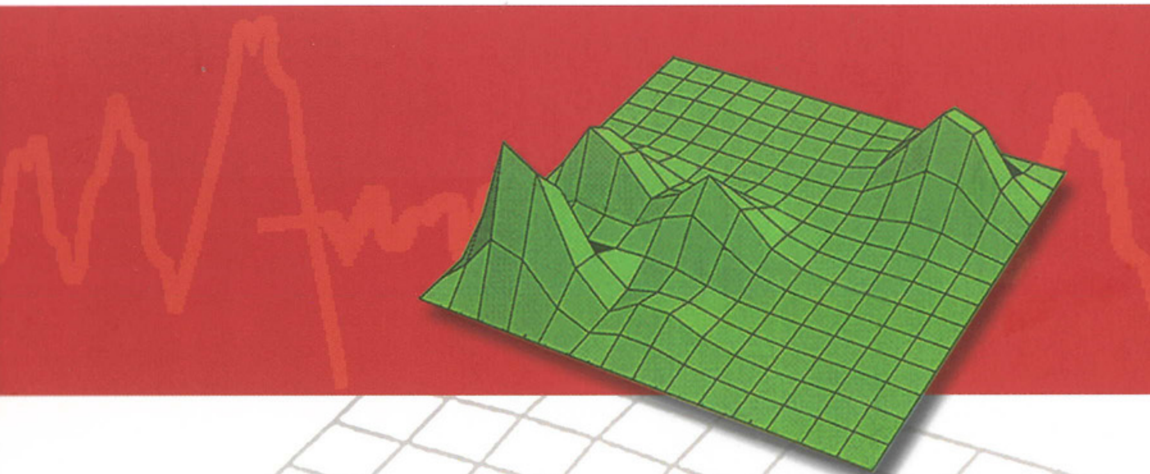
QUANTUM THEORY OF TUNNELING



MOHSEN RAZAVY

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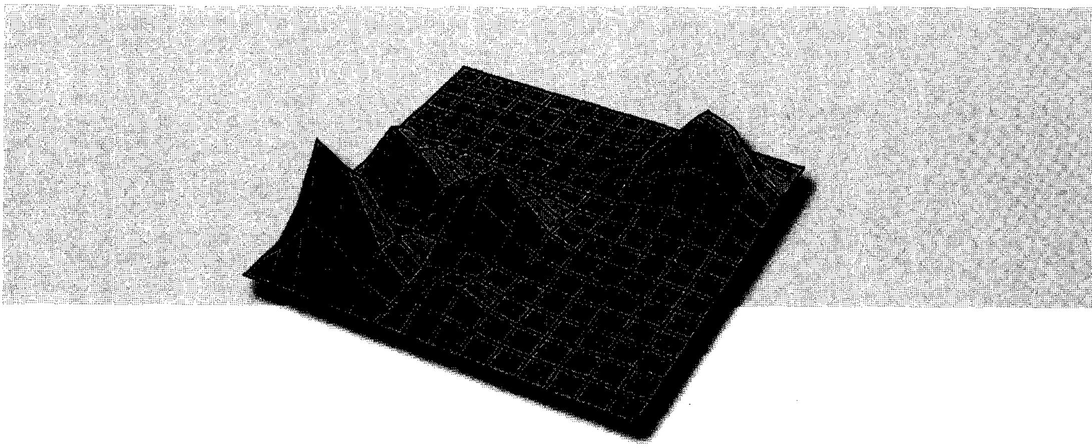

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Preface

The present book grew out of a lecture course given at the Institute for Advanced Studies in Basic Sciences, Zanjan, Iran in the summer of 1999. The intent at the outset was to present some of the basic results and methods of quantum theory of tunneling without concentrating on any particular application. It was difficult to decide what topics should be treated at length and which ones should be omitted from the discussion. Thus my main area of interest, the quantum theory of dissipative tunneling, was left out completely since even an introductory survey of the subject would have nearly doubled the size of the book.

I am indebted to my dear friends and colleagues Professors Y. Sobouti and M.R. Khajepour for giving me the opportunity of lecturing to a group of enthusiastic graduate students and also encouraging me to write this monograph. I have benefitted immensely from discussions with my colleague Professor A.Z. Capri and with Mr. Robert Teshima. Above all, I am indebted to my wife who never failed to support me.

Contents

Preface v

1 A Brief History of Quantum Tunneling 1

2 Some Basic Questions Concerning Quantum Tunneling 9

2.1 Tunneling and the Uncertainty Principle 9

2.2 Decay of a Quasistationary State 11

3 Semi-Classical Approximations 23

3.1 The WKB Approximation 23

3.2 Method of Miller and Good 31

3.3 Calculation of the Splitting of Levels in a Symmetric Double-Well Potential Using WKB Approximation 35

4 Generalization of the Bohr-Sommerfeld Quantization Rule and its Application to Quantum Tunneling 41

4.1 The Bohr-Sommerfeld Method for Tunneling in Symmetric and Asymmetric Wells 45

4.2 Numerical Examples 48

5 Gamow's Theory, Complex Eigenvalues, and the Wave Function of a Decaying State **53**

5.1 Solution of the Schrödinger Equation with Radiating Boundary Condition 53

5.2 The Time Development of a Wave PacketTrapped Behind a Barrier 57

5.3 A More Accurate Determination of the Wave Function of a Decaying State 61

5.4 Some Instances Where WKB Approximation and the Gamow Formula Do Not Work 66

6 Simple Solvable Problems **73**

6.1 Confining Double-Well Potentials 73

6.2 Time-dependent Tunneling for a δ-Function Barrier 79

6.3 Tunneling Through Barriers of Finite Extent 82

6.4 Tunneling Through a Series of Identical Rectangular Barriers 90

6.5 Eckart's Potential 96

6.6 Double-Well Morse Potential 99

7 Tunneling in Confining Symmetric and Asymmetric Double-Wells **105**

7.1 Tunneling When the Barrier is Nonlocal 112

7.2 Tunneling in Separable Potentials 116

7.3 A Solvable Asymmetric Double-Well Potential 119

7.4 Quasi-Solvable Examples of Symmetric and Asymmetric Double-Wells 121

7.5 Gel'fand-Levitan Method 124

7.6 Darboux's Method 127

7.7 Optical Potential Barrier Separating Two Symmetric or Asymmetric Wells 128

8 A Classical Description of Tunneling 139

9 Tunneling in Time-Dependent Barriers 149

9.1 Multi-Channel Schrödinger Equation for Periodic Potentials . 150

9.2 Tunneling Through an Oscillating Potential Barrier 152

9.3 Separable Tunneling Problems with Time-Dependent Barriers 157

9.4 Penetration of a Particle Inside a Time-Dependent Potential Barrier 162

10 Decay Width and the Scattering Theory 167

10.1 Scattering Theory and the Time-Dependent Schrödinger Equation 168

10.2 An Approximate Method of Calculating the Decay Widths . 173

10.3 Time-Dependent Perturbation Theory Applied to the Calculation of Decay Widths of Unstable States 176

10.4 Early Stages of Decay via Tunneling 181

10.5 An Alternative Way of Calculating the Decay Width Using the Second Order Perturbation Theory 184

10.6 Tunneling Through Two Barriers 186

10.7 Escape from a Potential Well by Tunneling Through both Sides . . . 191

10.8 Decay of the Initial State and the Jost Function . . . 196

11 The Method of Variable Reflection Amplitude Applied to Solve Multichannel Tunneling Problems 205

11.1 Mathematical Formulation . . . 206

11.2 Matrix Equations and Semi-classical Approximation for Many-Channel Problems . . . 212

12 Path Integral and Its Semi-Classical Approximation in Quantum Tunneling 219

12.1 Application to the S-Wave Tunneling of a Particle Through a Central Barrier . . . 222

12.2 Method of Euclidean Path Integral . . . 226

12.3 An Example of Application of the Path Integral Method in Tunneling . . . 231

12.4 Complex Time, Path Integrals and Quantum Tunneling . . . 237

12.5 Path Integral and the Hamilton-Jacobi Coordinates . . . 241

12.6 Remarks About the Semi-Classical Propagator and Tunneling Problem . . . 243

13 Heisenberg's Equations of Motion for Tunneling 251

13.1 The Heisenberg Equations of Motion for Tunneling in Symmetric and Asymmetric Double-Wells . . . 252

13.2 Tunneling in a Symmetric Double-Well . . . 258

13.3 Tunneling in an Asymmetric Double-Well . . . 259

13.4 Tunneling in a Potential Which Is the Sum of Inverse Powers of the Radial Distance 261

13.5 Klein's Method for the Calculation of the Eigenvalues of a Confining Double-Well Potential 267

14 Wigner Distribution Function in Quantum Tunneling 277

14.1 Wigner Distribution Function and Quantum Tunneling 281

14.2 Wigner Trajectory for Tunneling in Phase Space 284

14.3 Wigner Distribution Function for an Asymmetric Double-Well 290

14.4 Wigner Trajectory for an Oscillating Wave Packet 290

14.5 Margenau-Hill Distribution Function for a Double-Well Potential 292

15 Complex Scaling and Dilatation Transformation Applied to the Calculation of the Decay Width 297

16 Multidimensional Quantum Tunneling 307

16.1 The Semi-classical Approach of Kapur and Peierls 307

16.2 Wave Function for the Lowest Energy State 311

16.3 Calculation of the Low-Lying Wave Functions by Quadrature 313

16.4 Method of Quasilinearization Applied to the Problem of Multidimensional Tunneling 318

16.5 Solution of the General Two-Dimensional Problems 323

16.6 The Most Probable Escape Path 327

17 Group and Signal Velocities 339

18 Time-Delay, Reflection Time Operator and Minimum Tunneling Time 351

18.1 Time-Delay in Tunneling 352

18.2 Time-Delay for Tunneling of a Wave Packet 356

18.3 Landauer and Martin Criticism of theDefinition of the Time-Delay in Quantum Tunneling 365

18.4 Time-Delay in Multi-Channel Tunneling 368

18.5 Reflection Time in Quantum Tunneling 371

18.6 Minimum Tunneling Time 375

19 More about Tunneling Time 381

19.1 Dwell and Phase Tunneling Times 382

19.2 Büttiker and Landauer Time 385

19.3 Larmor Precession 388

19.4 Tunneling Time and its Determination Using the Internal Energy of a Simple Molecule 392

19.5 Intrinsic Time 394

19.6 A Critical Study of the Tunneling Time Determination by a Quantum Clock 398

19.7 Tunneling Time According to Low and Mende 402

20 Tunneling of a System with Internal Degrees of Freedom 411

20.1 Lifetime of Coupled-Channel Resonances 411

20.2 Two-Coupled Channel Problem with Spherically Symmetric Barriers 413

20.3 A Numerical Example 415

20.4 Tunneling of a Simple Molecule 418

20.5 Tunneling of a Molecule in Asymmetric Double-Wells 424

20.6 Tunneling of a Molecule Through a Potential Barrier 429

20.7 Antibound State of a Molecule 434

21 Motion of a Particle in a Space Bounded by a Surface of Revolution 439

21.1 Testing the Accuracy of the Present Method 444

21.2 Calculation of the Eigenvalues 445

22 Relativistic Formulation of Quantum Tunneling 453

22.1 One-Dimensional Tunneling of the Electrons 453

22.2 Tunneling of Spinless Particles in One Dimension 458

22.3 Tunneling Time in Special Relativity 461

23 The Inverse Problem of Quantum Tunneling 471

23.1 A Method for Finding the Potential from the Reflection Amplitude 472

23.2 Determination of the Shape of the Potential Barrier in One-Dimensional Tunneling 473

23.3 Prony's Method of Determination of Complex Energy Eigenvalues 476

23.4 A Numerical Example 478

23.5 The Inverse Problem of Tunneling for Gamow States 479

24 Some Examples of Quantum Tunneling in Atomic and Molecular Physics **485**

24.1 Torsional Vibration of a Molecule 485

24.2 Electron Emission from the Surface of Cold Metals 488

24.3 Ionization of Atoms in Very Strong Electric Field 491

24.4 A Time-Dependent Formulation of Ionization in an Electric Field 493

24.5 Ammonia Maser 497

24.6 Optical Isomers 500

24.7 Three-Dimensional Tunneling in the Presence of a Constant Field of Force 501

25 Examples from Condensed Matter Physics **511**

25.1 The Band Theory of Solids and the Kronig-Penney Model . . 511

25.2 Tunneling in Metal-Insulator-Metal Structures 515

25.3 Many Electron Formulation of the Current 516

25.4 Electron Tunneling Through Hetero-structures 525

26 Alpha Decay **531**

Index **541**

Introduction

Quantum tunneling is a microscopic phenomenon where a particle can penetrate and in most cases pass through a potential barrier. This barrier is assumed to be higher than the kinetic energy of the particle, therefore such a motion is not allowed by the laws of classical dynamics. The simplest problems in quantum tunneling are one-dimensional and most of the research is done on these problems. But the extension of one-dimensional tunneling to higher dimensions is not straightforward. In addition there are certain characteristics that appear in two- or three-dimensional tunneling which do not show up in the one-dimensional motion.

In most of the one-dimensional problems we study the motion of a particle in a potential $V(x)$, where $V(x)$ has a finite (or sometimes infinite) number of maxima. As long as the height of the barriers remain finite, the motion of the particle will not be restricted and we may choose the energy of the particle E to be greater than the asymptotic value of the potential say at $x = -\infty$. Then the simplest case will be that of a particle with energy $E > V(-\infty)$ approaching the barrier from the left and then penetrating the barrier. Now depending on whether $E > V(\infty)$ or $E < V(\infty)$ the particle can pass through the potential or be reflected back and move to $x = -\infty$. The value of E is arbitrary as long as these conditions or inequalities are met.

The other possibility is the one where the potential is finite on one side and tends to infinity on the other, e.g. $V(-\infty) = \infty$ and $V(\infty)$ is finite. In addition the potential has at least one local maximum say at $x = a$. Then depending on the boundary conditions of the problem we can have two different possibilities:

(i) - If the particle moves from $x = \infty$ in the direction of $x = -\infty$, then there is the possibility that by tunneling the particle can enter the region between a and $-\infty$ and stays there for a finite time (a metastable state).

(ii) - If the initial condition shows that the particle is in the region $-\infty < x < a$, then in the course of time by the process of tunneling the particle passes through the barrier and goes to $x = \infty$. This initial state has also a finite lifetime. In both of these cases there are characteristic energies for which the tunneling probability is large, whereas for other energies it is small.

The third possibility is when the potential $V(x)$ is a confining potential, i.e. $V(x)$ tends to infinity on both sides of the central maximum (or maxima), $V(x) \to \infty$ as $x \to \pm\infty$. In this case the motion of the particle will be restricted to a part of the x-axis. Depending on the number of maxima of $V(x)$, we can have the eigenvalue problem for a double- or multi-well potential. The motion of the wave packet for double-wells, due to their importance in applied physics have received extensive treatment.

The double-wells can be symmetric or asymmetric. The motion of a wave packet which represents the particle in a symmetric double-well, under certain conditions, can be obtained from the superposition of the eigenfunctions of the two lowest states of the system. When this happens then the wave packet oscillates between the two wells with a well defined frequency, and it also preserves its shape after successive back and forth tunneling. This very important case is called quantum coherence. For asymmetric wells, if the motion from one well to the other takes place by tunneling, then we have a situation which we call quantum hopping.

In two or three dimensions when the barrier is only a function of the distance from the origin of the coordinate system, i.e. $\rho = \sqrt{x^2 + y^2}$ or $r = \sqrt{x^2 + y^2 + z^2}$, we can separate the variables in the Schrödinger equation and thus reduce the problem to a one-dimensional motion but now with the boundary conditions imposed at $\rho = 0$ or $r = 0$ and at ρ and r infinity. For instance in three dimensions if we assume that $V(r \to \infty) \to 0$ and that $V(r)$ has a maximum at $r = a$, then if the particle is originally confined in the region $0 \le r < a$, it can tunnel through the barrier and go to infinity. These special cases of two- or three-dimensional tunneling can be regarded as one-dimensional but the potentials $V(\rho)$ and $V(r)$ are replaced by $V_{eff}(\rho)$ and $V_{eff}(r)$, with the boundary condition that the reduced radial wave function must vanish at the origin.

In the first chapter of this book we present a brief history of the subject of quantum tunneling and the role that a number of pioneers played in its development. In the second chapter we discuss the physics of tunneling and the solution to the problem of local kinetic energy provided by the uncertainty principle. Furthermore we show that the principles of wave mechanics imply that, in general, the decay of the system, either because of tunneling or by some other mechanism, is nonexponential. Following this argument, we consider a special solvable problem to show that the exponential decay law is a very good approximation except for very short initial time and also after a very long time, and only at these extremes there are departures from the exponential decay. In the third chapter we study the semi-classical or WKB approximation and the conditions under which this approximation is valid. In addition we discuss another approach proposed by Miller and Good. We apply the WKB technique to calculate the energy separation between the two lowest levels of a symmetric double-well potential. Another important semi-classical approximation is the quantization rule of Bohr and Sommerfeld which is of great historical significance in atomic physics. In Chapter 4 we generalize this rule to the problems of quantum tunneling and we find the well-known Gamow formula for the decay of a system by means of tunneling. The same Bohr-Sommerfeld rule can also be used to determine the energy levels of symmetric and asymmetric double-wells.

Gamow found his formula by employing the complex eigenvalues and the Gamow states. In Chapter 5 we show that even though Gamow's approach is in apparent contradiction with the principles of quantum theory and this is a result of the approximate nature of this approach, nonetheless it is a useful approximation. Realizing that Gamow's approach is an approximation, we find that there are certain systems for which this approximation breaks down. In addition to discussing these systems, we find that the method has another shortcoming, viz, for the wave functions corresponding to the complex eigenvalues, the integral $\int |\psi|^2 dx$ is divergent. A re-examination and resolution of this difficulty is also given in Chapter 5. In the next chapter (Chapter 6) we solve a number of simple problems for which analytic solutions are known, and we determine, in appropriate cases, the lifetime of the quasistationary states, and or the motion of the wave packets. Of special interest is the resonant tunneling from either two identical barriers or a group of barriers. In addition to these, we discuss the question of tunneling in nonlocal and separable potentials for which little is known. In Chapter 7 we return to the problem of tunneling in double-wells. Here we will discuss the possibility of tunneling of a wave packet which originally is localized in one of the wells to the second well. While for two symmetric wells, the tunneling is always possible, for asymmetric wells tunneling is possible only when certain conditions are satisfied, we discuss these conditions in this chapter. Chapter 8 deals with the interesting question of the classical description of tunneling. This is achieved by coupling the motion of the tunneling particle to a specific system with infinite degrees of freedom.

We assumed, up to this point, that the potential is time-independent. If the potential depends on space as well as on time, only for special cases the problem is exactly solvable. Because of the importance of this type of tunneling in the physics of layered semiconductors, we need a general method of formulating and solving the problem. In Chapter 9 we will investigate the simplest types of tunneling involving time-dependent potentials.

When quantum tunneling is three-dimensional with an effective potential $V(r) + \frac{\hbar^2 l(l+1)}{r^2}$, we can calculate the decay width or the lifetime from scattering theory. In Chapter 10 we first establish the connection between the quantum scattering theory and the width of the decaying states, and we formulate two parallel approaches to this subject. We show how for different potentials we can calculate the decay width exactly or approximately. This formulation also enables us to study the time-dependence of the decay of initial state by tunneling, both for early times and in the exponential regime. When the tunneling particle (or system of particles) has internal degrees of freedom, like a simple molecule, and also in some cases where the time-dependence of the potential is sinusoidal, we can decompose the Schrödinger equation into an infinite set of coupled equations. A simple and accurate method for solving a set of equations of this type (which can only be solved numerically) is the method of variable reflection coefficient. Chapter 11 is devoted to a study of this technique and its applications.

In three subsequent chapters 12-14 we study alternative ways of formulating the tunneling problem starting with Feynman's method of path integration. Most of the techniques based on Feynman's method such as instantons, Euclidean path integration and the introduction of complex time in the formulation are developed for use in subatomic and particle physics. However they can be applied to the simpler cases like systems of few degrees of freedom. The difficulty of generalizing these ideas to multi-dimensional systems is a serious limitation of the method, and at present it is not clear whether the introduction of complex time would enable one to overcome this difficulty or not. At the end of Chapter 12 we discuss an interesting method of using the Hamilton-Jacobi coordinates and path integration to solve a simple tunneling problem. But again it is not known whether this approach can be extended to other systems or not.

Continuing our discussion of the alternative methods of solving different tunneling situations, we investigate the solution of Heisenberg's equations of motion for quantum tunneling of a single particle. Up to now only few problems, namely those involving potentials expressible as polynomials in x (or in $\frac{1}{r}$) and of the form $\sum_n a_n x^n$ or $\sum_n b_n r^{-n}$ have been studied. The advantage of using operator equations for solving tunneling problems lies in the facts that (i) the initial wave packet does not change in time and (ii) since Heisenberg 's equation are similar to the classical equations of motion therefore the definition of some of the dynamical quantities such as tunneling time is clearer in this formulation.

The fourth approach which we study in Chapter 14 is a method based on the Wigner distribution function. Using this distribution function we can follow the motion of a wave packet in phase space. As an example we present the case of tunneling through two rectangular barriers and show how this can be used to determine a tunneling time. A related and interesting question is that of finding the Wigner trajectory for a wave packet formed from the superposition of the two lowest eigenfunctions. As we mentioned earlier this is a coherent (shape preserving) tunneling with a period $T = \frac{2\pi}{E_1 - E_0}$, where E_0 and E_1 are the two lowest eigenvalues of the system. Preliminary result suggests that the Wigner trajectory in the phase space for this motion does not have a fixed period and this is a strange result.

The method of complex scaling and the dilatation transformation for the calculation of the decay width is the subject of discussion in Chapter 15. In Chapter 16 we study the important and difficult problem of multidimensional tunneling when the wave equation is not separable. There is considerable amount of published work about this subject, but as yet a satisfactory and reliable technique for determining the motion of the particle has not been found. In particular, questions concerning the most probable escape path and the tunneling time need more careful investigation.

The three following chapters 17-19 deal with different aspects of the tunneling time. As a way of introducing the subject, we start by defining the physical concepts of group and signal velocities for a wave, and by following the works of Sommerfeld, Brillouin and Stevens, we calculate the tunneling time for a simple potential.

In Chapter 18 we continue our discussion of the tunneling time with an examination of the idea of time-delay. Starting with the classically well-defined concept of the time of flight over a barrier, we first develop a semi-classical formulation and later present a definition of the quantal time-delay and show its relationship with the Wigner inequality. We observe that the definition of the time-delay can be extended to the case of confining potentials. To this end we make use of the Schwinger work which relates the phase shift to the splitting of the energy levels and we find a connection between the time of oscillation from one well to the other and the derivative of phase shift with respect to energy. These formulations are mostly based on the form of classical travel time of the particle and do not have a proper defi-

Chapter 1

A Brief History of Quantum Tunneling

Three years after the discovery of natural radioactivity in 1896, Elster and Geitel [1] found the exponential decay rate of radioactive substances experimentally. In 1900 Rutherford [2] introduced the idea of half-life of these chemicals, i.e. the time that the number of radioactive nuclei reach one-half of their original number. In 1905 Schweidler [3] showed the statistical nature of the decay. This means that the probability of disintegration of a nucleus does not depend on the time of its formation and also the time that a particular nucleus decays can only be predicted statistically. This idea was verified empirically by Kohlrausch [4] in 1906. Later experiments showed that the decay width Γ (which is related to the half-life τ by $\tau = \frac{\ln 2}{\Gamma}$) does not depend on external variables such as pressure, temperature or chemical environment.

The exponential law of decay can be written either in differential form as

$$\frac{dN(t)}{dt} = -\Gamma N(t), \tag{1.1}$$

or as an integral of Eq. (1.1), i.e.

$$N(t) = N_0 \exp(-\Gamma t), \tag{1.2}$$

where N_0 is the original number of nuclei (at $t = 0$), $N(t)$ is their number at $t > 0$, and Γ is the decay probability per unit time. For the rate of decay one can use either $T = \frac{1}{\Gamma}$ or the half-life $\tau = T \ln 2$. It should be pointed out that $N(t)$ is not the result of a single measurement but it is the average over a group of measurements, therefore $P(t) = \frac{N(t)}{N_0}$ is the probability that certain nucleus has not decayed at the time t ($t > 0$) and has remained in its initial state. Instead of $N(t)$ we can use $P(t) = \frac{N(t)}{N_0} = e^{-\Gamma t}$ which is usually referred to as the law of exponential decay.

The theory of α-radioactivity on the basis of quantum tunneling was proposed by Gamow [5] [6] [7] who found the well-known Gamow formula. The story of this discovery is told by Rosenfeld [8] who was one of the leading nuclear physicist of the twentieth century. " In my experience nuclear physic starts with the sudden appearance, one morning in the library of the Göttingen Institute, of a fair-haired giant, with shortsighted, half-shut eyes behind his spectacles, who introduced himself, with a broad smile, by declaring " I am Gamow." This pronouncement, at that time, could not provoke very much excitement. As it turned out that Professor Born would not be in for some time, I proposed to Gamow to go out for a walk. It was during the walk that he told me what he was doing.

He wanted to understand alpha radioactivity. Now, this seemed to me- and I think most physicists then would have had the same reaction - quite fantastic idea. All we knew about nuclei was that they were very small and that they had spin; this had just emerged from Pauli's interpretation of the hyperfine structure which spectroscopists had detected in the spectra of the heaviest atoms".

Gamow's first attempt was a failure. In that he assumed that the α particle is a point particle located in the Coulomb field of the nucleus. He found a continuous spectrum for its emission, and this was in contradiction with the empirical fact that that there are certain characteristic energies with which the particles are emitted. Later Gamow thought of combining the attractive nuclear forces with the Coulomb repulsion and this combination provided an effective barrier for the α particle (Chapter 25). He solved the Schrödinger equation with this effective potential and he imposed the "outgoing" wave boundary condition for large distances from the center of the nucleus. Gamow found that this two-point boundary condition problem (for $r = 0$, ψ must be finite and for $r \to \infty$, $\psi \to \frac{\exp(ikr)}{kr}$, (Chapter 5)) does not have a solution for the real energies, but for complex energies there are solutions. He interpreted the complex part of the energy as the decay width $\frac{\Gamma}{2}$, (or decay constant) of the disintegration and in this way he found the Geiger-Nuttall formula [9] which is a relation between $\frac{\Gamma}{2}$ and the energy of the emitted α-particle (Chapter 25) [5] [6] [7]. This work was completed shortly after Gamow's arrival at Göttingen. When in a weekly seminar at the Institute he presented his result it attracted much attention. Max Born was among the audience and he realized the significance of the theory. Born noticed that this idea is not only applicable to nuclear physics, but it is a general feature that must be present in other physical systems. He noticed that the cold emission of electrons from a metallic surface (Chapter 23) can be another example of this phenomena. Born being one of the founders of modern quantum mechanics criticized the foundation of Gamow's work arguing that the Hamiltonian is a Hermitian operator and its eigenvalues must be real, not complex, as Gamow had assumed. However the success of Gamow's result could not have been ignored. Therefore Born worked on this problem for few weeks and obtained the same result by considering Hermitian operators and states with real eigenvalues [10]. For this Born assumed that inside the nucleus there are stationary and distinct states, and the Coulomb potential outside the nucleus has a continuous spectrum which overlaps with the discrete energies inside. Now one can consider these two sets of wave functions (inside and outside) as a complete set of states and expand the original wave packet in terms of these, to obtain essentially the same result as Gamow's [10] (see also [11]).

About the same time as Gamow published his work, Gurney and Condon also submitted an article to the periodical Nature about α-decay [12]. Years later (1969), E.U. Condon recalled the history of the theory of tunneling [13] which we will briefly mention here. In 1928 Condon was hired as an assistant professor at Princeton University. There he met R.W. Gurney, a former student of E. Rutherford. At that time there were two published papers, one by Oppenheimer [14] and the other by Fowler and Nordheim [15]. These scientists had observed certain interesting and unusual features in the quantum mechanics of one-dimensional systems, and they had applied this new mechanics to understand the physics of the cold emission of the electrons. By reading these articles Gurney thought of applying the same idea to solve the problem of α-decay. At first he asked the opinion of the physicist H.R. Robertson about this approach, but he received no encouragement. Later when Gurney discussed his idea with Condon, Condon realized the potential of this theory, and they decided to collaborate on this project. Very soon they observed that it is not essential to know the shape of the potential inside the nucleus, only one had to assume that the interior potential becomes zero at a distance equal to the nuclear radius. They also observed that they can use the semi-classical or WKB approximation (Chapter 3) to calculate the wave function under the barrier. In this way Gurney and Condon found the solution to the Schrödinger equation for the radial wave function with the condition that the amplitude of the wave function must be large inside and small outside the nucleus. From the solution of the wave equation they found the decay width and the energy of the emitted α-particle approximately. Within few days this work was submitted to the periodical Nature (July 1928) [12], and later they published a detailed account and sent it to the Physical Review, and this was published in February of 1929 [16].

After submitting this work for publication, Condon and Gurney thought of applying the result of their work to the question of artificial disintegration of the atomic nucleus. They realized that in quantum mechanics the penetration inside the nucleus is possible with the low energy protons or α-particles, whereas according to the laws of classical mechanics for penetration the energy of these particles must be higher than the maximum height of the barrier. But they regarded this as an obvious conclusion of their work and did not bother to publish it. On the other hand Gamow in 1928 and 1929 published papers pointing out this implication of quantum tunneling. About the same time Gurney was thinking about resonant tunneling i.e. how a particle having a low energy equal to one of the quasistationary energies of the nucleus can easily penetrate the barrier. This work of Gurney was published in Nature (1929), [17] and according to Condon it deserves more attention than what it has received so far.

In 1930's and 1940's there were many attempts to relate the dynamics of the electron current in a system of metal-semiconductor which was used in rectifying the current, to the tunneling of electrons in solids. But the models were not realistic enough and usually quantum theory was predicting a current in the opposite direction of the observed current. With the discovery of transistors in 1947, the tunneling of electrons received renewed attention. In 1950 the construction of semiconductors like Ge and Si had advanced to a point were it was possible to manufacture semiconductors of given characteristics.

In 1957 L. Esaki discovered tunnel diode and this discovery proved the electron tunneling in solids conclusively [18]. Three years later i.e. in 1960, I. Giaever observed that if one or both of the metals are superconducting then the voltage-current curve provides interesting information regarding the state of superconductor(s). This experiment of Giaever was sufficiently accurate that it enabled one to measure the energy gap in superconductors. This gap appears when electrons form Cooper pairs, and the gap plays an essential role in the BCS theory of superconductivity [19].

The other major discovery was the theoretical work of B.D. Josephson in 1962 in connection with the tunneling between two superconductors separated by a thin layer of insulating oxide which serves as the barrier. Taking all of this as a single system, Josephson was able to predict the existence of a second current, i.e. the supercurrent in addition to the current found by Giaever, and this he showed is due to the tunneling of electrons in pairs [20].

Only very recently the tunneling of an individual atom, e.g. hydrogen on a metal surface such as copper has been observed directly. A remarkable (non-classical) feature of the experiment is that the tunneling rate increases as the surface gets colder [21] [22].

For a brief history of time in quantum tunneling see the papers of Steiberg [23] [24].

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Chapter 2

Some Basic Questions Concerning Quantum Tunneling

We begin our study of quantum tunneling by investigating as to why tunneling is exclusively a quantum phenomena and does not have a classical counterpart [1]. Then we obtain a general result about the time dependence of the decay of a quasi-stationary system, and in particular the nonexponential nature of the decay [3] [4] [5] [6]. But if the decay is not exponential why the empirical results suggest otherwise? To explain this we study a solvable problem and show that an exponential decay, while is not exact, is a very good approximation.

2.1 Tunneling and the Uncertainty Principle

At the first sight the tunneling of a particle looks like a paradoxical problem, since if the height of the barrier is greater than the total energy of the particle,

$$E = \frac{1}{2m}p^2 + V(x) \tag{2.1}$$

then in the range b where $V(x) > E$, the kinetic energy $\frac{1}{2m}p^2$ is negative and p is imaginary, but this is not correct.

At the root of this paradox is our assumption that at each instant we know both the kinetic and the potential energy separately, or in other words we can assign values to the coordinate x and the momentum p simultaneously and this is in violation of the uncertainty principle. Here we want to know whether it is possible to determine the position of the particle when it is moving under the barrier or not. For this we observe that the particle can be at the point x where $E < V(x)$ but then according to the uncertainty principle its momentum is uncertain by an amount $\sqrt{\overline{\Delta p^2}}$. Thus if we know the position of the particle to be x, then its total energy cannot be E.

Since the transmission amplitude during tunneling is proportional to (see Chapters 3 and 4)

$$\exp\left[-\frac{1}{\hbar}\int_{x_0}^{x}\sqrt{2m(V(x)-E)}dx\right], \tag{2.2}$$

where x_0 is the classical turning point, then the probability of finding the particle which is coming from the left to be on the right of the barrier, i.e. $x_0 + b$ is proportional to the square of this amplitude or to the factor

$$\exp\left[-\frac{2}{\hbar}\int_{x_0}^{x_0+b}\sqrt{2m(V(x)-E)}dx\right]. \tag{2.3}$$

Now if we want a non-negligible probability then we must have

$$2\sqrt{2m(V_m - E)}\, b \approx \hbar. \tag{2.4}$$

where V_m is the maximum height of the potential. To find the position of the particle inside the barrier, we have to measure its coordinate with an accuracy $\Delta x < b$, therefore the uncertainty in momentum is

$$\overline{\Delta p^2} = \frac{\hbar^2}{4(\Delta x)^2} = \frac{\hbar^2}{4b^2}. \tag{2.5}$$

By substituting b from (2.4) in (2.5) we find

$$\frac{\overline{\Delta p^2}}{2m} = V_m - E. \tag{2.6}$$

Thus the kinetic energy of the particle must be greater than the difference between the height of the barrier V_m and the total energy E [1].

A result similar to (2.5) and (2.6) can be obtained from the time-energy uncertainty relation [2] i.e.

$$\Delta E \Delta t \approx \frac{\hbar}{2}. \tag{2.7}$$

Again let us denote the energy of the incident particle by E. For a very short time Δt, the uncertainty in the energy is ΔE, and for sufficiently small Δt, the energy of the particle $E + \Delta E$ is greater than the height of the barrier V_m. Tunneling takes place if in the time Δt the particle can traverse the barrier. For a rectangular barrier of width b this Δt is given by

$$\Delta t = \frac{b}{\sqrt{\left(\frac{2}{m}\right)(E + \Delta E - V_m)}}. \tag{2.8}$$

From Eqs. (2.7) and (2.8) we find ΔE to be the solution of the quadratic equation

$$(\Delta E)^2 - \frac{\hbar^2}{2mb^2}\Delta E + \frac{\hbar^2}{2mb^2}(V_m - E) = 0, \tag{2.9}$$

and the condition for ΔE to be real is given by

$$\frac{\hbar^2}{8mb^2} > V_m - E, \tag{2.10}$$

which is the same as Eq. (2.6).

2.2 Decay of a Quasistationary State

Consider a system with the initial wave function, Ψ_0, and let $\phi(E)$ be the eigenfunction of the Hamiltonian H of the system

$$H|\phi(E)\rangle = E|\phi(E)\rangle. \tag{2.11}$$

Let us denote the complete set of commuting observables of this system of which H is a member by (H, A), then we have

$$A|\phi(E)\rangle = a|\phi(E)\rangle, \tag{2.12}$$

and

$$\int |\phi(E,a)\rangle\langle\phi(E,a)|dEda = I, \tag{2.13}$$

where in Eq. (2.13) I is the unit operator. Since Ψ_0 is not an eigenstate of H, this initial state will decay in time. The probability amplitude for the decay of Ψ_0 is given by (we set $\hbar = 1$) [6]

$$C_0(t) = \int_{E_{min}}^{\infty} e^{-iEt} dE \int |\langle\phi(E,a)|\Psi_0\rangle|^2 da, \tag{2.14}$$

where E_{min} is the lowest energy state of the Hamiltonian H. Now if we define $\omega(E)$ by the following relation

$$\omega(E) = \int |\langle\phi(E,a)|\Psi\rangle|^2 da, \tag{2.15}$$

then we can write $C_0(t)$ as

$$C_0(t) = \int_{E_{min}}^{\infty} e^{-iEt}\omega(E)dE = \int_{-\infty}^{\infty} e^{-iEt}\tilde{\omega}(E)dE, \tag{2.16}$$

where in the last relation

$$\tilde{\omega}(E) = \begin{cases} \omega(E) & \text{for } E \geq E_{min} \\ 0 & \text{for } -\infty < E < E_{min} \end{cases}. \tag{2.17}$$

Since $\tilde{\omega}(E)$ is zero for $E < E_{min}$, therefore from Paley and Wiener theorem [7] [8] it follows that

$$\int_{-\infty}^{\infty} \frac{|\ln|C_0(t)||^2}{1+t^2} dt < \infty. \tag{2.18}$$

For the convergence of this integral as $t \to \infty$, it is necessary for $C_0(t)$ to behave as

$$|\ln|C_0(t)|| \to Bt^{2-p} \;\; \text{as} \;\; t \to \infty, \;\; p > 1, \tag{2.19}$$

and since $C_0(t) \to 0$ as $t \to \infty$, therefore $\ln|C_0(t)|$ is negative and

$$P(t) = |C_0(t)|^2 \to \exp[-Ct^q], \;\; \text{as} \;\; t \to \infty, \;\; q < 1, \tag{2.20}$$

where in this relation C is a positive constant. Equation (2.20) shows that asymptotically the decay is not exponential and the probability of finding the system in its initial state $P(t)$ tends to zero slower than an exponential [9] [10] [11]. This argument is quite general and is applicable to different decaying systems.

The reason for the breakdown of the exponential decay law after a long time is due to the fact that the part of the system that is decayed moves away from the decaying part so slowly that there is interference between these two parts. This interference is responsible for the behavior shown by

Eq. (2.20). However if the motion of the decayed part is accelerated, e.g. by the presence of a constant force, then asymptotically, the system can decay exponentially [13]. A model which shows this type of decay is discussed in Section(24.4).

Now let us examine the behavior of $P(t)$ at the initial stages of decay, i.e. as $t \to 0$. From Eq. (2.16) it follows that

$$\int_{E_{min}}^{\infty} |\omega(E)|\, dE = \int_{E_{min}}^{\infty} dE \int |\langle\phi(E,a)|\Psi_0\rangle|^2\, da = \langle\Psi_0|\Psi_0\rangle = 1. \tag{2.21}$$

Since

$$\int_{E_{min}}^{\infty} |\omega(E)|\, dE < \infty, \tag{2.22}$$

therefore $C_0(t)$ is uniformly convergent and is continuous for $-\infty < t < \infty$ [12]. The function $\omega(E)e^{-iEt}$ is differentiable at every point with respect to t and its derivative is continuous for $E_{min} \le E < \infty$ and $-\infty < t < \infty$ and has a uniformly convergent integral

$$\int_{E_{min}}^{\infty} \frac{\partial}{\partial t}\left[\omega(E)e^{-iEt}\right] dE < \infty, \tag{2.23}$$

provided that the mean energy in the state Ψ_0 is finite

$$\int_{E_{min}}^{\infty} E\omega(E)dE < \infty. \tag{2.24}$$

From the derivative of $C_0(t)$

$$\frac{dC_0(t)}{dt} = -i\int_{E_{min}}^{\infty} E\omega(E)e^{-iEt}dE, \tag{2.25}$$

it follows that

$$\left(\frac{dC_0(t)}{dt}\right)_{t=0^+} = \left(\frac{dC_0(t)}{dt}\right)_{t=0^-}. \tag{2.26}$$

Noting that $\omega(E)$ is real, therefore

$$C_0(-t) = \left(C_0(t)\right)^*, \tag{2.27}$$

and $P(t)$ can be written as

$$P(t) = C_0(t)C_0(-t). \tag{2.28}$$

By differentiating (2.28) with respect to t we find

$$\frac{dP(t)}{dt} = \frac{dC_0(t)}{dt}C_0(-t) + \frac{dC_0(-t)}{dt}C_0(t). \tag{2.29}$$

Thus in the limit of $t \to 0$, $C_0(\pm t) \to 1$ and we have

$$\left(\frac{dP(t)}{dt}\right)_{t=0^+} = \left(\frac{dC_0(t)}{dt}\right)_{t=0^+} - \left(\frac{dC_0(t)}{dt}\right)_{t=0^-} = 0. \tag{2.30}$$

Clearly this result is not compatible with purely exponential decay since if $P(t) = P(0)e^{-\Gamma t}$ then

$$\left(\frac{dP(t)}{dt}\right)_{t=0} = -\Gamma P(0) < 0. \tag{2.31}$$

Thus we conclude that at the early stages of decay $P(t)$ is greater than $P(0)\exp(-\Gamma t)$ [6]. A detailed analysis shows that at the early stages of decay, the probability $P(t)$ is proportional to $\cos^2(\sqrt{\mathcal{A}}t)$, where $\sqrt{\mathcal{A}}$ depends on the shape of the potential barrier [5] (see also the model discussed in Section (10.4)).

Now for the decay of a quasistationary system by the mechanism of tunneling we want to show that most of the decay can be approximated very well by the exponential law. For the decay by tunneling we can formulate the problem in the following way [14] [15]:
Let $\phi_p(r)$ be the solution of the radial Schrödinger equation for the $l = 0$ partial wave with the potential barrier $V(r)$,

$$H\phi_p(r) = \left(-\frac{1}{2m}\frac{d^2}{dr^2} + V(r)\right)\phi_p(r) = \frac{p^2}{2m}\phi_p(r), \quad (\hbar = 1) \tag{2.32}$$

and let $\Psi_0(r)$ represent the initial wave packet which is localized behind the barrier. To find the time evolution of this wave packet we expand it interms of $\phi_p(r)$,

$$\Psi_0(r) = \int_0^\infty c_p\phi_p(r)dp, \tag{2.33}$$

where

$$c_p = \int_0^\infty \Psi_0(r')\phi_p^*(r')dr'. \tag{2.34}$$

Since $\phi_p(r)$ is an eigenfunction of the Hamiltonian with the eigenvalue $\frac{p^2}{2m}$, therefore

$$\Psi(r,t) = \int_0^\infty c_p\phi_p(r)\exp\left[-i\frac{p^2t}{2m}\right]dp. \tag{2.35}$$

Substituting c_p from (2.34) in (2.35) we get

$$\Psi(r,t) = \int_0^\infty \exp\left[-i\frac{p^2t}{2m}\right]\phi_p(r)dp\int_0^\infty \Psi_0(r')\phi_p^*(r')dr'. \tag{2.36}$$

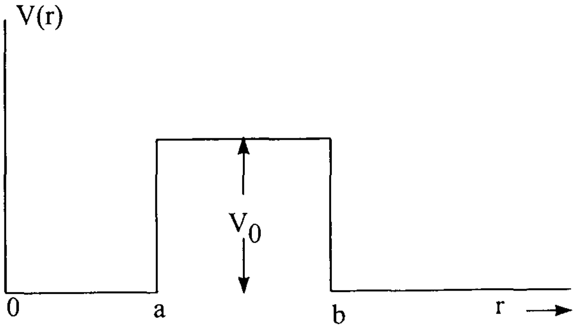

Figure 2.1: A particle trapped in the range $0 < x < a$ can escape to infinity by tunneling

Finally by multiplying (2.36) by $\Psi_0^*(r)$ and integrating over r we find $C_0(t)$ Eq. (2.14);

$$C_0(t) = \int_0^\infty \exp\left[-i\frac{p^2 t}{2m}\right] dp \left|\int_0^\infty \Psi_0(r')\phi_p^*(r')dr'\right|^2. \qquad (2.37)$$

Let us consider the specific problem where a wave packet is trapped behind a barrier and then by tunneling it escapes to infinity [16] [17] [18]. suppose that a particle of mass m is initially confined to a segment $0 \le x \le a$ behind a rectangular potential of height V_0 and width $b - a$. The wave function is obtained from the solution of the Schrödinger equation and is

$$\psi_p(r) = \begin{cases} \frac{2}{N(p)}\sin(pr) & \text{for } 0 \le r \le a \\ Ae^{\gamma r} + Be^{-\gamma r} & \text{for } a \le r \le b \\ Ce^{ipr} + De^{-ipr} & \text{for } b \le r \end{cases}, \qquad (2.38)$$

where $p^2 < 2mV_0$ and

$$\gamma = \sqrt{2mV_0 - p^2}. \qquad (2.39)$$

The normalization constant $N(p)$ is chosen so as to satisfy the relation

$$\int_0^\infty \psi^*{}_p(r)\psi_{p'}(r)dr = \delta(p - p'). \qquad (2.40)$$

By imposing the boundary conditions, i.e. the continuity of the logarithmic derivative of the wave function at the points $x = a$ and $x = b$, we can find the constants A, B, C and D in terms of $N(p)$

$$A = \frac{i}{N(p)}\left[\sin(pa) + \frac{p}{\gamma}\cos(pa)\right], \tag{2.41}$$

$$B = \frac{i}{N(p)}\left[\sin(pa) - \frac{p}{\gamma}\cos(pa)\right], \tag{2.42}$$

$$C = \frac{1}{2}\left(1 + \frac{\gamma}{ip}\right)Ae^{\frac{G}{2}} + \frac{1}{2}\left(1 - \frac{\gamma}{ip}\right)Be^{\frac{-G}{2}}, \tag{2.43}$$

$$D = \frac{1}{2}\left(1 - \frac{\gamma}{ip}\right)Ae^{\frac{G}{2}} + \frac{1}{2}\left(1 + \frac{\gamma}{ip}\right)Be^{\frac{-G}{2}}, \tag{2.44}$$

and

$$\begin{aligned} N^2(p) &= \frac{1}{2\pi}\left(1 + \frac{\gamma^2}{p^2}\right)\left\{\left[\sin(pa) + \frac{p}{\gamma}\cos(pa)\right]^2 e^G \right. \\ &+ \left.\left[\sin(pa) - \frac{p}{\gamma}\cos(pa)\right]^2 e^{-G}\right\} \\ &+ 2\left(1 - \frac{\gamma^2}{p^2}\right)\left[\sin^2(pa) - \frac{p^2}{\gamma^2}\cos^2(pa)\right], \end{aligned} \tag{2.45}$$

where

$$G = 2(b - a)\gamma. \tag{2.46}$$

The expression (2.45) is approximate since we have replaced the lower limit of the integral in Eq. (2.40), i.e. zero by b, and this is a very good approximation. In Fig. (2.2) a plot of $\ln N^2(p)$ versus $\ln p$ is shown (for this plot the parameters $a = 1L, b = 1.3L, V_0 = 200L^{-2}$ where L is a unit of length and $m = \frac{1}{2}$ have been used). For this set of numbers $G >> 1$ and is of the order of 8. Thus the wave function is very small outside the potential. From the above equations we conclude that $A \approx 0$ and hence

$$\sin(pa) + \frac{p}{\gamma}\cos(pa) = 0. \tag{2.47}$$

The roots of this equation are nearly at the same points where $\ln N^2(p)$ has a discontinuous derivative. The difference between the roots of (2.47) and these points are of the order e^{-G}.

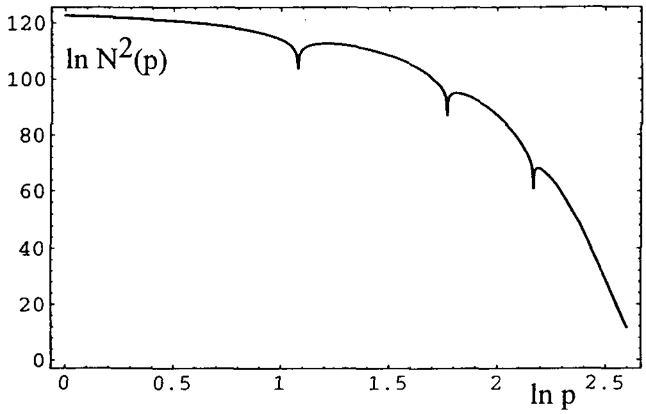

Figure 2.2: Plot of $\ln N^2(p)$ as a function of $\ln p$. Here $\frac{2}{N(p)}$ is the amplitude of the wave function behind the barrier (see Eq. (2.38)) and p is the wave number.

Treating p as a continuous variable, we can calculate $C_0(t)$. To this end we choose the initial wave packet to be

$$\Psi_0(r) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi r}{a}\right) & \text{for } r < a \\ 0 & \text{for } r > a \end{cases} . \tag{2.48}$$

Expanding this wave packet in terms of the wave function $\phi_p(r)$, Eq. (2.38), and substituting the result in Eq. (2.37) we find

$$C_0(t) = 8\pi^2 a \int_0^\infty \exp\left[\frac{-ip^2 t}{2m}\right] \frac{\sin^2(pa)}{N^2(p)(\pi^2 - p^2a^2)^2} dp. \tag{2.49}$$

When t is large then the main contribution to the integral (2.49) comes from the region where p is small. In this case we can write (2.49) as

$$C_0(t) = \frac{8a^3}{\pi^2} \int_0^\infty \exp\left[\frac{-ip^2 t}{2m}\right] \frac{p^2}{N^2(p)} dp. \tag{2.50}$$

Now we change the variables from p to E, where $p^2 = 2mE$, and we also expand $N^2(E)$ around its minimum (see Fig. (2.3)),

$$N^2(E) = (E_0 - E)^2 + \frac{1}{4}\Gamma^2. \tag{2.51}$$

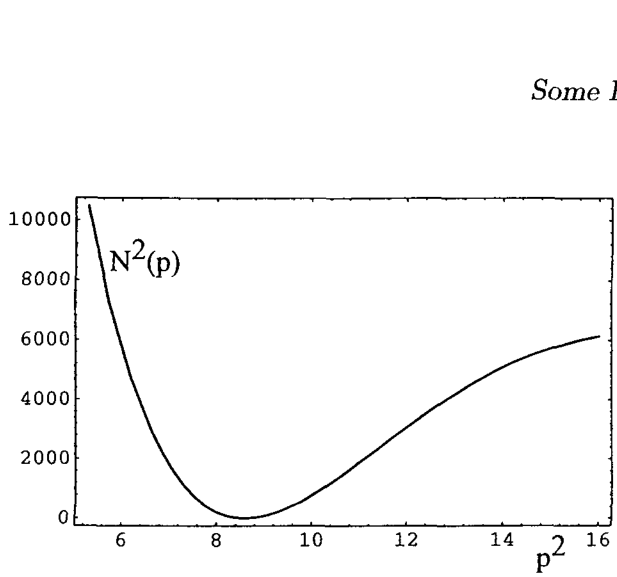

Figure 2.3: Plot of $N^2(p)$ versus p^2, see also Fig. (2.2).

Using this we can simplify (2.50)

$$C_0(t) = \frac{8a^3}{\pi^2}\sqrt{m}\left(\frac{\Gamma}{2}\right)\int_0^\infty \frac{1}{(E_0 - E)^2 + \frac{1}{4}\Gamma^2} e^{-iEt}\sqrt{E}dE. \tag{2.52}$$

To calculate this integral we rotate the contour of integration to coincide with the imaginary axis, and this enables us to calculate the part of the integral coming from the contribution of the pole at $E - \frac{i}{2}\Gamma$ analytically

$$\begin{aligned} C_0(t) &\approx \frac{8a^3}{\pi^2}\sqrt{m}\left\{2\pi\sqrt{E_0}\exp\left[-i(E_0 - \frac{i\Gamma}{2})t\right]\right. \\ &- \left. i^{\frac{3}{2}}\int_0^\infty \frac{\frac{\Gamma}{2}}{(E_0 + iE)^2 + \frac{1}{4}\Gamma^2} e^{-Et}\sqrt{E}dE\right\}. \end{aligned} \tag{2.53}$$

When t tends to infinity the largest terms in C_0 are;

$$C_0(t) \approx \frac{16a^3}{\pi}\sqrt{mE_0}\left\{\exp\left[-i\left(E_0 - \frac{i\Gamma}{2}\right)t\right] + \frac{1-i}{2\sqrt{\pi}}\left(\frac{\Gamma}{2E_0}\right)^{\frac{5}{2}}\left(\frac{2}{\Gamma t}\right)^{\frac{3}{2}}\right\}. \tag{2.54}$$

In Fig. (2.4) the probability of decay $P(t) = |\frac{C_0(t)}{C_0(0)}|^2$ is shown as a function of time. This curve is obtained from the numerical calculation of (2.52). The figure has been plotted for the values of $\Gamma = 0.2$ and $E_0 = 1$. In the same figure we have also shown $P_1(t) = \exp(-\Gamma t)$. The difference

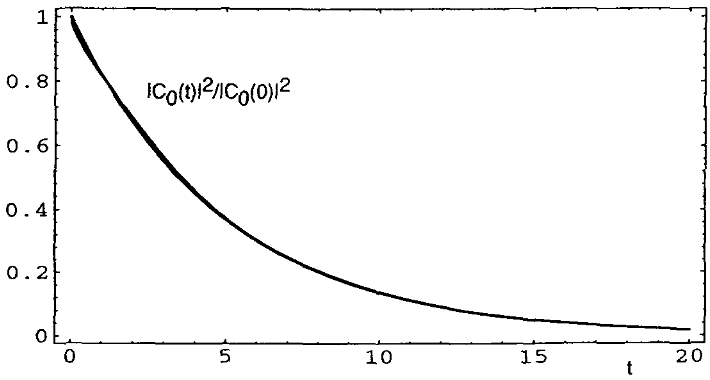

Figure 2.4: The decay probability $P(t)$ shown as a function of time. For comparison the exponential decay law $P_1(t) = \exp(-\Gamma t)$ is also shown.

between the two curves for the times shown in Fig. (2.4) are very small. When t tends to infinity, we can calculate this integral in terms of the erfc$\sqrt{t}$:

$$\int_0^\infty \frac{\sqrt{E}e^{-iEt}dE}{(E-E_0)^2+\frac{1}{4}\Gamma^2} = \frac{2\pi}{\Gamma}\left(E_0+\frac{i}{2}\Gamma\right)^{\frac{1}{2}} \exp\left[-\left(iE_0+\frac{1}{2}\Gamma\right)t\right] + \frac{\pi}{\Gamma}e^{-i\frac{\pi}{4}}\left\{F(E_0,\Gamma,t)-F(E_0,-\Gamma,t)\right\}, \quad (2.55)$$

where

$$F(E_0,\Gamma,t) = \left(-iE_0+\frac{\Gamma}{2}\right)^{\frac{1}{2}} \exp\left[\left(-iE_0+\frac{\Gamma}{2}\right)t\right] \operatorname{erfc}\sqrt{\left[\left(-iE_0+\frac{\Gamma}{2}\right)t\right]}. \quad (2.56)$$

Now if we use the expansion of the erfc (z), [19] then we find the result given in (2.54). A similar result can be found from the path integral formulation of quantum mechanics (see [20]). For very short times the decay of an initial state by tunneling is also nonexponential. This aspect of the decay was discussed earlier in this chapter and we will return to it again in Chapter 10. As we have seen earlier at the initial stages of decay $P(t) \approx 1 - \frac{At^2}{2}$. In the case of certain decays of atomic resonance states it is possible to confirm this quadratic time-dependence of $P(t)$ for short

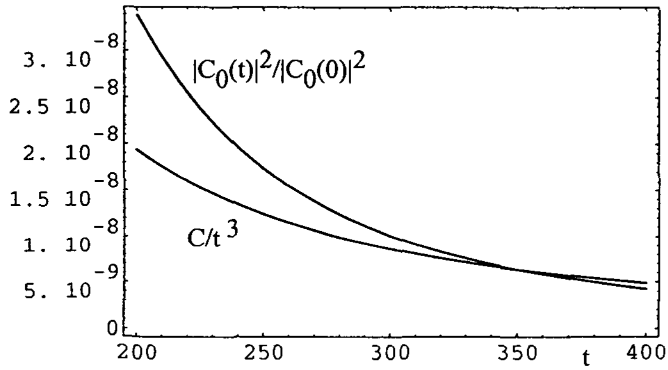

Figure 2.5: Long time behavior of the probability of decay showing $\frac{C}{t^3}$ behavior of $P(t)$.

times experimentally [21]. We have also the experimental verification of the nonexponential nature of decay by tunneling, where in a recent experiment ultra-cold sodium atoms were trapped in an alternating potential produced by light waves. The only way that these atoms could escape was by tunneling. The number of atoms left in the original state depended on the time of interaction if the depth of the potential and the acceleration were kept constant, and thus were measurable [22]. This experiment confirms the result that the decay rate remains constant for a very short time and then becomes exponential.

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Chapter 3

Semi-Classical Approximations

The WKB (Wentzel, Kramers and Brillouin) method is the most widely used approximation for solving tunneling problems [1] [2], and while it is often applied to one-dimensional cases [3] [4] [5], it is possible to modify it in different ways to solve two- or three-dimensional tunneling. In this chapter we discuss this approximate technique in some detail and find conditions for its validity [6], and then consider another semi-classical approximation, i.e. the Miller-Good method [7].

3.1 The WKB Approximation

Here the emphasis will be on the solution of one-dimensional problems, but later, we will see how this can be generalized to higher dimensions. Suppose that we want to find the approximate solution of the Schrödinger equation

$$\psi''(x) + Q(x)\psi(x) = 0, \tag{3.1}$$

where primes indicate derivatives with respect to x and

$$Q(x) = \frac{2m}{\hbar^2}(E - V(x)). \tag{3.2}$$

We first replace $\psi(x)$ by $\phi(x)$, where

$$\psi(x) = \exp[\phi(x)], \tag{3.3}$$

and substitute this in (3.1) to find

$$\phi''(x) + \phi'^2(x) + Q(x) = 0. \tag{3.4}$$

Now we can transform (3.4) to a Riccati equation [6] by changing ϕ to y';

$$\phi'(x) = y(x), \tag{3.5}$$

to obtain

$$y'(x) + y^2(x) + Q(x) = 0. \tag{3.6}$$

Remembering that in tunneling problems $y(x)$, in general, is a complex function, we write it as

$$y(x) = \alpha(x) + i\beta(x). \tag{3.7}$$

By substituting (3.7) in (3.6) and separating the real and imaginary parts we find two first order differential equations

$$\alpha' + \alpha^2 - \beta^2 + Q(x) = 0, \tag{3.8}$$

and

$$\beta' + 2\alpha\beta = 0. \tag{3.9}$$

Equation (3.9) can be integrated to yield

$$\int \alpha(x)dx = \ln\left(\frac{1}{\sqrt{\beta(x)}}\right) + C. \tag{3.10}$$

Thus from Eqs. (3.5), (3.7) and (3.10) we are able to find ϕ and ψ;

$$\phi(x) = \ln\left(\frac{1}{\sqrt{\beta(x)}}\right) + i\int \beta(x)dx, \tag{3.11}$$

and

$$\psi(x) = e^{\phi(x)} = \frac{1}{\sqrt{\beta(x)}}\left[A_1\cos\left(\int \beta(x)dx\right) + A_2\sin\left(\int \beta(x)dx\right)\right]. \tag{3.12}$$

This expression for $\psi(x)$ is the exact solution of Eq. (3.1). To find an approximate solution to (3.1) we observe that if in (3.8) we ignore α' and

α (we will see the conditions under which this is justified) then we have an algebraic equation for the unknown function β;

$$\beta(x) = \sqrt{Q(x)}. \tag{3.13}$$

Now if $Q(x)$ is positive from (3.12) and (3.13) we get

$$\psi(x) = \frac{1}{[Q(x)]^{\frac{1}{4}}} \exp\left[i\left(\int \sqrt{Q(x)}\, dx - \theta\right)\right]. \tag{3.14}$$

On the other hand if $Q(x)$ is negative, then we have

$$\psi(x) = \frac{1}{[-Q(x)]^{\frac{1}{4}}} \left\{A_1 \exp\left[\int \sqrt{-Q(x)}\, dx\right] + A_2 \exp\left[-\int \sqrt{-Q(x)}\, dx\right]\right\}. \tag{3.15}$$

Equations (3.8) and (3.9) show that this approximation is not valid at those points where $Q(x)$ is small or zero, but it is acceptable whenever $Q(x)$ is large. In order to estimate the error in this approximation we go back to Riccati equation (3.6) and write $y(x)$ as

$$y(x) = y_0(x) + \eta(x), \tag{3.16}$$

where $y_0(x)$ is the solution of the Riccati equation in the WKB approximation, i.e.

$$y_0(x) = i\sqrt{Q(x)} - \frac{1}{4}\frac{Q'(x)}{Q(x)}. \tag{3.17}$$

From Eqs. (3.16), (3.17) and (3.6) it follows that

$$\eta'(x) + \eta^2(x) + 2y_0(x)\eta(x) + \frac{1}{16}\left[(\ln Q(x))'\right]^2 - \frac{1}{4}(\ln Q(x))'' = 0. \tag{3.18}$$

Since we have assumed that $\eta(x)$ is a small function compared to $y(x)$, we can ignore $\eta^2(x)$ and $\eta'(x)$ in (3.18) and find $\eta(x)$ as

$$\eta(x) = \frac{(\ln Q(x))'' - \frac{1}{4}\left[(\ln Q(x))'\right]^2}{8i\sqrt{Q(x)}}, \tag{3.19}$$

where in the denominator we have replaced y_0, Eq. (3.17), by its largest part $i\sqrt{Q(x)}$. Equation (3.19) shows that the WKB approximation is valid when the right hand side of (3.19) is small. But in all tunneling problems $Q(x)$ changes sign, thus we have a region where $Q(x)$ is positive (oscillatory solution) and a part where $Q(x)$ is negative (exponential solution). Hence

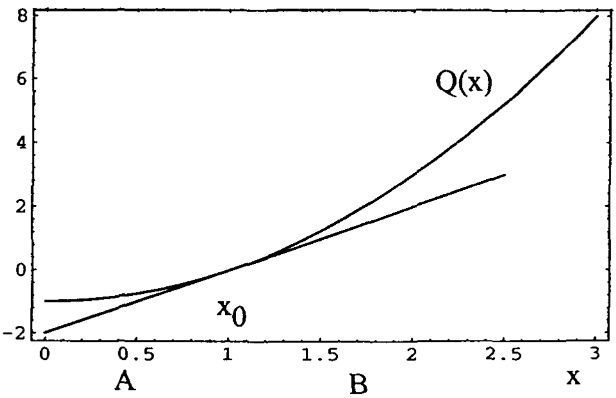

Figure 3.1: Approximating the potential by a linear function between the points A and B.

if Q is continuous it passes through zero.

When $Q(x) = 0$, or it is small, this method breaks down and we have to find another way of determining the solution. Let us assume that the WKB method is not valid for all points on the x-axis between A and B, and between these points $Q(x)$ changes sign. If $Q(x)$ is a smoothly varying function, we can approximate it by a straight line, i.e.

$$Q(x) = a(x - x_0), \quad A \leq x \leq B. \tag{3.20}$$

We also choose the origin of the coordinate system so that it coincides with x_0, then the Schrödinger equation for the segment AB can be written as

$$\psi''(x) + ax\psi(x) = 0, \quad A \leq x \leq B. \tag{3.21}$$

This differential equation can be integrated and the solution is given as the Bessel function. First we observe that if

$$\psi(x) = x^{\nu} J_p(\beta x^{\alpha}), \tag{3.22}$$

where J_p is the Bessel function of order p, then $\psi(x)$ satisfies the differential equation [8] [9]

$$\psi''(x) + \left(\frac{1 - 2\gamma}{x}\right)\psi'(x) + \left(\alpha^2\beta^2 x^{2\alpha-2} + \frac{\gamma^2 - \alpha^2 p^2}{x^2}\right)\psi(x) = 0. \tag{3.23}$$

Ncw if we compare Eq. (3.21) with Eq. (3.23) we conclude that the latter simplifies to the former provided that

$$\alpha = \frac{3}{2}, \quad \gamma = \frac{1}{2}, \quad p = \frac{1}{3} \text{ and } \alpha^2\beta^2 = a. \tag{3.24}$$

We set $\beta = 1$ and therefore we have $a = \frac{9}{4}$. Thus we can write the solution of (3.21) in terms of the Bessel function,

$$\psi(x) = \sqrt{x}\left\{A_1 J_{\frac{1}{3}}\left(x^{\frac{3}{2}}\right) + A_2 J_{\frac{-1}{3}}\left(x^{\frac{3}{2}}\right)\right\}. \tag{3.25}$$

Alternatively we can write ψ as a linear combination of $f(x)$ and $g(x)$, where

$$f(x) = \sqrt{x}\left[J_{\frac{1}{3}}\left(x^{\frac{3}{2}}\right) + J_{\frac{-1}{3}}\left(x^{\frac{3}{2}}\right)\right], \tag{3.26}$$

and

$$g(x) = \sqrt{x}\left[-J_{\frac{1}{3}}\left(x^{\frac{3}{2}}\right) + J_{\frac{-1}{3}}\left(x^{\frac{3}{2}}\right)\right]. \tag{3.27}$$

From the asymptotic expansion of the Bessel function we can find the asymptotic forms of $f(x)$ and $g(x)$ to be [6] [8]

$$f(x) \to 2\sqrt{\frac{2}{\pi}} x^{-\frac{1}{4}} \cos\left(\frac{\pi}{6}\right) \cos\left(x^{\frac{3}{2}} - \frac{\pi}{4}\right), \quad \text{as} \quad x \to \infty, \tag{3.28}$$

and

$$g(x) \to -2\sqrt{\frac{2}{\pi}} x^{-\frac{1}{4}} \sin\left(\frac{\pi}{6}\right) \sin\left(x^{\frac{3}{2}} - \frac{\pi}{4}\right), \quad \text{as} \quad x \to \infty. \tag{3.29}$$

To find the asymptotic form when x tends to $-\infty$, we first change the variable from x to t;

$$t^2 = x^3. \tag{3.30}$$

In terms of this new variable we have

$$f(-x) = t^{\frac{1}{3}} K_{\frac{1}{3}}(it), \tag{3.31}$$

and the asymptotic expansion of $f(-x)$ becomes

$$f(-x) \to t^{\frac{1}{3}}\sqrt{\frac{2}{\pi t}} e^{-t} \sin\left(\frac{\pi}{3}\right) = \sqrt{\frac{2}{\pi}} x^{-\frac{1}{4}} \sin\left(\frac{\pi}{3}\right) \exp\left(-\frac{x^3}{2}\right). \tag{3.32}$$

In the same way for $g(-x)$ we find

$$g(-x) \to \sqrt{\frac{2}{\pi}} x^{-\frac{1}{4}} \exp\left(\frac{x^3}{2}\right). \tag{3.33}$$

With the aid of these relations we find the connection formula for the wave function from a region where $Q(x)$ is negative to a part where $Q(x)$ is positive.

First we observe that

$$Q(x) = \frac{9}{4}x, \tag{3.34}$$

and

$$\int_0^x \sqrt{Q(x)}dx = x^{\frac{3}{2}}. \tag{3.35}$$

Similarly if $Q(x) < 0$, we take $x = -z$, then we have

$$\sqrt{-Q(x)} = \frac{3}{2}z^{\frac{1}{2}}, \tag{3.36}$$

and

$$\int_0^{-x} \sqrt{-Q(x)}dx = -z^{\frac{3}{2}}. \tag{3.37}$$

Now we choose the point $x = x_0$ at which $Q(x_0) = 0$ as a reference point and for negative $Q(x)$ we write $\psi(x)$ as

$$\begin{aligned} \psi(x) &= \frac{1}{[-Q(x)]^{\frac{1}{4}}}\left\{A_1 \exp\left[\int_{x_0}^x \sqrt{-Q(x)}dx\right]\right. \\ &+ \left. A_2 \exp\left[-\int_{x_0}^x \sqrt{-Q(x)}dx\right]\right\}, \end{aligned} \tag{3.38}$$

and in a similar way for positive $Q(x)$ we write

$$\begin{aligned} \psi(x) &= \frac{1}{[Q(x)]^{\frac{1}{4}}}\left\{A_1' \exp\left[i\int_{x_0}^x \sqrt{Q(x)}dx\right]\right. \\ &+ \left. A_2' \exp\left[-i\int_{x_0}^x \sqrt{Q(x)}dx\right]\right\}. \end{aligned} \tag{3.39}$$

But the four constants A_1, A_2, A_1' and A_2' are related to each other. For joining $\psi(x)$ on the two sides of $x = x_0$, we use $f(x)$ to find A_1 and $g(x)$ to obtain A_2. Thus by comparing Eqs. (3.32) and (3.28), writing the latter in terms of complex functions we find

$$A_1' = \exp\left(-i\frac{\pi}{4}\right)A_1, \tag{3.40}$$

and

$$A_2' = \exp\left(i\frac{\pi}{4}\right)A_1. \tag{3.41}$$

In the same way by writing (3.33) and (3.29) where the second equation is written in terms of complex function we obtain the following expressions

$$A_1{}' = \frac{i}{2}\exp\left(-i\frac{\pi}{4}\right)A_2, \tag{3.42}$$

and

$$A_2{}' = \frac{-i}{2}\exp\left(i\frac{\pi}{4}\right)A_2. \tag{3.43}$$

Thus the relations between A_i's and $A_i{}'$'s are

$$A_1{}' = \exp\left(-i\frac{\pi}{4}\right)\left[A_1 + \frac{i}{2}A_2\right], \tag{3.44}$$

and

$$A_2{}' = \exp\left(i\frac{\pi}{4}\right)\left[A_1 - \frac{i}{2}A_2\right]. \tag{3.45}$$

We can simplify these two and write them as

$$A_1{}' = \frac{1}{\sqrt{2}}\left[(1-i)A_1 + \frac{1}{2}(1+i)A_2\right], \tag{3.46}$$

and

$$A_2{}' = \frac{1}{\sqrt{2}}\left[(1+i)A_1 + \frac{1}{2}(1-i)A_2\right]. \tag{3.47}$$

In what we have discussed so far, we have assumed that $Q(x)$ goes from negative to positive. For cases where $Q(x)$ goes from positive to negative values, we can use the same arguments as above and find

$$A_1{}' = \frac{1}{\sqrt{2}}\left[\frac{1}{2}(1-i)A_1 + (1+i)A_2\right], \tag{3.48}$$

and

$$A_2{}' = \frac{1}{\sqrt{2}}\left[\frac{1}{2}(1+i)A_1 + (1-i)A_2\right]. \tag{3.49}$$

If needed we can invert the above relations and write A_1 and A_2 in terms of $A_1{}'$ and $A_2{}'$.

For those cases where a real wave function is desirable, e.g. for a double-well potential we can simplify the result:

(i) -We note that for regions where $\psi(x)$ is the sum of two exponentials, it is sufficient to take the coefficients of the two exponentials as real quantities.

(ii) -For the region where $\psi(x)$ is oscillatory we need real functions, and for this when $Q(x)$ is positive we write $\psi(x)$ as

$$\psi(x) = \frac{C}{[Q(x)]^{\frac{1}{4}}} \cos\left[\int_{x_0}^{x} \sqrt{Q(x)}dx - \theta\right], \tag{3.50}$$

i.e. we replace the two constant C and θ for A_1' and A_2' in (3.39). By comparing (3.39) and (3.50) we find

$$A_1' = \frac{C}{2}e^{-i\theta}, \quad A_2' = \frac{C}{2}e^{i\theta}. \tag{3.51}$$

Having expressed A_1' and A_2' in terms of C and θ, we can use Eqs. (3.48) and (3.49) to go from the region of positive $Q(x)$ (exponential) to the region of negative $Q(x)$ (sinusoidal) and find A_1 and A_2 in terms of C and θ;

$$A_1 = \frac{C}{2}\cos\left(\theta - \frac{\pi}{4}\right), \tag{3.52}$$

and

$$A_2 = -C\sin\left(\theta - \frac{\pi}{4}\right). \tag{3.53}$$

Also by solving for θ and C we have

$$\tan\left(\theta - \frac{\pi}{4}\right) = -\frac{A_2}{2A_1},. \tag{3.54}$$

and

$$C = \sqrt{4{A_1}^2 + {A_2}^2}. \tag{3.55}$$

This completes the problem of finding the connection formula for the WKB approximation [6].

As an application of the WKB approximation let us consider the tunneling of a particle of mass m and energy E through an arbitrary potential barrier $V(x)$. Denoting the classical turning points by a and b, the approximate solution of the Schrödinger equation can be written as

$$\begin{aligned}\psi_1(x) &= \frac{A_1}{(Q(x))^{\frac{1}{4}}}\exp\left[i\int_a^x \sqrt{Q(x')}dx'\right] \\ &+ \frac{B_1}{(Q(x))^{\frac{1}{4}}}\exp\left[-i\int_a^x \sqrt{Q(x')}dx'\right], \quad x < a,\end{aligned} \tag{3.56}$$

$$\begin{aligned}\psi_2(x) &= \frac{A_2}{(-Q(x))^{\frac{1}{4}}}\exp\left[-\int_a^x \sqrt{-Q(x')}dx'\right] \\ &+ \frac{B_2}{(-Q(x))^{\frac{1}{4}}}\exp\left[\int_a^x \sqrt{-Q(x')}dx'\right], \quad a < x < b,\end{aligned} \tag{3.57}$$

and

$$\begin{aligned}\psi_3(x) &= \frac{A_3}{(Q(x))^{\frac{1}{4}}}\exp\left[i\int_b^x \sqrt{Q(x')}dx'\right] \\ &+ \frac{B_3}{(Q(x))^{\frac{1}{4}}}\exp\left[-i\int_b^x \sqrt{Q(x')}dx'\right], \quad x > b.\end{aligned} \tag{3.58}$$

Using the connection formula for joining the three wave functions and then eliminating the constants A_2 and B_2 from these formulae we find

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 2e^{\sigma} + \frac{1}{2}e^{-\sigma} & i(2e^{\sigma} - \frac{1}{2}e^{-\sigma}) \\ -i(2e^{\sigma} - \frac{1}{2}e^{-\sigma}) & 2e^{\sigma} + \frac{1}{2}e^{-\sigma} \end{bmatrix}\begin{bmatrix} A_3 \\ B_3 \end{bmatrix}, \tag{3.59}$$

where

$$\sigma = \int_a^b \sqrt{-Q(x)}dx. \tag{3.60}$$

The transmission coefficient is defined by the relation $\left|\frac{A_3}{A_1}\right|^2$, i.e.

$$T(E) = \left|\frac{A_3}{A_1}\right|^2 = \frac{e^{-2\sigma}}{\left(1 + \frac{1}{4}e^{-2\sigma}\right)^2}. \tag{3.61}$$

3.2 Method of Miller and Good

This is a semi-classical method similar to the WKB approximation and is a useful way of studying tunneling problems [7]. Let us assume that the general solution of the linear differential equation

$$\frac{d^2\Phi(S)}{dS^2} + P^2(S)\Phi(S) = 0, \tag{3.62}$$

is known analytically. Furthermore the function $P^2(S)$ is a function of S with the same number of zeros as $Q(x)$, Eq. (3.2), and with the same degrees.

Now we define $\psi(x)$ in the following way

$$\psi(x) = T(x)\Phi[S(x)], \tag{3.63}$$

and find its first derivative

$$\psi''(x) = T''\Phi[S(x)] + \left[2T'S' + TS''\right]\frac{d\Phi}{dS} + T\left(S'\right)^2\frac{d^2\Phi}{dS^2}, \tag{3.64}$$

where primes denote derivatives with respect to x. If we choose T to be

$$T = \frac{1}{\sqrt{\frac{dS}{dx}}}, \tag{3.65}$$

then (3.64) can be written as

$$\psi''(x) = \left\{T'' - T(S')^2P^2[S(x)]\right\}\Phi[S(x)] = -Q(x)\psi(x). \tag{3.66}$$

By ignoring T'' in (3.66), we find the following condition for this transformation

$$P[S(x)]S'(x) = \sqrt{Q(x)}. \tag{3.67}$$

We can also write (3.67) as an integral

$$\int_{S(x_0)}^{S(x)} P(\sigma)d\sigma = \int_{x_0}^{x}\sqrt{Q(x)}dx. \tag{3.68}$$

Equation (3.68) can be regarded as the definition of $S(x)$. Thus we can write $\psi(x)$ as

$$\psi(x) = \frac{1}{\sqrt{\frac{dS}{dx}}}\Phi[S(x)], \tag{3.69}$$

and this function is continuous even at the points where $Q(x)$ is zero as long as $S'(x)$ is not zero at these points. From (3.68) it follows that if at $x = x_0$, the function $\sqrt{Q(x)}$ has a zero of order n, i.e. $\sqrt{Q(x)}$ is proportional to $(x - x_0)^n$, $P(S)$ also must have a zero of order n at this point. Thus if for a certain range of x, $Q(x)$ does not have a zero, we set $P(S) = 1$, and the result will be the same as we would get from the simple WKB approximation. On the other hand if $Q(x)$ about the point $x = x_0$ behaves as $Q(x) = a(x - x_0)$, then we choose $P^2(S) = S$, and Eq. (3.62) can be integrated to yield

$$\Phi(S) = Ai(-S) \quad \text{or} \quad \Phi(S) = Bi(-S), \tag{3.70}$$

where Ai and Bi are Airy functions [8]. From Eq. (3.68) we find the relation between S and x to be

$$S(x) = (a)^{\frac{1}{3}}(x - x_0), \tag{3.71}$$

and

$$\left(\frac{dS}{dx}\right)_{x_0} = (a)^{\frac{1}{3}} \neq 0. \tag{3.72}$$

Thus the wave function for this problem is

$$\psi(x) = \frac{C_1}{(a)^{\frac{1}{6}}} Ai\left[-(3a)^{\frac{1}{3}}(x - x_0)\right] + \frac{C_2}{(a)^{\frac{1}{6}}} Bi\left[-(3a)^{\frac{1}{3}}(x - x_0)\right], \tag{3.73}$$

where C_1 and C_2 are constants.

Next as an application of the method of Miller and Good we consider the problem of determination of the transmission coefficient through a barrier. Here $Q(x)$ will have two zeros of first order which we denote by x_1 and x_2 and since $Q(x)$ is real, the turning points will be complex conjugate of each other. We take x_1 to be the root with positive imaginary part and x_2 the other root. We write Eq. (3.62) as

$$\frac{d^2\Phi}{dS^2} + (F + S^2)\Phi(S) = 0, \tag{3.74}$$

in which F is a positive quantity. We denote the roots of $F + S^2$ in the following way

$$s_1 = -\sqrt{-F}, \quad s_2 = \sqrt{-F}, \quad \text{if } F < 0, \tag{3.75}$$

$$s_1 = i\sqrt{F}, \quad s_2 = -i\sqrt{F} \quad \text{if } F > 0. \tag{3.76}$$

Using the method just described we can write the approximate solution for ψ as

$$\psi \approx \frac{1}{\sqrt{\frac{dS}{dx}}} D_{\frac{1}{2}(iF-1)}\left(\sqrt{2}Se^{-i\frac{\pi}{4}}\right), \tag{3.77}$$

and

$$\psi \approx \frac{1}{\sqrt{\frac{dS}{dx}}} D_{\frac{1}{2}(-iF-1)}\left(\sqrt{2}Se^{i\frac{\pi}{4}}\right), \tag{3.78}$$

respectively, where $D_\nu(z)$ is the parabolic cylinder function of order ν [9] , and

$$\int_{S_1}^{S(x)} (F + \sigma^2)^{\frac{1}{2}} d\sigma = \int_{x_1}^{x} \sqrt{Q(x)}dx. \tag{3.79}$$

The parameter F is chosen in such a way that it satisfies the equality

$$\int_{x_1}^{x_2} \sqrt{Q(x)}dx = \int_{S_1}^{S_2} (F + \sigma^2)^{\frac{1}{2}} d\sigma = -\frac{1}{2}i\pi F. \tag{3.80}$$

In the integration over σ, for $F > 0$ and S real, we choose a branch of the square root for which $\arg\sqrt{F+S^2} = 0$, and for the same branch when $F \le 0$ and S is real then the choice is

$$\arg\sqrt{F+S^2} = \begin{cases} 0 & \text{for } S < s_1 \\ \frac{\pi}{2} & \text{for } s_1 < S < s_2 \\ 0 & \text{for } s_2 < S \end{cases} . \tag{3.81}$$

We have to use this same branch for integrating over x. From Eq. (3.80) it follows that F is real and positive if $k^2 = \frac{2mE}{\hbar^2}$ is greater than the maximum of $\frac{2mV(x)}{\hbar^2}$ and F is real and negative if k^2 is less than $\frac{2mV(x)}{\hbar^2}$. Also from Eqs. (3.79) and (3.80) it follows that when x is real, S is also real. For calculating the transmission coefficient, we need to know the asymptotic form of $\psi(x)$. Eq. (3.79) shows us that

$$\lim_{x\to\pm\infty} S(x) \to \pm\infty. \tag{3.82}$$

In addition we know the asymptotic form of $D_n(z)$, which is given by the following relations:

If $\arg z = 0$ or $\arg z = -\frac{\pi}{4}$ we have

$$D_n(z) \sim z^n \exp\left(-\frac{1}{4}z^2\right), \tag{3.83}$$

and if $\arg z = \frac{3\pi}{4}$, we have

$$D_n(z) \sim z^n \exp(-\frac{1}{4}z^2) - \frac{\sqrt{2\pi}}{\Gamma(-n)} e^{in\pi} \exp\left(\frac{1}{4}z^2\right) z^{-n-1}. \tag{3.84}$$

Therefore if

$$I = \left(2e^{-i\frac{\pi}{2}}\right)^{\frac{1}{4}} \left[\frac{|F|e^{\frac{3\pi i}{2}}}{2e}\right]^{\frac{-iF}{4}} \frac{1}{\sqrt{S'}} D_{\frac{1}{2}(iF-1)}\left(\sqrt{2}e^{-i\frac{\pi}{4}}S\right), \tag{3.85}$$

then

$$\begin{aligned} \lim_{x\to-\infty} I \quad &\to \quad \left\{\sqrt{\frac{2}{\pi}}\left(\frac{|F|}{2e}\right)^{-\frac{1}{2}iF} \Gamma\left[\frac{1}{2}(iF+1)\right] \cosh\left(\frac{F\pi}{2}\right) \exp\left(\frac{F\pi}{4}\right)\right\} \\ &\times \quad \left\{\frac{1}{[Q(x)]^{\frac{1}{4}}} \exp\left[-i\mathrm{Re}\int_x^{x_1} \sqrt{Q(x)}dx\right]\right\} \\ &+ \quad \left\{\frac{e^{-i\frac{\pi}{2}}}{[Q(x)]^{\frac{1}{4}}} \exp\left[i\mathrm{Re}\int_x^{x_1} \sqrt{Q(x)}dx\right]\right\}, \end{aligned} \tag{3.86}$$

and

$$\lim_{x\to\infty} I \to \frac{e^{F\frac{\pi}{2}}}{[Q(x)]^{\frac{1}{4}}} \exp\left[i\mathrm{Re}\int_{x_2}^{x} \sqrt{Q(x)}dx\right]. \tag{3.87}$$

From these equations it follows that the ratio of the current transmitted to the incident current is given by [7]

$$|T|^2 = \frac{1}{|1+\exp(-F\pi)|} = \frac{1}{|1+\exp[-2i\int_{x_1}^{x_2}\sqrt{Q(x)}dx]|}, \tag{3.88}$$

and for the tunneling problem we have

$$|T|^2 = \frac{1}{1+\exp[2\int_{x_1}^{x_2}\sqrt{\frac{2m}{\hbar^2}(V(x)-E)}dx]}. \tag{3.89}$$

When the exponential term in (3.89) is much larger than one, then

$$|T|^2 = \exp\left[-2\int_{x_1}^{x_2}\sqrt{\frac{2m}{\hbar^2}(V(x)-E)}dx\right]. \tag{3.90}$$

which agrees with the WKB result when in Eq. (3.61) $\sigma > 1$.

3.3 Calculation of the Splitting of Levels in a Symmetric Double-Well Potential Using WKB Approximation

As an application of the method that we have discussed in this chapter let us find the energy splitting for the lowest eigenvalues of a symmetric double-well caused by tunneling [2] [10].

Consider the double well shown in Fig. (3.2) where the two wells are separated by the central barrier. If the barrier were impenetrable (i.e. its maximum height was infinite), then the energy levels would correspond to the motion of a particle in one of the two wells. But since for a finite barrier tunneling is possible, each energy level splits into two and these two levels correspond to the motion of the particle in the two wells at the same time.

Let us denote the lowest eigenvalue and its corresponding eigenfunction in the well to the left of the barrier by E_0 and ψ_0 respectively. Since the wave function becomes exponentially small to the left of the well and also

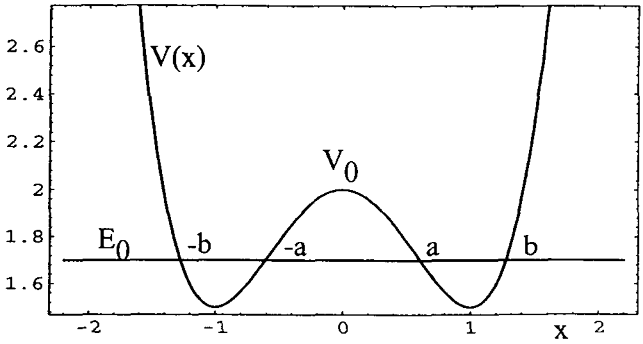

Figure 3.2: A symmetric double-well potential $V(x)$ is shown which for the energy E_0 has four turning points. If either V_0 or a is large then the particle will be either in the left well or in the right well.

inside the central barrier, the eigenfunction between the two turning points is given by

$$\psi_0(x) = \frac{C}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_{-b}^{x} p(x)dx + \frac{\pi}{4}\right], \quad -b \le x \le -a, \tag{3.91}$$

and inside the barrier it is

$$\psi_0(x) = \frac{-iC}{\sqrt{|p(x)|}} \exp\left[\frac{1}{\hbar}\left|\int_{-a}^{x} p(x)dx\right|\right], \quad x \ge -a, \tag{3.92}$$

where

$$p(x) = \sqrt{2m(E - V(x))}. \tag{3.93}$$

The constant C can be determined from the normalization condition

$$\int_{-b}^{-a} |\psi_0(x)|^2 dx = 1. \tag{3.94}$$

From Eqs. (3.91) and (3.94) we have

$$C^2 \int_{-b}^{-a} \frac{dx}{p(x)} \sin^2\left\{\frac{1}{\hbar}\int_{-b}^{x} p(x)dx + \frac{\pi}{4}\right\} = 1. \tag{3.95}$$

Since the quantity inside the curly bracket changes very rapidly, we can replace it by its average value, $\frac{1}{2}$, to get

$$\frac{1}{2}C^2\int_{-b}^{-a}\frac{dx}{p(x)} = 1. \tag{3.96}$$

Now let us define T_0 by the relation

$$T_0 = 2m\int_{-b}^{-a}\frac{dx}{p(x)}, \tag{3.97}$$

where T_0 is the period and $\omega = \frac{2\pi}{T_0}$ is the angular frequency for oscillation of the particle in the left well [11]. Thus we note that $\psi_0(x)$ is very small in the right well and $\psi_0(-x)$ is very small in the left well. If the probability of the penetration in the central barrier is small, we can construct a symmetric and an antisymmetric wave function from $\psi_0(x)$;

$$\psi_S(x) = \frac{1}{\sqrt{2}}[\psi_0(x) + \psi_0(-x)], \tag{3.98}$$

and

$$\psi_A(x) = \frac{1}{\sqrt{2}}[\psi_0(x) - \psi_0(-x)]. \tag{3.99}$$

From these relations it follows that at $x = 0$, $\psi_S{}' = 0$, $\psi_S(0) = \sqrt{2}\psi_0(0)$ and

$$\int_0^\infty \psi_0(x)\psi_S(x) \approx \frac{1}{\sqrt{2}}\int_0^\infty \psi_0{}^2(x)dx = \frac{1}{\sqrt{2}}. \tag{3.100}$$

Let us denote the eigenvalues of (3.98) and (3.99) by E_S and E_A respectively. To find these we write the Schrödinger equations

$$\frac{d^2\psi_0(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E_0 - V(x)\right)\psi_0(x) = 0, \tag{3.101}$$

and

$$\frac{d^2\psi_S(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E_S - V(x)\right)\psi_S(x) = 0. \tag{3.102}$$

By multiplying (3.101) by $\psi_S(x)$ and (3.102) by $\psi_0(x)$ and subtracting from each other using $\psi_S{}'(0) = 0$, $\psi_S(0) = \sqrt{2}\psi_0(0)$ and Eq. (3.100) we find

$$E_S - E_0 = -\frac{\hbar^2}{m}\psi_0(0)\psi_0{}'(0). \tag{3.103}$$

Similarly for $E_A - E_0$, we find

$$E_A - E_0 = \frac{\hbar^2}{m}\psi_0(0)\psi_0'(0). \tag{3.104}$$

Again by subtracting (3.104) from (3.103) we find

$$E_A - E_S = \frac{2\hbar^2}{m}\psi_0(0)\psi_0'(0). \tag{3.105}$$

The right hand side of this relation can be calculated from (3.92). Thus we have

$$\psi_0(x) = \sqrt{\frac{\omega}{2\pi v_0}} \exp\left[-\frac{1}{\hbar}\int_{-a}^{0} |p(x)|\, dx\right], \tag{3.106}$$

and

$$\psi_0'(0) = \frac{m v_0}{\hbar}\psi_0(0) \tag{3.107}$$

where

$$v_0 = \sqrt{\left[\frac{2}{m}\left(V(x=0) - E_0\right)\right]}. \tag{3.108}$$

Substituting these in (3.105) we have the following equation for the splitting between the two levels E_S and E_A [2];

$$E_A - E_S = \frac{\omega\hbar}{\pi}\exp\left[-\frac{1}{\hbar}\int_{-a}^{a} |p(x)| dx\right]. \tag{3.109}$$

To test the accuracy of this approximation let us consider the potential

$$V(x) = \left[\frac{1}{8}\xi^2\cosh(4x) - 4\xi\cosh(2x) - \frac{1}{8}\xi^2\right] + V_0. \tag{3.110}$$

This potential has a minimum at the points $x_m = \pm\frac{1}{2}\cosh^{-1}(\frac{8}{\xi})$, and we choose V_0 so that $V(x_m) = 0$. If we expand $V(x)$ around one of these two points we find that $V(x)$ can be approximated by a simple harmonic potential

$$V_a(x) = \frac{1}{2}K(x + x_m)^2. \tag{3.111}$$

The energy levels of this oscillator are given by:

$$E'_n = \frac{\sqrt{K}}{2}(2n+1). \tag{3.112}$$

Next we set $\xi = (\frac{8}{\cosh 2})$ so that $x_m = \pm 1$, then we find $E'_0 = 5.453$. The exact eigenvalues for the four lowest levels of this potential is known analytically (see Chapter 7), and the ground and the first excited states energies are ϵ_0 =5.8718 and ϵ_1 =7.1085 respectively. Thus the exact energy difference between these two levels is $\Delta\epsilon = 1.2368$, whereas the approximate value for $\Delta E = E_A - E_S$ calculated from (3.109) is 0.84.

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Chapter 4

Generalization of the Bohr-Sommerfeld Quantization Rule and its Application to Quantum Tunneling

In addition to the semi-classical methods that we studied in the previous chapter, there is the well known technique of the Bohr and Sommerfeld which can be applied to solve the problems of quantum tunneling. In this chapter we first discuss the application of this method to the problem of decay of a particle trapped behind a barrier and the approximate determination of the decay width Γ [1]. Then we show how in the case of the double-well potentials, the approximate energies of the low-lying states can be calculated.

In what follows, unless otherwise stated, we use the units where $\hbar = m = 1$. Let us assume that the potential $V(x)$ is continuous but otherwise arbitrary function of x, and let us denote the point $x = x_m$ as the point where the potential is maximum. We expand $V(x)$ around this point and we write the local momentum of the particle as a function of $x - x_m$;

$$p(x) = \sqrt{\frac{1}{4}\rho^2 - a}, \quad a = \frac{1}{\omega}\left(V(x_m) - E\right), \tag{4.1}$$

where ρ is a dimensionless variable which is defined by

$$\rho = \alpha(x - x_m), \quad \alpha = \sqrt{\frac{m\omega}{\hbar}} = \sqrt{\omega}, \tag{4.2}$$

and in these relations ω is given by

$$\omega = \sqrt{-V''(x_m)}. \tag{4.3}$$

By replacing the terms $(E - V(x))$ in the Schrödinger equation by its approximate form (4.1), we can find the solution of the wave equation with the outgoing boundary condition to be

$$\psi_1(x) = C_1 D_{-\frac{1}{2}-ia}\left[\rho \exp\left(\frac{-i\pi}{4}\right)\right], \tag{4.4}$$

where $D_\nu(z)$ is the parabolic cylinder function [2]. From the left side of the barrier, i.e. for $\rho < 0$ and $|\rho| >> a$ this function must join the semi-classical wave function (see also Eq. (3.91))

$$\psi_2(x) = \frac{C_2}{\sqrt{p(x)}} \sin\left[\theta(x) + \frac{\pi}{4}\right], \tag{4.5}$$

where

$$\theta(x) = \int_{x_0}^{x} p(x)dx. \tag{4.6}$$

In Eqs. (4.4) and (4.5), C_1 and C_2 are constants and x_0 is the classical turning point located to the left of the barrier. According to the Bohr-Sommerfeld rule of quantization, the phase difference between the wave functions (4.4) and (4.5) in the region where they overlap i.e. $a << |\rho| << \alpha x_m$ is $n\pi$. Now using the asymptotic form of $D_\nu(z)$ as $z \to \infty$ we find the following relation

$$\int_{x_0}^{x_1} p(x, E)dx = \left[n + \frac{1}{2} - \frac{1}{2\pi}\phi(a)\right]\pi, \tag{4.7}$$

where

$$\phi(a) = \frac{1}{2i}\ln\left\{\frac{\Gamma(\frac{1}{2} + ia)}{\Gamma(\frac{1}{2} - ia)[1 + \exp(-2\pi a)]}\right\} + a(1 - \ln a), \tag{4.8}$$

and

$$a = \frac{1}{\pi}\int_{x_0}^{x_1} \sqrt{-p^2(x, E)}dx. \tag{4.9}$$

Here $\Gamma(z)$ in Eq. (4.8) is the gamma function . For a barrier with the shape of an inverted parabola we can integrate (4.9) in closed form with the result given in (4.1). However (4.9) can be used for any arbitrary potential with a maximum between the two turning points x_1 and x_2. When E is a real number (i.e. the energy eigenvalue for a stationary problem) a is also real.

As an application of the above method let us consider the three-dimensional problem of escape of a particle trapped behind the barrier when the effective potential is given by

$$V_{eff} = V(r) + \frac{(l+\frac{1}{2})^2}{2r^2}. \tag{4.10}$$

In this case

$$p(r) = \left[2\left(E_r - \frac{i}{2}\Gamma - V_{eff}\right)\right]^{\frac{1}{2}}. \tag{4.11}$$

If the penetration under the barrier is small, i.e. $a >> 1$, then to simplify the result we use the expanded form of $\phi(a)$, Eq. (4.8),

$$\phi(a) = \frac{1}{24a} + \frac{7}{2880a^3} + \ldots.. + \frac{i}{2}e^{-2\pi a}, \tag{4.12}$$

and from Eq. (4.7) we find the following results:

$$\Gamma = \frac{1}{T_0}\exp\left[-2\int_{r_1}^{r_2}|p(r)|dr\right], \tag{4.13}$$

and

$$T_0 = 2\int_{r_0}^{r_1}\frac{dr}{p(r)}, \tag{4.14}$$

where T_0 is the period of oscillation in the well between the turning points $r_0 < r < r_1$ [3]. Equation (4.13) is the well-known Gamow's formula for the decay width (Chapter 5).

Let us emphasize that (4.13) is valid not only for small a but also for $a >> 1$, as can be seen from Eqs. (4.1) and (4.12), therefore it may be argued that the method is valid even for $a \approx 1$. When it is used for stationary problems, this approach yields real E, but in the case of quasi-stationary states, e.g. a particle trapped behind a barrier which can escape to infinity, E would be complex.

Equations (4.7) - (4.9) are the generalized form of the Bohr-Sommerfeld rule. For a more accurate approximation we observe that for a small, when (4.1) is valid we can define J as

$$J = \frac{1}{\omega}(V(x_m) - E). \tag{4.15}$$

For quadratic potentials $a = J$, but from the definition of a, Eq. (4.9) it is evident that

$$\frac{da(J)}{dJ} = \frac{\omega}{\pi}\int_{x_1}^{x_2} \frac{1}{\sqrt{2\left(V(x)-E\right)}}dx, \quad a(0) = 0. \tag{4.16}$$

Since we have assumed that $V(x)$ is a continuous and differentiable function of x, we can expand it as

$$V(x) = V(x_m) - \frac{1}{2}\omega^2(x-x_m)^2[1 + v_1\rho + v_2\rho^2 + ...], \tag{4.17}$$

where

$$\rho = \alpha(x - x_m) = \sqrt{\omega}(x - x_m), \tag{4.18}$$

and $v_1, v_2......$ are the coefficients of expansion of $V(x)$ around $x = x_m$. From (4.16) and (4.17) we conclude that

$$a = J + c_2 J^2 + ..., \tag{4.19}$$

where

$$c_2 = -\frac{3}{4}\left(v_2 - \frac{5}{4}{v_1}^2\right). \tag{4.20}$$

As an example of this formulation let us consider the case where the central potential is given by

$$V_{eff} = \begin{cases} 0 & \text{for } 0 < r < L \\ V_0 & \text{for } L < r < L + a \\ 0 & \text{for } r > R + L \end{cases}. \tag{4.21}$$

Here we want to determine the decay width for the S-wave. For this potential the Schrödinger equation for a particle trapped in the region $0 < r < L$ with the outgoing boundary condition, $\psi(r) \to \exp(ikr)$, as $r \to \infty$ is exactly solvable and the solution gives us the quasi-stationary levels as the roots of the complex eigenvalue equation (see Chapter 6),

$$\frac{(q - ik)[q + k\cot(kL)]}{(q + ik)[q - k\cot(kL)]} = \exp(-2qa), \tag{4.22}$$

where $k = \sqrt{2E}$ and $q = \sqrt{2(V_0 - E)}$. If we have a relatively thick barrier so that $\exp(-2qa) << 1$, then for (4.22) we find the roots $E = E_r + \Delta E_r - \frac{i}{2}\Gamma$;

$$\frac{\Delta E_r}{E_r} = \frac{4\varepsilon(1-2\varepsilon)}{1 + q_r L}\exp(-2q_r a), \tag{4.23}$$

and

$$\frac{\Gamma}{E_r} = \frac{16\sqrt{\varepsilon(1-\varepsilon)}}{1+q_r L}\exp(-2q_r a). \tag{4.24}$$

In these equations we have used the following symbols

$$\varepsilon = \frac{V_0 - E}{V_0}, \quad (0 < \varepsilon < 1), \;\; E = E_r + \Delta E_r - \frac{i}{2}\Gamma, \tag{4.25}$$

and where the quantities q_r and $E_r = \frac{1}{2}{k_r}^2$ are found from the lowest root of

$$k_r \cot(k_r L) = -q_r = -\sqrt{2\left(V_0 - \frac{1}{2}{k_r}^2\right)}. \tag{4.26}$$

Now the exact solution of the transmission coefficient $|T|^2$ for a rectangular barrier (4.21) is given by (see Eq. (6.71))

$$|T|^2 = \frac{4k^2\gamma^2}{(k^2+q^2)^2 \sinh^2(qa) + 4k^2q^2}. \tag{4.27}$$

When the condition $\exp(-2qa) << 1$ is satisfied, we can expand $|T|^2$ in powers of $\exp(-2qa) << 1$ and find

$$|T|^2 = 16\varepsilon(1-\varepsilon)\exp(-2q_r a) + O(\exp(-4q_r a)). \tag{4.28}$$

Also we note that the time of oscillation of a particle behind the barrier, i.e. in the region $0 < r < L$ is given by $T_0 = \frac{2L}{k_r}$, therefore Γ satisfies the equation

$$\Gamma = \frac{q_r L}{1+q_r L}\left\{\frac{|T|^2}{T_0}\right\} + O(|T|^4). \tag{4.29}$$

This equation agrees with Gamow's result (see Chapter 5) when $L >> \frac{1}{q_r}$. Note that the difference between Eqs. (4.13) and (4.14) and Eq. (4.29) is due to the fact that in this example $V(r)$ is not a continuous and differentiable function of r.

4.1 The Bohr-Sommerfeld Method for Tunneling in Symmetric and Asymmetric Wells

As a next application of this rule we want to calculate the energy levels of a double-well potential. Let us consider a particle of mass m moving

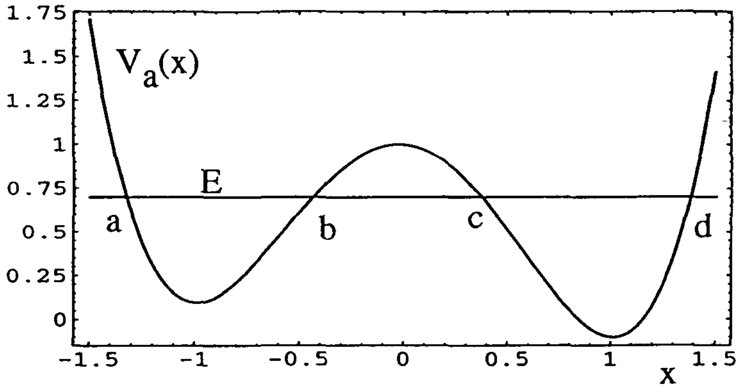

Figure 4.1: An asymmetric potential $V_a(x)$ and four turning points for the energy E.

in a confining potential $V(x)$, i.e. a potential which goes to infinity as $x \to \pm\infty$. For this problem we derive the Bohr-Sommerfeld rule from the WKB approximation . In Fig. (4.1) we have plotted an asymmetric double-well to show that for the low-lying levels, there are four turning points, these are denoted by a, b, c and d respectively. Now making use of the WKB method we write the wave function for the different regions in the following way:

For $x > d$ we write

$$\psi_1(x) = \frac{1}{2\sqrt{|p(x)|}} \exp\left[-\int_d^x |p(x)|dx\right], \quad x > d, \tag{4.30}$$

where $p(x) = \sqrt{2m(E - V(x))}$ and we have set $\hbar = 1$.

For $c < x < d$, we have

$$\psi_2(x) = \frac{1}{\sqrt{p(x)}} \cos\left[\int_x^d p(x)dx - \frac{\pi}{4}\right], \quad c < x < d. \tag{4.31}$$

This last equation can also be written as the sum of two exponentials:

$$\begin{aligned}\psi_2(x) &= \frac{\exp\left[i(\phi_2 - \frac{\pi}{2})\right]}{2\sqrt{p(x)}} \exp\left[-i\int_c^x p(x)dx - \frac{i}{2}g(\gamma) + i\frac{\pi}{2}\right] \\ &+ \text{ complex conjugate of the first term}, \quad c < x < d. \qquad (4.32)\end{aligned}$$

Here

$$\gamma = \frac{1}{\pi}\int_b^c |p(x)|dx, \tag{4.33}$$

and

$$\phi_2 = \int_c^d p(x)dx + \frac{1}{2}g(\gamma). \tag{4.34}$$

The function $g(\gamma)$ is a real function defined by

$$g(\gamma) = \arg\Gamma\left(\frac{1}{2} + i\gamma\right) - \gamma \ln|\gamma| + \gamma. \tag{4.35}$$

For the third region $b < x < c$, the wave function $\psi_3(x)$ is composed of two terms

$$\psi_3(x) = A\exp\left[-\int_x^c |p(x)|dx\right] + B\exp\left[\int_x^c |p(x)|dx\right], \quad b < x < c. \tag{4.36}$$

This $\psi_3(x)$ should join $\psi_4(x)$ for the part $a < x < b$ with the WKB condition. Imposing this joining condition we write $\psi_4(x)$ as

$$\begin{aligned}
\psi_4(x) &= \frac{1}{\sqrt{p(x)}}\left[\sqrt{1+\exp(2\pi\gamma)}\sin(\phi_1+\phi_2) + e^{\pi\gamma}\sin(\phi_1-\phi_2)\right] \\
&\times \cos\left(\int_a^x p(x)dx - \frac{\pi}{4}\right) \\
&- \frac{1}{\sqrt{p(x)}}\left[\sqrt{1+\exp(2\pi\gamma)}\cos(\phi_1+\phi_2) + e^{\pi\gamma}\cos(\phi_1-\phi_2)\right] \\
&\times \sin\left(\int_a^x p(x)dx - \frac{\pi}{4}\right), \quad a < x < b.
\end{aligned} \tag{4.37}$$

Here the phase ϕ_1 is obtained from the condition of continuity of ψ_3 and ψ_4 at $x = b$, and is given by

$$\phi_1 = \int_a^b p(x)dx + \frac{1}{2}g(\gamma). \tag{4.38}$$

For the last part, $x < a$, the wave function $\psi_5(x)$ is a damped exponential;

$$\psi_5(x) = N\exp\left[-\int_x^a |p(x)|dx\right], \quad x < a, \tag{4.39}$$

and this should join $\psi_4(x)$ at $x = a$. The last condition is met if the coefficient of the last term in (4.37) is zero, i.e.

$$\left[\sqrt{1+\exp(2\pi\gamma)}\cos(\phi_1+\phi_2) + e^{\pi\gamma}\cos(\phi_1-\phi_2)\right] = 0. \tag{4.40}$$

Then N in (4.39) is obtained by setting $\psi_4(a) = \psi_5(a)$.

The roots of (4.40) are the eigenvalues of the problem when there are four turning points. By substituting the expressions for ϕ_1 and ϕ_2, Eqs. (4.34) and (4.38) in (4.40) we can write the latter in the more familiar form of

$$\frac{1}{\pi}\int_a^b p(x)dx + \frac{1}{\pi}\int_c^d p(x)dx = n + \frac{1}{2} + \delta_n, \quad E < V(c), \quad n = 0, 1, 2.... \tag{4.41}$$

where δ_n is given by

$$\begin{aligned}\delta_n &= \frac{(-1)^n}{\pi}\sin^{-1}\left\{\frac{1}{\sqrt{1+\exp(-2\pi\gamma)}}\cos\left[\int_a^b p(x)dx - \int_c^d p(x)dx\right]\right\} \\ &- \frac{1}{\pi}g(\gamma).\end{aligned} \tag{4.42}$$

For a symmetric potential we can simplify (4.41) further and write it as

$$\begin{aligned}\frac{1}{\pi}\int_a^b p(x)dx &= s + \frac{1}{2} + \frac{1}{2\pi}\left[-g(\gamma) \pm \tan^{-1}(e^{-\pi\gamma})\right], \\ E < V(c), \; s &= 0, 1, 2, ...\end{aligned} \tag{4.43}$$

4.2 Numerical Examples

Equations (4.41) and (4.43) are the semi-classical quantization rule for the double-well potentials . Chebotarev who has found these generalization of the Bohr-Sommerfeld rule has also applied them to calculate the low-lying energy levels of the following potentials [4]:
(i) - An asymmetric potential of the form

$$V_a(x) = \frac{V_0}{L^4}\left[\left(x^2 - L^2\right)^2 - \frac{1}{10}xL^3\right]. \tag{4.44}$$

(ii) - A symmetric potential which is given by

$$V_s(x) = \frac{V_0}{L^4}\left(x^2 - L^2\right)^2. \tag{4.45}$$

He has found the energy levels for $n = 0$, 1, and 2. Expressing the results in units of V_0 and choosing L to be $\frac{5}{\sqrt{2mV_0}}$, the energy levels for the symmetric potential are: $E_0 = 0.377$, $E_1 = 0.382$ and $E_2 = 0.946$. These should be compared to $E_0 = 0.374$, $E_1 = 0.380$ and $E_2 = 0.942$, the exact results obtained from the numerical solution of the Schrödinger equation. For the asymmetric potential $V_a(x)$, the Bohr-Sommerfeld rules gives $E_0 = 0.288$, $E_1 = 0.469$ and $E_2 = 0.921$, whereas the exact results are $E_0 = 0.285$, $E_1 = 0.467$ and $E_2 = 0.917$. Thus this method is a very accurate way of calculating the low-lying eigenvalues.

The splitting caused by the tunneling through the central part of a symmetric potential $V_s(x)$, can be found by first writing Eq. (4.43) for $E + \Delta E$ and for $E - \Delta E$ keeping the same s, i.e.

$$\begin{aligned} & \frac{1}{\pi}\int_a^b p(x, E \pm \Delta E)dx \\ = \quad & (s + \frac{1}{2}) + \frac{1}{2\pi}\left\{-g[\gamma(E \pm \Delta E)] \pm \tan^{-1}(\exp[-\pi\gamma(E)])\right\}. \end{aligned} \quad (4.46)$$

Then by expanding (4.46) for both $E + \Delta E$ and $E - \Delta E$ and assuming that $\frac{\Delta E}{E} << 1$, and also noting that the contributions from the changes in a, b and c are zero, we find the following expression for ΔE;

$$\Delta E \approx \frac{\tan^{-1}(\exp[-\pi\gamma(E)])}{\int_a^b \frac{\partial p}{\partial E}dx + \frac{\partial g}{\partial \gamma}\int_c^b \frac{\partial |p|}{\partial E}dx}. \quad (4.47)$$

If we ignore the second term in the denominator and if we approximate $\tan^{-1}(x)$ by x, then this ΔE will be the same as the one given by Eq. (3.109).

The level splitting ΔE for the symmetric potential (4.45) calculated from (4.47) is about 0.0057 whereas the exact numerical calculation yields 0.0060. In addition to the approximate techniques of calculating the splitting between the ground and the first excited state that we have discussed in this and in the previous chapter, there are other methods among which we should mention the iterative method which has been recently proposed by Friedberg *et al* [5].

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Chapter 5

Gamow's Theory, Complex Eigenvalues, and the Wave Function of a Decaying State

The theory of the α-decay of a nucleus by tunneling through the Coulomb potential was developed by Gamow [1] [2] who solved the Schrödinger equation approximately with outgoing wave boundary condition and found complex discrete eigenvalues [3].

In this chapter we study Gamow's theory, first by using the complex eigenstates, and later with the help of the wave packets. In the last part of this chapter we consider very special cases where the approximate method of Gamow fails completely.

5.1 Solution of the Schrödinger Equation with Radiating Boundary Condition

This method which was proposed by Gamow to explain α-radioactivity is a simple way of solving the Schrödinger equation with radiating boundary condition . For simplicity let us consider the zero angular momentum state

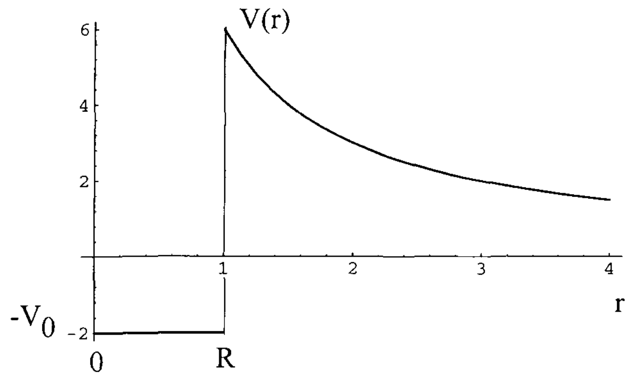

Figure 5.1: A simplified picture of the potential for studying the α-decay and the Gamow states.

(or S-wave) and replace $\psi(r)$ by the reduced wave function $u(r)$ [3] [4]

$$\psi(r) = \frac{u(r)}{r}, \tag{5.1}$$

then the Schrödinger equation can be written as

$$-\frac{1}{2m}\frac{d^2u(r)}{dr^2} + V(r)u(r) = Eu(r), \quad \hbar = 1, \tag{5.2}$$

where $V(r)$ is the potential barrier. In general for problems like α-decay we can choose a very simple potential to explain the main features of the decay process. For instance we can assume a barrier of the form

$$V(r) = \begin{cases} -V_0 & \text{for } r < R \\ V(r) & \text{for } R < r < b \end{cases} \tag{5.3}$$

like the one shown in Fig. (5.1). Now using the WKB approximation for $r > R$, we find $u(r)$ in the three regions to be

$$\begin{cases} N\sin(Kr) & \text{for } r < R \\ \frac{N}{\sqrt{|p(r)|}}\left[A\exp\left(\int_R^r |p(\rho)|d\rho\right) + B\exp\left(-\int_R^r |p(\rho)|d\rho\right)\right] & \text{for } R < r < b \\ \frac{N}{\sqrt{p(r)}}C\exp\left[i\int_b^r p(\rho)d\rho - i\frac{\pi}{4}\right] & \text{for } r > b \end{cases}. \tag{5.4}$$

The phase $\left(-\frac{i\pi}{4}\right)$ in the last part of Eq. (5.4) comes from the joining condition in the WKB approximation Eqs. (3.38), (3.39) and (3.40). In these relations N is the normalization constant, b is the classical turning point, i.e. $V(b) = E$ and K and $p(r)$ are defined by

$$K = \sqrt{2m(E+V_0)}, \quad p(r) = \sqrt{2m(E-V(r))}. \tag{5.5}$$

We note that in the solution (5.4) only the outgoing wave is present as $r \to \infty$. In the absence of the incoming wave there are only three constants A, B and C in $u(r)$, but there are four boundary conditions. These are the continuity of $u(r)$ and $\frac{du(r)}{dr}$ at $r = R$ and $r = b$ respectively. These conditions cannot be satisfied for arbitrary values of E, but E has to have one of the discrete values $E(0), E(1)$...
If we denote the penetration in the barrier by σ, i.e.

$$\sigma = \int_R^b |p(r)|dr, \tag{5.6}$$

then the eigenvalues are given by

$$\tan(KR) + \frac{K}{|p(R)|} = \frac{i}{2}\exp(-2\sigma)\left[\tan(KR) - \frac{K}{|p(R)|}\right]. \tag{5.7}$$

This complex eigenvalue equation can be solved numerically, and the roots are complex. An approximate way of solving (5.7) is to consider the situations where $e^{-2\sigma} << 1$, i.e. the height and the width of the barrier are large enough so that $2\sigma > 1$. Then in Eq. (5.7) we can ignore the right hand side in the zeroth order of approximation and find the eigenvalues from the transcendental equation

$$\tan(K_r R) + \frac{K_r}{|p(K_r, R)|} = 0. \tag{5.8}$$

Here the energy eigenvalues are given by $E_r = \frac{K_r{}^2}{2m} - V_0$. Now to calculate the contribution of the right hand side of (5.7) approximately, we replace K_r by $K_r - i\Delta K_r$, and expand the resulting equation and simplify it using (5.8). This gives us

$$\Delta K_r = \frac{K_r}{R|p(K_r, R)|}\exp[-2\sigma(K_r)]. \tag{5.9}$$

In this way we can write the energy levels as

$$E = \frac{1}{2m}(K_r - i\Delta K_r)^2 - V_0 \approx E_r - \frac{i}{2}\Gamma, \tag{5.10}$$

where the decay width Γ is given by

$$\Gamma \approx \frac{2K_r^{\,2}}{mR|p(K_r, R)|}\exp[-2\sigma(K_r)], \tag{5.11}$$

and is a positive quantity. This is essentially Gamow's formula which relates the decay width Γ to the energy of the emitted particle E_r [5] (see also Eq. (4.13) and Chapter 26).

Gamow's theory of decay can be criticized for two reasons:
(i) - The first difficulty is that why a Hermitian Hamiltonian for the Schrödinge equation (5.2) has complex eigenvalues.
(ii) - The time-dependent wave function shows exponential growth as a function of radial distance from the origin which, at first sight seems unphysical. We have already seen that the eigenvalues, due to the choice of outgoing boundary condition, are complex numbers, let us now concentrate on the second problem before resolving both difficulties. The time-dependent wave function for the problem that we have just solved is of the form

$$\begin{aligned}
\psi(r,t) &= \frac{1}{r}u(r)e^{-iEt} \\
&= \frac{C\exp(-i\frac{\pi}{4})}{r\sqrt{p(r)}}\exp\left[i\int_b^r p_r(\rho)d\rho + \frac{\Gamma}{2}\int_b^r \frac{m}{p_r(\rho)}d\rho\right] \\
&\times \exp\left[-iE_r t - \frac{1}{2}\Gamma t\right], \quad r > b,
\end{aligned} \tag{5.12}$$

where in arriving at this equation we have used the following approximation

$$\int_b^r p(\rho)d\rho = \int_b^r \left[p_r(\rho) + (E - E_r)\frac{2m}{p_r(\rho)}\right] d\rho. \tag{5.13}$$

From Eq. (5.12) it follows that in the limit of $r \to \infty$, $\psi(r,t)$ also tends to infinity.

This difficulty can be resolved by noting that the probability of finding a particle at a distance r from the source of radioactivity (which is centered about the origin), depends on the strength of this source at the earlier time $\frac{r}{v_0}$, where v_0 is the speed of the particle. But at that earlier time the source was stronger by a factor $\exp[\frac{\Gamma}{2}\int_b^r \frac{m}{p_r(\rho)}d\rho]$ and this is precisely the factor that has caused the growth of $|\psi(r,t)|^2$.
A more convincing way to deal with the problem of decay is to consider the time evolution of a wave packet rather than working with the eigenfunctions of the decaying system.

5.2 The Time Development of a Wave Packet Trapped Behind a Barrier

Here again we consider the decay problem for the $l = 0$ partial wave and we start with the Schrödinger equation

$$\frac{d^2u(r)}{dr^2} + [k^2 - v(r)]u(r) = 0, \tag{5.14}$$

where

$$k^2 = \frac{2m}{\hbar^2}E \text{ and } v(r) = \frac{2m}{\hbar^2}V(r). \tag{5.15}$$

The asymptotic solution of this equation as $r \to \infty$ is given by

$$u(E, r) = A(C, E)e^{-ikr} + B(C, E)e^{ikr}. \tag{5.16}$$

This solution is valid for all points $r > R$, provided that $v(r > R) = 0$. In Eq. (5.16) C is the first nonzero coefficient in the expansion of $u(r)$ in powers of r, when r is very small. But the dependence of either A or B on E is more complicated. If E and C are real quantities, then we can choose $u(r)$ to be a real function, this follows from the fact that for $r > 0$, $u(r+dr)$ can be obtained from $u(r)$ and $\frac{du(r)}{dr}$ by Taylor expansion, and these involve only real quantities. Since $u(r)$ is a real function therefore

$$A^* = B, \tag{5.17}$$

and this relation shows that when E is real we cannot find a solution in which either A or B is zero except for the trivial case of $u(r) = 0$ [7]. Now let us assume that E is complex

$$E = E_r - \frac{i}{2}\Gamma, \quad \Gamma > 0. \tag{5.18}$$

If this is the case, then we can choose A and B so that $A = 0$ and $B \neq 0$ and this is the radioactive state of Gamow. Since we want $A(E_r - \frac{i}{2}\Gamma)$ to be zero, we expand $A(E)$ around this point

$$A(E) = \left(E - E_r + \frac{i}{2}\Gamma\right)\left[\frac{dA}{dE}\right]_{A=0} + \dots \tag{5.19}$$

When Γ is very small, then the most important values of E in determining the form of decay comes from a strip of width Γ, therefore we can ignore higher order terms in expansion (5.19). From Eqs. (5.17) and (5.19) it follows that

$$B(E) = \left(E - E_r - \frac{i}{2}\Gamma\right)\left[\frac{dA^*}{dE}\right]_{A=0} + \dots \tag{5.20}$$

From the expanded forms of $A(E)$ and $B(E)$, Eqs. (5.19) and (5.20) and Eq. (5.16) we find that for $r > R$

$$|u|^2 = 2\left|\frac{dA}{dE}\right|^2_{A=0}\left\{(E - E_r)^2 + \frac{1}{4}\Gamma^2\right\}. \tag{5.21}$$

This relation shows that for $r > R$, $|u|^2$ is very small for $E = E_r$, and with $|E - E_r| >> \frac{1}{2}\Gamma$, $|u|^2$ increases quadratically with $E - E_r$. But we have to remember that for the values of E such that $E - E_r >> \frac{1}{2}\Gamma$, we have to keep higher order terms in the expansions (5.19) and (5.20). For intermediate energies both of the expansions for A and B are valid. Now if instead of $|u|^2$, Eq. (5.21), we choose $| Nu|^2$ so that

$$|Nu|^2 = \frac{1}{2}, \quad r > R, \tag{5.22}$$

then we find N^2 to be

$$N^2 = \frac{\frac{1}{4}\left(\left|\frac{dA}{dE}\right|^{-2}\right)_{A=0}}{(E - E_r)^2 + \frac{1}{4}\Gamma^2}. \tag{5.23}$$

This N^2 is the probability of finding the particle inside a sphere of radius r, where $r < b$, and as we see from Eq. (5.23) N^2 has a resonance for $E = E_r$. Let us now construct a wave packet which initially is localized within a sphere of radius R. Using the superposition principle we can write the wave packet as

$$U(r,t) = \int_0^\infty u(E,r)e^{-iEt}g(E)dE, \quad \hbar = 1, \tag{5.24}$$

where $g(E)$ is a function of E of the Breit-Wigner form [7] [8]

$$g(E) = \left(\frac{\Gamma}{2\pi}\right)\frac{1}{(E - E_r)^2 + \frac{1}{4}\Gamma^2}. \tag{5.25}$$

For $r > R$ we can use Eqs. (5.16), (5.19) and (5.20) and write $U(r,t)$ as an integral over e^{ikr} and e^{-ikr}

$$\begin{aligned} U(r,t) &= \frac{\Gamma}{2\pi}\int_0^\infty\left[\left(\frac{dA}{dE}\right)_{A=0}\frac{\exp(-ikr)}{E - E_r - \frac{i}{2}\Gamma}\right]e^{-iEt}dE \\ &+ \frac{\Gamma}{2\pi}\int_0^\infty\left[\left(\frac{dA^*}{dE}\right)_{A=0}\frac{\exp(ikr)}{E - E_r + \frac{i}{2}\Gamma}\right]e^{-iEt}dE. \end{aligned} \tag{5.26}$$

The quantity in the brackets in (5.26) has its maximum at $E = E_r$. To evaluate the integral analytically, we use the approximation where the lower limit of the integral is changed from zero to $-\infty$. The added value to the integral from the range $-\infty$ to zero of E is quite small, since most of the contribution comes from the neighborhood of $E = E_r$. For the following calculation we need the complex integrals

$$\int_{-\infty}^{\infty} \frac{\exp(-ixt')}{x - \frac{i}{2}\Gamma} dx = \begin{cases} 0 & \text{for } t' > 0 \\ 2\pi i \exp(\frac{\Gamma t'}{2}) & \text{for } t' < 0 \end{cases}, \tag{5.27}$$

and

$$\int_{-\infty}^{\infty} \frac{\exp(-ixt')}{x + \frac{i}{2}\Gamma} dx = \begin{cases} -2\pi i \exp(\frac{-\Gamma t'}{2}) & \text{for } t' > 0 \\ 0 & \text{for } t' < 0 \end{cases}. \tag{5.28}$$

Returning to Eq. (5.26) we expand the exponential in powers of $(E - E_r)$ and keep only the first term of the expansion. Thus the first integral is proportional to

$$\exp\left[-i(E - E_r)\left(t + \frac{r}{v_0}\right)\right], \tag{5.29}$$

where $v_0 = \frac{k}{m}$ is the velocity of the particle. Since

$$t' = t + \frac{r}{v_0} > 0, \tag{5.30}$$

therefore the part $(\frac{dA}{dE})_{A=0}$ does not contribute to the integral. We also note that the second integral in (5.26) can be written as

$$\frac{\Gamma}{2\pi} \exp\left[-i\left(E_r t + p_r r\right)\right] \left(\frac{dA^*}{dE}\right)_{A=0} \times \int_{-\infty}^{\infty} \frac{\exp\left[-i\left(E - E_r\right)\left(t - \frac{r}{v_0}\right)\right]}{E - E_r + \frac{i}{2}\Gamma} dE. \tag{5.31}$$

In the exponential appearing in the integral we have the variable

$$t'' = t - \frac{r}{v_0}, \tag{5.32}$$

which can be greater or less than zero. The integral (5.31) is of the same type as (5.28), therefore if $t > \frac{r}{v_0}$ it has the value

$$-i\Gamma\left(\frac{dA^*}{dE}\right)_{A=0} \exp\left[-\frac{1}{2}\Gamma\left(t - \frac{r}{v_0}\right)\right], \quad t > \frac{r}{v_0} \tag{5.33}$$

otherwise it is zero. Now according to Eq. (5.20)

$$B\left(E_r + \frac{i}{2}\Gamma\right) = 0, \tag{5.34}$$

and

$$\left(\frac{dB}{dE}\right)_{B=0} = \left(\frac{dA^*}{dE}\right)_{A=0}. \tag{5.35}$$

From these and the relation

$$-i\Gamma\left(\frac{dB}{dE}\right)_{B=0} = B\left(E_r - \frac{i}{2}\Gamma\right), \tag{5.36}$$

we find the wave packet to be

$$U(r,t) = \begin{cases} B\left(E_r - \frac{i}{2}\Gamma\right)\exp\left[-i\left(E_r t - p_r r\right) - \frac{\Gamma}{2}\left(t - \frac{r}{v_0}\right)\right] & \text{for } t > \frac{r}{v_0},\ \ r > R \\ 0 & \text{for } t < \frac{r}{v_0},\ \ r > R \end{cases} \tag{5.37}$$

The wave packet that we have found in this way is localized in the part where $r < v_0 t$, and in this volume the dependence of U on t has a factor $\exp(-\frac{\Gamma t}{2})$. Hence the probability of finding the particle within a radius $r < R$ decreases as $\exp(-\Gamma t)$.

The solution (5.37) is not an eigenfunction of the Schrödinger equation for a given E, but if we look for the continuation of (5.37) from very small r to $v_0 t$, then essentially we have the same solution as Gamow's radioactive wave function, but unlike the Gamow's solution this one has an acceptable limit as $r \to \infty$.

In order to find the law of conservation of probability, we write the time-dependent equations for $U(r,t)$ and $U^*(r,t)$

$$-i\frac{\partial U(r,t)}{\partial t} + \left[-\frac{1}{2m}\frac{\partial^2}{\partial r^2} + V(r)\right]U(r,t) = 0, \tag{5.38}$$

and

$$i\frac{\partial U^*(r,t)}{\partial t} + \left[-\frac{1}{2m}\frac{\partial^2}{\partial r^2} + V(r)\right]U^*(r,t) = 0. \tag{5.39}$$

Since both $U(r,t)$ and $U^*(r,t)$ are zero at $r = 0$, we can use Green's theorem and from these equations we deduce the following result:

$$-i\frac{d}{dt}\int_0^R |U(r,t)|^2 dr + \frac{1}{2m}\left[U(r,t)\frac{\partial U^*}{\partial r} - U(r,t)^*\frac{\partial U}{\partial r}\right]_{r=R} = 0. \tag{5.40}$$

At $r = R$ and for $t > 0$, the function U depends on r like e^{ikr}, therefore

$$\frac{d}{dt}\int_0^R |U(r,t)|^2 dr = -v_0|U(R)|^2. \tag{5.41}$$

From Eqs. (5.37) and (5.41) we find the following expression for the decay width Γ,

$$\Gamma = \frac{v_0[|U|^2]_{r=R}}{\int_0^R |U(r,t)|^2 dr}. \tag{5.42}$$

This is another way of expressing Γ in terms of the wave function.

The accuracy of the time-dependent wave function (5.37) has been tested by van Dijk *et al* [9] using a narrow square well potential with its center at $r = R$, and with the normalization $|B|^2 = \frac{\Gamma}{v_0}$. By direct numerical integration of the Schrödinger equation, these authors were able to show that when the decay rate is very small, i.e. the potential is strong, then $U(r,t)$ is a good approximation for all r except for the points around $r = v_0 t$ (see also the next section).

5.3 A More Accurate Determination of the Wave Function of a Decaying State

In the previous section we expanded the wave function $U(r,t)$ in terms of plane waves, Eq. (5.26). van Dijk and Nogami [10] [?] have observed that a more accurate description of the time-dependent wave function can be obtained if instead of plane wave approximation, we use an expansion in terms of Moshinsky function [12] [13] [14] which will be defined below (see also Chapter 6). Let us start with the time-dependent Schrödinger equation (5.38) and set $m = \frac{1}{2}$. We want to solve Eq. (5.38) subject to the condition that $U(r,0)$ is known and is a wave packet localized inside the barrier. The time independent solution of the problem is given by $u(k,r)$, Eq. (5.14), which we can write as

$$u(k,r) = \frac{1}{2ik}\left[f(k)f(-k,r) - f(-k)f(k,r)\right]. \tag{5.43}$$

In this relation $f(k) = f(k, r = 0)$ is the Jost function [15] [16] (see also section (10.8)). The wave function $u(k,r)$ is real and satisfies the boundary conditions

$$u(k,0) = 0, \quad \text{and} \quad \left(\frac{du(k,r)}{dr}\right)_{r=0} = 1, \tag{5.44}$$

and $f(k,r)$ is the solution of the Schrödinger equation but with the boundary condition

$$\lim_{r\to\infty} e^{ikr} f(k,r) \to 1. \tag{5.45}$$

The set of $\{u(k,r)\}$ form a complete set of orthogonal states,

$$\int_0^\infty u^*(k,r)u(k',r)dr = \frac{\pi}{2k^2}|f(k)|^2\delta(k-k'), \tag{5.46}$$

and thus we can expand $U(r,t)$ in terms of $u(k,r)$;

$$U(r,t) = \frac{2}{\pi}\int_0^\infty \frac{k^2}{|f(k)|^2} C(k)\exp\left(-ik^2t\right)u(k,r)dk, \tag{5.47}$$

where

$$C(k) = \int_0^\infty u^*(k,r)U(r,0)dr. \tag{5.48}$$

From (5.43) and (5.48) it follows that $C(k) = C(-k)$. We can also write (5.47) as

$$\begin{aligned} U(r,t) &= \int_0^\infty \exp\left(-k^2t\right)\left[e^{ikr}h(k,r) + e^{-ikr}h(-k,r)\right]dk \\ &= \int_{-\infty}^\infty \exp\left(-k^2t\right)e^{ikr}h(k,r)dk. \end{aligned} \tag{5.49}$$

Here $h(k,r)$ is defined by

$$h(k,r) = \frac{-ik}{\pi}C(k)\frac{e^{-ikr}f(-k,r)}{f(-k)}. \tag{5.50}$$

Equation (5.49) also shows that the boundary condition $U(0,t) = 0$ is satisfied. The Jost function $f(-k)$ has infinite number of zeros in the lower half of the complex k plane [15] [16] [17]. Thus $h(k,r)$ has infinite number of poles, but has no other singularities for finite $|k|$. If $h(k,r)$ has no essential singularity as $k\to\infty$, then we can expand $h(k,r)$ as

$$h(k,r) = \lim_{N\to\infty}\sum_{\nu=-N}^{N}\frac{a_\nu(r)}{k-k_\nu}, \quad \nu\neq 0, \tag{5.51}$$

according to Mittag-Leffeler's theorem [18] [19]. Here we have used the fact that the poles are located symmetrically about the Im k axis. If we have a cut-off potential of range R, so that $v(r>R)\equiv 0$, then instead of expanding

$h(k,r)$ we choose the function $e^{ikR}h(k,r)$ which is meromorphic in the lower half of the complex k plane and for $r > R$ we replace (5.51) by

$$\lim_{N\to\infty}\sum_{\nu=-N}^{N}\frac{a_\nu(r)e^{ik_\nu R}}{k-k_\nu}, \quad \nu \neq 0. \tag{5.52}$$

From Eqs. (5.49) and (5.51) we have

$$U(r,t) \approx -2\pi i\sum_{\nu=-N}^{N} a_\nu(r)M\left(k_\nu,r,t\right), \tag{5.53}$$

where $M\left(k_\nu,r,t\right)$ is the Moshinsky function

$$M\left(k_\nu,r,t\right) = \frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{\exp\left[-ip^2t+ipr\right]}{p-k+i\epsilon}dp, \quad \epsilon > 0. \tag{5.54}$$

Carrying out the integration in (5.54) over p we find

$$M\left(k_\nu,r,t\right) = \frac{1}{2}\exp\left[-ik^2t+ikr\right]\operatorname{erfc}\left[\frac{e^{\frac{-i\pi}{4}}}{2\sqrt{t}}(r-v_0t)\right], \tag{5.55}$$

where in this equation v_0 which is the speed of the particle is defined by

$$v_0 = \frac{k}{m} = 2k. \tag{5.56}$$

Equations (5.53) and (5.55) give us $U(r,t)$. Thus starting with the solution of (5.14) with the boundary condition (5.45) we find $f(k,r)$, and from $f(k,r)$ we determine $u(k,r)$, Eq. (5.43). Since $U(r,0)$ is known we can find $C(k)$ from (5.48), and $h(k,r)$ and $a_\nu(r)$ from Eqs. (5.50) and (5.51) respectively.

Let us consider the following simple example which is studied by van Dijk and Nogami [10]. We assume the barrier is a delta function;

$$v(x) = s\delta(r-R), \tag{5.57}$$

and the initial wave packet is given by

$$U(r,0) = \begin{cases}\sqrt{\frac{2}{R}}\sin\left(\frac{\pi r}{R}\right) & \text{for } r < R \\ 0 & \text{for } r > R\end{cases}. \tag{5.58}$$

Then $h(k,r)$ is given by

$$\begin{aligned} h(k,r) &= i\sqrt{2R}\frac{ke^{-ikr}}{(k^2R^2-\pi^2)} \\ &\times \frac{\left[1+\frac{s}{2ik}\left(e^{2ik(R-r)}-1\right)\right]\theta(R-r)}{[k\cot(kR)+(s-ik)]}. \end{aligned} \tag{5.59}$$

The poles of $h(k,r)$ in the lower half k plane are the roots of

$$k\cot(kR)+(s-ik)=0, \tag{5.60}$$

and the residues $a_\nu(r)$ are

$$\begin{aligned} a_\nu &= \frac{i\sqrt{2R}\exp\left(-ik_\nu R\right)}{(k_\nu^2R^2-\pi^2)} \\ &\times \left(\frac{k_\nu+\left[\frac{s}{2i}\left(e^{2ik_\nu(R-r)}-1\right)\right]\theta(R-r)}{[(1+Rs-ik_\nu R)\cot(k_\nu R)-(i+k_\nu R)]}\right). \end{aligned} \tag{5.61}$$

We note that for this example $a_\nu(r)$ has an essential singularity as $k\to\infty$ due to the factor e^{-ikR}, therefore for $r>R$ we replace $h(k,r)$ by $e^{-ikR}h(k,r)$ and apply the Mittag-Leffler's expansion to the latter function. This gives us

$$U(r,t)\approx -2\pi i\sum_{-N}^{N}a_\nu(r)e^{ik_\nu R}M(k_\nu,r-R,t). \tag{5.62}$$

In Fig. (5.2) the norm of the wave function $|U(r,t)|$ for $r>R$ is shown at two different times. In this calculation we have used the parameters $R=1L$, $s=100L^{-1}$ and the wave function is shown at $t=5$ and $t=15L^2$. We have included six terms in the summation (5.62), i.e. used $N=3$. The difference between summing over four or six poles in the calculation is quite small.

Similarly for the wave function inside the barrier, $r<R$, we find [9]

$$U(r,t)\approx -2\pi i\sum_{-N}^{N}a_\nu\left[\left(1+\frac{is}{2k_\nu R}\right)\mathcal{M}(k_\nu,r-R,t)-\frac{is}{2k_\nu R}\mathcal{M}(k_\nu,R-r,t)\right], \tag{5.63}$$

where $\mathcal{M}(k_\nu,R-r,t)$ is defined by

$$\mathcal{M}(k,r,t)=M(k,r,t)+\frac{1}{2k}\frac{e^{\frac{i\pi}{4}}}{\sqrt{\pi t}}\exp\left(\frac{ir^2}{4t}\right). \tag{5.64}$$

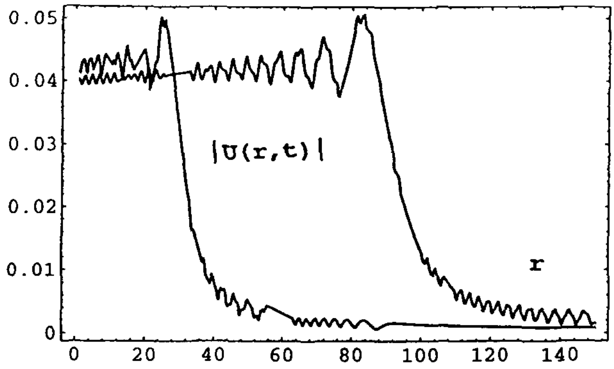

Figure 5.2: The norm of the wave function $|U(r,t)|$ of a decaying state outside the barrier calculated using the expansion Eq. (5.53).

We note that $\mathcal{M}(k_\nu, R-r, t) \to t^{\frac{3}{2}}$ as $t \to \infty$, and therefore $U(r,t)$ behaves in the same way for large t (see also Chapter 2).
From $U(r,t)$, Eq. (5.63), we can calculate the probability for decay $P^-(t)$, which is given by

$$P^-(t) = \left| \int_0^R U(r,t)\sqrt{\frac{2}{R}} \sin\left(\frac{\pi r}{R}\right) dr \right|^2 . \tag{5.65}$$

For the parameters given above with $N = 3$, this probability is plotted as a function of time in Fig. (5.3). Other solvable examples are given in the paper of van Dijk and Nogami [11]. The asymptotic form of the time-dependent wave function for the transmitted wave in one-dimensional tunneling can be calculated for an incident wave packet. In the case of a rectangular barrier of width a and height V_0 this exact transmitted wave function is given by

$$\psi_{tr}(x,t) = \frac{1}{\sqrt{\pi}} \int_0^\infty A(k) \frac{\exp\left[-ika + ikx - \frac{\hbar k^2 t}{2m}\right]}{(q+k)^2 e^{-iqa} - (q-k)^2 e^{iqa}} dk, \tag{5.66}$$

where

$$\hbar q = \sqrt{\hbar^2 k^2 - 2mV_0}. \tag{5.67}$$

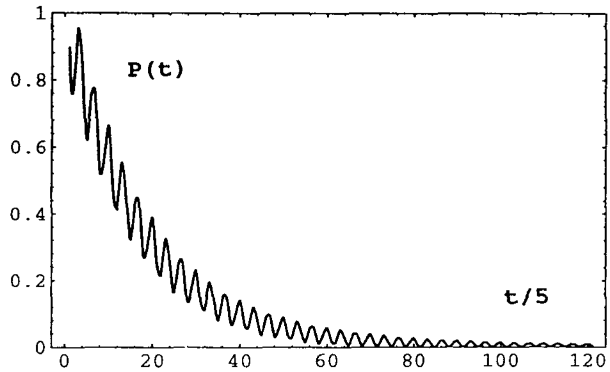

Figure 5.3: The decay probability $P^{-}(t)$ of a particle trapped behind a δ-function barrier, Eq. (5.65), as a function of time t.

For $t \to \infty$ Eq. (5.66) can be calculated using the method of stationary phase. Petrillo and Refaldi have compared this asymptotic solution with the numerical solution of the Schrödinger equation for a Gaussian wave packet and have concluded that the approximate wave function agrees with the exact solution [20].

5.4 Some Instances Where WKB Approximation and the Gamow Formula Do Not Work

For most of the tunneling problems the semi-classical approximations (WKB or Miller-Good) and the Gamow formula derived by applying these approximations are reliable. But in exceptional cases they completely fail. Here we will study examples where this failure is quite pronounced.

As we will see in detail in Chapter 26 that in a number of problems the barrier has a Coulomb tail, i.e. $V(r) \to \frac{1}{r}$ as $r \to \infty$. Therefore here we also consider those central potentials which asymptotically have the $r^{-\alpha}$ $(\alpha > 0)$ dependence on r. These potentials have bound states for positive energy states. The wave function corresponding to the bound state tends to zero as $r \to \infty$ and is normalizable, i.e.

$$\int_0^\infty |\psi(r)|^2 r^2 dr = 1. \tag{5.68}$$

von Neumann and Wigner [21] [22] found these potentials from the special solution of the Schrödinger equation in the following way:

The wave equation written in units of $\hbar = m = 1$ is

$$\frac{-1}{2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi(r)}{dr}\right) + v(r)\psi(r) = \frac{1}{2}k^2\psi(r), \tag{5.69}$$

where $E = \frac{k^2}{2}$. When $v(r) = 0$, i.e. for a free particle the solution of Eq. (5.69) is given by

$$\psi_0(r) = \frac{\sin(kr)}{kr}. \tag{5.70}$$

This wave function is not normalizable in the sense of (5.68). Now let us assume that there is a function $f(r)$ which relates $\psi(r)$ to $\psi_0(r)$;

$$\psi(r) = f(r)\psi_0(r). \tag{5.71}$$

For $\psi(r)$ to satisfy the normalization condition (5.68), $f(r)$ has to go to zero faster than $\frac{1}{\sqrt{r}}$. By substituting $\psi(r)$, Eq. (5.71), in (5.69), we find $v(r)$ to be

$$v(r) = k\cot(kr)\frac{f'(r)}{f(r)} + \frac{f''(r)}{2f(r)}, \tag{5.72}$$

where primes denote derivatives with respect to r. For $v(r)$ to remain finite for all r values the ratio $\frac{f'(r)}{f(r)}$ must vanish at the poles of $\cot(kr)$ (or zeros of $\sin(kr)$). Thus we can choose $f(r)$ to be a differentiable function of the variable

$$k\int_0^r \sin^2(kr')dr' = \frac{1}{2}kr - \frac{1}{4}\sin(2kr). \tag{5.73}$$

For instance we can take $f(r)$ to be of the form

$$f(r) = \frac{1}{a^2k^4 + [2kr - \sin(2kr)]^2} \tag{5.74}$$

where a is a constant quantity. Once $f(r)$ is determined the corresponding potential is obtained by substituting $f(r)$ in (5.72). In Figs. (5.4) and (5.5) the wave function and the potentials are shown for $a = 1$ and two different k values, $k = 0.01$ and $k = \sqrt{2}$ respectively. We observe that the potential

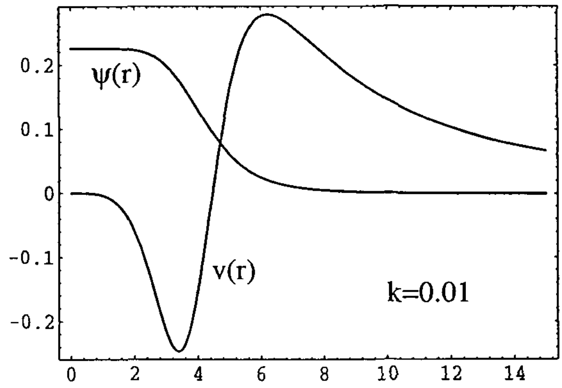

Figure 5.4: Bound state with positive energy . The potential $v(r)$ is similar to the potential of Fig. (5.1) but here the particle remains in the well indefinitely.

$v(r)$, Fig (5.4), starts as an attractive well followed by a repulsive barrier, very similar to the potential (5.3) which we studied earlier in this chapter.

Now if we apply the semi-classical approximation to the Schrödinger equation for this potential, we find a finite lifetime for the particle which at $t = 0$ is located in the attractive part of the well and has an original wave function shown in Fig. (5.4). Of course the exact solution of the Schrödinger equation shows that there is a bound state with infinite lifetime.

In the same way for the l-th partial wave we can find a potential of the form

$$v_l(r) = \left\{\frac{kj_l'(kr)}{j_l(kr)} + \frac{1}{r}\right\}\frac{f_l'(r)}{f_l(r)} + \frac{f_l''(r)}{2f_l(r)}, \tag{5.75}$$

and for this case the wave function is given by

$$\psi_l = N_l f_l(r) j_l(kr) Y_{lm}(\theta, \phi), \tag{5.76}$$

where N_l is the normalization constant and $Y_{lm}(\theta, \phi)$ is the spherical harmonics of order l and m.

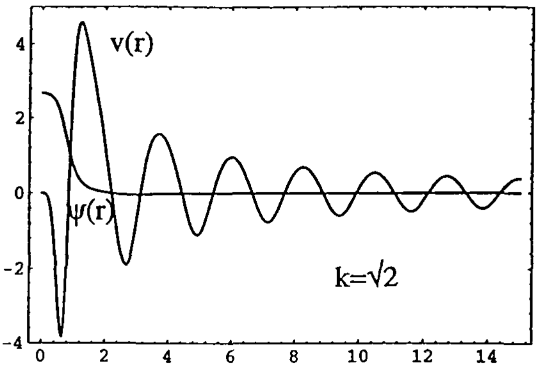

Figure 5.5: Same as in Fig. (5.4) but for a different energy.

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Chapter 6

Simple Solvable Problems

In this chapter we study a number of analytically solvable problems, all one-dimensional or reducible to one-dimensional Schrödinger equation. These solvable problems can be grouped as follows:
(i) - Confining and nonconfining potentials with central barriers.
(ii) - One-dimensional problems when the motion of the particle is not restricted along the direction of motion.
(iii) - Those situations where a particle is initially trapped behind a barrier and in the course of time escapes to infinity.

6.1 Confining Double-Well Potentials

One of the simplest cases where the Schrödinger equation can be solved exactly is shown in Fig. (6.1). This is the case of a confining double-well potential

$$V(x) = \frac{\hbar^2}{2m}\begin{cases} +\infty & \text{for } x < -a \\ 0 & \text{for } -a < x < 0 \\ V_1 & \text{for } 0 < x < b \\ -V_0 & \text{for } b \le x < c \\ +\infty & \text{for } x > c \end{cases} . \tag{6.1}$$

If the energy of the particle E is less than the height of the potential $\frac{\hbar^2}{2m}V_1$, the wave functions and the eigenvalues are given by the following

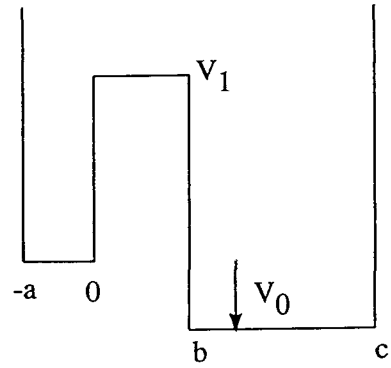

Figure 6.1: An asymmetric confining double-well potential for which the Schrödinger equation is exactly solvable.

equations:

$$\psi_1(x) = A\sin[k(x+a)], \quad -a < x < 0, \tag{6.2}$$

$$\begin{aligned}\psi_2(x) &= \frac{1}{2}A\left\{\left[\sin(ka) + \frac{k}{q}\cos(ka)\right]e^{qx}\right.\\ &+ \left.\left[\sin(ka) - \frac{k}{q}\cos(ka)\right]e^{-qx}\right\}, \quad 0 < x < b,\end{aligned} \tag{6.3}$$

$$\psi_3(x) = Ae^{qb}\frac{\sin(ka) + \frac{k}{q}\cos(ka)}{\sin[\kappa(c-b)] - \frac{\kappa}{q}\cos[\kappa(c-b)]}\sin[\kappa(c-x)], \quad b < x < c, \tag{6.4}$$

and

$$\begin{aligned}&\left\{\sin[\kappa(c-b)] - \frac{\kappa}{q}\cos[\kappa(c-b)\right\}\left\{\sin(ka) + \frac{k}{q}\cos(ka)\right\}\\ -\ &\exp(-2qb)\left\{\sin[\kappa(c-b)] + \frac{\kappa}{q}\cos[\kappa(c-b)\right\}\\ \times\ &\left\{\sin(ka) + \frac{k}{q}\cos(ka)\right\} = 0.\end{aligned} \tag{6.5}$$

In these equations q and κ are functions of $k = \sqrt{\frac{2mE}{\hbar^2}}$;

$$q = \sqrt{V_1 - k^2} \quad \text{and} \quad \kappa = \sqrt{k^2 + V_0}, \tag{6.6}$$

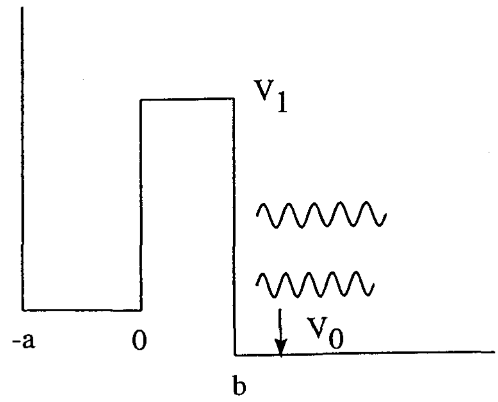

Figure 6.2: The limiting case of the potential given by (6.1) when $c \to \infty$.

and the roots of Eq. (6.5) determine the eigenvalues. The constant A is found from the normalization condition

$$\int_{-a}^{c} |\psi(x)|^2 dx = 1. \tag{6.7}$$

In the limit of $c \to \infty$, the potential is no longer confining (see Fig. (6.2)) and the initially trapped particle can escape to infinity. In this limit $\psi_1(x)$ and $\psi_2(x)$ will retain their forms however $\psi_3(x)$ will change to

$$\psi_3(x) = D\exp(i\kappa x) + F\exp(-i\kappa x), \tag{6.8}$$

where the two coefficients D and F are functions of the energy;

$$\begin{aligned} D &= F^* = \frac{1}{4}A\exp(-i\kappa b)\left\{\left[\left(\sin(ka) + \frac{k}{q}\cos(ka)\right)\left(1 + \frac{q}{ik}\right)e^{qb}\right]\right. \\ &+ \left.\left[\left(\sin(ka) - \frac{k}{q}\cos(ka)\right)\left(1 - \frac{q}{ik}\right)e^{-qb}\right]\right\}. \end{aligned} \tag{6.9}$$

Here $\psi_3(x)$ is a real function, but unlike the finite c case, k can take arbitrary values. In general the wave function outside the barrier, i.e. for $b < x < \infty$ is large, and only a small fraction of it is in the space $-a < x < 0$. In Fig. (6.3) this wave function for two values of k, $k = 1$ and $k = 4$ for the

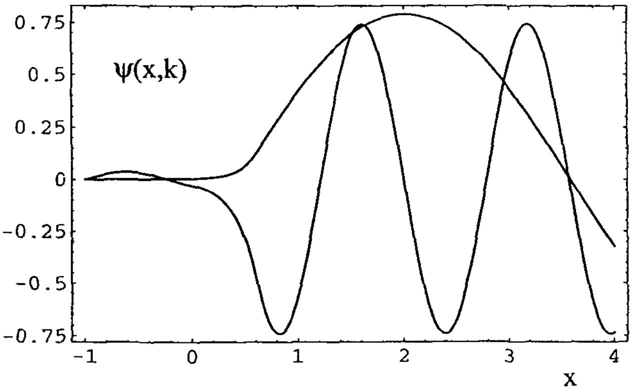

Figure 6.3: The wave function (6.8) plotted for two arbitrary wave numbers $k = 1L^{-1}$ and $k = 4L^{-1}$ (L is a unit of length). Here the wave function inside the well is much smaller than the wave function outside the well.

potential (6.1) is shown.

Taking the ratio $|\frac{A}{D}|^2$ as a function of k, we observe that only for certain values of k this ratio is appreciable and that these characteristic values of k are functions of the parameters of the potential, $V_1, a, \ldots$ To make $|\frac{A}{D}|^2$ as large as possible we have to make the denominator D as small as possible. Suppose that in Eq. (6.9) qb is greater than one, then the first term in the right hand side of (6.9) is larger than the second term, and the first term has its minimum value if k satisfies the equation

$$\sin(ka) + \frac{k}{q}\cos(ka) = 0. \tag{6.10}$$

The roots of this equation are the characteristic values for the quasi-stationary states of the problem. For these values of k, the wave function inside the potential is larger than outside (see Fig. (6.4)).

Next let us consider the simpler problem where the barrier is a δ-function, i.e.

$$V(x) = \frac{\hbar^2}{2m}\begin{cases} +\infty & \text{for } x < -a \\ s\delta(x) & \text{for } -a < x < \epsilon \\ -V_0 & \text{for } \epsilon < x < c \\ +\infty & \text{for } x > c \end{cases}, \tag{6.11}$$

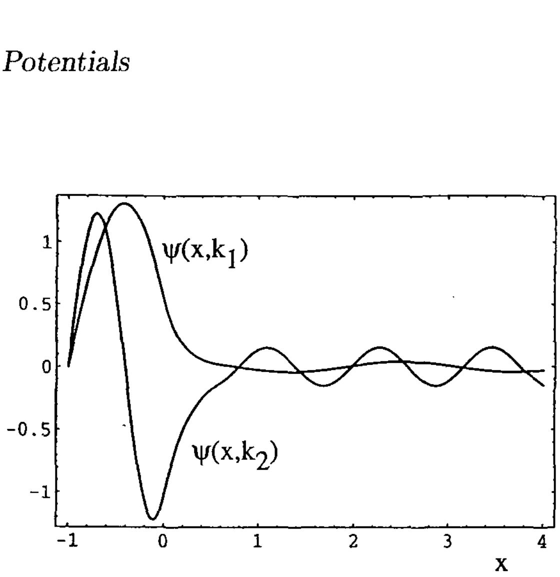

Figure 6.4: The same wave function as in Fig. (6.3) but now shown for quasi-stationary energies. The wave numbers k_1 and k_2 are the two lowest roots of Eq. (6.10).

where ϵ is a positive small number. The wave function for the two wells can be written as

$$\psi_1(x) = A\sin[k(x+a)], \quad -a < x < 0, \tag{6.12}$$

and

$$\begin{aligned} \psi_2(x) &= B\sin[\kappa(c-x)] \\ &= -A\left\{\frac{k\cos(ka)+s\sin(ka)}{\kappa\cos(\kappa c)}\right\}\sin[\kappa(c-x)], \quad 0 < x < c. \end{aligned} \tag{6.13}$$

Here the ratio of the wave function inside the first well to the wave function in the second well is;

$$\left(\frac{A}{B}\right)^2 = \left[\frac{\kappa\cos(\kappa c)}{k\cos(ka)+s\sin(ka)}\right]^2, \tag{6.14}$$

where $\kappa = \sqrt{k^2+V_0}$. The dependence of $\left(\frac{A}{B}\right)^2$ on k is shown in Fig. (6.5) for finite but large c, $c >> a$. If c tends to infinity $\psi_2(x)$ becomes

$$\psi_2(x) = Be^{i\kappa x} + B^*e^{-i\kappa x}. \tag{6.15}$$

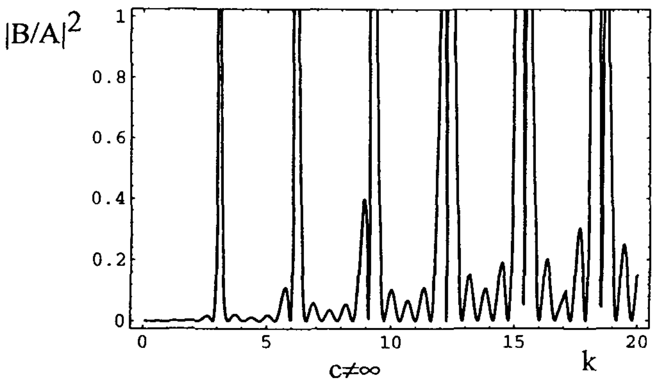

Figure 6.5: The squares of the modulus of the ratio of the amplitudes of wave functions inside the well to that of the outside well when c is large but not infinite.

In the latter case, i.e. for $c \to \infty$, the ratio $(\frac{A}{B})^2$ is given by

$$\left(\frac{A}{B}\right)^2 = \frac{4k^2}{k^2\sin^2(ka) + [s\sin(ka) + k\cos(ka)]^2}, \tag{6.16}$$

and the plot of $(\frac{A}{B})^2$ versus k is shown in Fig. (6.6).

A comparison of Fig. (6.5) and Fig. (6.6) shows that the tunneling when $c >> a$ and when $c \to \infty$ are not qualitatively different and in both the condition for $(\frac{A}{B})^2$ to be large is given by the roots of

$$k\cos(ka) + s\sin(ka) = 0. \tag{6.17}$$

We note that when c is finite the discrete eigenvalues k_n for the eigenfunctions (6.12) and (6.13) which is obtained by setting $\psi_1(0,k) = \psi_2(0,k)$ is given by the equation

$$\kappa\cot(\kappa c) + [k\cot(ka) + s] = 0, \tag{6.18}$$

which for $\frac{c}{a} >> 1$ gives the same roots as (6.17).

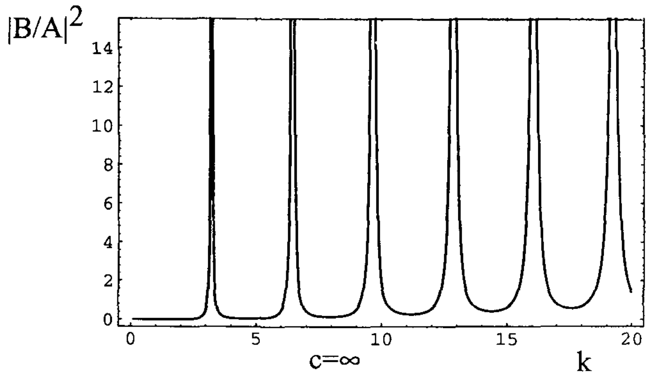

Figure 6.6: Same as in Fig. (6.5) but now for the limit of $c \to \infty$.

6.2 Time-dependent Tunneling for a δ-Function Barrier

A simple and analytically solvable time-dependent problem is the case of one-dimensional tunneling through a δ-function barrier [1]. Let us consider the potential $V(x) = \frac{\hbar^2}{2m} s\delta(x-b)$, for which the Schrödinger equation is

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x,t) = V(x)\psi(x,t), \tag{6.19}$$

and let us denote the initial wave function by $\psi_0(x,t_0)$. Then at the time t, $\psi(x,t)$ is obtained from the integral [2]

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,t;x',t_0)\psi_0(x,t_0)dx', \tag{6.20}$$

where $K(x,t;x',t_0)$ is the Green function which is a solution of the integral equation

$$\begin{aligned} K(x,t;x',t_0) &= K_0(x,t;x',t_0) \\ - \quad \frac{i}{\hbar}\int_{t'}^{t} dt'' &\int_{-\infty}^{\infty} K_0(x,t;x'',t'')V(x'')K(x'',t'';x',t_0)dx''. \end{aligned} \tag{6.21}$$

In this equation K_0 is the free particle Green's function [2];

$$K_0(x,t;x',t') = \left[\frac{m}{2\pi i\hbar(t-t')}\right]^{\frac{1}{2}} \exp\left[\frac{im(x-x')^2}{2\hbar(t-t')}\right]. \tag{6.22}$$

Since the barrier $V(x)$ does not depend on time, the dependence of K on t is of the form $t-t'$, therefore we can set $t' = t_0 = 0$ and define two functions U_0 and U by

$$U_0(x-x';t) = K_0(x,t;x',0), \tag{6.23}$$

$$U(x,x';t) = K(x,t;x',0). \tag{6.24}$$

By substituting for K and K_0 in terms of U_0 and U in Eq. (6.21) and noting that $V(x) = \frac{\hbar^2}{2m}s\delta(x-b)$ we find the following integral equation for U;

$$U(x,x';t) = U_0(x-x';t) - \frac{i\hbar s}{2m}\int_0^t U_0(x-b;t-t'')U(b,x';t'')dt''. \tag{6.25}$$

In order to solve this last equation for U, we use the Laplace transform technique. Denoting the transform of $f(t)$ by $\tilde{f}(z)$ where

$$\tilde{f}(z) = \mathcal{L}[f(t)] = \int_0^z e^{-zt}f(t)dt, \tag{6.26}$$

and by utilizing the convolution theorem,

$$\mathcal{L}\left[\int_0^z f_1(t-\tau)f_2(\tau)d\tau\right] = \tilde{f}_1(z)\tilde{f}_2(z), \tag{6.27}$$

we find the Laplace transform of U at $x=b$;

$$\tilde{U}(b,x';\sigma) = \frac{\tilde{U}_0(b-x';\sigma)}{1+\frac{i\hbar s}{2m}\tilde{U}_0(0;\sigma)}. \tag{6.28}$$

Next we find the Laplace transform of K_0 from Eqs. (6.22), (6.23) and (6.26)

$$\tilde{U}_0(z;\sigma) = \sqrt{\frac{m}{2i\hbar\sigma}}\exp\left[-\sqrt{\frac{2m\sigma}{i\hbar}}|z|\right]. \tag{6.29}$$

Therefore we can write the Laplace transform of Eq. (6.25) as

$$\tilde{U}(x,x';\sigma) = \tilde{U}_0(x-x';\sigma) - \left(\frac{i\hbar s}{2m}\right)\frac{\tilde{U}_0(x-b;\sigma)\tilde{U}_0(b-x';\sigma)}{1+\frac{i\hbar s}{2m}\tilde{U}(0;\sigma)}. \tag{6.30}$$

Having obtained a solution for $\tilde{U}$, we apply the inverse transform to find U;

$$U(x,x';t)=U_0(x-x';t)-\frac{s}{2}M\left(|x-b|+|b-x'|;-i\frac{s}{2};\frac{\hbar}{m}t\right), \qquad (6.31)$$

where $U_0(x-x';t)$ is given by (6.23) and M is the Moshinsky function [3] which is expressible in terms of the error function [4] :

$$M(x;k;t)=\frac{1}{2}\exp\left[i\left(kx-\frac{\hbar k^2 t}{2m}\right)\right]\left\{\operatorname{erfc}\left[\frac{x-\frac{\hbar kt}{m}}{\sqrt{\frac{2i\hbar t}{m}}}\right]\right\}. \qquad (6.32)$$

The Moshinsky function satisfies the following relations:

$$\frac{\partial}{\partial x}M(x;k;t)=ikM(x;k;t)-U_0(x;t) \qquad (6.33)$$

and

$$\begin{aligned}&\int_0^x e^{ikx'}M(ax'+b;c;t)dx'\\ &= \frac{e^{ikx}}{i(k+ca)}\left[M\left(ax+b;c;t\right)-M\left(ax+b;-\frac{k}{a};t\right)\right]. \qquad (6.34)\end{aligned}$$

From Eqs. (6.21), (6.24) and (6.31) we find the following integral equation for $\psi(x,t)$;

$$\psi(x,t)=\psi_0(x,t)-\frac{\hbar^2 s}{2m}\int_{-\infty}^{\infty}M\left(|x|+|x'|;\frac{-i\hbar^2 s}{2m};t\right)\psi(x',0)dx', \qquad (6.35)$$

in which $\psi_0(x,t)$ is the wave function for a free particle

$$\psi_0(x,t)=\int_{-\infty}^{\infty}K_0(x,t;x',0)\psi(x',0)dx'. \qquad (6.36)$$

For the rest of our discussion we will use the units where $\hbar=m=1$, and write the initial wave function as

$$\psi(x,0)=\sqrt{\alpha}\exp[-\alpha|x+x_0|]\exp[ik(x+x_0)], \qquad (6.37)$$

then from Eqs. (6.35) and (6.36) we find $\psi(x,t)$

$$\begin{aligned}\psi(x,t)&=\sqrt{\alpha}[M(x+x_0;k-i\alpha;t)+M(-x-x_0;-k-i\alpha;t)] \;+\\ &\frac{s\sqrt{\alpha}}{2}\left\{J(x_0,\lambda^*)-J(x_0,-\lambda)+e^{-\lambda x_0}[J(0,-\lambda)+J(0,\lambda)]\right\}, \qquad (6.38)\end{aligned}$$

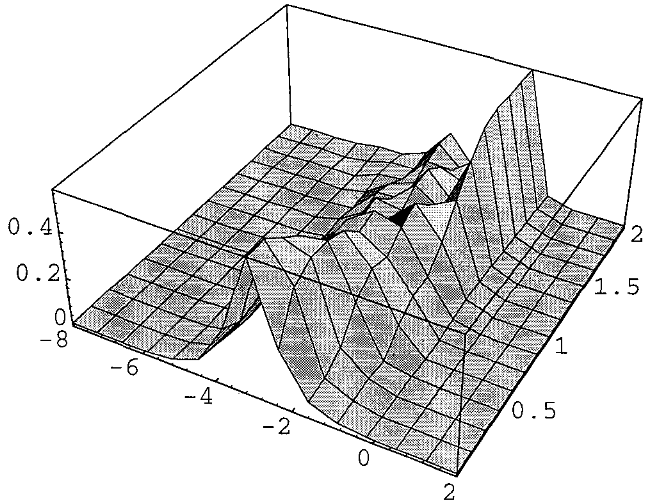

Figure 6.7: Two-dimensional plot of $|\psi(x,t)|^2$ as a function of x and t, (Eq. (6.38)).

where in these relations

$$\lambda = \alpha - ik, \tag{6.39}$$

and

$$J(\xi,\lambda) = \frac{2}{s-2\lambda}\left[M\left(|x|+\xi;-i\frac{s}{2};t\right) - M\left(|x|+\xi;-i\lambda;t\right)\right]. \tag{6.40}$$

The probability density $|\psi(x,t)|^2$ as a function of x and t for the tunneling through a δ-function potential is shown in Fig. (6.7). For this calculation the parameters $s = 100\ L^{-1}, \alpha = k = 1\ L^{-1}$ and $x_0 = 3\ L$ have been used.

6.3 Tunneling Through Barriers of Finite Extent

Let us consider a particle of mass m with the energy E which is moving in the direction of positive x-axis. The Schrödinger equation for this motion is given by

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x), \tag{6.41}$$

where the function $V(x)$ represents the barrier. We write this equation in the simpler form of

$$\frac{d^2\psi(x)}{dx^2}+[k^2-v(x)]\psi(x)=0, \tag{6.42}$$

where $k^2=\frac{2mE}{\hbar^2}$ and $v(x)=\frac{2mV(x)}{\hbar^2}$, both having the dimension of $(\text{length})^{-2}$.

In the limit of $x\to\infty$, $v(x)$ is zero and we have only the transmitted wave which is moving in the positive x direction

$$\psi(x)=T(k)\exp(ikx), \quad \text{as } x\to\infty. \tag{6.43}$$

Here $T(k)$ is the transmission amplitude which is a function of the energy of the particle. When $x\to-\infty$, in addition to the incoming wave, i.e. Ae^{ikx}, we have a reflected wave, the reflection caused by the presence of the barrier. Thus in this limit

$$\psi(x)=A\exp(ikx)+R(k)\exp(-ikx) \quad \text{as } x\to-\infty. \tag{6.44}$$

The two ratios $|\frac{R}{A}|^2$ and $|\frac{T}{A}|^2$, the reflection and the transmission coefficients are important quantities in quantum tunneling. Before we study in detail various methods of calculating these ratios, we consider few simple cases where $|\frac{R}{A}|^2$ and $|\frac{T}{A}|^2$ can be determined analytically. In what follows we assume that the incident wave has a unit amplitude, i.e. $A=1$.

The simplest solvable case is a δ-function barrier $v(x)=s\delta(x)$, where s is the strength of the potential. In this problem we can easily find $R(k)$ and $T(k)$ by matching the solutions (6.43) and (6.44). Thus the transmission and the reflection coefficient are found to be

$$|T(k)|^2=\frac{4k^2}{4k^2+s^2}, \tag{6.45}$$

and

$$|R(k)|^2=\frac{s^2}{4k^2+s^2}. \tag{6.46}$$

The sum of these two, i.e. the result

$$|T(k)|^2+|R(k)|^2=1, \tag{6.47}$$

follows from the law of conservation of the probability. For any shape of barrier this conservation law holds, unless the tunneling takes place in a dissipative environment. In the absence of the barrier, i.e. for $s = 0$, $|T(k)|^2 = 1$, and thus the presence of the barrier causes a reduction of the transmission coefficient to a number less than one. Now if instead of a single barrier, two or a number of barriers are in the path of the particle [5], in general, the transmission coefficient is less than a single barrier unless the second barrier facilitates the transmission and then we have resonant tunneling.

To illustrate this point let us consider the tunneling through two δ-function potentials;

$$v(x) = s_1\delta(x) + s_2\delta(x-a). \tag{6.48}$$

The transmission coefficient obtained for this case from the solution of the Schrödinger equation is given by

$$|T(k)|^2 = \left|\frac{4k^2}{4k^2 + 2ik(s_1+s_2) - [1-\exp(2ika)]s_1s_2}\right|^2. \tag{6.49}$$

This transmission coefficient is a function of the parameters s_1, s_2, k and a. If we keep a and s_1 fixed and vary s_2 and k, we find the surface which is shown in Fig. (6.8). We observe that $|T(k)|^2$ has maxima for certain values of k and s_2 , and these are at points where s_2 is not zero. This means that for a particle with the energy $E = \frac{\hbar^2k^2}{2m}$, there are certain values of k and s_2 for which the second barrier facilitates tunneling. For instance if we take $s_1 = s_2 = s$, then for perfect transmission $|T(k_r)|^2 = 1$ and k_r is one of the roots of the transcendental equation

$$(s^2 - 4k^2)(1 - \cos(2ka)) + 4ks\sin(2ka) + 8k^2 = 0. \tag{6.50}$$

If L denotes an arbitrary unit of length, for $a = 1L$ and $s_1 = s_2 = 24L^{-1}$, in Fig. (6.9) we have plotted $|T(k)|^2$ as a function of k. Here we have a resonance at the value of $k = 2.906L^{-1}$, and for this wave number $|T(k_r)|^2 = 1$, i.e. we have perfect transmission. Next suppose that we have a number of δ-function barriers located at $x = a, b, c, \ldots\ldots..$ For this case also we can calculate $|T(k)|^2$ from the Schrödinger equation. The result shows that while there are resonances for certain k values, the transmission coefficient $|T(k)|^2$ usually remains less than one.

The delta function barriers used in the above examples are not only convenient for finding analytic expressions for $T(k)$, but for all values of k

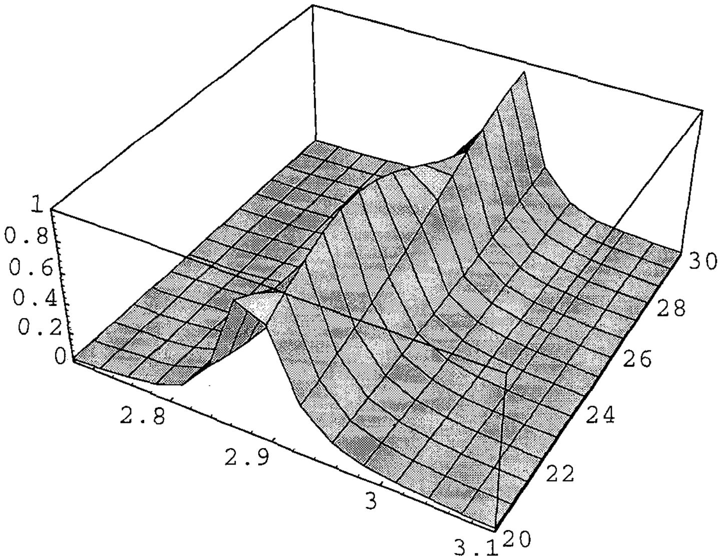

Figure 6.8: Variation of the transmission coefficient as a function of the wave number k and the strength of one of the potentials s_2 showing the condition for resonant tunneling in the case of two δ-function barriers .

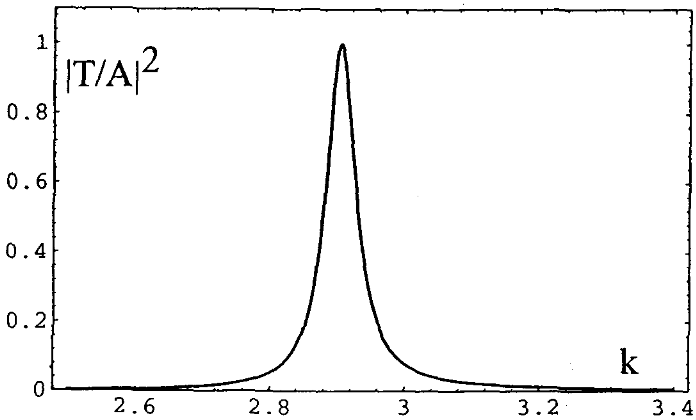

Figure 6.9: The transmission coefficient $|\frac{T}{A}|^2$ as a function of the wave number k.

the particle can pass the barrier only by tunneling, and for this reason we can change s_1 and s_2 between zero and arbitrary values, without imposing conditions on the k values.

Another solvable example is given by the potential

$$v(x) = v_0 e^{\mu x}\theta(-x), \tag{6.51}$$

where $\theta(x)$ is the step function. The solution of the Schrödinger equation with this potential for $k^2 < v_0$ is given by [6] (see also Section 10.6)

$$\psi_1(x) = Cf_1(x) + Dg_1(x), \quad x < 0, \tag{6.52}$$

and

$$\psi_2(x) = T(k)e^{ikx}, \quad x > 0, \tag{6.53}$$

where

$$f_1(x) = J_{-\frac{2ik}{\mu}}\left(\frac{-i\sqrt{2v_0}}{\mu}e^{\frac{\mu x}{2}}\right), \tag{6.54}$$

and

$$g_1(x) = J_{\frac{2ik}{\mu}}\left(\frac{i\sqrt{2v_0}}{\mu}e^{\frac{\mu x}{2}}\right). \tag{6.55}$$

By joining these two wave functions smoothly at $x = 0$, we find the reflection coefficient to be

$$R(k) = \left(\frac{\sqrt{2v_0}}{2\mu}\right)^{-\frac{2ik}{\mu}} \frac{\Gamma\left(1+\frac{2ik}{\mu}\right)}{\Gamma\left(1-\frac{2ik}{\mu}\right)}\left(\frac{ikg_1(0)-g_1'(0)}{f_1'(0)-ikf_1(0)}\right), \tag{6.56}$$

where

$$g_1'(0) = \left(\frac{dg_1(x)}{dx}\right)_{x=0} \quad \text{and} \quad f_1'(0) = \left(\frac{df_1(x)}{dx}\right)_{x=0}. \tag{6.57}$$

Next let us consider a barrier which is zero outside the interval $0 < x < a$, and denote the potential by $V(x)$. Let us further assume that the Schrödinger equation for this potential is solvable and the two independent solutions are $\psi_1(x)$ and $\psi_2(x)$. Outside the interval $(0, a)$ the solution of the wave equation is given by (6.43) and (6.44), where for simplicity in (6.44) we have set $A = 1$. By imposing the conditions of the continuity of the wave function and its derivative at $x = 0$ and at $x = a$, we find:

$$1 + R(k) = C_1\psi_1(0) + C_2\psi_2(0), \tag{6.58}$$

$$ik(1 - R(k)) = C_1\psi_1'(0) + C_2\psi_2'(0), \tag{6.59}$$

$$T(k) = C_1\psi_1(a) + C_2\psi_2(a), \tag{6.60}$$

and

$$ikT(k)e^{ika} = C_1\psi_1'(a) + C_2\psi_2'(a), \tag{6.61}$$

where C_1 and C_2 are constants and primes denote derivatives with respect to x. Solving these equations for $T(k)$, we find

$$T(k) = \frac{2ike^{-ika}W[\psi_1(a), \psi_2(a)]}{\mathcal{D}(k)}, \tag{6.62}$$

where $W[\psi_1(a), \psi_2(a)]$ is the Wronskian and $\mathcal{D}(k)$ is given by

$$\begin{aligned} \mathcal{D}(k) &= \left[\psi_1'(0) + ik\psi_1(0)\right]\left[\psi_2'(a) - ik\psi_2(a)\right] \\ &- \left[\psi_1'(a) - ik\psi_1(a)\right]\left[\psi_2'(0) + ik\psi_2(0)\right]. \end{aligned} \tag{6.63}$$

As a first example, let us determine the transmission amplitude for a linear potential

$$V(x) = \begin{cases} \mathcal{E}x & \text{for } 0 < x < a \\ 0 & \text{otherwise} \end{cases}. \tag{6.64}$$

In this case the two solutions of the wave equation inside the barrier are given by

$$\psi_1(x) = Ai\left[\left(\frac{2m\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E}{\mathcal{E}}\right)\right], \quad 0 < x < a, \tag{6.65}$$

and

$$\psi_2(x) = Bi\left[\left(\frac{2m\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E}{\mathcal{E}}\right)\right], \quad 0 < x < a, \tag{6.66}$$

where Ai and Bi are two independent solutions (Airy functions) [7] . The Wronskian in this case is

$$W[\psi_1(a), \psi_2(a)] = \psi_1(a)\psi_2'(a) - \psi_2(a)\psi_1'(a) = \frac{1}{\pi}\left(\frac{2m\mathcal{E}}{\hbar^2}\right)^{-\frac{1}{3}}. \tag{6.67}$$

Thus by substituting (6.65) and (6.66) in (6.63) we find $\mathcal{D}(k)$, and then we can calculate $T(k)$ from $\mathcal{D}(k)$ and (6.62).

As a second example consider the rectangular barrier where

$$v(x) = \begin{cases} 0 & \text{for } x < 0 \\ v_2 & \text{for } 0 < x < a \\ 0 & \text{for } x > a \end{cases}. \tag{6.68}$$

Here also T can be found analytically;

$$T(k) = \frac{e^{-ika}}{\cosh(qa) + \frac{i}{2}(\frac{q}{k} - \frac{k}{q})\sinh(qa)}. \tag{6.69}$$

where

$$q = \sqrt{v_2 - k^2}. \tag{6.70}$$

From (6.69) we find the transmission coefficient $|T(k)|^2$;

$$|T(k)|^2 = \frac{1}{1 + \frac{(k^2+q^2)^2}{4k^2q^2}\sinh^2(qa)}. \tag{6.71}$$

When k^2 is greater than v_2 then

$$T(k) = \frac{4kpe^{i(p-k)a}}{(p+k)^2}\left[1 - \left(\frac{p-k}{p+k}\right)^2 e^{2ipa}\right]^{-1}. \tag{6.72}$$

where

$$p = \sqrt{k^2 - v_0}. \tag{6.73}$$

If the barrier consists of two rectangular potentials separated by a distance b, i.e.

$$v(x) = \begin{cases} 0 & \text{for } x < 0 \\ v_2 & \text{for } 0 < x < a \\ 0 & \text{for } a < x < b \\ v_4 & \text{for } b < x < c \\ 0 & \text{for } x > c \end{cases}, \tag{6.74}$$

then the transmission amplitude T is given by [8]

$$T(k) = \frac{16q_2q_4k^2}{(v_2v_4Q)}, \tag{6.75}$$

where

$$\begin{aligned} Q &= e^{-aq_2-cq_4}\left[e^{ikb} - e^{-i(kb+2\phi_2+2\phi_4)}\right] \\ &+ e^{aq_2+cq_4}\left[e^{ikb} - e^{i(-kb+2\phi_2+2\phi_4)}\right] \\ &+ e^{aq_2-cq_4}\left[-e^{ikb} + e^{i(-kb+2\phi_2-2\phi_4)}\right] \\ &+ e^{-aq_2+cq_4}\left[-e^{ikb} + e^{i(-kb-2\phi_2+2\phi_4)}\right], \end{aligned} \tag{6.76}$$

and

$$q_2 = \sqrt{v_2 - k^2} \text{ and } q_4 = \sqrt{v_4 - k^2}, \tag{6.77}$$

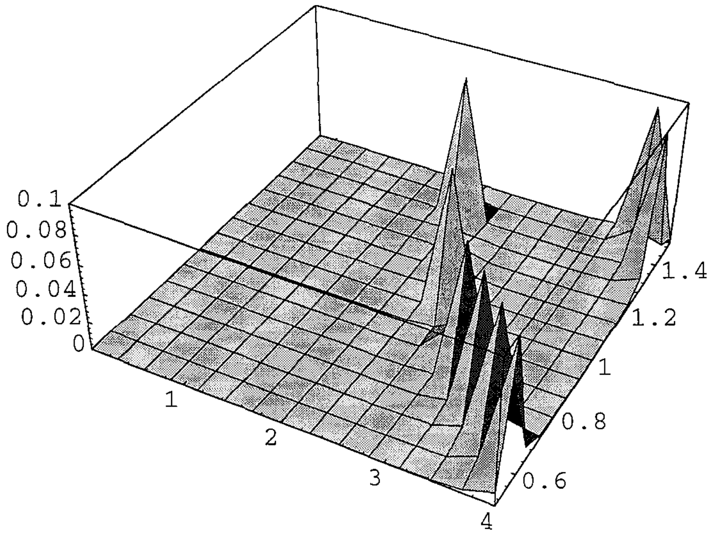

Figure 6.10: Two-dimensional plot of the transmission coefficient for the two rectangular barrier separated by a distance b.

with the phases ϕ_2 and ϕ_4 defined by

$$\phi_2 = \tan^{-1}\frac{q_2}{k} \tag{6.78}$$

and

$$\phi_4 = \tan^{-1}\frac{q_4}{k}. \tag{6.79}$$

In Fig. (6.10), $|T(k)|^2$ is plotted as a function of k and b For this calculation the parameters $a = c = 0.2L^{-1}$ and $v_2 = v_4 = 100L^{-2}$ have been used. If we choose $b = 1L$ and plot this $|T|^2$ as a function of k, we find the resonance shown in Fig. (6.11). This resonance has a narrower width than the one shown in Fig. (6.9), and the maximum transmission ($|T|^2 = 1$) occurs for the wave number $k = 2.598L^{-1}$.
For a time-dependent study of resonant tunneling through two rectangular barriers see [9].

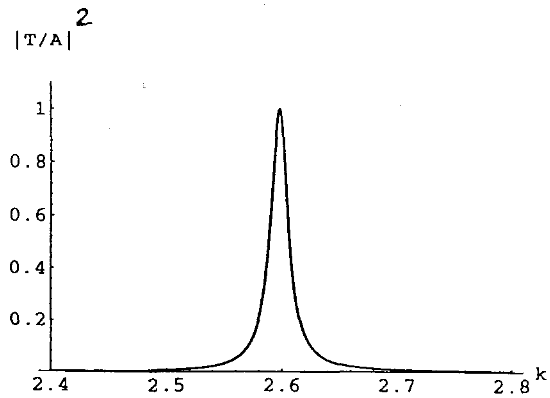

Figure 6.11: The transmission coefficient for resonance case when $b = 1L$.

6.4 Tunneling Through a Series of Identical Rectangular Barriers

Let us assume that there are N rectangular barriers each of height V_0 and width b, and the distance between the two barriers is a, Fig. (6.12). For solving this problem we first find the transfer matrix M [10] [11] [12] [13] for a single barrier of Fig. (6.12). The wave function for the three regions I, II and III are

$$\psi_I = A_I e^{ikx} + B_I e^{-ikx}, \tag{6.80}$$

$$\psi_{II} = A_{II} e^{-qx} + B_{II} e^{qx}, \tag{6.81}$$

and

$$\psi_{III} = A_{III} e^{ikx} + B_{III} e^{-ikx}, \tag{6.82}$$

where

$$k^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad q^2 = \frac{2m(V_0 - E)}{\hbar^2}, \quad E < V_0. \tag{6.83}$$

Now we take the center of the barrier as the origin of the coordinate system and we impose the continuity condition of the wave function at $x = -\frac{b}{2}$ and $x = \frac{b}{2}$ on Eqs. (6.80- 6.82). If M represents a 2 by 2 matrix

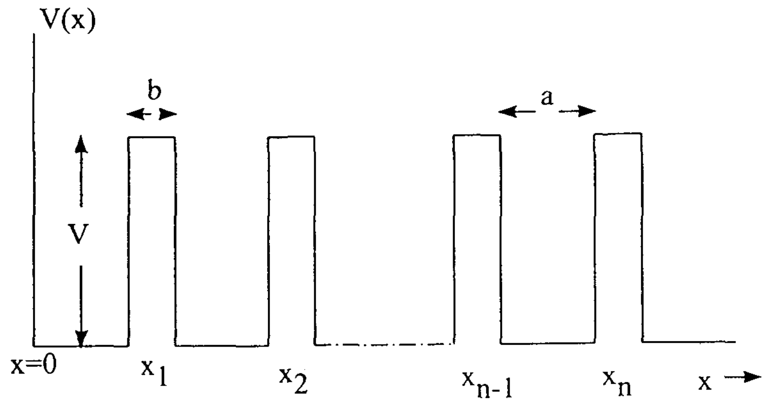

Figure 6.12: A series of identical rectangular barriers.

which is defined by

$$\begin{bmatrix} A_{III} \\ B_{III} \end{bmatrix} = M \begin{bmatrix} A_I \\ B_I \end{bmatrix}, \tag{6.84}$$

then the matrix elements of M calculated from Eqs. (6.80)-(6.82) are:

$$M_{11} = {M_{22}}^* = \exp(-ikb)\left[\cosh(qb) + \frac{i}{2kq}(k^2 - q^2)\sinh(qb)\right], \tag{6.85}$$

$$M_{12} = {M_{21}}^* = -\frac{i}{2kq}(k^2 + q^2)\sinh(qb). \tag{6.86}$$

From these matrix elements we find that

$$\det M = 1. \tag{6.87}$$

Next we generalize the transfer matrix to the case of N barriers. We write the wave function for the n-th zero of the potential as ψ_n;

$$\psi_n = A_n \exp(ikx) + B_n \exp(-ikx), \tag{6.88}$$

where $n = 0$ refers to the interval where $V(x) = 0$ to the left of the first barrier, and $n = N$ is for $V(x) = 0$ to the right of the N-th barrier, with

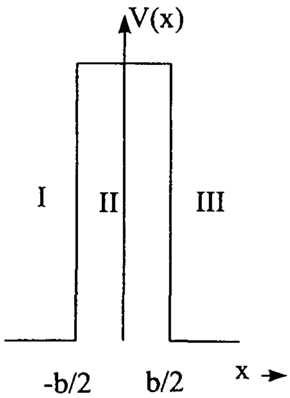

Figure 6.13: One of the rectangular barriers which is located at $x = 0$.

$n = 1$ to $n = N - 1$ referring to the parts where $V(x) = 0$ between the first and the last barriers. Let us define the matrix W_N by

$$\begin{bmatrix} A_N \\ B_N \end{bmatrix} = W_N \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}, \tag{6.89}$$

and thus find the relation between W_N and M as

$$W_N = (F^*)^N G^N, \tag{6.90}$$

where

$$F = \begin{bmatrix} \exp[ik(a+b)] & 0 \\ 0 & \exp[-ik(a+b)] \end{bmatrix}, \tag{6.91}$$

and

$$G = MF. \tag{6.92}$$

With the help of Eqs. (6.85)-(6.87) and the diagonal form of F we find the following properties for the matrix elements of W_N and G;

$$W_N(11) = W_N^*(22), \tag{6.93}$$

$$W_N(12) = W_N^*(21), \tag{6.94}$$

$$\det W_N = 1, \tag{6.95}$$

$$G_{11} = G^*{}_{22} = \exp(ika)\left[\cosh(qb) + \frac{i(k^2 - q^2)}{2kq}\sinh(qb)\right], \tag{6.96}$$

$$G_{12} = G^*{}_{21} = -i\exp[ik(a+b)]\left(\frac{(k^2+q^2)}{2kq}\right)\sinh(qb), \tag{6.97}$$

and

$$\det G = 1. \tag{6.98}$$

To simplify Eq. (6.89), we first diagonalize the matrix G;

$$Q^{-1}GQ = S, \tag{6.99}$$

where

$$S = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}. \tag{6.100}$$

We will see shortly that λ_1 and λ_2 are two distinct eigenvalues. In Eq. (6.99), Q and Q^{-1} are two matrices defined by

$$Q = \begin{bmatrix} G_{12} & G_{12} \\ \lambda_1 - G_{11} & \lambda_2 - G_{11} \end{bmatrix}, \tag{6.101}$$

and

$$Q^{-1} = \begin{bmatrix} \frac{\lambda_2 - G_{11}}{G_{12}(\lambda_2-\lambda_1)} & \frac{-1}{(\lambda_2-\lambda_1)} \\ \frac{G_{11}-\lambda_1}{G_{12}(\lambda_2-\lambda_1)} & \frac{1}{(\lambda_2-\lambda_1)} \end{bmatrix}. \tag{6.102}$$

From Eqs. (6.89), (6.90) and (6.99) - (6.102) we find the matrix elements of W_N;

$$\begin{aligned} W_N(11) &= W_N{}^*(22) \\ &= \frac{\exp[-ikN(a+b)]}{(\lambda_2-\lambda_1)}\left\{\lambda_1{}^N(\lambda_2 - G_{11}) - \lambda_2{}^N(\lambda_1 - G_{11})\right\}, \end{aligned} \tag{6.103}$$

$$W_N(12) = W_N{}^*(21) = \frac{\exp[-ikN(a+b)]}{(\lambda_2-\lambda_1)}\left(\lambda_2{}^N - \lambda_1{}^N\right)G_{12}. \tag{6.104}$$

Finally from these equations we calculate λ_1 and λ_2;

$$\lambda_1 = \frac{1}{2}\left[d + \sqrt{d^2-4}\right], \quad \lambda_2 = \frac{1}{\lambda_1} = \frac{1}{2}\left[d - \sqrt{d^2-4}\right], \tag{6.105}$$

where

$$d = G_{11} + G_{22}. \tag{6.106}$$

Depending on whether $|d| < 2$ or $|d| > 2$, we can rewrite λ_1 and λ_2 in the following ways: If $|d| < 2$, then

$$\lambda_1 = \frac{1}{\lambda_2} = e^{i\theta}, \quad \cos\theta = \frac{d}{2}, \tag{6.107}$$

and if $|d| > 2$, then

$$\lambda_1 = \frac{1}{\lambda_2} = e^{\phi}, \quad \cosh\phi = \frac{d}{2}. \tag{6.108}$$

Now we try to determine the reflection coefficient which in the present case is given by

$$|T_N|^2 = \left|\frac{A_N}{A_1}\right|^2 . \tag{6.109}$$

This is obtained from the assumption that the particles are moving from the left to the right, and after successive tunneling they exit from the right side of the last barrier. Since $B_n \exp(-ikx)$ shows the motion of the particles in the opposite direction, and after passing the last barrier there is no reflection, therefore $B_N = 0$. Using this condition and Eqs. (6.88), (6.93)-(6.95) and (6.109) we find $|T_N|^2$;

$$|T_N|^2 = \frac{1}{|W_N(11)|^2}. \tag{6.110}$$

With the help of Eqs. (6.104), (6.107) and (6.108) we find the reflection coefficient for the two cases:

$$|T_N{}^{(1)}|^2 = \frac{1}{1 + |M_{12}|^2 [U_{N-1}(\cos\theta)]^2}, \quad |d| < 2, \tag{6.111}$$

and

$$|T_N{}^{(2)}|^2 = \frac{1}{1 + |M_{12}|^2 [t_{N-1}(\cosh\phi)]^2}, \quad |d| > 2. \tag{6.112}$$

In these equations U_{N-1} and t_{N-1} are given by the relations

$$U_{N-1}(\cos\theta) = \frac{\sin(N\theta)}{\sin\theta}, \tag{6.113}$$

and

$$t_{N-1}(\cosh\phi) = \frac{\sinh(N\phi)}{\sinh\phi}. \tag{6.114}$$

The function $U_{N-1}(\cos\theta)$ is the Chebyshev polynomial [4] which is the solution of the difference equation

$$U_N(\cos\theta) = 2\cos\theta U_{N-1}(\cos\theta) - U_{N-2}(\cos\theta), \tag{6.115}$$

with the conditions

$$U_{-1}(\cos\theta) = 0, \quad U_0(\cos\theta) = 1. \tag{6.116}$$

Remembering that $\cos\theta = \frac{1}{2}d$, we can write U_N for N even and N odd as

$$U_{N-1}(\cos\theta) = \mu_N(d) = d \sum_{j=0}^{\frac{1}{2}(N-2)} \alpha_{2j} d^{2j} \quad (N = \text{even}), \tag{6.117}$$

and

$$U_{N-1}(\cos\theta) = \nu_N(d) = \sum_{j=0}^{\frac{1}{2}(N-1)} \beta_{2j} d^{2j} \quad (N = \text{odd}), \tag{6.118}$$

respectively, where the coefficients α_{2j} and β_{2j} can be determined from the difference equation (6.115).

By calculating these coefficients we can find the condition for resonant tunneling, i.e. for $|T_N|^2 = 1$. If we consider the case of $d > 2$, then we observe that $|M_{12}|^2[t_{N-1}(\cosh\phi)]^2$ is always greater than zero, and Eq. (6.112) shows that $|T_N|^2$ will always be less than one. On the other hand if $|d| < 2$, we can have one of the following possibilities [14]:

(i) - If $N = 1$, $\nu_1(d) = U_0(\cos\theta) = 1$ and resonance is not possible.

(ii) - When $N = 2, 4, 6....$ then the condition for resonance is $d = 0$ or $\mu_N(d) = 0$.

(iii) - For $N = 3, 5, ...$ the condition is $\nu_N(d) = 0$.

Since $U_{N-1}(\cos\theta)$ is a polynomial of degree $N - 1$ of $\cos\theta$, therefore the equation $U_{N-1}(\cos\theta) = 0$ has $N - 1$ roots for $d < 2$, and these roots are

$$\theta = \frac{p\pi}{N}, \quad p = 1, 2, ...N - 1, \tag{6.119}$$

or

$$d = 2\cos(\frac{p\pi}{N}). \tag{6.120}$$

Each of these roots correspond to a group of energies and for these energies we have perfect transmission, $|T|^2 = 1$.

For a number of applications of tunneling in arrays of potentials see references [5] [15] and [16].

The transfer matrix method discussed here can be modified and applied to the numerical solution of quantum mechanical tunneling. This is achieved by approximating the given potential by a series of rectangular barriers with variable heights and then using the appropriate boundary conditions to match the solution of the wave equation within the barrier with

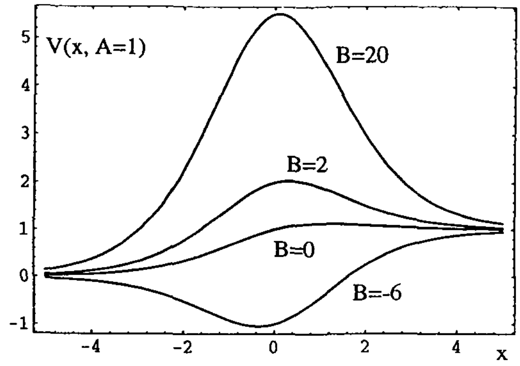

Figure 6.14: The Eckart potential shown as a function of x when the parameter A is fixed, $(A = 1)$, and B is changing.

those of the adjacent barriers. As the number of the rectangular barriers grow the solution tends to the exact solution of the Schrödinger equation [17].

6.5 Eckart's Potential

One of the most useful potentials for which the Schrödinger equation is solvable for tunneling is the Eckart potential [18] [19]:

$$V(x) = \frac{\hbar^2}{2m}\left\{\frac{Ae^x}{1+e^x} + \frac{Be^x}{(1+e^x)^2}\right\}. \tag{6.121}$$

In this potential there are two arbitrary parameters A and B, each can be positive, negative or zero. If we choose $A = 0$, then $V(x)$ will be symmetric, otherwise it is asymmetric. The shapes of this potential for $A = 1$ and different values of B are shown in Fig. (6.14). If $|B| > |A|$ then the potential has a maximum at the point

$$x_m = \ln\left(\frac{B+A}{B-A}\right), \tag{6.122}$$

and this maximum is

$$V(x_m) = \left(\frac{\hbar^2}{2m}\right)\frac{(A+B)^2}{4B}. \tag{6.123}$$

In what follows we choose B to be positive, and we start with the Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \left\{\frac{2mE}{\hbar^2} - \frac{Ae^x}{1+e^x} - \frac{Be^x}{(1+e^x)^2}\right\}\psi = 0. \tag{6.124}$$

By changing the variable from x to ξ, where

$$\xi = -\exp(x), \tag{6.125}$$

we can write the Schrödinger equation as

$$\xi^2\frac{d^2\psi}{d\xi^2} + \xi\frac{d\psi}{d\xi} + \left\{k^2 + \frac{A\xi}{1-\xi} + \frac{B\xi}{(1-\xi)^2}\right\}\psi = 0, \quad k^2 = \frac{2mE}{\hbar^2}. \tag{6.126}$$

Equation (6.126) is a differential equation for the hypergeometric function

$$\begin{aligned}\psi &= (1-\xi)^{i\beta}\left(\frac{-\xi}{1-\xi}\right)^{ik} \\ &\times\ {}_2F_1\left[\frac{1}{2} + i(k-\beta+\delta),\ -\frac{1}{2} + i(k-\beta-\delta),\ 1-2i\beta,\ \frac{1}{1-\xi}\right],\end{aligned} \tag{6.127}$$

where β and δ are defined by

$$\beta = \sqrt{k^2 - A}, \quad \delta = \sqrt{B - \frac{1}{4}}. \tag{6.128}$$

In the limit of $x \to \infty$, i.e. $\xi \to -\infty$, the asymptotic form of this wave function is

$$\psi \to (-\xi)^{i\beta} = \exp(i\beta x), \tag{6.129}$$

and in the limit of $x \to -\infty$, i.e. $\xi \to 0$, using the identities between different ${}_2F_1$'s, we can write ψ as

$$\begin{aligned}\psi(\xi) &= a_1(1-\xi)^{i\beta}\left(\frac{\xi}{\xi-1}\right)^{ik}\\ \times &\ {}_2F_1\left[\frac{1}{2}+i(k-\beta+\delta),\ -\frac{1}{2}+i(k-\beta-\delta),\ 1+2ik,\ \frac{\xi}{1-\xi}\right]\\ + &\ a_2(1-\xi)^{i\beta}\left(\frac{\xi}{\xi-1}\right)^{-ik}\\ \times &\ {}_2F_1\left[\frac{1}{2}+i(-k-\beta+\delta),\ -\frac{1}{2}+i(-k-\beta-\delta),\ 1-2ik,\ \frac{\xi}{1-\xi}\right].\end{aligned} \tag{6.130}$$

In this equation a_1 and a_2 are functions of the energy of the particle $\frac{\hbar^2k^2}{2m}$;

$$a_1 = \frac{\Gamma(1-2i\beta)\Gamma(-2ik)}{\Gamma[\frac{1}{2}+i(-k-\beta-\delta)]\Gamma[\frac{1}{2}+i(-k-\beta+\delta)]}, \tag{6.131}$$

and

$$a_2 = \frac{\Gamma(1-2i\beta)\Gamma(2ik)}{\Gamma[\frac{1}{2}+i(k-\beta-\delta)]\Gamma[\frac{1}{2}+i(k-\beta+\delta)]}. \tag{6.132}$$

From the asymptotic form of (6.130) for $\xi \to 0$ we find that in the limit of $x \to -\infty$, the asymptotic form of $\psi(x)$ is given by

$$\psi(x) \to a_1e^{ikx} + a_2e^{-ikx} \quad \text{as} \quad x \to -\infty. \tag{6.133}$$

Therefore the reflection coefficient $|R(k)|^2$ for this potential is

$$|R(k)|^2 = \left|\frac{a_2}{a_1}\right|^2 = \left|\frac{\Gamma[\frac{1}{2}+i(\delta-\beta-k)]\Gamma[\frac{1}{2}+i(-\delta-\beta-k)]}{\Gamma[\frac{1}{2}+i(\delta-\beta+k)]\Gamma[\frac{1}{2}+i(-\delta-\beta+k)]}\right|^2. \tag{6.134}$$

We can simplify this result by noting that [4]

$$\left|\Gamma\left(\frac{1}{2}+iy\right)\right|^2 = \frac{\pi}{\cosh(\pi y)}. \tag{6.135}$$

If $B > \frac{1}{4}$, then

$$|R(k)|^2 = \frac{\cosh[2\pi(k-\beta)] + \cosh(2\pi\delta)}{\cosh[2\pi(k+\beta)] + \cosh(2\pi\delta)}, \tag{6.136}$$

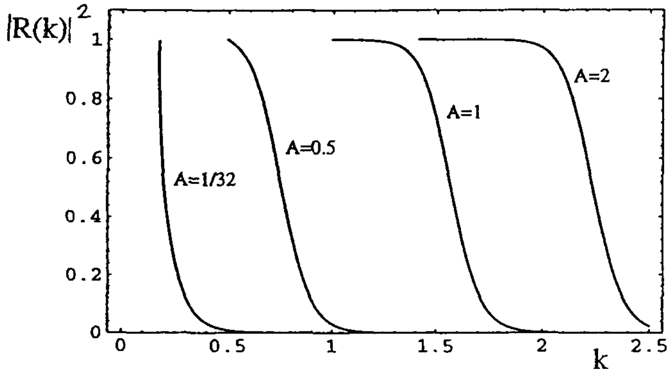

Figure 6.15: The reflection coefficient $|R(k)|^2$ for the Eckart potential is shown as a function of the wave number of the incident particle k and for different values of A.

and when $B < \frac{1}{4}$ the reflection coefficient is

$$|R(k)|^2 = \frac{\cosh[2\pi(k-\beta)] + \cos(2\pi|\delta|)}{\cosh[2\pi(k+\beta)] + \cos(2\pi|\delta|)}. \tag{6.137}$$

For the first case i.e. $B > \frac{1}{4}$, taking $B = 8A$, we have plotted, in Fig (6.15), $|R(k)|^2$ as a function of k, where $\sqrt{A} \le k < \infty$.

6.6 Double-Well Morse Potential

At the beginning of this chapter we studied a confining double-well potential. For certain applications [20] a non-confining double-well may be a more realist form of interaction. The double-well Morse potential is a solvable example of such potential [20]:

$$V(x) = D\exp[-2\alpha(|x| - x_0)] - 2D|\exp[-\alpha(|x| - x_0)], \quad -\infty < x < \infty. \tag{6.138}$$

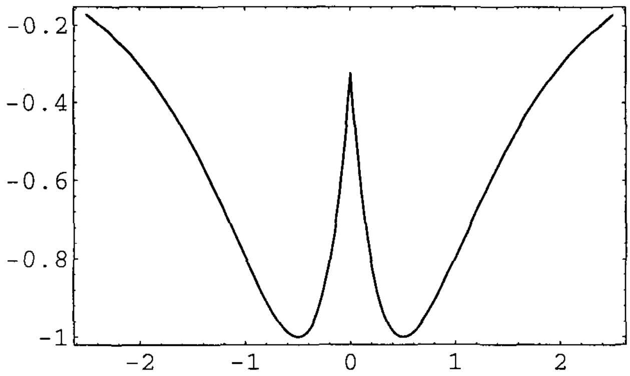

Figure 6.16: The double-well Morse potential given by Eq.(6.138).

Since $V(x)$ is symmetric about the origin we only need to find the wave function for the positive values of x. To solve the wave equation we write

$$\xi = x - x_0, \quad d = \frac{(2mD)^{\frac{1}{2}}}{\alpha\hbar}, \quad E = -\frac{(\alpha\hbar\epsilon)^2}{8m}, \quad B = \frac{2m}{\hbar^2}, \quad z = 2d\exp(-\alpha\xi), \tag{6.139}$$

and then express the wave function $\psi(x)$ as

$$\psi = \exp\left(-\frac{1}{2}z\right) z^{\frac{\epsilon}{2}} F(z), \quad 0 \le z < \infty. \tag{6.140}$$

By substituting (6.140) in the Schrödinger equation and simplifying the result we find $F(z)$ to be the solution of the Kummer equation [21]

$$z\frac{d^2F(z)}{dz^2} + (\epsilon + 1 - z)\frac{dF(z)}{dz} + \left(\frac{DB}{\alpha^2 d} - \frac{\epsilon}{2} - \frac{1}{2}\right)F(z) = 0. \tag{6.141}$$

We choose the solution of (6.141) which is well-behaved as $x \to +\infty$, and then the eigenvalue equations corresponding to the symmetric and antisymmetric wave functions are obtained from the boundary conditions

$$\psi(x)_{x=0} = 0, \tag{6.142}$$

and

$$\left(\frac{d\psi(x)}{dx}\right)_{x=0} = 0, \tag{6.143}$$

respectively.

Additional solvable examples where the barrier is nonlocal or is separable will be discussed in the next chapter.

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Chapter 7

Tunneling in Confining Symmetric and Asymmetric Double-Wells

In the previous chapter we studied some solvable examples where the wave functions were found analytically. Now we want to study the energy splitting and the motion of a wave packet in a double-well confining potential, and in particular to see the difference between the tunneling in a symmetric and an asymmetric potential. The level splitting caused by tunneling is an important feature of these potentials and plays an essential role in a large number of problems of molecular physics [1] [2] and chemical physics [3] [4] [5].

In this chapter we start by studying few simple solvable problems and the conditions for coherent tunneling, then we discuss tunneling by nonlocal and separable barriers and by quasi-solvable local potentials. Finally we show that by some simple transformations we can generate infinitely many solvable or quasi-solvable symmetric or asymmetric local potentials depending on the form of the transformation. Here we start with a simple example where the potential is given by

$$V(x) = \frac{\hbar^2}{2m}\begin{cases} +\infty & \text{for } x < 0 \\ v & \text{for } 0 < x < a \\ v_1 & \text{for } a < x < b, \quad v_1 > v\,. \\ 0 & \text{for } b < x < c \\ +\infty & \text{for } x > c \end{cases} \tag{7.1}$$

We set $\frac{\hbar^2}{2m} = 1$ so that $E = k^2$, and write the wave function for the three different parts of the well as

$$\psi_1(k,x) = N\sin(Kx), \quad 0 < x < a, \tag{7.2}$$

$$\begin{aligned} \psi_2(k,x) &= N\left[\sin(Ka) + \frac{K}{q}\cos(Ka)\right]e^{-q(a-x)} \\ &+ N\left[\sin(Ka) - \frac{K}{q}\cos(Ka)\right]e^{q(a-x)}, \quad a < x < b, \end{aligned} \tag{7.3}$$

and

$$\psi_3(k,x) = N\frac{\left[\sin(Ka) + \frac{K}{q}\cos(Ka)\right]e^{q(b-a)}}{\sin[k(b-c)] + \frac{k}{q}\cos[k(b-c)]}\sin[k(x-c)], \quad b < x < c, \tag{7.4}$$

where N is the normalization constant which can be determined from

$$\int_0^c |\psi(k,x)|^2 dx = 1, \tag{7.5}$$

and K and q are functions of k;

$$q = \sqrt{v_1 - k^2} \text{ and } K = \sqrt{k^2 - v}. \tag{7.6}$$

By imposing the conditions for the continuity of the wave function and its derivative at $x = a$ and at $x = b$, we find the eigenvalue equation for k;

$$\begin{aligned} f(k,v) &= \exp[-2q(b-a)]\left[\sin k(b-c) + \frac{k}{q}\cos k(b-c)\right] \\ &\times \left[\sin(Ka) - \frac{K}{q}\cos(Ka)\right] \\ &- \left[\sin k(b-c) - \frac{k}{q}\cos k(b-c)\right]\left[\sin(Ka) + \frac{K}{q}\cos(Ka)\right]. \end{aligned} \tag{7.7}$$

It should be noted that by changing v the eigenvalues will change, and in particular, for the lowest energy levels K may become imaginary. If this happens, we replace N in Eqs. (7.1)-(7.3) by iN, so that the wave function stays real. If the two wells are symmetric, i.e. $v = 0$, and $c = a+b$, and if we denote the lowest roots of (7.7) by $k_1, k_2, k_3...$, then we have the following relations

$$\begin{aligned} k_2 - k_1 &<< k_3 - k_2, \\ k_4 - k_3 &<< k_5 - k_4. \end{aligned} \tag{7.8}$$

Thus the eigenvalues form doublets $(k_1, k_2), (k_3, k_4)$.... well separated from each other. Since each doublet is composed of states of opposite parity, electromagnetic dipole radiation causes transition between them and this allows for accurate measurement of the splitting of the energy levels (see also Chapter 24) [1].

Next let us study the motion of a wave packet [6] [7] [8] [9] [10]. For the case of two symmetrical wells, from the wave functions $\psi(k_1, x)$ and $\psi(k_2, x)$, we can construct wave packets $\Psi_\pm(x)$ in the following way [10]:

$$\Psi_\pm(x) = \frac{1}{\sqrt{2}}\left[\psi\left(k_1, x\right) \pm \psi\left(k_2, x\right)\right], \tag{7.9}$$

where depending on the $(\pm)$ signs in Eq. (7.9) we can have a wave packet localized to the left or to the right of the barrier. The time evolution of $\Psi_\pm(x)$ is given by the solution of the time-dependent Schrödinger equation;

$$\Psi_\pm(x,t) = \frac{1}{\sqrt{2}}\left[\psi(k_1, x)\exp\left(-ik_1{}^2 t\right) \pm \psi(k_1, x)\exp\left(-ik_2{}^2 t\right)\right]. \tag{7.10}$$

From the time-dependence of (7.10) it follows that each of $|\Psi_+(x,t)|^2$ or $|\Psi_-(x,t)|^2$ is a wave packet which oscillates between the two wells with a fixed period of

$$T = \frac{2\pi}{k_2{}^2 - k_1{}^2}, \tag{7.11}$$

and while oscillating, each wave packet preserves its shape (coherent tunneling) [6].

Now let us solve this problem for an asymmetric double-well. First we take v to have an arbitrary value less than v_1. We choose the initial wave packet to be of the form

$$\Psi(x,0) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) & \text{for } 0 < x < a \\ 0 & \text{for } x > a \end{cases}, \tag{7.12}$$

and then expand $\Psi(x,0)$ in terms of $\psi(k_1, x), \psi(k_2, x), \psi(k_3, x)$..... The coefficients of this expansion are:

$$c_j = \int_0^a \Psi(x,0)\psi(k_j, x)dx. \tag{7.13}$$

Once the c_j's are determined the motion of the wave packet can be expressed as

$$\Psi_a(x,t) = \sum_j c_j\psi(k_j, x)\exp\left(-ik_j{}^2 t\right). \tag{7.14}$$

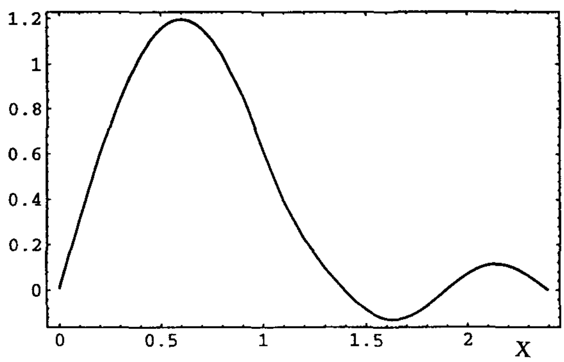

Figure 7.1: An approximate wave packet obtained from the superposition of the first three eigenfunctions. The barrier starts at $x = 1$ and extends to $x = 1.4$.

If we approximate (7.14) by the sum of a finite number of terms (e.g. three or four) then we find a wave packet $\Psi_a(x, 0)$ which is shown in Fig. (7.1). Because of this approximation $\Psi_a(x, 0)$ does not vanish outside of the left well, but only a very small fraction of this wave packet will be in the range $x > a$. Let us denote the probability of finding the wave packet to the left of the barrier by $P^-(t)$, i.e.

$$P^-(t) = \int_0^a |\Psi_a(x,t)|^2 dx, \tag{7.15}$$

then for an arbitrary value of v, $v \neq 0$ this probability remains large for all times. For instance if we choose the parameters $a = 1L, b = 1.4L, c = 2.4L$, $v_1 = 40L^{-2}$ and $v_1 = 4L^{-2}$ (L is an arbitrary unit of length), and carry out the summation in (7.14) with four terms, we find the time-dependence of the probability $P^-(t)$ calculated from (7.15) as shown in Fig. (7.2).

We note that in this case $P^-(t)$ oscillates between 0.86 and 1. The conclusion here is that unlike the case of symmetric double-wells, for asymmetric double-wells tunneling in general is improbable. But as we will see shortly, for a specific choice of $v \neq 0$, we have a resonant condition and the tunneling becomes possible. Let us take the height of the well to the left, i.e. v, in Eq. (7.1) as a variable, then we can find the variation of the

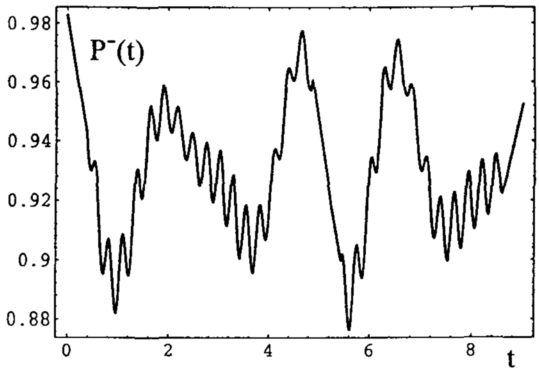

Figure 7.2: The probability $P^-(t)$ for the wave packet to remain in the left well as a function of time.

wave numbers k_i for the lowest energy levels from (7.7). In Fig. (7.3) the dependence of k_i $(i = 1, 2, 3)$ on v is shown, when $c = a + b$. As this simple calculation shows, for a certain value of v, the difference $k_3 - k_2$ has a minimum. For instance for the parameters given above, the minimum of $k_3 - k_2$ is at $v = 21.56L^{-2}$. This particular value of v gives us the condition for resonant tunneling in this asymmetric potential.
If we calculate $P^-(t)$, this probability at the time

$$t = \frac{T_0}{2} = \frac{\pi}{{k_3}^2 - {k_2}^2}, \tag{7.16}$$

will have its minimum value, and this minimum is less than 0.5, which means that the wave packet has tunneled to the second well. The essential difference between this resonant tunneling and the coherent tunneling in a symmetric double well is that in the former case the wave packet after passing the barrier has two peaks, not one.

After a time $\frac{T_0}{2}$ given by Eq. (7.16) this wave packet tunnels through the barrier and appears to the right of the barrier. But this tunneling affects the shape of the wave packet, and $|\Psi_a\left(x, \frac{T_0}{2}\right)|^2$ is composed of two similar peaks, shown in Fig. (7.4) [6]. The asymmetry of the double-well

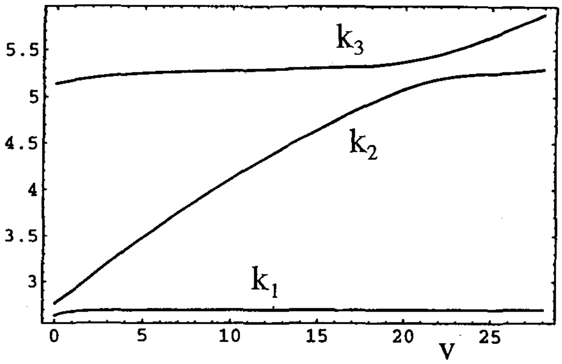

Figure 7.3: Variation of the lowest three wave numbers with the hight v of the left well when $c = a + b$.

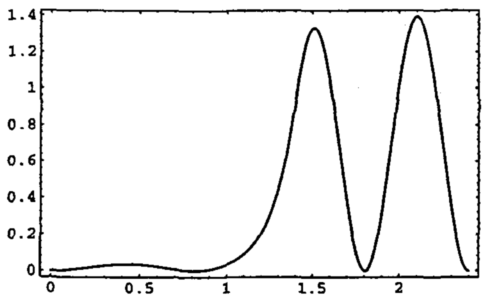

Figure 7.4: The probability density $|\Psi_a(x, \frac{T_0}{2})|^2$ as a function of x showing the two peaks for the case of resonant tunneling.

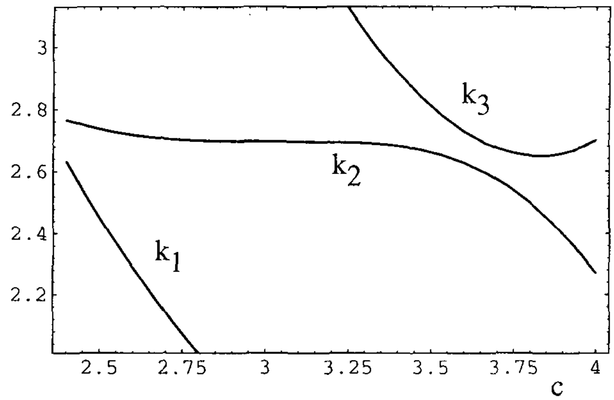

Figure 7.5: The three lowest eigenvalues k_j, $j = 1, 2$ and 3 are shown as a function of the width of the second well c.

which we studied is due to different depths of the two wells. But the same phenomena appears for the case of a double-well where the asymmetry is due to the widths of the wells. For this situation we set v in Eq. (7.7) equal to zero and determine the eigenvalues k_j as a function of c. The variations of k_1, k_2, and k_3 for $v = 0$ and as a function of c are shown in Fig. (7.5).

Just as the case of previous asymmetric double-well we observe that for the parameters $a = 1L, b = 1.4L$ and $v = 40L^{-2}$, the condition for the resonance which corresponds to the minimum of $k_3 - k_2$ occurs for the value of $c = 3.65L$ (Fig. (7.5)), when the depths of the two wells are the same. Here a wave packet which is initially located to the left of the barrier, after a time $t = \frac{T_0}{2} = \frac{\pi}{k_3^2 - k_2^2}$ tunnels to the right of the barrier but unlike the former problem, in this case, $P^-(\frac{T_0}{2})$ is not small and has a peak in the left well, as well as two peaks to the right of the barrier (Fig. (7.6)).

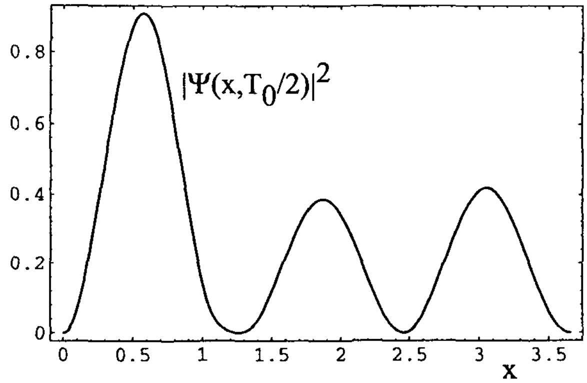

Figure 7.6: The probability density $|\Psi\left(x, \frac{T_0}{2}\right)|^2$ as a function of x.

7.1 Tunneling When the Barrier is Nonlocal

In nuclear physics the potential that a nucleon feels inside a nucleus may be (i) velocity-dependent [11] or (ii) may be nonlocal [12] [13]. The velocity-dependent force is a special case of the nonlocal potential [14]. When the potential is nonlocal, the term $V(x)\psi(x)$ in the Schrödinger equation is replaced by $\int \Gamma(x,x')\psi(x')dx'$, therefore a local potential that we have been assuming so far, can be regarded as a special nonlocal potential with the kernel $\Gamma(x,x') = V(x')\delta(x-x')$.
In general $\Gamma(x,x')$ is a real symmetric function of x and x', and usually it is assumed that it is independent of the energy of the particle.

A wave packet which tunnels through a nonlocal barrier evolves differently from the one that tunnels through a local potential. The reason for the difference can be attributed to the following properties of a local double-well potential in one dimension [15]:
(i) - The eigenvalues are all distinct . This is not always true for nonlocal potentials.
(ii) - The lowest eigenvalues for symmetric double-wells are paired, each pair is well separated from other pairs (see the inequality (7.7)).
(iii) - The lowest eigenfunction is , i.e. it does not vanish except at $x \to \pm\infty$.

For nonlocal potentials one, two or all of these may not be true.

The simplest example that we can investigate is the case of a particle oscillating between two rectangular wells separated by a nonlocal barrier. Thus we have a local potential

$$V(x) = \begin{cases} \infty & \text{for } |x| > b \\ 0 & \text{for } -b < x < -a \\ \frac{-\hbar^2}{2m} w_0 & \text{for } a < x < b \end{cases}, \tag{7.17}$$

everywhere except for the interval $-a < x < a$, where the Schrödinger equation is given by

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) - \int_{-a}^{a} v(x, x')\psi(x')dx' = 0. \tag{7.18}$$

Let us consider a specific model of nonlocality in the form of [12] [13]

$$\begin{aligned} v(x, x') &= \frac{v_0\beta}{\sinh(2\beta a)} \\ &\times \begin{cases} \sinh[\beta(x + a)\sinh[\beta(a - x')] & \text{for } -a \le x \le x' \le a \\ \sinh[\beta(a - x)\sinh[\beta(x' + a)] & \text{for } -a \le x' \le x \le a \end{cases}, \end{aligned} \tag{7.19}$$

where v_0 is the strength of the potential and β^{-1} is the range of the nonlocality. To see the latter point we observe that $v(x, x')$ is the Green function for the differential equation

$$\frac{d^2v(x, x')}{dx^2} - \beta^2 v(x, x') = -\beta^2\delta(x - x'). \tag{7.20}$$

From Eqs. (7.18) and (7.20) it follows that $\psi(x)$ satisfies a differential equation of the fourth order:

$$\frac{d^4\psi(x)}{dx^4} - \left(\beta^2 - k^2\right)\frac{d^2\psi(x)}{dx^2} - \beta^2(k^2 - v_0)\psi(x) = 0. \tag{7.21}$$

Both of the Eqs. (7.20) and (7.21) show that when $\beta^{-1} \to 0$, we have a local interaction, i.e. (7.21) reduces to

$$\frac{d^2\psi(x)}{dx^2} - \left(k^2 - v_0\right)\psi(x) = 0. \tag{7.22}$$

The boundary condition for solving the differential equation (7.21) can be found from (7.18) and (7.19), and they are:

$$v(-a, x') = v(a, x) = 0. \tag{7.23}$$

This relation together with Eq. (7.18) show that at $x = \pm a$, we have

$$\left[\frac{d^2\psi(x)}{dx^2} + k^2\psi(x)\right]_{x=\pm a} = 0. \tag{7.24}$$

This boundary condition plus the conditions for continuity of $\frac{d\ln(\psi(x))}{dx}$ at $x = \pm a$, and the vanishing of ψ at $x = \pm b$ give us the following eigenvalue equation

$$\frac{k\varepsilon(a)\cot[k(b-a)] + \varepsilon'(a)}{p\varepsilon(a)\cot[p(a-b)] - \varepsilon'(a)} = \frac{kO(a)\cot[k(b-a)] + O'(a)}{O'(a) - pO(a)\cot[p(a-b)]}, \tag{7.25}$$

where in this equation

$$p^2 = k^2 + w_0, \tag{7.26}$$

$$\varepsilon(x) = \cosh(\nu x) - \frac{(\nu^2 + k^2)\cosh(\nu a)\cosh(\mu x)}{(\mu^2 + k^2)\cosh(\mu a)}, \tag{7.27}$$

and

$$O(x) = \sinh(\nu x) - \frac{(\nu^2 + k^2)\sinh(\nu a)\sinh(\mu x)}{(\mu^2 + k^2)\sinh(\mu a)}. \tag{7.28}$$

The two parameters μ and ν are dependent on k^2, β^2 and v_0

$$\begin{pmatrix}\mu\\ \nu\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\left(\beta^2 - k^2\right) \pm \sqrt{\left(\beta^2 + k^2\right)^2 - 4\beta^2 v_0}\right]^{\frac{1}{2}}, \tag{7.29}$$

and in Eq. (7.25) we have used the notations:

$$\varepsilon'(a) = \left(\frac{d\varepsilon}{dx}\right)_a \quad \text{and} \quad O'(a) = \left(\frac{dO}{dx}\right)_a. \tag{7.30}$$

The wave function for asymmetric double-well (when $w_0 \neq 0$) and symmetric double-well (when $w_0 = 0$) can be found from the following relations

$$\psi_I(x) = A\sin[k(x+a)] \quad -b \le x \le -a, \tag{7.31}$$

$$\psi_{II}(x) = A\frac{\mathcal{N}_{II}(x)}{\mathcal{D}}, \tag{7.32}$$

and

$$\psi_{III}(x) = A\frac{\mathcal{N}_{III}(x)}{\sin[p(a-b)]\mathcal{D}}, \tag{7.33}$$

where

$$\begin{aligned}\mathcal{N}_{II}(x) &= k\cos[k(b-a)][\varepsilon(a)O(x)+O(a)\varepsilon(x)] \\ &+ \sin[k(b-a)][\varepsilon'(a)O(x)+O'(a)\varepsilon(x)], \quad -a \le x \le a,\end{aligned} \tag{7.34}$$

$$\begin{aligned}&\mathcal{N}_{III}(x) = \sin[p(x-b)] \\ \times\ &\left\{2k\cos[k(b-a)]\varepsilon(a)O(a) + \sin[k(b-a)][\varepsilon'(a)O(a)+O'(a)\varepsilon(a)]\right\}, \\ &a \le x \le b,\end{aligned} \tag{7.35}$$

and

$$\mathcal{D} = [O'(a)\varepsilon(a) - \varepsilon'(a)O(a)]. \tag{7.36}$$

Finally the constant A is determined from the normalization of the wave function

$$\int_{-b}^{b} |\psi(x)|^2 dx = 1. \tag{7.37}$$

Knowing the eigenvalues and the eigenfunctions, from Eqs. (7.14) and (7.15) we can find the time development of a wave packet with the wave profile which satisfies the initial condition

$$\Psi(x,0) = 0, \quad x > -a. \tag{7.38}$$

Once we have obtained $\Psi(x,t)$, we can determine the probability of finding the particle to be on the left of the barrier at time t , i.e. $P^-(t)$ from the equation

$$P^-(t) = \int_{-b}^{-a} |\Psi(x,t)|^2 dx. \tag{7.39}$$

In Fig. (7.7), $P^-(t)$ for nonlocal (dashed line) and the corresponding local potential, $\beta^{-1} = 0$, (solid line) are shown. These are calculated from Eq. (7.39). In this calculation we have used the following parameters $a = 1.5L, b = 4.5L, w_0 = 2.2L^{-2}, v_0 = 2L^{-2}$ and $\beta = 4L^{-1}$ for nonlocal and $\beta = \infty$ for the local potential. These are given in units where L is an arbitrary measure of length and $\hbar = 2m = 1$, and for the initial wave profile we have assumed a superposition of the two lowest eigenfunctions like Eq. (7.9). For this nonlocal barrier the eigenvalues are smaller than the corresponding local barrier. For this reason the nonlocality in this case lowers the effective height of the barrier. As we can see in Fig. (7.7), $P^-(t)$ for nonlocal barrier has a longer period, i.e. even though the apparent height of the potential has been reduced due to nonlocality, nonetheless this nonlocality impedes tunneling.

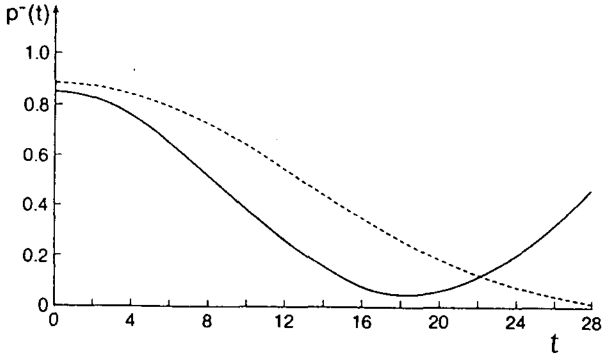

Figure 7.7: The probability of finding the particle to the left of the barrier given as a function of time. The solid line shows the result for local and the dashed line shows the result for nonlocal barrier.

7.2 Tunneling in Separable Potentials

While in one limit nonlocal potentials become local, there is another limit in which they can become separable, i.e. when $\Gamma(x, x')$ can be written as a product $g(x)g(x')$. In the latter case it is difficult to distinguish between the regime where the particle tunnels, and when it flies over the barrier. Since the effective potential acting on an electron in a solid or the potential that is felt by neutron or proton inside a nucleus are generally nonlocal potentials found for example from the Hartree-Fock or Brueckner type calculations, therefore there is the possibility of tunneling through nonlocal potentials in realistic physical systems.

The merit of working with separable potentials compared to other types of nonlocal potentials is the fact that for the separable potentials we can find the solution of the Schrödinger equation analytically. As in the case of the nonlocal potential of the last section we can use a separable barrier inside a box with rigid boundaries. However when the boundaries are at $\pm\infty$ the problem is simpler and more interesting.

For instance let us consider the Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = \lambda e^{-\mu|x|} \int_{-\infty}^{\infty} e^{-\mu|x'|}\psi(x')dx'. \tag{7.40}$$

An incoming plane wave from the left e^{ikx} will partly be reflected and partly transmitted by the barrier. We can write the solution of (7.40) for this case as

$$\psi_1(x) = e^{ikx} + R(k)e^{-ikx} + \frac{\lambda C}{\mu^2 + k^2}e^{\mu x}, \quad x < 0, \tag{7.41}$$

and

$$\psi_2(x) = T(k)e^{ikx} + \frac{\lambda C}{\mu^2 + k^2}e^{-\mu x}, \quad x > 0, \tag{7.42}$$

where

$$C = \int_{-\infty}^{\infty} e^{-\mu|x'|}\psi(x')dx'. \tag{7.43}$$

At the point $x = 0$, we have the boundary condition

$$\frac{\psi_1'(0)}{\psi_1(0)} = \frac{\psi_2'(0)}{\psi_2(0)}. \tag{7.44}$$

Using Eqs. (7.41)-(7.44), we find the transmission and reflection amplitudes $T(k)$ and $R(k)$;

$$T(k) = R(k) + 1, \tag{7.45}$$

$$R(k) = \frac{2\lambda\mu^3(\mu - ik)}{(\mu^2 + k^2)[ik(\mu - ik)(\mu^3 + \mu k^2 - \lambda) - 2\mu^2\lambda]}. \tag{7.46}$$

The wave function can be written in terms of $R(k)$;

$$\psi_1(x) = e^{ikx} + R(k)\left(e^{-ikx} + \frac{ik}{\mu}e^{\mu x}\right) \quad x < 0, \tag{7.47}$$

and

$$\psi_2(x) = [1 + R(k)]e^{ikx} + \frac{ikR(k)}{\mu}e^{-\mu x}, \quad x > 0. \tag{7.48}$$

From (7.45) and the conservation of probability , $|T(k)|^2 + |R(k)|^2 = 1$, Eq. (6.47), we find that

$$2|R(k)|^2 = -[R(k) + R^*(k)], \tag{7.49}$$

a relation which can easily be verified for Eq. (7.46). The dependence of the transmission coefficient $|T(k)|^2$ on k is shown in Fig. (7.8), where the

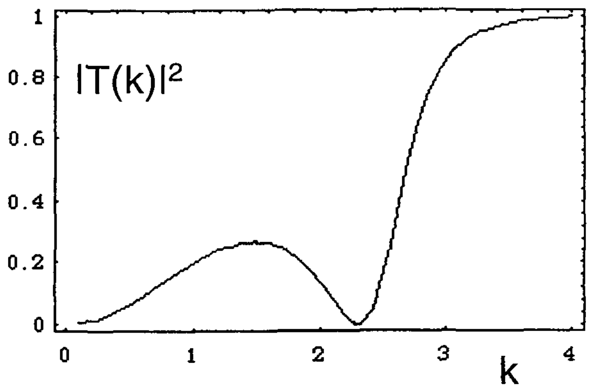

Figure 7.8: The transmission coefficient for the separable potential Eq. (7.40) is plotted as a function of k.

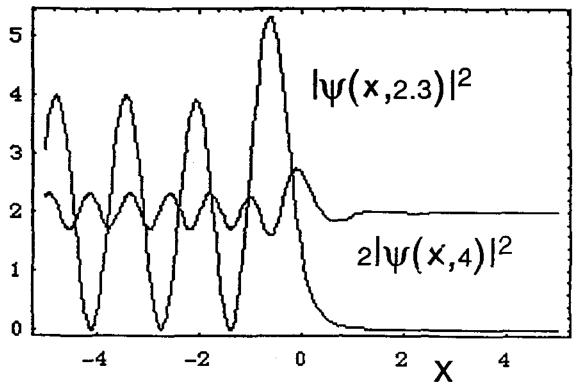

Figure 7.9: The probability density $|\psi(k,x)|^2$ for tunneling in a separable potential.

parameters $\mu = 2L^{-1}$ and $\lambda = 10L^{-3}$ have been used. In Fig. (7.8), the probability density $|\psi(k,x)|^2$ is shown as a function of x, for two values of k, $k = 2.3L^{-1}$ and $k = 4L^{-1}$. In the case of separable potentials it is difficult to distinguish between tunneling and flight over the barrier by examining $|T(k)|^2$ or $|\psi(k,x)|^2$. What is interesting about these separable potentials is that the transmission coefficient is zero not only for $k = 0$ but also for a different k (in our example $k = 2.3L^{-1}$). Thus for this wave number, the separable barrier acts as a rigid wall and is a complete reflector (see Figs. (7.7) and (7.8)).

7.3 A Solvable Asymmetric Double-Well Potential

Another problem for which the wave function can be determined analytically is for the potential which is given by [6]

$$V(x) = \begin{cases} \frac{1}{2m}\Omega^2\left[(x+a)^2 + b^2\right] & \text{for } x \le 0 \\ \frac{1}{2m}\Omega^2\left[x - \sqrt{a^2+b^2}\right]^2 & \text{for } x \ge 0 \end{cases}. \tag{7.50}$$

This potential is shown in Fig. (7.10). The Schrödinger equation for this potential can be written as

$$\frac{d^2\psi_1}{d\eta^2} + \left[\left(\frac{E}{\hbar\Omega} - \frac{m\omega b^2}{2\hbar}\right) - \frac{1}{4}\eta^2\right]\psi_1 = 0, \tag{7.51}$$

and

$$\frac{d^2\psi_2}{d\xi^2} + \left(\frac{E}{\hbar\Omega} - \frac{1}{4}\xi^2\right)\psi_2 = 0, \tag{7.52}$$

where

$$\eta = \sqrt{\frac{2m\Omega}{\hbar}}(x+a), \quad x \le 0, \tag{7.53}$$

and

$$\xi = \sqrt{\frac{2m\Omega}{\hbar}}\left(x - \sqrt{a^2+b^2}\right), \quad x \ge 0. \tag{7.54}$$

Equations (7.51) and (7.52) both have solutions in terms of the parabolic cylinder functions;

$$\psi_1(x) = N_1 D_{\nu'}\left[-\sqrt{\frac{2m\Omega}{\hbar}}(x+a)\right], \quad x \le 0, \tag{7.55}$$

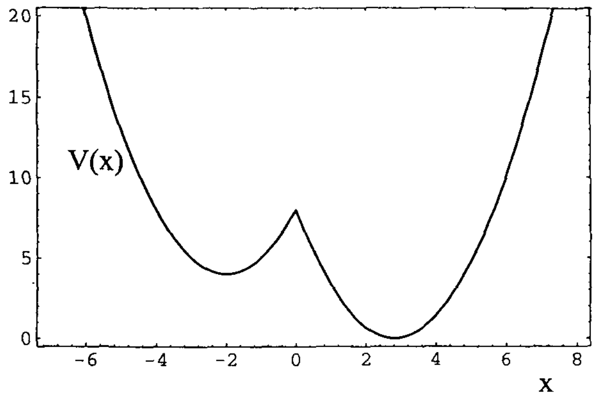

Figure 7.10: The double-well potential (7.50) shown for the values of $\frac{1}{2m}\Omega^2 = 1, a = 2$ and $b = 2$.

and

$$\psi_2(x) = N_2 D_\nu \left[\sqrt{\frac{2m\Omega}{\hbar}}\left(x - \sqrt{a^2+b^2}\right)\right], \quad x \geq 0, \tag{7.56}$$

where

$$\nu' = \nu - \frac{m\Omega b^2}{2\hbar}, \tag{7.57}$$

and

$$\frac{E}{\hbar\Omega} = \nu + \frac{1}{2}. \tag{7.58}$$

Joining the two wave functions ψ_1 and ψ_2 at $x = 0$ smoothly by requiring that the logarithmic derivatives of these two be equal at this point, gives us

$$\left(\frac{\psi_1'}{\psi_1}\right)_{x=0} = \left(\frac{\psi_2'}{\psi_2}\right)_{x=0}. \tag{7.59}$$

This is the eigenvalue equation which can be solved for ν.

If we choose $b = 0$ in (7.50) then we have a symmetric double-well with the eigenvalue equations [16]

$$D_\nu'\left(-\sqrt{\frac{2m\Omega}{\hbar}}\,a\right) = 0, \tag{7.60}$$

for even states and

$$D_\nu\left(-\sqrt{\frac{2m\Omega}{\hbar}}\,a\right)=0, \tag{7.61}$$

for odd states. In Eq. (7.60) prime denotes derivative with respect to the argument of D_ν.

7.4 Quasi-Solvable Examples of Symmetric and Asymmetric Double-Wells

The simple examples that we have so far considered are completely solvable. By this we mean that all of the eigenfunctions can be found analytically, and all of the eigenvalues can be found from a set of eigenvalue equations. Whether we have a confining or non-confining potentials would not have made any difference in obtaining the various physical quantities for these barriers. However, as we have seen earlier in this chapter, for a confining double-well potential only the few low-lying eigenfunctions and eigenvalues are needed to study the tunneling of a particle. Thus if we require the problem to be solvable only for a finite number of low-lying states but not for all, the so called quasi-solvable cases [17], we can still find a good description of the tunneling problems.

Here we start with a special quasi-solvable symmetric potential and then show how to construct other asymmetric potentials, once we have the analytic solution of the Schrödinger equation. Let us consider the potential [18]

$$V(x)=\frac{\hbar^2}{2m}\left[\frac{1}{8}\xi^2\cosh(4x)-(n+1)\xi\cosh(2x)-\frac{1}{8}\xi^2\right], \tag{7.62}$$

where ξ is a constant, n is an integer and x is a dimensionless variable. Noting that the minima of this potential are at the points

$$x_0=\pm\frac{1}{2}\cosh^{-1}\left[\frac{2(n+1)}{\xi}\right], \tag{7.63}$$

we can add a constant to the potential so that $V(x_0)=0$. Thus we have

$$V_1(x)=\frac{\hbar^2}{2m}\left[\frac{1}{8}\xi^2\cosh(4x)-(n+1)\xi\cosh(2x)-\frac{1}{8}\xi^2+(n+1)^2+\frac{\xi^2}{4}\right]. \tag{7.64}$$

The Schrödinger equation for the potential $V(x)$ is given by

$$\frac{d^2\psi(x)}{dx^2} + \left[\epsilon + \frac{1}{8}\xi^2 + (n+1)\xi\cosh(2x) - \frac{1}{8}\xi^2\cosh(4x)\right]\psi(x) = 0. \quad (7.65)$$

We note that the asymptotic form of this equation as $x \to \pm\infty$ is the same as

$$\frac{d^2\psi_a(x)}{dx^2} - \left[\frac{1}{8}\xi^2\left(\cosh(4x) - 1\right) - \xi\cosh(2x)\right]\psi_a(x) = 0. \quad (7.66)$$

But Eq. (7.66) has an acceptable solution, i.e. the one which goes to zero for $x \to \pm\infty$ and that is

$$\psi_a(x) = \exp\left[-\frac{1}{4}\xi\cosh(2x)\right]. \quad (7.67)$$

We write $\psi(x)$ as a product

$$\psi(x) = \psi_a(x)\phi(x), \quad (7.68)$$

and substitute this in Eq. (7.65) to find a differential equation for $\phi(x)$;

$$\frac{d^2\phi(x)}{dx^2} - \xi\sinh(2x)\frac{d\phi(x)}{dx} + [\epsilon + n\xi\cosh(2x)]\phi(x) = 0. \quad (7.69)$$

Now let us seek those solutions of (7.69) which can be expressed in terms of finite sums involving $\sinh(jx)$ and $\cosh(jx)$. For even states we have

$$\phi(x) = \sum_{j=0}^{k} C_{2j+1}\cosh[(2j+1)x], \quad (n = 2k+1), \quad (7.70)$$

$$\phi(x) = \sum_{j=0}^{k} C_{2j}\cosh(2jx), \quad (n = 2k), \quad (7.71)$$

and for odd states we write

$$\phi(x) = \sum_{j=0}^{k} S_{2j+1}\sinh[(2j+1)x], \quad (n = 2k+1), \quad (7.72)$$

$$\phi(x) = \sum_{j=0}^{k} S_{2j}\sinh(2jx), \quad (n = 2k). \quad (7.73)$$

By substituting Eqs.(7.70)-(7.73) in (7.69) we find three term recurrence relations for the coefficients $C_{2j+1}, C_{2j}, S_{2j+1}$ and S_{2j}. For instance for even states we have

$$\left\{\frac{n+1}{2}\xi\delta_{j0} + \left[(2j+1)^2 + \epsilon\right]\right\} C_{2j+1} + \frac{\xi}{2}(n+1-2j)C_{2j-1} + \frac{\xi}{2}(n+3+2j)C_{2j+3} = 0, \tag{7.74}$$

and

$$\left[(2j)^2 + \epsilon\right] C_{2j} + \xi\left[\frac{n}{2}(1+\delta_{j1}) + 1 - j\right] C_{2j-2} + \xi\left[\frac{n}{2} + 1 + j\right] C_{2j+2} = 0, \tag{7.75}$$

with similar relations for S_{2j} and S_{2j+1}. The boundary conditions for the difference equations (7.74) and (7.75) are

$$C_{-2} = C_{n+2} = 0, \quad (n \ \text{even}), \tag{7.76}$$

and

$$C_{-1} = C_{n+3} = 0, \quad (n \ \text{odd}). \tag{7.77}$$

If we choose $n = 3$, then we can find the four lowest levels from Eqs. (7.65), (7.68) and (7.69). Thus the four ϕ_i's are

$$\phi_0 = N_0\left\{3\xi\cosh x + \left[4 - \xi + 2\sqrt{4 - 2\xi + \xi^2}\right]\cosh(3x)\right\}, \tag{7.78}$$

$$\phi_1 = N_1\left\{3\xi\sinh x + \left[4 + \xi + 2\sqrt{4 + 2\xi + \xi^2}\right]\sinh(3x)\right\}, \tag{7.79}$$

$$\phi_2 = N_2\left\{3\xi\cosh x + \left[4 - \xi - 2\sqrt{4 - 2\xi + \xi^2}\right]\cosh(3x)\right\}, \tag{7.80}$$

and

$$\phi_3 = N_3\left\{3\xi\sinh x + \left[4 + \xi - 2\sqrt{4 + 2\xi + \xi^2}\right]\sinh(3x)\right\}, \tag{7.81}$$

where N_i's in these equations are found from the normalization condition;

$$\int_{-\infty}^{\infty}[\phi_i]^2\exp\left[-\frac{1}{2}\xi\cosh(2x)\right]dx = 1. \tag{7.82}$$

The eigenvalues corresponding to these eigenfunctions are:

$$\epsilon_0 = -5 - \xi - 2\sqrt{4 - 2\xi + \xi^2}, \tag{7.83}$$

$$\epsilon_1 = -5 + \xi - 2\sqrt{4 + 2\xi + \xi^2}, \tag{7.84}$$

$$\epsilon_2 = -5 - \xi + 2\sqrt{4 - 2\xi + \xi^2}, \tag{7.85}$$

and

$$\epsilon_3 = -5 + \xi + 2\sqrt{4 + 2\xi + \xi^2}. \tag{7.86}$$

The energy differences between ϵ_0 and ϵ_1 and ϵ_2 and ϵ_3 satisfies the inequality

$$\epsilon_1 - \epsilon_0 < \epsilon_3 - \epsilon_2, \tag{7.87}$$

so that the energy levels are paired together. This inequality can also be obtained from the WKB approximation. But it should be pointed out that the inequalities of this type are only true for one-dimensional tunneling, and in two or three dimensions they are not generally valid. For instance Carbonell and Kostin [19] by solving the Schrödinger equation numerically for the case of a potential with cylindrical symmetry have shown that (7.87) is not true.

7.5 Gel'fand-Levitan Method

From the symmetric potential (7.62) or any other solvable examples we can construct asymmetric solvable potentials. The starting point is the Schrödinger equation which we write as

$$\frac{d^2u_j}{dx^2} + [E_j - V(x)]\, u_j = 0, \tag{7.88}$$

where E_j and $V(x)$ are measured in units of $\frac{\hbar^2}{2m}$ and $V(x)$ is a symmetric potential for which (7.88) is solvable for a finite or infinite number of eigenfunctions $\{u_j\}$, $j = 0, 1, \ldots\ldots$

From the ground state wave function u_0 we construct the kernel $K(x,y)$, the so called Gel'fand-Levitan kernel [20] [21] [22]

$$K(x,y) = \frac{\lambda u_0(x) u_0(y)}{1 - \lambda \int_{-\infty}^{x} [u_0(\xi)]^2 d\xi}, \tag{7.89}$$

where λ is a constant. From this kernel we can find the asymmetric potential $W(x)$ [20] [21] [22]

$$W(x) = V(x) + 2\frac{dK(x,x)}{dx}, \tag{7.90}$$

for which the eigenfunctions are also known. Thus if we write the Schrödinger equation as

$$\frac{d^2\psi_j}{dx^2} + [E_j - W(x)]\,\psi_j = 0, \quad j = 0, 1, 2, ... \tag{7.91}$$

then the ψ_j's are determined from the integral

$$\psi_j(x) = u_j(x) + \int_{-\infty}^{x} K(x,y)u_j(y)dy, \quad j = 0, 1, 2, ... \tag{7.92}$$

where $\{u_j(x)\}$'s are the solutions of the Schrödinger equation with the old potential $V(x)$. The new set $\{\psi_j(x)\}$ form an orthonormal set, i.e.

$$\int_{-\infty}^{\infty} \psi_j(x)\psi_n(x)dx = \delta_{jn}, \quad j, n = 0, 1, 2, ... \tag{7.93}$$

Now let us study the motion of a wave packet $\Psi(x,0)$ in an asymmetric double-well potential. We expand $\Psi(x,0)$ in terms of the set $\{\psi_j(x)\}$;

$$\Psi(x,0) = \sum_{j=0} C_j\psi_j(x), \tag{7.94}$$

where the coefficients C_j's are given by

$$C_j = \int_{-\infty}^{\infty} \Psi(x,0)\psi_j(x)dx. \tag{7.95}$$

If only n lowest eigenfunctions $\{\psi_j\}$ are known, then the sum in (7.94) will be a finite sum, but one should include enough terms in (7.94) to get a fairly localized wave packet.

For $\lambda = 0$, i.e. for a symmetric well, as we have already seen, even when the sum contains the ground and the first excited state, we have a wave packet localized in one of the wells. Here an arbitrary but localized wave packet oscillates between the two wells with a period of $T_0 = \frac{2\pi}{E_1 - E_0}$. By adding more terms to the sum (7.94) we observe that the period of oscillation does not change. This is because when $\lambda = 0$, for such a wave packet C_0 and C_1 in (7.94) are large and $C_2, C_3....$ are all small. But this is not true about the expansion (7.94) for asymmetric double-wells.

The time development of $\Psi(x,0)$ is given by

$$\Psi(x,t) = \sum_{j=0} C_j\psi_j(x)\exp(-iE_jt), \tag{7.96}$$

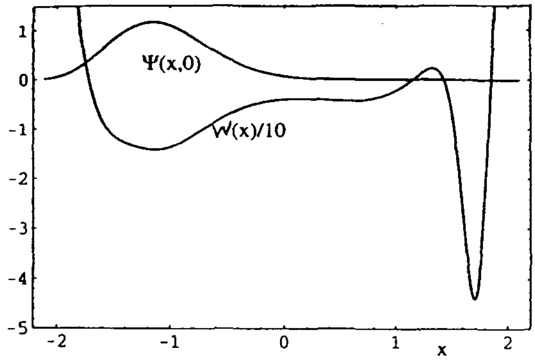

Figure 7.11: The asymmetric double-well constructed from the symmetric potential (7.62) using the Gel'fand-Levitan method. The constants $n = 3$, $\xi = 1$ and $\lambda = 0.98$ have been used in this calculation. In this figure the initial wave packet $\Psi(x, 0)$ is also shown.

and to study the tunneling in this situation, we determine $\Psi(x, t)$. From $\Psi(x, t)$ we calculate the motion of the center- and the average momentum of this wave packet;

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} |\Psi(x, t)|^2 x dx \tag{7.97}$$

and

$$\langle p(t)\rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \left(-i\frac{\partial \Psi(x, t)}{\partial x}\right) dx. \tag{7.98}$$

With the passage of time the position and the momentum $\langle x(t)\rangle$ and $\langle p(t)\rangle$ move in a part of the phase space. If the initial wave packet which we take to be a Gaussian, (Fig.(7.11)), is centered about the minimum of the left well (shallower well), then the motion fills the circular part of the phase space shown in Fig. (7.12). However if we place the same Gaussian wave packet in the deeper well to the right of the barrier, the motion of the trajectory in phase space will be limited to the region shown at the right of Fig. (7.12) [22].

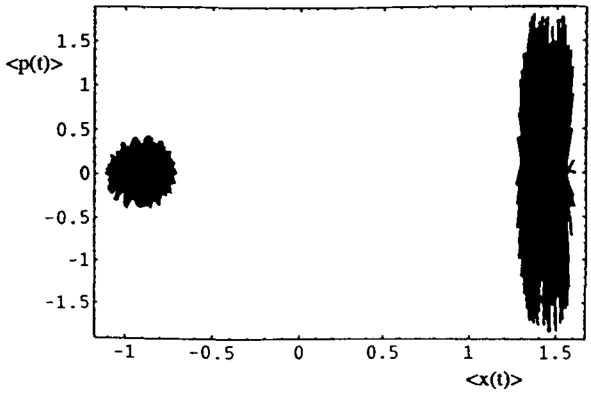

Figure 7.12: Phase space trajectory for the motion of the center and the momentum of a Gaussian wave packet in an asymmetric potential shown in Fig. (7.11).

7.6 Darboux's Method

From a solvable symmetric double-well potential we can construct other symmetric potentials with the help of the Darboux method [23]. Darboux has shown that if u_0 is an eigenfunction of the differential equation (7.88) and E_0 its corresponding eigenvalue, then $w_{j-1}(x)$ is a solution of the differential equation

$$\frac{d^2 w_{j-1}}{dx^2} + \left[E_j - E_0 - u_0\left(\frac{1}{u_0}\right)''\right] w_{j-1} = 0, \quad j = 1, 2, ... \tag{7.99}$$

where primes denote derivatives with respect to x. We can find w_{j-1} directly from u_j;

$$w_{j-1} = u_0 \frac{d}{dx}\left(\frac{u_j}{u_0}\right), \quad j = 1, 2, ... \tag{7.100}$$

These relations show that in the Darboux method the lowest energy level and its corresponding eigenfunction are eliminated from the spectrum. The new spectrum consists of one level $E_1 - E_0$ and two levels close to each other $E_2 - E_0$ and $E_3 - E_0$, but these two are far from $E_1 - E_0$, i.e.

$$E_3 - E_2 < E_2 - E_1, \tag{7.101}$$

therefore the new potential

$$V_1(x) = u_0 \left(\frac{1}{u_0}\right)'', \tag{7.102}$$

is not a symmetric double-well . But we can repeat the process and eliminate two levels. After applying Darboux's method twice, we obtain the Schrödinger equation

$$\frac{d^2 y_{j-2}}{dx^2} + \left[E_j - E_0 - E_1 - w_0 \left(\frac{1}{w_0}\right)''\right] y_{j-2} = 0, \quad j = 2, 3...... \tag{7.103}$$

The spectrum of this equation consists of levels $\epsilon_0 = E_2 - E_0 - E_1$ and $\epsilon_1 = E_3 - E_0 - E_1 ....$ etc. But ϵ_0 and ϵ_1 are close to each other and far from ϵ_2. Thus the new potential

$$V_2(x) = w_0 \left(\frac{1}{w_0}\right)'', \tag{7.104}$$

is usually of the form of double-well. The eigenfunctions $y_{j-2}(x)$ are related to $w_j(x)$ and $u_j(x)$ by the Darboux relation (7.100) and

$$y_{j-2}(x) = w_0 \frac{d}{dx}\left(\frac{w_{j-1}}{w_0}\right). \tag{7.105}$$

In Fig. (7.13) the potential $V_2(x)$ is shown. This is found from (7.62) by two consecutive Darboux transformations . Here the parameter $\xi = 0.6$ has been used. For this case both of the energies E_3 and E_4 are higher than the height of the barrier $V(0)$, therefore ϵ_0 and ϵ_1, the lowest eigenvalues of $V_2(x)$ are higher than $V_2(0)$.

7.7 Optical Potential Barrier Separating Two Symmetric or Asymmetric Wells

Let us consider a model where a particle which is confined to move between two wells has to pass through a complex potential barrier. The probability of finding the particle within this confined space is one if the barrier is not absorbing the particle, but only reducing its energy.

A model with these properties is described by the evolution equation [15] [22] [24],

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = H\Psi(x,t) + i\left[W(x) - \langle\Psi|W(x)|\Psi\rangle\right]\Psi(x,t), \tag{7.106}$$

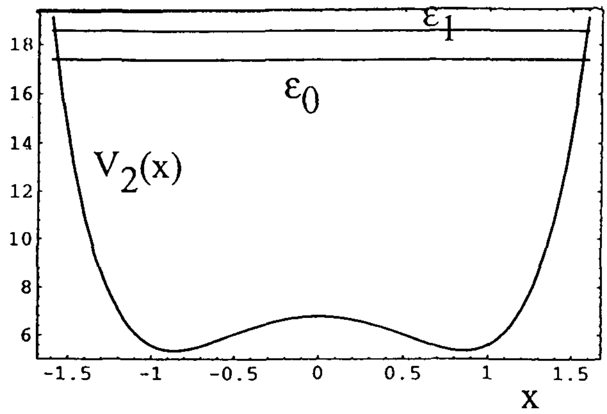

Figure 7.13: The potential $V_2(x)$ obtained by applying the Darboux transformation twice on $V(x)$, Eq. (7.62), ($\xi = 0.6$).

where H is an Hermitian Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \tag{7.107}$$

and $W(x)$ is the optical potential. A well known result of the optical potential theory states that [25]

$$\text{Im } W(x) \le 0, \quad \text{for all values of } x. \tag{7.108}$$

From Eq. (7.106) and its complex conjugate we can verify that

$$\frac{d}{dt}\langle\Psi|\Psi\rangle = 0, \tag{7.109}$$

and thus the probability is conserved. To solve (7.106) we first introduce another wave function $\Phi(x,t)$ by

$$\Psi(x,t) = \Phi(x,t)\exp\left[-\int_0^t \langle\Psi|W(x)|\Psi\rangle\, dt\right]. \tag{7.110}$$

Substituting for $\Psi(x,t)$ from (7.110) in (7.106) we find $\Phi(x,t)$ to be the solution of the linear differential equation

$$i\hbar\frac{\partial\Phi(x,t)}{\partial t} = H\Phi(x,t) + iW(x)\Phi(x,t). \tag{7.111}$$

In the next step we define the wave function $\phi_n(x)$ by

$$[H + iW(x)]\,\phi_n(x) = \left(E_n - \frac{i\Gamma_n}{2}\right)\phi_n(x), \tag{7.112}$$

where E_n's and Γ_n's are real quantities and $\Gamma_n \geq 0$ for all n. From the Hamiltonian (7.107), Eq. (7.112) and a similar equation for $\phi_j(x)$ we find that these $\phi_n(x)$'s satisfy the orthogonality relation

$$\int_{-\infty}^{\infty} \phi_n(x)\phi_j(x)dx = 0, \quad n \neq j. \tag{7.113}$$

We write $\Phi(x,t)$ as an infinite series in terms of $\phi_n(x)$;

$$\Phi(x,t) \approx \sum_n C_n \exp\left[-i\left(E_n - \frac{i\Gamma_n}{2}\right)t\right]\phi_n(x), \tag{7.114}$$

where C_n's are the coefficients of expansion and are determined from the initial wave packet $\Psi(x,0)$

$$C_n \approx \frac{\int_{-\infty}^{\infty}\Psi(x,0)\phi_n(x)dx}{\int_{-\infty}^{\infty}\left[\phi_n(x)\right]^2 dx}. \tag{7.115}$$

Equations (7.109), (7.114) and (7.115) give us the time development of the wave packet.

The time dependence of the center of the wave packet is given by

$$\langle x(t)\rangle \approx \int_{-\infty}^{\infty} x\,|\Psi(x,t)|^2\,dx, \tag{7.116}$$

or in terms of $\phi_n(x)$'s

$$\langle x(t)\rangle \approx \frac{\sum_{n,j}\langle\phi_j|x|\phi_n\rangle C_k C_j^* \exp\left[-\frac{i}{\hbar}(E_n - E_j)t - \frac{1}{2\hbar}(\Gamma_n + \Gamma_j)t\right]}{\sum_{n,j}\langle\phi_j|\phi_n\rangle C_k C_j^* \exp\left[-\frac{i}{\hbar}(E_n - E_j)t - \frac{1}{2\hbar}(\Gamma_n + \Gamma_j)t\right]}. \tag{7.117}$$

If Γ_j is the smallest member of Γ_n's then as $t \to \infty$, we have

$$\langle x(t)\rangle \to \langle\phi_j|x|\phi_j\rangle\,. \tag{7.118}$$

As an example consider the simple case where

$$V(x) = \begin{cases} +\infty & \text{for } x \leq -1 \\ \frac{\hbar^2}{2m}s_1\delta(x) & \\ \frac{\hbar^2}{2m}v_0 & \text{for } 0 < x < 1 \\ +\infty & \text{for } x \geq 1 \end{cases}, \tag{7.119}$$

and

$$W(x) = -\frac{\hbar^2}{2m} s_2 \delta(x). \tag{7.120}$$

Here s_1 and s_2 are real constants with the dimension of L^{-1}. By solving the Schrödinger equation for this potential we find the following eigenvalue equation

$$\sqrt{\varepsilon - v_0} \cot \sqrt{\varepsilon - v_0} + \sqrt{\varepsilon} \cot \sqrt{\varepsilon} + s_1 - i s_2 = 0, \tag{7.121}$$

where $\varepsilon = \frac{2m}{\hbar^2} E$ is the complex eigenvalue with the negative imaginary part. Let us denote the $(n+1)$-th root of (7.121) by $\lambda_n = \varepsilon_n - \frac{i}{2}\gamma_n$ ($\gamma_n > 0$) then the wave function ϕ_n is given by

$$\phi_n(x) = \begin{cases} N_n \sin\left[\sqrt{\lambda_n}(x+1)\right] & \text{for } -1 \le x \le 0 \\ -N_n \frac{\sin\sqrt{\lambda_n}}{\sin\sqrt{\lambda_n - v_0}} \sin\left[\sqrt{\lambda_n - v_0}(x-1)\right] & \text{for } 0 \le x \le 1 \end{cases}. \tag{7.122}$$

We choose the initial wave function to be

$$\Psi(x,0) = \Phi(x,0) = \begin{cases} \sqrt{2}\sin(\pi x) & \text{for } -1 \le x \le 0 \\ 0 & \text{for } 0 < x \le 1 \end{cases}, \tag{7.123}$$

and we find that $\langle x(0) \rangle = -0.5$ for all values of v_0. Next we expand (7.123) in terms of ϕ_n's, Eq. (7.122), using the parameters $s_1 = 4L^{-1}$ and $s_2 = 0.4L^{-1}$ for the potential and then calculate the time evolution of the center of the wave packet from (7.117). First we consider the case of $v_0 = 0$, i.e. a symmetric double well potential separated by a thin optical potential barrier. In Fig. (7.14) the oscillations of the center of the wave packet in this potential are shown in the presence of the optical potential barrier. We observe that in this case the center of the wave packet comes to rest at the middle of the two wells, i.e. $\langle x(\infty) \rangle = 0$.

As we mentioned earlier in this section, unless resonant conditions are met, a wave packet originally located in one of the wells of an asymmetric double-well potential is unlikely to tunnel through the barrier to the other well. But the presence of an optical potential barrier facilitates this tunneling. Here we have two possibilities (i) when the wave packet is in the shallower well and (ii) when it is in the deeper well. For the first case we choose $v_0 = -4L^{-2}$, so the the deeper well is to the right and the wave packet is to the left of the barrier. Initially the center of the wave packet $\langle x(0) \rangle$ is at $x = -0.5L$. In Fig. (7.15) $\langle x(t) \rangle$ is plotted as a function of time, and this figure shows that the center moves from the left well to the right of the barrier and after a large number of oscillations it assumes a constant

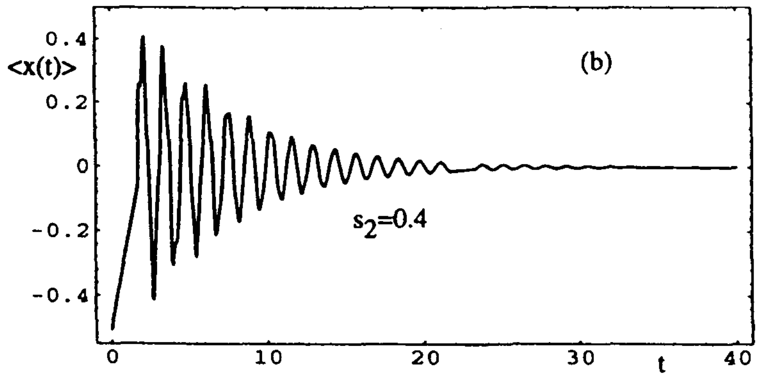

Figure 7.14: The motion of the center of the wave packet in a symmetric double-well when the barrier is complex with negative imaginary part. The time is measured in units of L^2.

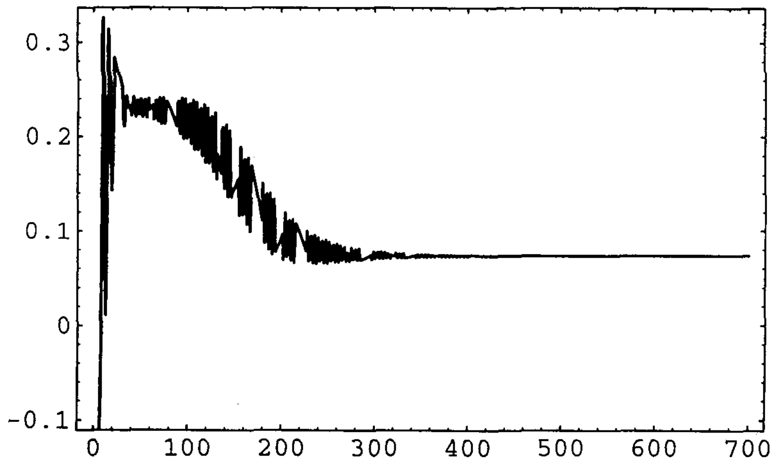

Figure 7.15: The motion of the center of the wave packet as a function of time t when the wave packet is initially in the shallower well.

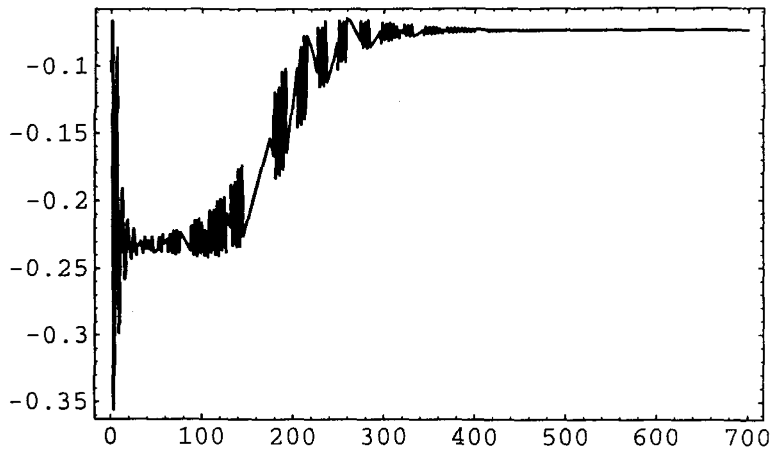

Figure 7.16: The time dependence of the center of wave packet when at $t = 0$ this center is in the middle of the deeper well.

value and remains in the deeper well.

The other possibility is to have the initial wave packet in the deeper well. For this case we choose $v_0 = 4L^{-2}$ and repeat the calculation to find that again $\langle x(t) \rangle$ oscillates very rapidly for a long time before reaching its asymptotic value. This time $\langle x(\infty) \rangle$ is to the right of the barrier whereas $\langle x(0) \rangle$ was to the left (Fig. (7.16)). We conclude that the presence of the imaginary part in $V(x)$ makes it possible for a wave packet to tunnel through the barrier which otherwise would have been very improbable.

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Chapter 8

A Classical Description of Tunneling

At the beginning of Chapter 2, we defined tunneling as a quantal process which is forbidden by the laws of classical dynamics. But we can describe the tunneling phenomena either partially, [1] [2] [3] [4] (see also Section 12.5), or completely in terms of the laws of classical dynamics provided that we replace the simple system by a complicated interacting system [5].

Here we will study the latter case where we assume that a specific system with infinite number of degrees of freedom is coupled to the tunneling particle [6]. Let us consider the motion of a particle with N degrees of freedom whose motion is governed by the Hamiltonian operator $H(\mathbf{P}, \mathbf{Q})$, where P_n and Q_n $(n = 1, 2, \ldots N)$ are the momentum and coordinate operators.

The wave function at the time t for the particle is

$$\Psi(t) = U \sum_j B_j(t)\phi_j, \tag{8.1}$$

where U is given by

$$U = \exp\left(i\frac{S}{\hbar}\right) \exp\left[-\frac{i}{\hbar}\left(\mathbf{q} - \langle\mathbf{Q}\rangle\right).\mathbf{P}\right] \exp\left[\frac{i}{\hbar}\left(\mathbf{p} - \langle\mathbf{P}\rangle\right).\mathbf{Q}\right], \tag{8.2}$$

and ϕ_j's form a complete set of orthonormal wave functions. Each of the vectors $\mathbf{P}$ and $\mathbf{Q}$ have N components and $\mathbf{p}$ and $\mathbf{q}$ are real vectors which depend on time, and $B_j(t)$'s are an infinite set of complex functions of time.

In Eq. (8.2) the symbol $\langle\rangle$ is used to denote the inner product of any operator A;

$$\langle A\rangle = \sum_j \sum_k B_j{}^* A_{jk} B_k, \tag{8.3}$$

where

$$A_{jk} = \langle \phi_j | A | \phi_k \rangle . \tag{8.4}$$

Returning to Eq. (8.2), the phase $S(t)$ is defined by

$$S(t) = \int_{t_0}^{t} (\mathbf{p} - \langle \mathbf{P} \rangle) . \frac{d\mathbf{q}}{dt'} dt', \tag{8.5}$$

where t_0 is the arbitrary initial time. We choose the coefficients $B_j(t)$ in such a way that $\Psi(t)$, Eq. (8.1), is properly normalized, or

$$\sum_j \langle B_j(t) | B_j(t) \rangle = 1. \tag{8.6}$$

If this condition is fulfilled at an arbitrary time t_0, then the time-dependent Schrödinger equation guarantees its validity at other times. Now using the identity

$$U^\dagger (a\mathbf{P} + b\mathbf{Q}) U = a\,(\mathbf{p} + \mathbf{P} - \langle \mathbf{P} \rangle) + b\,(\mathbf{q} + \mathbf{Q} - \langle \mathbf{Q} \rangle)\,, \tag{8.7}$$

we can show that

$$\mathbf{q} = \langle \Psi | \mathbf{Q} | \Psi \rangle\,, \tag{8.8}$$

and

$$\mathbf{p} = \langle \Psi | \mathbf{P} | \Psi \rangle\,. \tag{8.9}$$

Since ϕ_j's are orthogonal to each other, then from (8.1) it follows that

$$B_j = \left\langle \phi_j | U^\dagger | \Psi \right\rangle . \tag{8.10}$$

By differentiating (8.8) and (8.10) with respect to time and using (8.7), we find the following equations for $\frac{d\mathbf{q}}{dt}$ and $\frac{d\mathbf{p}}{dt}$;

$$\frac{d\mathbf{p}}{dt} = -\langle \Psi | \nabla_Q H | \Psi \rangle = -\nabla_q \mathcal{H}, \tag{8.11}$$

and

$$\frac{d\mathbf{q}}{dt} = \langle \Psi | \nabla_P H | \Psi \rangle = \nabla_p \mathcal{H}, \tag{8.12}$$

where

$$\mathcal{H} = \langle \Psi | H(P, Q) | \Psi \rangle = \langle H\,(p + P - \langle P \rangle\,, q + Q - \langle Q \rangle) \rangle\,. \tag{8.13}$$

In addition we get

$$
\begin{aligned}
i\hbar\frac{dB_j}{dt} &= -\frac{d\langle\mathbf{Q}\rangle}{dt}.\left(\mathbf{p}-\langle\mathbf{P}\rangle\right)B_j - \left[\nabla_q\mathcal{H}+\frac{d}{dt}\langle\mathbf{P}\rangle\right].\sum_j \mathbf{Q}_{jk}B_k \\
&- \left[\nabla_p\mathcal{H}-\frac{d}{dt}\langle\mathbf{Q}\rangle\right].\sum_j \mathbf{P}_{jk}B_k \\
&+ \sum_k \left[H\left(p+P-\langle P\rangle, q+Q-\langle Q\rangle\right)\right]_{jk}B_k.
\end{aligned}
\tag{8.14}
$$

In this last expression we have the terms $\frac{d\langle\mathbf{P}\rangle}{dt}$ and $\frac{d\langle\mathbf{Q}\rangle}{dt}$. If we start with Eq. (8.3) and write for $\langle\mathbf{Q}\rangle$

$$
\langle\mathbf{Q}\rangle = \sum_j\sum_k B_j{}^*\left\langle\phi_j|\mathbf{Q}|\phi_k\right\rangle B_k, \tag{8.15}
$$

then differentiate (8.15) with respect to t, and eliminate $\frac{dB_j{}^*}{dt}$ and $\frac{dB_k}{dt}$ using Eq. (8.14) we get the trivial result $\frac{d\langle\mathbf{Q}\rangle}{dt}=\frac{d\langle\mathbf{Q}\rangle}{dt}$ and a similar result for $\frac{d\langle\mathbf{P}\rangle}{dt}$. This means that we can assign arbitrary values to these quantities, and in particular we can set them equal to zero

$$
\frac{d\langle\mathbf{Q}\rangle}{dt} = \frac{d\langle\mathbf{P}\rangle}{dt} = 0. \tag{8.16}
$$

Having obtained the essential equations for this formulation we choose the following canonical coordinates and momenta for the classical Hamiltonian.

In addition to the N pairs of conjugate variables (q_n, p_n) defined by (8.11) and (8.12) we have an infinite set of pairs (ξ_j, π_j) given by

$$
\pi_j = \sqrt{2\hbar}\,\mathrm{Im}\,B_j, \quad \xi_j = \sqrt{2\hbar}\,\mathrm{Re}\,B_j. \tag{8.17}
$$

Now the classical Hamiltonian $\mathcal{H}(q,p,:\xi,\pi)$ defined by (8.13) gives the time development of q and p as well as those of ξ and π according to the Hamilton's canonical equations [7]

$$
\frac{dp_j}{dt} = -\frac{\partial\mathcal{H}}{\partial q_j}, \quad \frac{dq_j}{dt} = \frac{\partial\mathcal{H}}{\partial p_j}, \tag{8.18}
$$

and

$$
\frac{d\pi_j}{dt} = -\frac{\partial\mathcal{H}}{\partial\xi_j}, \quad \frac{d\xi_j}{dt} = \frac{\partial\mathcal{H}}{\partial\pi_j}, \tag{8.19}
$$

which follows from the variation of (8.13), and these are exactly the same equations as those given by (8.11), (8.12) and (8.14).

Now let us apply this idea to the tunneling of a particle in a one-dimensional confining potential, for instance, a double-well. Here the Hamiltonian (8.13) can be written as

$$\begin{aligned}\mathcal{H}(q,p;\xi,\pi) &= \frac{1}{2m}\left\langle (p+P-\langle P\rangle)^2\right\rangle + \langle V(q+Q-\langle Q\rangle)\rangle \\ &= \frac{p^2}{2m}+\frac{1}{2m}\left[(p-\langle P\rangle)^2\left(\sum_j B_j{}^*B_j-1\right)+\left(\left\langle P^2\right\rangle-\langle P\rangle^2\right)\right] \\ &+ \langle V\left(q+Q-\langle Q\rangle\right)\rangle .\end{aligned} \tag{8.20}$$

The Hamiltonian in (8.20) gives us the equation of motion for q, p, π and ξ. Along the trajectory of the particle $(\sum_j B_j{}^*B_j - 1) = 0$, therefore we can set the second term on the right hand side of (8.20) equal to zero although for the calculation of $\frac{dB_j^*}{dt}$ and $\frac{dB_j}{dt}$ we have to keep $\mathcal{H}$ in the original form of (8.20). Keeping this point in mind we can simplify (8.20) and write $\mathcal{H}$ as

$$\mathcal{H}_{eff}(p,q;\pi_0,\xi_0) = \frac{p^2}{2m} + V_{eff}(q;\pi_0,\xi_0). \tag{8.21}$$

This Hamiltonian can be used to generate the equations of motion for q and p, provided that we replace ξ and π by ξ_0 and π_0 and assume that the latter pair does not change with changes in p and q. By this we mean that once the solutions of (8.19) are found, and we denote these by $\xi_0(t)$ and $\pi_0(t)$, they will be used in (8.21). Then the effective potential in (8.21) will be given by

$$V_{eff} = \mathcal{H}_{eff}(p=0,q;\pi_0,\xi_0) = \frac{1}{2m}\left\langle P^2-\langle P\rangle^2\right\rangle + \langle V\left(q+Q-\langle Q\rangle\right)\rangle , \tag{8.22}$$

and this V_{eff} will depend on the two functions of time $\xi_0(t)$ and $\pi_0(t)$.

A simple way of determining V_{eff} is to write those quantities which we have denoted by the inner product $\langle\rangle$ in terms of the expectation value

$$\langle A\rangle = \left\langle \Psi_0|U_0AU_0{}^\dagger|\Psi_0\right\rangle , \tag{8.23}$$

where Ψ_0 and U_0 are Ψ and U in which ξ and π have been replaced by ξ_0 and π_0. In this way the effective potential becomes

$$V_{eff}(q:\pi_0;\xi_0) = \frac{1}{2m}\left(\left\langle\Psi_0|P^2|\Psi_0\right\rangle - {p_0}^2\right) + \langle\Psi_0\left|V(q+Q-x_0)\right|\Psi_0\rangle . \tag{8.24}$$

Thus the potential is found by calculating the expectation value of $V(Q+q-x_0)$ with the wave function $\Psi_0(Q,\pi_0,\xi_0)$ and then adding the quantity $\frac{1}{2m}(\langle\Psi_0|P^2|\Psi_0\rangle - {p_0}^2)$ which is independent of q to it. The position x_0 and the momentum p_0 in the above relations are the expectation values of (8.8) and (8.9) in which we have used $\Psi_0(x,t)$ instead of $\Psi(x,t)$.

As an example let us consider the symmetric potential (7.62) with $n=3$ for which the lowest eigenfunctions are given by (7.68) and (7.78)-(7.81) . For the wave packet we choose a Gaussian function

$$\Psi(x) = \left(\frac{\Omega}{\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{1}{4}\Omega\,(q+a)^2\right]. \tag{8.25}$$

We expand this wave packet in terms of the $\psi_j(x)$'s Eqs. (7.68) and (7.78)-(7.81) to find the approximate wave packet $\Psi_0(x,t)$

$$\Psi_0(x,t) = \sum_j c_j \psi_j(q) \exp\left(-iE_j t\right), \tag{8.26}$$

where we have replaced x in $\psi_j(x)$ by q, and E_j's are given by Eqs. (7.83)-(7.86). Using this wave packet we can determine x_0 and p_0 from Eqs. (7.97) and (7.98). In Fig. (8.1) both x_0 and p_0 are shown as functions of time. Here unlike the case of asymmetric well the center of the wave packet oscillates between the two wells.

In Figs. (8.2), (8.3) and (8.4) we have plotted the classical potential in which the particle moves at three different times.
First at $t=0$, $x_0(t=0) = -0.965$ and the potential $\langle V(Q+q-x(0)\rangle$ has the shape shown in Fig. (8.2) and the oscillation of the particle starts in the left well. At a later time $t=1.27$, $x_0(t=1.27) = -0.344$ and now the potential changes its shape becoming a wide well shown in Fig. (8.3). But after passing the barrier, the particle enters the well to the right. For this case we have the effective potential which is shown in Fig (8.4). This is obtained for the time $t=2.28$ and $x_0=0.91$. Since we have superimposed four wave functions to get $\Psi_0(q,t)$ and the ratios of the energies $\frac{E_1}{E_0}$, $\frac{E_2}{E_0}$... are not all integers, it takes a very long time for the trajectory in the phase space to return to its original point, i.e. $x_0(T)=x_0(0)$ and $p_0(T)=p_0(0)$, and for this reason the period of oscillations of $\langle V(Q+q-x(0)\rangle$ is very long.

In Fig. (8.5) the parametric curve $p_0(t)$, $x_0(t)$ for the oscillations of the particle between the two points is shown. Some of the differences between the motion in symmetric and and in asymmetric wells can be seen by comparing Fig. (8.5) and Fig. (7.12).

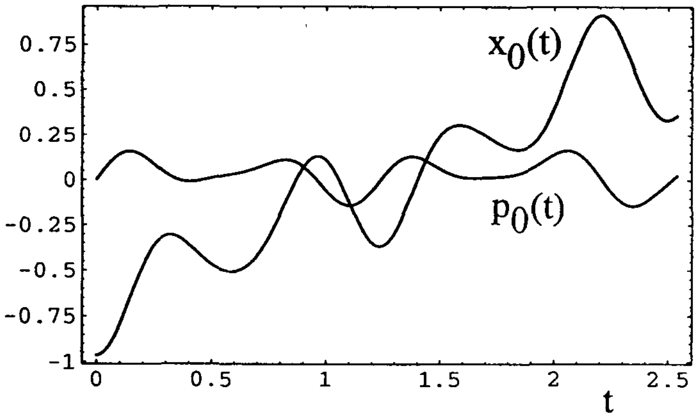

Figure 8.1: The motion of the center and the momentum of the Gaussian wave packet (8.25) in the double-well (7.62) shown as a function of time. The parameters $n = 3$, $a = 1$,, $\Omega = 10.907$ and $\xi = \frac{8}{\cosh 2}$ have been used in this calculation.

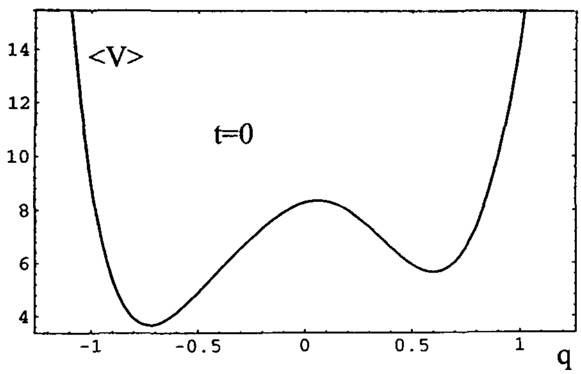

Figure 8.2: The average potential felt by the particle at $t = 0$.

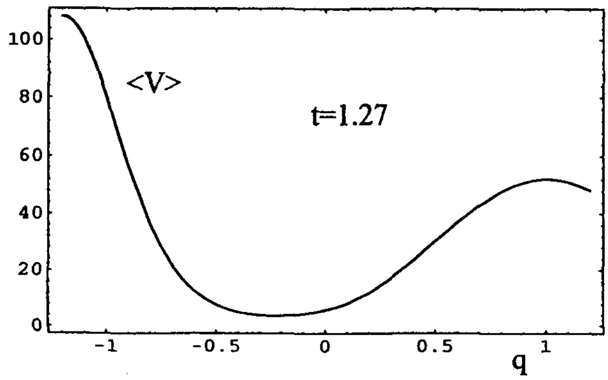

Figure 8.3: Same as in Fig. (8.2) but for the time $t = 1.27$.

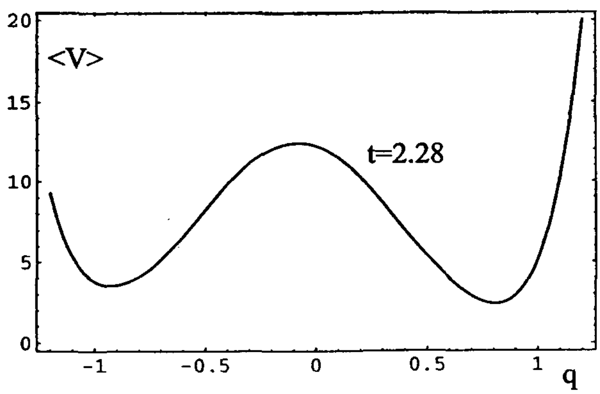

Figure 8.4: The classical potential affecting the particle at $t = 2.28$.

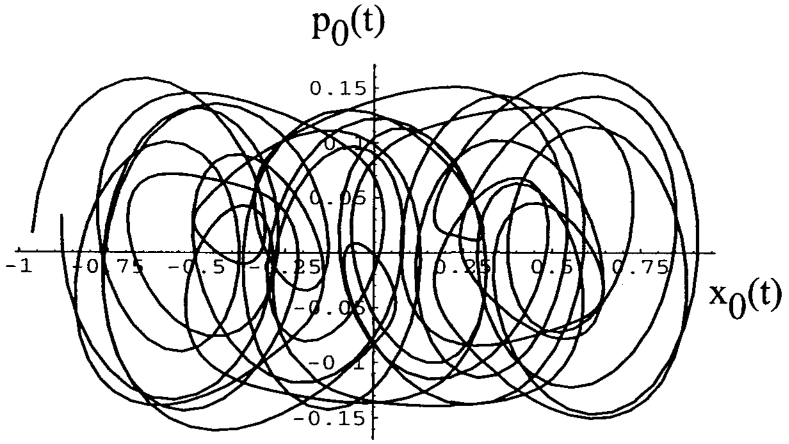

Figure 8.5: The phase space trajectory for $p_0(t)$ and $x_0(t)$ for a symmetric double-well potential.

Bibliography

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Chapter 9

Tunneling in Time-Dependent Barriers

In condensed matter physics, the technology of molecular beam epitaxy and layer by layer growth of semiconductor heterostructures have given rise to numerous tunneling applications. In these structures the time-dependent barriers appear in two ways: An explicit time-dependence arises due to the applied a.c. fields with frequencies reaching into microwaves ($10^7 - 10^{11}$ Hz). Secondly, resonant tunneling occurs in a small energy range and this can be modeled by considering an oscillating barrier [1] [2] [3]. In these problems mostly one-dimensional tunneling is important and therefore we study the motion of a particle of mass m in a barrier $V(x,t)$, where we assume that

$$V(x,t) \to 0 \quad \text{as} \quad x \to \pm\infty. \tag{9.1}$$

Thus the problem is that of the solution of the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{9.2}$$

with the initial and boundary conditions that will be specified shortly.

9.1 Multi-Channel Schrödinger Equation for Periodic Potentials

In most of the problems in condensed matter physics $V(x,t)$ is a periodic function of time with a period T_0, and for these we expand $V(x,t)$ in terms of the Fourier series

$$V(x,t) = V(x,t+T_0) = \sum_{n=-\infty}^{\infty} V_n(x)\exp(in\omega t), \tag{9.3}$$

where $\omega = \frac{2\pi}{T_0}$ is the angular frequency. Since in the differential equation (9.2), $V(x,t)$ is periodic we can make use of Floquet's theorem [4] and write the wave function ψ as

$$\psi_E(x,t) = \exp\left(-i\frac{Et}{\hbar}\right)\phi_E(x,t), \tag{9.4}$$

in which $\phi_E(x,t)$ is periodic with a period T_0

$$\phi_E(x,t+T_0) = \phi_E(x,t). \tag{9.5}$$

The function $\phi_E(x,t)$ which is periodic in time, can be expanded as a Fourier series

$$\phi_E(x,t) = \sum_{-\infty}^{\infty}\phi_{nE}(x)e^{in\omega t}. \tag{9.6}$$

Now if we substitute Eqs. (9.3), (9.4) and (9.6) in (9.2) and eliminate the time-dependence we find that $\phi_{nE}(x)$ satisfies the set of coupled differential equations;

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_{nE}}{dx^2} + \sum_{p=-\infty}^{\infty} V_{n-p}(x)\phi_{pE} = (E - \hbar n\omega)\phi_{nE}. \tag{9.7}$$

To simplify this set of equations we omit the subscript E and write ϕ_n instead of ϕ_{nE} and as usual define ${k_n}^2$ and $v_{np}(x)$ by

$${k_n}^2 = \frac{2m}{\hbar^2}(E - \hbar n\omega), \tag{9.8}$$

and

$$v_{np} = \frac{2m}{\hbar^2}V_{n-p}, \tag{9.9}$$

and thus we get the following set of coupled differential equations

$$\frac{d^2\phi_n}{dx^2} + k_n{}^2\phi_n = \sum_p v_{np}\phi_p. \tag{9.10}$$

When the potential $V_{n-p}(x)$ is real and symmetric matrix, then $v_{np}(x) = v^*_{pn}(x)$ and also from Eq. (9.1) $v_{np}(x) \to 0$ as $x \to \pm\infty$. Thus boundary conditions for the system are:

$$\lim_{x\to\pm\infty} \phi_n(x) \to \exp(\pm i k_n x) \quad \text{as} \quad x \to \pm\infty, \quad k_n^2 > 0, \tag{9.11}$$

and

$$\lim_{x\to\pm\infty} \phi_n(x) \to \exp(-|k_n|x) \quad \text{as} \quad x \to \pm\infty, \quad k_n^2 < 0. \tag{9.12}$$

In general the wave functions $\{\phi_n(x)\}$ are not orthogonal to each other, i.e. $\langle\phi_n|\phi_p\rangle \neq 0$, however the matrix composed of the elements $\langle\phi_n|\phi_p\rangle \neq 0$ is related to the scattering matrix. Since the particle at $x \to -\infty$ may be in a state n and at $x \to \infty$ in another state p, we write Eq. (9.10) as a matrix equation

$$\frac{d^2\phi_{np}}{dx^2} + k_n{}^2\phi_{np} = \sum_p v_{nq}\phi_{qp}. \tag{9.13}$$

Here n indicates the incident and p the exit channel. With this convention we can write the reflection and the transmission amplitudes as

$$R_{np} = \sum_q \frac{1}{2ik_n}\int_{-\infty}^{\infty} \exp(ik_n x')v_{nq}(x')\phi_{qp}(x')dx', \tag{9.14}$$

and

$$T_{np} = \delta_{np} + \sum_q \frac{1}{2ik_n}\int_{-\infty}^{\infty} \exp(-ik_n x')v_{nq}(x')\phi_{qp}(x')dx', \tag{9.15}$$

where R_{np} is the reflection amplitude when n and p are the incident and the exit channels. In Chapter 11 we will study the direct method of calculating R_{np} and T_{np}. But for the present we find the solution of some simple examples of tunneling in time-dependent barriers (see also [6] and [7] and Section (24.4)).

9.2 Tunneling Through an Oscillating Potential Barrier

Let us consider the potential

$$v(x,t) = \frac{s}{2}\delta\left[x - a\cos(\omega t)\right], \tag{9.16}$$

and choose the units so that $\hbar = m = 1$. The wave functions for $x < a\cos(\omega t)$ and $x > a\cos(\omega t)$ will be denoted by ψ_1 and ψ_2 respectively. Then at $x = a\cos(\omega t)$ we have the conditions of continuity

$$\psi_1\left[x = a\cos(\omega t)\right] = \psi_2\left[x = a\cos(\omega t)\right], \tag{9.17}$$

and

$$\left(\frac{\partial\psi_2}{\partial x}\right)_{x=a\cos(\omega t)} - \left(\frac{\partial\psi_1}{\partial x}\right)_{x=a\cos(\omega t)} = s\psi_1\left[x - a\cos(\omega t)\right]. \tag{9.18}$$

Now let us assume that in the incident channel the particle has the energy $E = \frac{1}{2}k^2$, thus

$$\psi_{in}(x,t) = \exp[i(kx - Et)]. \tag{9.19}$$

From what we have seen earlier, we know that the complete solution of the Schrödinger equation for this case is

$$\begin{aligned}\psi_1(x,t) &= \exp[i(kx - Et)] \\ &+ \sum_{j=-\infty}^{\infty} R_j \exp[-ik_jx - i(E + j\omega)t], \quad x < a\cos(\omega t),\end{aligned} \tag{9.20}$$

and

$$\psi_2(x,t) = \sum_{j=-\infty}^{\infty} T_j \exp[ik_jx - i(E + j\omega)t], \quad x > a\cos(\omega t), \tag{9.21}$$

where in these relations k_j's are defined by

$$E_j = \frac{1}{2}{k_j}^2 = E + j\omega = \frac{1}{2}k^2 + j\omega. \tag{9.22}$$

For those values of j when ${k_j}^2$ becomes negative and k_j imaginary, we write

$$k_j \to i|k_j| = i(2|j|\omega - k^2)^{\frac{1}{2}}. \tag{9.23}$$

By substituting (9.20) and (9.21) in (9.17) and (9.18) and making use of the integral [8]

$$\int_{-\infty}^{\infty} \exp\left[i(ka\cos(\omega t) - j\omega t\right] dt = \left(\frac{2\pi}{\omega}\right) \sum_{n=-\infty}^{\infty} i^n J_n(ka)\delta(n-j), \quad (9.24)$$

we find the following set of linear equations for T_j and R_j;

$$J_n(ka) = \sum_{j=-\infty}^{\infty} i^j J_{n+j}(k_j a)\left\{T_j - (-1)^{n+j} R_j\right\}, \quad (9.25)$$

and

$$kJ_n(ka) = \sum_{j=-\infty}^{\infty} i^j J_{n+j}(k_j a)\left\{(k_j + is)T_j + (-1)^{n+j} k_j R_j\right\}. \quad (9.26)$$

When k_j is imaginary, in these equations we replace J_n by

$$J_n(i|k_j|a) = i^n I_n(|k_j|a). \quad (9.27)$$

From Eqs. (9.25) and (9.26) we can find T_j's and R_j's. An approximate way of solving these equations is to truncate the infinite sums in (9.25) and (9.26) to finite sums. To this end we set all the Bessel functions $J_{p+j}(z)$ for which $|p+j| > n$ equal to zero, and also set all $J_n(k_q a)$ when $|q| > n$ equal to zero. As a numerical example let us consider the case where $a = 1L, k^2 = \omega = 1L^{-2}$. By truncating the sums in Eqs. (9.25) and (9.26) to 21 terms, we find the values of T_j and R_j displayed in Table I.

TABLE I - The real and imaginary parts of the transmission amplitude T_j and the reflection amplitude R_j calculated for tunneling through an oscillating delta function potential Eqs. (9.25) and (9.26). For this calculation we have used $a = 1L, s = 1L^{-1}$ and $k^2 = \omega = 1L^{-2}$.

j	-3	-2	-1	0	1	2	3
Re T_j	-0.025	-0.069	-0.198	0.834	-0.076	0.019	0.010
Im T_j	0.047	0.080	0.112	0.420	0.046	0.030	0.007
Re R_j	0.010	-0.041	0.147	-0.104	0.120	0.043	-0.087
Im R_j	0.066	0.137	0.287	0.127	0.066	0.097	0.032

We can calculate the probability current in terms of T_m's from $\psi_2(x,t)$. For instance at $x=0$, the current is given by

$$j_2(x=0,t) = \mathrm{Im}\left\{\sum_n\sum_m ik_n T_m{}^* T_n \exp[-i(n-m)\omega t]\right\}. \tag{9.28}$$

The very important result, the conservation of probability for this problem can be stated as

$$\sum_m{}' \left(\frac{k_m}{k_0}\right)\left\{|T_m|^2 + |R_m|^2\right\} = 1, \tag{9.29}$$

where $\sum_m'$ denotes a sum over those values of m for which k_m is real. This relation can be used to check the accuracy of the solution of Eqs. (9.25) and (9.26).

Next we want to solve the problem of tunneling of a particle through an arbitrary one-dimensional potential $V(x)$ when the particle is charged and in addition to $V(x)$, there is an oscillating applied electric field $\mathcal{E} = \omega A_0 \sin(\omega t)$. In this case the Schrödinger equation is given by

$$i\frac{\partial\psi(x,t)}{\partial t} = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + iA_0\cos(\omega t)\frac{\partial}{\partial x} + V(x)\right]\psi(x,t). \tag{9.30}$$

When $V(x)$ is constant the solution of this equation has the simple form of

$$\psi(x,t) = \exp\left[i\left(\pm kx - Et \pm \frac{A_0 k\sin(\omega t)}{\omega}\right)\right], \tag{9.31}$$

where

$$k = \sqrt{2(E-V)}. \tag{9.32}$$

We can approximate $V(x)$ by a large number of rectangular potentials of different heights. Thus we need to solve (9.30) for one rectangular barrier for all times and then match the solution for a given barrier to the solution of the two adjacent barriers. At the boundary X_i separating two regions of constant potentials the wave functions to the left $\Psi^l(x,t)$ and to the right $\Psi^r(x,t)$ each can be written as a linear combination of the solutions like (9.31),

$$\begin{aligned}\Psi^l(x,t) &= \sum_{n=-\infty}^{\infty}\left\{T_n^l \exp\left[i\left(k_n^l x - E_n t + \frac{A_0 k_n^l\sin(\omega t)}{\omega}\right)\right]\right.\\ &+ \left. R_n^l \exp\left[-i\left(k_n^l x + E_n t + \frac{A_0 k_n^l \sin(\omega t)}{\omega}\right)\right]\right\},\end{aligned} \tag{9.33}$$

and

$$\begin{aligned}\Psi^r(x,t) &= \sum_{n=-\infty}^{\infty} \left\{ T_n^r \exp\left[i\left(k_n^r x - E_n t + \frac{A_0 k_n^r \sin(\omega t)}{\omega} \right) \right] \right. \\ &+ \left. R_n^r \exp\left[-i\left(k_n^r x + E_n t + \frac{A_0 k_n^r \sin(\omega t)}{\omega} \right) \right] \right\}. \qquad (9.34)\end{aligned}$$

In these expressions $E_n = E + n\omega$ where E is the initial energy of the particle. The wavenumbers $k_n^{l,r}$ depend on the values of the potential to the left or to the right of the discontinuity

$$k_n^{l,r} = \sqrt{2(E_n - V^{l,r})}, \qquad (9.35)$$

where $k_n^{l,n}$ can be real or imaginary for the open and closed channels respectively. For the numerical calculation we truncate the infinite sums in (9.33) and (9.34) by summing from $n = -N$ to $n = N$. Then we have $2N(N+1)$ unknowns $T_n^{l,r}$ and $R_n^{l,r}$which should be determined by matching the solutions. Since these matchings must be satisfied at all times, therefore we proceed by matching the Fourier components. To this end we observe that using the identity Eq. (9.26)

$$\exp\left[\pm \frac{iA_0 k_n}{\omega} \sin(\omega t) \right] = \sum_{j=-\infty}^{\infty} J_j\left(\pm \frac{A_0 k_n}{\omega} \right) \exp[ij\omega t], \qquad (9.36)$$

we can decompose $\psi(x,t)$, Eq. (9.31) into an infinite number of Fourier components. Again we replace the infinite sums by finite sums (from $n = -N$ to $n = N$ in (9.26)), and we find $2(2N+1)$ equations for $2(2N+1)$ amplitudes, $T_n^{l,r}$ and $R_n^{l,r}$. We can write these equations in matrix form by defining a^l and a^r by

$$a^l = \begin{bmatrix} T_{-N}^l \\ \cdots \\ T_0^l \\ \cdots\cdot \\ T_N^l \\ R_{-N}^l \\ \cdots\cdot \\ R_0^l \\ \cdots\cdot \\ R_N^l \end{bmatrix} \quad \text{and} \quad a^r = \begin{bmatrix} T_{-N}^r \\ \cdots \\ T_0^r \\ \cdots\cdot \\ T_N^r \\ R_{-N}^r \\ \cdots\cdot \\ R_0^r \\ \cdots\cdot \\ R_N^r \end{bmatrix}. \qquad (9.37)$$

Then the matching condition can be expressed as the matrix equation

$$M^l(X_i)a^l = M^r(X_i)a^r, \tag{9.38}$$

where $M^{l,r}(X_i)$'s are given by

$$M^{l,r}(X_i) =$$
$$\left[\begin{array}{ccc|ccc} .... & e^{ik_nX_i}J_p\left(\frac{A_0k_n}{\omega}\right) & ... & .... & e^{-ik_nX_i}J_p\left(-\frac{A_0k_n}{\omega}\right) & ... \\ ... & ... & ... & ... & ... & ... \\ ... & ik_ne^{ik_nX_i}J_p\left(\frac{A_0k_n}{\omega}\right) & ... & ... & -ik_ne^{-ik_nX_i}J_p\left(-\frac{A_0k_n}{\omega}\right) & ... \end{array}\right]. \tag{9.39}$$

Here by k_n we mean k_n^l for $M^l(X_i)$ and k_n^r for $M^r(X_i)$. On the upper left side of this $M(X_i)$ matrix are the coefficients of the Fourier components of the transmitted wave and on the lower side their derivatives. The right side of $M(X_i)$ is composed of the Fourier components of the reflected wave and its derivative.
By the matrix inversion of (9.38) we find the column matrix

$$a^r = [M^r(X_i)]^{-1} M^l(X_i)a^l = \mathcal{M}(X_i)a^l. \tag{9.40}$$

This relation gives us the transfer matrix $\mathcal{M}$ for crossing the discontinuity at X_i. Next we consider a number of discontinuities at $X_1, X_2......X_p$ respectively and we denote the matrix formed of the amplitudes to the left of the barrier, i.e. where $V(x) = 0$ by a^{in} and the matrix of amplitudes to the right of the potential barrier by a^{out}. Then we can connect a^{out} to a^{in} by the transfer matrix method of Chapter 7;

$$a^{out} = \mathcal{M}(X_1)\mathcal{M}(X_2)......\mathcal{M}(X_p)a^{in}. \tag{9.41}$$

The boundary conditions of the problem implies that in a^{in}, $T_0 = 1$ and all other transmission amplitudes are zero, whereas in a^{out} all the reflections amplitudes R_n are zero. Thus we have $2N+1$ unknowns for the transmission amplitudes, and the same number of unknowns for the reflection amplitudes, and altogether we have $2(2N+1)$ inhomogeneous linear equations which can be solved for these unknowns. The same test that we discussed earlier, Eq. (9.29) can be used here to determine the accuracy of the method for a given N. For the numerical results of this procedure see the paper of Lefebvre [5].

9.3 Separable Tunneling Problems with Time-Dependent Barriers

We start this section by studying the motion of a particle of unit mass which is tunneling through a potential with a special dependence on time of the form $v(\lambda(t)x)$, where $\lambda(t)$ is a dimensionless function of time. We want to find those potentials of this form where we can reduce the time-dependent Schrödinger equation to an ordinary differential equation [9].

If H represents the Hamiltonian operator for the particle;

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + v(\lambda(t)x), \tag{9.42}$$

then the time-dependent Schrödinger equation is of the form

$$\left(H - i\frac{\partial}{\partial t}\right)\psi_1 = 0, \tag{9.43}$$

where we have set $\hbar = m = 1$. The space- and time-dependence of ψ_1, in general, cannot be separated from each other, but there are special cases where this is possible. To study these we start with the unitary transformation

$$U_1 = -\frac{1}{2}(xp + px)\ln\lambda(t), \tag{9.44}$$

where x and p are the coordinate and momentum operator of the particle.

With this transformation x and p are transformed to

$$x \to \exp(-iU_1)\, x \exp(iU_1) = \lambda(t)x, \tag{9.45}$$

and

$$p \to \exp(-iU_1)\, p \exp(iU_1) = \frac{p}{\lambda(t)}. \tag{9.46}$$

Thus $\lambda(t)$ is a time-dependent scale transformation. Next we observe that the Schrödinger operator $H - i\frac{\partial}{\partial t}$ transforms to

$$\left(H - i\frac{\partial}{\partial t}\right) \to \exp(-iU_1)\left(H - i\frac{\partial}{\partial t}\right)\exp(iU_1) = \left(K - i\frac{\partial}{\partial t}\right), \tag{9.47}$$

where K is the Hamiltonian operator after transformation;

$$K = -\frac{1}{2\lambda^2(t)}\frac{\partial^2}{\partial x^2} + \frac{i}{2}\frac{d\ln(\lambda(t))}{dt}\left(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\right) + v(\lambda^2(t)x). \tag{9.48}$$

To simplify the problem further, we apply a second transformation to the operator (9.48). The unitary operator for this transformation is

$$U_2 = \exp\left[\frac{i}{2}\lambda(t)\frac{d\lambda(t)}{dt}x^2\right]. \tag{9.49}$$

Using this with Eq. (9.48) we obtain the Schrödinger equation

$$\left\{-\left(\frac{1}{2\lambda^2(t)}\right)\frac{\partial^2}{\partial x^2}+\frac{1}{2}\lambda(t)\frac{d^2\lambda(t)}{dt^2}x^2+v\left[\lambda^2(t)x\right]\right\}\psi=i\frac{\partial\psi}{\partial t}, \tag{9.50}$$

where in this equation ψ is the wave function after the two successive transformations. In Eq. (9.50) we can separate the space and time variables if the following conditions are met:

$$\lambda(t)\frac{d^2\lambda(t)}{dt^2}=\pm\left(\frac{\omega}{\lambda(t)}\right)^2, \tag{9.51}$$

and

$$v\left(\lambda^2(t)x\right)=\frac{w(x)}{\lambda^2(t)}. \tag{9.52}$$

In (9.51) ω^2 is the separation constant which has the dimension of $(\text{time})^{-2}$. By integrating (9.51) we find $\lambda(t)$;

$$\lambda(t)=\left[{\lambda_0}^2+2\lambda_0\dot{\lambda}_0 t+\left({\dot{\lambda}_0}^2\pm\frac{\omega^2}{{\lambda_0}^2}\right)t^2\right]^{\frac{1}{2}}, \tag{9.53}$$

with λ_0 and $\dot{\lambda}_0$ being the integration constants,

$$\dot{\lambda}_0=\left(\frac{d\lambda}{dt}\right)_{t=0}, \quad \lambda_0=\lambda(t=0). \tag{9.54}$$

From Eq. (9.52) it follows that apart from the trivial case of v=constant, only for two forms of v this equation is separable

$$v(x)=\left(\frac{s}{2}\right)\delta(x), \tag{9.55}$$

and

$$v(x)=\frac{s'}{x}, \tag{9.56}$$

If we assume a potential of the form (9.55) we can solve the Schrödinger equation by writing $\psi(x,t)$ as

$$\psi(x,t)=\phi(x)f(t). \tag{9.57}$$

By substituting (9.57) in (9.50) and separating the variables we find

$$i\frac{df}{dt}=\frac{k^2 f}{2\lambda^2(t)}, \tag{9.58}$$

and

$$\frac{d^2\phi}{dx^2}-\left(-k^2\pm\omega^2x^2\right)\phi=s\delta(x)\phi(x), \tag{9.59}$$

where in these equations $\frac{1}{2}k^2$ is the separation constant. The function f obtained from (9.58) is

$$f(t)=f(0)\exp\left[-\frac{i}{2}k^2\int_0^t\frac{dt'}{\lambda^2(t')}\right], \tag{9.60}$$

The other equation (9.59) can be solved in terms of the parabolic cylinder function [10] :

$$\phi(x<0)=\phi_1=A_1D_\nu(-z)+B_1D_\nu(z), \tag{9.61}$$

$$\phi(x>0)=\phi_2=A_2D_\nu(-z)+B_2D_\nu(z), \tag{9.62}$$

where z and ν are defined by

$$z=\sqrt{2\omega}x,\quad k^2=(2\nu+1)\omega. \tag{9.63}$$

After finding ϕ with the proper boundary conditions we can write the wave function in terms of the original variables ;

$$\psi_1(x,t)=\frac{1}{\sqrt{\lambda(t)}}\exp\left[\frac{i}{2}x^2\frac{d\ln\lambda(t)}{dt}\right]\phi\left(\frac{x}{\lambda(t)}\right)f(t). \tag{9.64}$$

For the special case of $\omega=0$, we can write $\phi(x)$ in terms of the trigonometric functions. If we assume that the boundary conditions are such that the particle is constrained to move in the interval $-b\lambda(t)\le x\le b\lambda(t)$, then k can take only discrete values. These are given by the equations

$$2k\cot(kb)=-s,\quad \text{for even states}, \tag{9.65}$$

and

$$\sin(kb)=0,\quad \text{for odd states}. \tag{9.66}$$

In this case $\lambda(t)$ is a linear function of time

$$\lambda(t)=\lambda_0+\dot{\lambda}_0t, \tag{9.67}$$

and $\psi(x,t)$ is composed of two parts, one for $x<0$ and the other for $x>0$. For instance for $x>0$ this wave function is of the following form

$$\psi_1(x>0,t)=\left\{\frac{B}{\sqrt{\lambda(t)}}\exp\left[\frac{i\dot{\lambda}_0x^2}{2\lambda(t)}\right]\exp\left[\frac{-i}{2}k^2\int_0^t\frac{dt'}{\lambda^2(t')}\right]\sin\left[\frac{kx}{\lambda(t)}\right]\right\}. \tag{9.68}$$

This wave function is interesting for the following reason: Here we have the one-dimensional motion of a particle between the two walls, but since these walls are moving, we have a current associated with the motion,

$$j(x,t)=\frac{\lambda_0B^2f^2(0)x}{\lambda^2(t)}\sin^2\left(\frac{kx}{\lambda(t)}\right). \tag{9.69}$$

If the boundary condition in this problem allows for a part of the incident wave from the left to pass through the barrier, then for the part which emerges on the right we have

$$\begin{aligned}\psi_1(x>0,t) &= \frac{2k}{(2k+is)\sqrt{\lambda(t)}}\exp\left[\frac{i}{2}\frac{d\ln\lambda(t)}{dt}x^2\right]\exp\left(\frac{ikx}{\lambda(t)}\right)\\ &\times \exp\left[\frac{-i}{2}k^2\int_0^t\frac{dt'}{\lambda^2(t')}\right].\end{aligned} \tag{9.70}$$

For the special case of

$$\lambda_0\dot{\lambda}_0\to\omega,\quad \text{and}\quad \lambda_0\to 0,\quad \text{i.e.}\ \ \lambda(t)=\sqrt{2\omega t}, \tag{9.71}$$

Scheitler and Kleber [6] have found an exact solution for the tunneling through a time-dependent δ-function potential of the form

$$v\left(\lambda(t)x\right)=\frac{s}{2\omega t}\delta(x). \tag{9.72}$$

In this relation s is the strength of the barrier and ω is a constant.

To find the solution of this problem when the initial wave function is given by $\psi(x,0)$ we first determine the propagator $K(x,t;x',0)$;

$$K(x,t;x',0)=U_0(x-x';t)-\frac{is}{2\omega|x'|+is}U(|x|,|x'|;t), \tag{9.73}$$

where $U_0(x-x';t)=K_0(x,t;x',0)$ is given by Eq. (6.22) and $U(|x|,|x'|;t)$ is defined by

$$U(|x|,|x'|;t)=\frac{1}{\sqrt{2\pi it}}\exp\left[\frac{i\left(|x|+|x'|\right)^2}{2t}\right]. \tag{9.74}$$

This last kernel is the solution of the wave equation

$$\left(i\frac{\partial}{\partial x}+\frac{1}{2}\frac{\partial^2}{\partial x^2}\right)U(|x|,|x'|;t)=\frac{i|x'|\delta(x)}{t}U(|x|,|x'|;t), \tag{9.75}$$

and this can be verified by direct substitution. With the help of the propagator (9.73) we can find the wave function at time t if $\psi(x,0)$ is known;

$$\begin{aligned}\psi(x,t) &= \int_{-\infty}^{\infty}U_0(x-x';t)\psi_0(x',0)dx' \\ &- is\int_{-\infty}^{\infty}\frac{2\omega}{2\omega|x'|+is}U(|x|,|x'|;t)\psi_0(x',0)dx'.\end{aligned} \tag{9.76}$$

Now let us consider the initial wave function $\psi_0(x,0)$. We assume that for $t\le 0$ the stream of noninteracting particles coming from left cannot penetrate the barrier and are reflected back, i.e.

$$\psi_0(x,0)=\theta(-x)\left(e^{ikx}-e^{-ikx}\right). \tag{9.77}$$

By substituting (9.77) in (9.76) we have the wave function $\psi(x,t)$ at time t. The first integral in Eq. (9.76) can be carried out with the result that

$$\int_{-\infty}^{\infty}U_0(x-x';t)\theta(-x)\left(e^{ikx}-e^{-ikx}\right)dx' = M(x;k;t)-M(x;-k;t), \tag{9.78}$$

where $M(x;k;t)$ is the Moshinsky function (see Eq. (6.32)) [11].

In order to evaluate the second integral in (9.76), we change the variable and write

$$\begin{aligned} &-\frac{is}{\sqrt{2\pi it}}\int_{-\infty}^{0}\frac{2\omega}{2\omega|x'|+is}\exp\left[i\frac{\left(|x|+|x'|\right)^2}{2t}\right]e^{ikx'}dx' \\ &= -\frac{is}{\sqrt{\pi}}\exp\left(kx-\frac{1}{2}k^2t\right)\int_{\frac{(x-kt)}{\sqrt{2it}}}^{\infty}\frac{e^{-z^2}}{\left(z-2ikt-x+\frac{is}{2\omega}\right)}dz, \\ &x\ge 0. \end{aligned} \tag{9.79}$$

This last integral can be carried out numerically. In Fig. (9.1), $|\psi(x,t)|^2$ which is calculated from (9.76) is plotted as a function of time for a point just to the right of the δ-function. For this calculation the parameters ω and k and the strength of the δ-function s are chosen as $0.5L^{-2}$, $0.4L^{-1}$ and $4L^{-1}$ respectively. The time in this graph is measured in units of L^2.

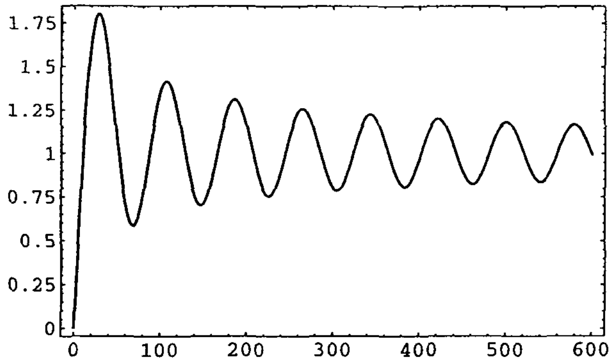

Figure 9.1: The square of the absolute value of the wave function $|\psi(x,t)|^2$ calculated from Eq. (9.76) for a point just outside and to the right of the δ-function.

9.4 Penetration of a Particle Inside a Time-Dependent Potential Barrier

For a potential barrier of the form

$$V(z,t) = G(t)z\theta(z)\theta(t), \quad G(t) > 0 \;\text{ for all t}, \tag{9.80}$$

where θ is the step function, the Schrödinger equation for $\psi(z,t)$ can be solved exactly. We write $\psi(z,t)$ as

$$\psi(z,t) = \exp\left[\frac{i}{\hbar}\left\{zf(t) + g(t)\right\}\right], \tag{9.81}$$

and substitute it in the Schrödinger equation and find the following equations for $f(t)$ and $g(t)$;

$$\frac{df(t)}{dt} = -G(t) \quad \text{and} \quad \frac{dg(t)}{dt} = -\frac{1}{2m}f^2(t). \tag{9.82}$$

Thus

$$f(t) = \hbar k - \int_0^t G(t')dt' \quad \text{and} \quad g(t) = -\frac{1}{2m}\int_0^t \left[\hbar k - \int_0^{t'} G(t'')dt''\right]^2 dt', \tag{9.83}$$

where $\hbar k$ is the constant of integration.

For small t, i.e. when $\hbar k >> \int_0^t G(t^{'})^{'} dt^{'}$, the wave function is

$$\psi(z,t) = \exp\left(ikz - \frac{i\hbar k^2}{2m}t\right). \tag{9.84}$$

This is a plane wave which is approaching the barrier from left. Now as Eqs. (9.81) and (9.83) show for times such that

$$\int_0^t G(t^{'})dt^{'} \geq \hbar k, \tag{9.85}$$

the particle is reflected and moves in the opposite direction. As is expected the transmission coefficient for this case is zero.

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Chapter 10

Decay Width and the Scattering Theory

The close connection between quantum scattering theory and the decay of a quasi-stationary state by tunneling is the topic that we want to discuss in this chapter.

Quantum scattering theory provides a powerful tool for calculating the decay width of a particle trapped behind a barrier. Here we consider two similar approaches to study the connection between scattering formalism and tunneling. In the first one the starting point is the time-dependent Schrödinger equation [1] and in the second is the time-dependent perturbation theory [2]. Both of these formulations are for three-dimensional tunneling when the barriers are central potentials.

In the case of one-dimensional tunneling when the particle is trapped between two barriers and can escape from one or both of these barriers, then the method of the variable S-matrix [3] can be used to find the complex eigenvalues of the system.

In the last two sections we study the connection between the Jost function [4] and the decay of the initial state and discuss the problem of antibound states [5].

10.1 Scattering Theory and the Time-Dependent Schrödinger Equation

In this chapter we study in some detail the connection between quantum tunneling and the quantum theory of scattering, and show how the latter theory can be used as a powerful tool for calculating the decay rates of the unstable states. For simplicity of discussion we assume three-dimensional tunneling but with central barriers. We define the effective potential $V_{eff}(r)$ as the sum of the central potential $V(r)$ and the centrifugal potential $\frac{\hbar^2 l(l+1)}{2mr^2}$;

$$V_{eff}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}. \tag{10.1}$$

Here the aim is to obtain the Gamow formula and the decay width Γ (see Chapter 5), which for $V_{eff}(r)$ can be written as

$$\Gamma = \frac{\hbar}{2m\int_{r_0}^{r_1} \frac{dr}{\sqrt{2m(E_0 - V_{eff}(r))}}} \exp[-2\sigma(E_0)], \tag{10.2}$$

where E_0 is the initial energy of the particle trapped behind the barrier $V_{eff}(r)$, and r_0 and r_1 are the turning points (for $l = 0$ usually we have $r_0 = 0$). The function $\sigma(E_0)$ is given by

$$\sigma(E_0) = \frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m(V_{eff}(r) - E_0)}dr. \tag{10.3}$$

The points r_1 and r_2 are the turning points inside the barrier i.e. they are the roots of $V_{eff}(r_{1,2}) = E_0$.

We start with the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}, \tag{10.4}$$

where the initial state is the wave packet $\Phi_0(\mathbf{r})$ which we assume is given for a fixed partial wave l;

$$\Phi_0(\mathbf{r}) = \Psi(\mathbf{r},0) = \frac{\phi(r)}{r}Y_{lm}(\theta,\phi)\exp(-\frac{i}{\hbar}E_0 t). \tag{10.5}$$

At any other time t, we can write $\Psi(\mathbf{r},t)$ as

$$\Psi(\mathbf{r},t) = \frac{\chi(r,t)}{r}Y_{lm}(\theta,\phi), \tag{10.6}$$

where $\chi(r,t)$ is the solution of the wave equation

$$i\hbar\frac{\partial\chi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\chi(r,t)}{\partial r^2} + V_{eff}(r)\chi(r,t). \tag{10.7}$$

Thus at $t=0$, we have the initial condition

$$\chi(r,t=0) = \phi(r). \tag{10.8}$$

Next we write $\chi(r,t)$ as

$$\chi(r,t) = A(t)\left\{\phi(r)\exp\left(-\frac{i}{\hbar}E_0 t\right) + Z(r,t)\right\}, \tag{10.9}$$

where from the initial form of the wave function (10.8) and (10.9) we find the following conditions that A and Z must satisfy:

$$A(0) = 1, \quad Z(r,0) = 0. \tag{10.10}$$

Noting that we have two new functions in the definition of $\chi(r,t)$, Eq. (10.9), i.e. $A(t)$ and $Z(r,t)$, we can impose a further condition on one or both of them. It is convenient to have the condition of orthogonality

$$\int_0^\infty \phi^*(r)Z(r,t)dr = 0, \tag{10.11}$$

imposed on $Z(r,t)$. Now if we substitute (10.9) in (10.7) and use Eq. (10.11) we obtain the following equation for $A(t)$;

$$i\hbar\frac{\partial A(t)}{\partial t} = y^*(t)A(t), \tag{10.12}$$

where

$$y^*(t) = \int_0^\infty \phi^*(r)V_1(r)\phi(r)dr + e^{\frac{i}{\hbar}E_0 t}\int_0^\infty \phi^*(r)V_1(r)Z(r,t)dr, \tag{10.13}$$

and $V_1(r)$ is given by

$$V_1(r) = \begin{cases} 0 & \text{for } r \le R \\ V_{eff}(r) - V_{eff}(R) & \text{for } r > R \end{cases}. \tag{10.14}$$

Here R is the point where $V(r)$ is maximum (see Fig. (10.1)).

By solving Eq. (10.12), we can find $A(t)$ in terms of $y^*(t)$;

$$A(t) = \exp\left[\frac{-i}{\hbar}\int_0^t y^*(t')dt'\right]. \tag{10.15}$$

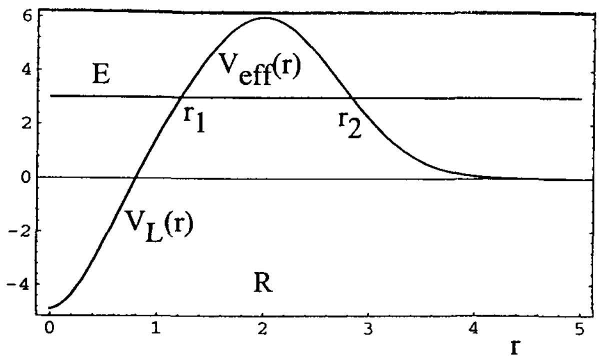

Figure 10.1: The effective potential for S-wave plotted as a function of r, showing the turning points r_1 and r_2.

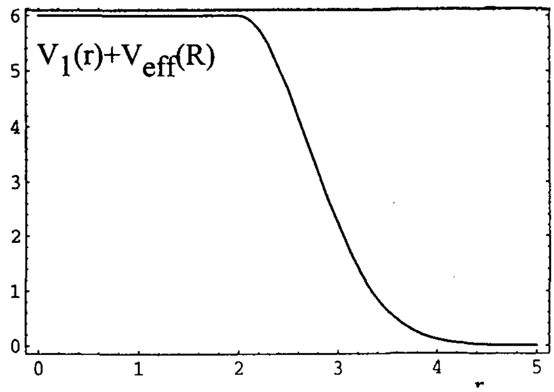

Figure 10.2: The sum of $V_1(r)$ and $V_{eff}(R)$ shown as a function of r, see Eq. (10.14).

Since $y^*(t)$ is a complex quantity we can write it as

$$y^*(t) = \mathrm{Re}\ \ y(t) - i\,\mathrm{Im}\ \ y(t), \quad \mathrm{Im}\, y(t) > 0, \tag{10.16}$$

and from this we can determine the probability of finding the system at the time t in the state $\phi(r)$;

$$P(t) = \left|\int_0^\infty \phi^*(r)\chi(r,t)dr\right|^2 = \exp\left[-\frac{2}{\hbar}\int_0^t \mathrm{Im}\ \ y(t')dt'\right]. \tag{10.17}$$

In the same way we obtain the probability of finding the system at the time t in the state

$$Z_0(r,t) = A(t)Z(r,t), \tag{10.18}$$

to be

$$W(t) = 1 - \exp\left[-\frac{2}{\hbar}\int_0^t \mathrm{Im}\, y(t')dt'\right]. \tag{10.19}$$

From Eqs. (10.7), (10.9) and (10.13) we find the differential equation which is satisfied by $Z_0(r,t)$;

$$\begin{aligned} & i\hbar\frac{\partial Z_0}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2 Z_0}{\partial r^2} - V(r)Z_0 \\ = \;& [V_1(r) - y^*(t)]\phi(r)\exp\left[-\frac{i}{\hbar}E_0 t - \frac{i}{\hbar}\int_0^t y^*(t')dt'\right]. \end{aligned} \tag{10.20}$$

We can write the solution of (10.20) with the boundary condition (10.10) as an integral equation

$$\begin{aligned} Z_0(r,t) \;=\; & -\frac{i}{\hbar}\int_0^t dt_1 \int_0^\infty G(r,t;r_1,t_1)[V_0(r_1) - V_{eff}(R)]Z_0(r_1,t_1)dr_1 \\ & - \frac{i}{\hbar}\int_0^t dt_1 \int_0^\infty G(r,t;r_1,t_1)\,[V_1(r_1) - y^*(t_1)]\,\phi(r_1) \\ & \times \exp\left[-\frac{i}{\hbar}E_0 t_1 - \frac{i}{\hbar}\int_0^{t_1} y^*(t_2)dt_2\right], \end{aligned} \tag{10.21}$$

where the potential $V_0(r)$ is defined by

$$V_0(r) = \begin{cases} V_{eff}(r) & \text{for } r \le R \\ V_{eff}(R) & \text{for } r > R \end{cases}, \tag{10.22}$$

and $G(r,t;r_1,t_1)$ is the Green function

$$\begin{aligned} & \left\{i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} - V_1(r) - V_{eff}(R)\right\} G(r,t;r_1,t_1) \\ = \;& i\hbar\delta(r - r_1)\delta(t - t_1). \end{aligned} \tag{10.23}$$

Now we express $G(r,t;r_1,t_1)$ in terms of its Fourier transform

$$G(r,t;r_1,t_1) = -\frac{i}{2\pi}\int_{-\infty}^{\infty} G(E;r,r_1)\exp\left[-\frac{i}{\hbar}E(t-t_1)\right]dE. \tag{10.24}$$

From (10.23) and (10.24) it follows that $G(E;r,r_1)$ is the solution of the differential equation

$$\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V_1(r) + V_{eff}(R)\right\}G(E;r,r_1) = EG(E;r,r_1) + \delta(r-r_1). \tag{10.25}$$

This Green's function is expressible in terms of the solution of the homogeneous differential equation for $\chi(r)$ [6]

$$\begin{aligned} G(E;r,r_1) &= -\frac{2m}{\hbar^2}\int_0^{\infty}\frac{\chi_q{}^{(+)}(r)\chi_q{}^{(*)}(r_1)}{k^2-q^2+i\epsilon}dq \\ &= \frac{2m}{\hbar^2 k}\sqrt{\frac{\pi}{2}}\begin{cases}\chi_k(r)\chi_k{}^{(+)}(r_1) & \text{for } r<r_1 \\ \chi_k(r_1)\chi_k{}^{(+)}(r) & \text{for } r>r_1.\end{cases}\end{aligned} \tag{10.26}$$

In this equation $k^2 = \frac{2mE}{\hbar^2}$ and $\chi_k{}^{(+)}(r)$ and $\chi_k(r)$ are the eigenfunctions of the Schrödinger equation for positive energies and for the potential

$$V_1(r) + V_{eff}(R) = \begin{cases} V_{eff}(R) & \text{for } r \le R \\ V_{eff}(r) & \text{for } r > R\end{cases}, \tag{10.27}$$

and have the following properties:

$$\chi_k(r) = \left(\frac{1}{2i}\right)\sqrt{\frac{2}{\pi}}\left[\chi_k{}^{(+)}(r) - \chi_k{}^{(-)}(r)\right], \tag{10.28}$$

and

$$\chi_k{}^{\pm}(r) \to \exp\left[\pm i\left(kr - \frac{\pi l}{2} + \delta_l\right)\right], \quad \text{as } r\to\infty. \tag{10.29}$$

Here δ_l is the phase shift which is a function of the energy E. By substituting (10.24) in (10.21) and making use of (10.25) and (10.26) we can write $Z_0(r,t)$ as

$$\begin{aligned} Z_0(r,t) &= \int_0^{\infty} G(r,t;r_1,t_1)\phi(r_1)dr_1 \\ &- \phi(r)\exp\left[-\frac{i}{\hbar}E_0 t - \frac{i}{\hbar}\int_0^t y^*(t_1)dt_1\right] \\ &- \left(\frac{1}{2\pi\hbar}\right)\int_0^t dt_1\int_0^{\infty}dr_1\int_{-\infty}^{\infty} G(E;r,r_1) \\ &\times \left[V_0(r_1) - V_{eff}(R)\right]\chi(r_1,t_1)\exp\left[-\frac{i}{\hbar}E\,(t-t_1)\right]dE. \end{aligned} \tag{10.30}$$

From Eqs. (10.9), (10.18) and (10.30) we conclude that

$$\begin{aligned}\chi(r,t) &\rightarrow \int_0^\infty G(r,t;r_1,0)\phi(r_1)dr_1 \\ &- \left(\frac{1}{2\pi\hbar}\right)\left(\frac{2m}{\hbar^2}\right)\sqrt{\frac{\pi}{2}}\int_0^t dt_1 \int_{-\infty}^{\infty}\frac{dE}{k}\chi_k{}^{(+)}(r)\int_0^R \chi_k(r_1)[V_0(r_1) \\ &- V_{eff}(R)]\chi(r_1,t_1)\exp\left[-\frac{i}{\hbar}E(t-t_1)\right]dr_1, \quad \text{for } r>R. \quad (10.31)\end{aligned}$$

We note that in (10.31) $[V_0 - V_{eff}(R)]_{r_1>R} = 0$, therefore $\chi(r,t)$ for $r > R$ is determined from the knowledge of $\chi(r,t)$ for $r < R$. No approximation has been made in arriving at Eq. (10.31).

10.2 An Approximate Method of Calculating the Decay Widths

When the decay is gradual, the state of the system is quasi-stationary and this is the case when

$$\alpha^2 = \left|\frac{y^*(t)}{E_0}\right| << 1, \quad (10.32)$$

for all values of $t > 0$ [1]. Once this inequality is satisfied then from the equation

$$\left\{i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} - V_0(r)\right\} Z(r,t) = -y^*(t)\left[Z(r,t) + \phi(r)\exp\left(-\frac{iE_0t}{\hbar}\right)\right], \quad (10.33)$$

and the initial conditions (10.10) we conclude that

$$Z(r,t)|_{r<R} = O\left(\frac{y^*(t)}{E_0}\right), \quad (10.34)$$

and thus

$$\chi(r,t)|_{r<R} = A(t)\left[\phi(r)e^{-\frac{i}{\hbar}E_0t} + O\left(\frac{y^*(t)}{E_0}\right)\right]. \quad (10.35)$$

By examining (10.31) we notice that for $r > R$, the first term of this equation decreases like $\frac{1}{\sqrt{t}}$ in time, and the second term is the quasi-stationary wave function of the system for times $t > \frac{\hbar}{E_0}$, provided that t is less than the lifetime of the original state $\phi(r)$. This second term, i.e. the quasi-stationary state of the system is approximately equal to

$$\begin{aligned}\chi(r,t)|_{r>R} &= -\frac{m}{\hbar^3}\sqrt{\frac{1}{2\pi}}\int_0^t dt_1\int_{-\infty}^{\infty}\frac{dE}{k}\chi_k{}^{(+)}(r)\exp\left(-\frac{i}{\hbar}E(t-t_1)\right)\\ &\times \int_0^R \chi_k(r_1)\left[V_0(r_1)-V_{eff}(R)\right]\left[\phi(r_1)\exp\left(-\frac{i}{\hbar}E_0t_1\right)+O\left(\frac{y^*(t_1)}{E_0}\right)\right]\\ &\times \exp\left[-\frac{i}{\hbar}\int_0^{t_1}y^*(t_2)dt_2\right]dr_1. \end{aligned} \tag{10.36}$$

Now we substitute Eq. (10.36) in (10.13) and calculate $y^*(t)$ in the first order of approximation (assuming α to be much less than one, Eq. (10.32)),

$$\begin{aligned} y^*(t) &\approx y_0{}^* = -\frac{2m}{\hbar^2k_0}\sqrt{\frac{\pi}{2}}\int_0^R \phi^*(r)V_1(r)\chi_{k_0}{}^{(+)}(r)dr\\ &\times \int_0^{\infty}\chi_{k_0}(r_1)[V_0(r_1)-V_{eff}(R)]\phi(r_1)dr_1, \end{aligned} \tag{10.37}$$

where $k_0=\sqrt{\frac{2mE_0}{\hbar^2}}$. The real and imaginary parts of $y_0{}^*$ give us the shift in the initial energy level and the decay width of the original state $\phi(r)$ respectively. From Eqs. (10.28) and (10.29) and the relation

$$\begin{aligned} &\int_0^{\infty}\chi_{k_0}(r_1)[V_0(r_1)-V_{eff}(R)]\phi(r_1)dr_1\\ &= \frac{\hbar^2}{2m}\left\{\chi_{k_0}\left(\frac{\partial\phi}{\partial r}\right)-\phi\left(\frac{\partial\chi_{k_0}}{\partial r}\right)\right\}_R, \end{aligned} \tag{10.38}$$

we find the following expression for Γ;

$$\begin{aligned} \Gamma &= \frac{2\pi m}{\hbar^2k_0}\left|\int_0^{\infty}\phi^*(r)V_1(r)\chi_{k_0}(r)dr\right|^2\\ &= \frac{\pi\hbar^2}{2mk_0}\left|\chi_{k_0}(r)\left(\frac{\partial\phi(r)}{\partial r}\right)-\phi(r)\left(\frac{\partial\chi_{k_0}(r)}{\partial r}\right)\right|_R^2. \end{aligned} \tag{10.39}$$

Similarly we can obtain the wave function for the quasi-stationary state and for $r>R$ in the first order approximation in α from Eq. (10.36);

$$\begin{aligned} \chi(r,t)|_{r>R} &= -\frac{m}{\pi\hbar^3}\sqrt{\frac{\pi}{2}}\int_0^t dt_1\int_{-\infty}^{\infty}\frac{dE}{k}\chi_k{}^{(+)}(r)\int_0^{\infty}\chi_k(r_1)[V_0(r_1)\\ &- V_{eff}(R)]\phi(r_1)dr_1\exp\left[-\frac{i}{\hbar}(E_0t_1+Et-Et_1)-\frac{1}{2\hbar}\Gamma t_1\right]. \end{aligned} \tag{10.40}$$

The asymptotic form of $\xi(r,t)$ as $r \to \infty$ is given by

$$\chi(r,t)|_{r\to\infty} = \frac{im}{\pi\hbar^2}\sqrt{\frac{\pi}{2}}\exp\left(-\frac{i}{\hbar}E_0t\right)\int_{-\infty}^{\infty}\left(\frac{dE}{k}\right)\frac{1}{E-iE_0+\frac{i}{2}\Gamma}$$
$$\times\left[\exp\left(-\frac{\Gamma t}{2\hbar}\right)-\exp\left(\frac{-i}{\hbar}(E-E_0)t\right)\right]$$
$$\times\exp\left[i\left(kr-\frac{l\pi}{2}+\delta_l\right)\right]\int_0^{\infty}\chi_k(r_1)\left[V_0(r_1)-V_{eff}(R)\right]\phi(r_1)dr_1. \tag{10.41}$$

Noting that the major contribution to the integral in (10.41) comes from the neighborhood of $E-E_0$, we can simplify this asymptotic form

$$\chi(r,t) = -\frac{2m}{\hbar^2}\sqrt{\frac{\pi}{2}}\frac{1}{k_0}\left[\int_0^{\infty}\chi_{k_0}(r)V_1(r)\phi(r)dr\right]$$
$$\times\exp\left[i\left(k_0r-\frac{\pi l}{2}+\delta_l\right)-\frac{i}{\hbar}E_0t-\frac{\Gamma}{2\hbar}\left(t-\frac{r}{v_0}\right)\right]\quad\text{for}\quad t>\frac{r}{v_0}, \tag{10.42}$$

and

$$\chi(r,t) = 0,\quad \text{for}\quad t<\frac{r}{v_0}, \tag{10.43}$$

where $v_0 = \frac{\hbar k_0}{m}$. Compare these with the results found in Section 5.2.

We can determine the number density of the particles at $t=\infty$ from Eq. (10.42), and its value is

$$j = \frac{1}{\hbar}\Gamma. \tag{10.44}$$

To calculate Γ we note that

$$\left[V_1(r)+V_{eff}(R)\right]_{r<R} = V_{eff}(R),\quad \text{and}\quad V_0|_{r>R} = V_{eff}(R), \tag{10.45}$$

and with the help of these relations we find $\phi(r)$ and $\chi_{k_0}(r)$ to be

$$\phi(r)|_{r>R} \approx A\exp\left\{-\frac{1}{\hbar}\int_{r_1}^{r}\sqrt{2m[V_0(r)-E_0]}\,dr\right\}, \tag{10.46}$$

and

$$\chi_{k_0}(r)|_{r<R} \approx B\exp\left\{-\frac{1}{\hbar}\int_{r}^{r_1}\sqrt{2m[V_1(r)+V_{eff}(R)-E_0]}\,dr\right\}. \tag{10.47}$$

If we substitute these two expressions in Eq. (10.39) and simplify the result we find

$$\Gamma = C\exp[-2\sigma(E_0)], \tag{10.48}$$

where C is a constant and $\sigma(E_0)$ is defined by Eq. (10.2). This approximation is valid whenever the inequality (10.32) is satisfied or

$$\alpha = \exp[-\sigma(E_0)] << 1. \tag{10.49}$$

Therefore the condition $\sigma(E_0) >> 1$ is needed for the validity of (10.2).

In the semi-classical (WKB) approximation we find that $\phi(r)$ is given by

$$\phi(r)|_{r>r_1} = \frac{A}{\sqrt{|p(r)|}} \exp\left[-\frac{1}{\hbar}\int_{r_1}^{r} |p(r)|dr\right], \tag{10.50}$$

where

$$p(r) = \sqrt{2m[E_0 - V_0(r)]}, \tag{10.51}$$

and

$$|A|^2 = \frac{1}{2\int_{r_0}^{r_1} \frac{dr}{p(r)}}. \tag{10.52}$$

Using the same approximation when (10.49) is satisfied, $\chi_{k_0}(r)$ can be written as

$$\begin{aligned} \chi_{k_0}(r)|_{r<r_2} &= \frac{B}{\sqrt{|p(r_1)|}} \exp\left[-\frac{1}{\hbar}\int_{r}^{r_2} |p_1(r)|dr\right] \\ &- \frac{B}{\sqrt{|p_1(r)|}} \exp\left[\frac{1}{\hbar}\int_{r}^{r_2} |p_1(r)|dr - \frac{2}{\hbar}\int_{r_0}^{r_2} |p_1(r)|dr\right]. \end{aligned} \tag{10.53}$$

Here $p_1(r)$ and B are defined by

$$p_1(r) = \sqrt{2m[E_0 - V_1(r) - V_{eff}(R)]}, \tag{10.54}$$

and

$$|B|^2 = \frac{\hbar k_0}{2\pi}. \tag{10.55}$$

respectively. If we substitute Eqs. (10.50) and (10.53) in (10.39) and simplify it we find Eq. (10.3) for Γ. For other methods of obtaining the decay width see Chapters 4, 5 and 12 and reference [7].

10.3 Time-Dependent Perturbation Theory Applied to the Calculation of Decay Widths of Unstable States

The same results that we have derived in the first part of this chapter can be obtained in a more elegant way using the time-dependent perturbation theory.

Let us denote the central potential as before by $V(r)$, but now introduce another potential $W_1(r)$ by

$$W_1(r) = \begin{cases} 0 & \text{for } r \le R \\ V(r) - V(R) & \text{for } r > R \end{cases}, \qquad (10.56)$$

where again $V(R)$ represents the maximum height of the barrier which is located at the point $r = R$. The difference between $V(r)$ and $W_1(r)$ is the potential $V_0(r)$

$$V_0(r) = V(r) - W_1(r). \qquad (10.57)$$

Thus the total Hamiltonian of the system can be written as

$$H = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(r)\right] + W_1(r) = H_0 + W_1(r), \qquad (10.58)$$

where H_0 has a spectrum with one or more bound states. If $\Phi_0(\mathbf{r})$ represents an eigenfunction of H_0 with the eigenvalue E_0, such that $E_0 < V(R)$, then this eigenstate under the action of the potential $W_1(r)\theta(t)$ becomes unstable.

The initial state Φ_0 is not an eigenstate of the Hamiltonian H. To find its time-development we expand $\Psi_0(\mathbf{r}, t)$, which is the time-dependent wave function for the total Hamiltonian H in terms of $\Phi_0(\mathbf{r})$ and $\{\Phi_{\mathbf{k}}(\mathbf{r})\}$;

$$\begin{aligned} \Psi_0(\mathbf{r}, t) &= b_0(t) \exp\left(-\frac{i}{\hbar}E_0 t\right) \Phi_0(\mathbf{r}) \\ &+ \int \frac{d^3k}{(2\pi)^3} b_{\mathbf{k}}(t) \exp\left(-\frac{i}{\hbar}E_{\mathbf{k}} t\right) \Phi_{\mathbf{k}}(\mathbf{r}). \end{aligned} \qquad (10.59)$$

In this expression we have assumed that H_0 has just a single bound state with energy E_0, and the eigenfunctions $\Phi_{\mathbf{k}}(\mathbf{r})$ are the solutions of the Schrödinger equation

$$H_0\Phi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\Phi_{\mathbf{k}}(\mathbf{r}) = \left(V(R) + \frac{\hbar^2 k^2}{2m}\Phi_{\mathbf{k}}(\mathbf{r})\right). \qquad (10.60)$$

The coefficients $b_0(t)$ and $b_{\mathbf{k}}(t)$ satisfy the initial conditions:

$$b_0(0) = 1, \quad b_{\mathbf{k}}(0) = 0. \qquad (10.61)$$

By substituting (10.59) in (10.58) we find the following equations [2]:

$$\begin{aligned} i\hbar\frac{db_0(t)}{dt} &= b_0(t) \langle\Phi_0|W_1|\Phi_0\rangle \\ &+ \int \frac{d^3k}{(2\pi)^3} b_{\mathbf{k}}(t) \exp\left[\frac{i}{\hbar}(E_0 - E_{\mathbf{k}})t\right] \langle\Phi_0|W_1|\Phi_{\mathbf{k}}\rangle, \end{aligned} \qquad (10.62)$$

and

$$i\hbar\frac{db_{\mathbf{k}}(t)}{dt} = b_0(t)\langle\Phi_{\mathbf{k}}|W_1|\Phi_0\rangle \exp\left[\frac{i}{\hbar}(E_{\mathbf{k}} - E_0)t\right]$$
$$+ \int \frac{d^3q}{(2\pi)^3} b_{\mathbf{q}}(t)\exp\left[-\frac{i}{\hbar}(E_{\mathbf{q}} - E_{\mathbf{k}})t\right]\langle\Phi_{\mathbf{k}}|W_1|\Phi_{\mathbf{q}}\rangle . \quad (10.63)$$

However in solving these equations we encounter the following problem. Since $W_1(r) \to -V(R)$ as $r \to \infty$, therefore

$$\begin{aligned}\langle\Phi_{\mathbf{k}}|W_1|\Phi_{\mathbf{q}}\rangle &\sim \int \exp(i\mathbf{k}.\mathbf{r})(-V(R))\exp(-i\mathbf{q}.\mathbf{r})d^3r \\ &= -V(R)(2\pi)^3\delta(\mathbf{k}-\mathbf{q}). \end{aligned} \quad (10.64)$$

In order to bypass this difficulty we replace $\langle\Phi_{\mathbf{k}}|W_1|\Phi_{\mathbf{q}}\rangle$ by

$$\langle\Phi_{\mathbf{k}}|W|\Phi_{\mathbf{q}}\rangle = \langle\Phi_{\mathbf{k}}|W_1 + V(R)|\Phi_{\mathbf{q}}\rangle - V(R)(2\pi)^3\delta(\mathbf{k}-\mathbf{q}), \quad (10.65)$$

in Eq. (10.63) and instead of $b_{\mathbf{k}}(t)$ introduce $\tilde{b}_{\mathbf{k}}(t)$;

$$\tilde{b}_{\mathbf{k}}(t) = b_{\mathbf{k}}(t)\exp\left[-\frac{i}{\hbar}V(R)t\right]. \quad (10.66)$$

With these replacements we rewrite (10.62) and (10.63) as

$$i\hbar\frac{db_0(t)}{dt} = b_0(t)\langle\Phi_0|W_1|\Phi_0\rangle$$
$$+ \int \frac{d^3k}{(2\pi)^3}\tilde{b}_{\mathbf{k}}(t)\exp\left[\frac{i}{\hbar}(E_0 + V(R) - E_{\mathbf{k}})t\right]\langle\Phi_0|W_1|\Phi_{\mathbf{k}}\rangle , \quad (10.67)$$

and

$$i\hbar\frac{d\tilde{b}_{\mathbf{k}}(t)}{dt} = b_0(t)\langle\Phi_{\mathbf{k}}|W_1|\Phi_0\rangle \exp\left[\frac{i}{\hbar}(E_{\mathbf{k}} - V(R) - E_0)t\right]$$
$$+ \int \frac{d^3q}{(2\pi)^3}\tilde{b}_{\mathbf{q}}(t)\exp\left[-\frac{i}{\hbar}(E_{\mathbf{q}} - E_{\mathbf{k}})t\right]\langle\Phi_{\mathbf{k}}|W_1 + V(R)|\Phi_{\mathbf{q}}\rangle . \quad (10.68)$$

Now we use Fermi's golden rule to find Γ from Φ_0 and $\Phi_{\mathbf{k}}$;

$$\Gamma = 2\pi\int |\langle\Phi_0|W_1|\Phi_{\mathbf{k}}\rangle|^2\rho(E_{\mathbf{k}})\delta\left[E_0 + V(R) - E_{\mathbf{k}}\right]dE_{\mathbf{k}}, \quad (10.69)$$

where $\rho(E_k)$ is the density of final states.

The presence of the delta-function in (10.69) indicates the conservation of energy, i.e. the initial kinetic energy is equal to the sum $V(R)+\frac{\hbar^2k^2}{2m}$ which is the final total energy of the particle. For the complete solution of Eqs. (10.67) and (10.68) we use the Laplace transform technique and introduce $b(\varepsilon)$ by

$$b(\varepsilon) = \int_0^\infty \exp\left(i\frac{\varepsilon t}{\hbar}\right) b(t)dt. \tag{10.70}$$

By applying this transform to Eqs. (10.67) and (10.68) and using the initial conditions (10.61) we find

$$-i\hbar + \varepsilon b_0(\varepsilon) = W_1(0,0)b_0(\varepsilon) + \int \frac{d^3k}{(2\pi)^3} W_1(0,\mathbf{k})\tilde{b}_{\mathbf{k}}(\varepsilon_{\mathbf{k}}), \tag{10.71}$$

and

$$\varepsilon_{\mathbf{k}}\tilde{b}_{\mathbf{k}}(\varepsilon_{\mathbf{k}}) = W_1(\mathbf{k},0)b_0(\varepsilon) + \int \frac{d^3q}{(2\pi)^3}\left[W_1 + V(R)\right](\mathbf{k},\mathbf{q})\tilde{b}_{\mathbf{q}}(\varepsilon_{\mathbf{q}}). \tag{10.72}$$

Here we have used the following symbols:

$$W_1(\mathbf{k},\mathbf{q}) = \langle \Phi_{\mathbf{k}}|W_1|\Phi_{\mathbf{q}}\rangle, \tag{10.73}$$

and

$$\varepsilon_{\mathbf{k}} = \varepsilon + E_0 + V(R) - E_{\mathbf{k}}. \tag{10.74}$$

By solving Eqs. (10.72) and (10.73) we find the following series for $b_0(\varepsilon)$,

$$\begin{aligned}
- \quad & i\hbar + \varepsilon b_0(\varepsilon) = W_1(0,0)b_0(\varepsilon) \\
+ \quad & \int \frac{d^3k}{(2\pi)^3} W_1(0,\mathbf{k}) \frac{1}{\varepsilon + E_0 + V(R) - E_{\mathbf{k}}} W_1(\mathbf{k},0)b_0(\varepsilon) \\
+ \quad & \int \frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3} W_1(0,\mathbf{k}) \frac{1}{\varepsilon + E_0 + V(R) - E_{\mathbf{k}}} (W_1 + V(R))(\mathbf{k},\mathbf{q}) \\
\times \quad & \frac{1}{\varepsilon + E_0 + V(R) - E_{\mathbf{q}}} W_1(\mathbf{q},0)b_0(\varepsilon) + \ldots.
\end{aligned} \tag{10.75}$$

We can write this series as

$$-i\hbar + \varepsilon b_0(\varepsilon) = \left\langle \Phi_0|W_1 + W_1\tilde{G}W_1|\Phi_0\right\rangle b_0(\varepsilon), \tag{10.76}$$

in which $\tilde{G}$ is the Green function which can be obtained from the solution of

$$\tilde{G} = \tilde{G}_0 + \tilde{G}_0(W_1 + V(R))\tilde{G}. \tag{10.77}$$

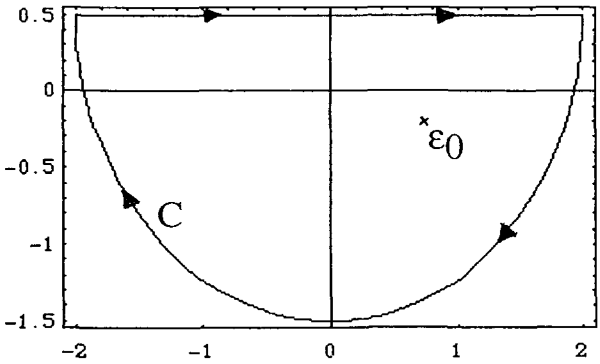

Figure 10.3: The contour C for integration of Eq. (10.80), assuming that $b_0(\varepsilon)$ has a pole at $\varepsilon = \varepsilon_0$.

Here $\tilde{G}_0$ denotes another Green function which is defined by

$$\tilde{G}_0 = \sum_{\mathbf{k}} \frac{|\Phi_{\mathbf{k}}\rangle\langle\Phi_{\mathbf{k}}|}{\varepsilon + E_0 + V(R) - E_{\mathbf{k}}} = \frac{(1 - |\Phi_0\rangle\langle\Phi_0|)}{\varepsilon + E_0 + V(R) - H_0}. \tag{10.78}$$

From Eq. (10.71) we find $b_0(\varepsilon)$ to be

$$b_0(\varepsilon) = \frac{i\hbar}{\varepsilon - \left\langle \Phi_0 | W_1 + W_1 \tilde{G} W_1 | \Phi_0 \right\rangle} \tag{10.79}$$

Having found $b_0(\varepsilon)$ we can use the inverse Laplace transform to obtain $b_0(t)$;

$$b_0(t) = \mathcal{L}^{-1}[b_0(\varepsilon)] = \frac{1}{2\pi\hbar} \oint_C d\varepsilon \exp\left(-i\frac{\varepsilon t}{\hbar}\right) b_0(\varepsilon), \tag{10.80}$$

where C is the contour of integration in the complex ε-plane which is shown in Fig. (10.3). Assuming that $b_0(\varepsilon)$ has a pole in the lower-half of the ε-plane at $\varepsilon = \varepsilon_0$, then $b_0(t)$ decays exponentially in time, i.e. $b_0(t) = \exp(-\frac{\Gamma t}{2\hbar})$ where Γ is related to ε_0 by

$$\Gamma = -2 \ \mathrm{Im} \ \varepsilon_0. \tag{10.81}$$

This pole which appears in the second Riemann sheet is a root of the denominator of (10.79)

$$\varepsilon_0 = \left\langle \Phi_0 | W_1 + W_1 \tilde{G}(\varepsilon_0) W_1 | \Phi_0 \right\rangle. \tag{10.82}$$

Equation (10.82) is exact, but it is convenient to find an approximate method of calculating ε_0. For this purpose we define the Green function G as

$$G = \frac{1}{E + \frac{\hbar^2}{2m}\nabla^2 - (W_1(r) + V(R))}. \tag{10.83}$$

This is the same Green function which in Eq. (10.26) was given for the partial wave l. Now we expand $\tilde{G}$ in terms of G and in the first order we find

$$\tilde{G}(\varepsilon) \approx G(E_0). \tag{10.84}$$

By substituting from Eqs. (10.26) and (10.29) in (10.82) for the partial wave l we find

$$\begin{aligned} \varepsilon_0 &= \pi \int_R^\infty W_1(r)|\phi_0(r)|^2 dr \\ &- \frac{\sqrt{2}m\pi^{\frac{3}{2}}}{\hbar^2 k} \int_R^\infty dr \int_R^r \phi_0(r) W_1(r) \chi_k^{(+)}(r) \chi_k(r') W_1(r') \phi_0(r') dr' \\ &+ \frac{\sqrt{2}m\pi^{\frac{3}{2}}}{\hbar^2 k} \int_R^\infty dr \int_r^\infty \phi_0(r) W_1(r) \chi_k(r) \chi_k^{(+)}(r') W_1(r') \phi_0(r') dr'. \end{aligned} \tag{10.85}$$

But

$$\mathrm{Im}\chi_k^{(+)} = \sqrt{\frac{2}{\pi}}\chi_k, \tag{10.86}$$

therefore for the width Γ, we find the same equation (10.39) that we found earlier, viz,

$$\Gamma = \frac{2\pi m}{\hbar^2 k}\left|\int_R^\infty \phi_0(r) W_1(r) \chi_k(r) dr\right|^2. \tag{10.87}$$

10.4 Early Stages of Decay via Tunneling

Since Eqs. (10.67)-(10.68) are not exactly solvable, let us consider the special case where the dominant contribution to the integrals in these equations comes from the matrix elements $\langle\Phi_0|W_1|\Phi_{\mathbf{k}}\rangle$, i.e. the matrix elements $\langle\Phi_{\mathbf{q}}|W_1 + V(R)|\Phi_{\mathbf{k}}\rangle$ in (10.68) can be ignored. Then introducing the symbols

$$W_1(i,j) = \hbar\mathcal{V}_{ij} = \hbar\mathcal{V}_{ji}, \quad \hbar\omega_{0\mathbf{k}} = E_0 - E_{\mathbf{k}} \quad \text{and} \quad V(R) = \hbar\beta, \tag{10.88}$$

we write (10.67) and (10.68) as

$$i\frac{db_0(t)}{dt} = \mathcal{V}_{00}b_0(t) + \int \frac{d^3k}{(2\pi)^3} \exp\left[i(\omega_{0\mathbf{k}} + \beta)t\right] \mathcal{V}_{0\mathbf{k}}\tilde{b}_{\mathbf{k}}(t), \tag{10.89}$$

and

$$i\frac{d\tilde{b}_{\mathbf{k}}(t)}{dt} = \mathcal{V}_{\mathbf{k}0}b_0(t) \exp\left[-i(\omega_{0\mathbf{k}} + \beta)t\right]. \tag{10.90}$$

Let us define $a_0(t)$ by

$$b_0(t) = a_0(t) \exp\left(-i\mathcal{V}_{00}t\right), \tag{10.91}$$

then we have two coupled equations for $a_0(t)$ and $\tilde{b}_{\mathbf{k}}(t)$;

$$i\frac{da_0(t)}{dt} = \int \frac{d^3k}{(2\pi)^3} \exp\left[i\Omega_{\mathbf{k}}t\right] \mathcal{V}_{0\mathbf{k}}\tilde{b}_{\mathbf{k}}(t), \tag{10.92}$$

and

$$i\frac{d\tilde{b}_{\mathbf{k}}(t)}{dt} = \mathcal{V}_{\mathbf{k}0} \exp\left[i\Omega_{\mathbf{k}}t\right] a_0(t), \tag{10.93}$$

where

$$\Omega_{\mathbf{k}} = \omega_{0\mathbf{k}} + \beta + \mathcal{V}_{00}. \tag{10.94}$$

By integrating (10.93) and then substituting in (10.92) we find an integro-differential equation for $a_0(t)$,

$$i\frac{da_0(t)}{dt} = -\int_0^t g(t-t')a_0(t')dt', \tag{10.95}$$

where

$$g(t-t') = \int \frac{d^3k}{(2\pi)^3} \left|\mathcal{V}_{0\mathbf{k}}\right|^2 \exp\left[i\Omega_{\mathbf{k}}(t-t')\right]. \tag{10.96}$$

We can also write (10.95) as

$$i\frac{da_0(t)}{dt} = -\int_0^t g(t')a_0(t-t')dt'. \tag{10.97}$$

Equations (10.96) and (10.97) can be used to determine both the early time behavior and also the exponential nature of the decay law of the system [8].

We have already seen the long time behavior of the probability of finding the particle in its initial state, i.e. $|a_0(t)|^2$. Here let us consider the onset of the decay [5]. To this end let us introduce the function $f(t)$ by

$$a_0(t) = \exp[-f(t)] \tag{10.98}$$

and substitute this in (10.98) to find

$$\frac{df(t)}{dt} = \int_0^t g(t')\exp\left[f(t) - f(t-t')\right] dt'. \tag{10.99}$$

From the initial condition $a(0) = 1$ and Eqs. (10.98)-(10.99) it follows that $f(0) = 0$ and $\left(\frac{df(t)}{dt}\right)_0 = 0$. Using these results we expand both $f(t)$ and $g(t)$, Eq. (10.96), for short times as

$$f(t) = \mathcal{A}t^2 + \mathcal{B}t^3 + \mathcal{C}t^4 + ..., \tag{10.100}$$

and

$$\begin{aligned} g(t) &= \int \frac{d^3k}{(2\pi)^3}\left|\mathcal{V}_{0\mathbf{k}}\right|^2 + it\int \frac{d^3k}{(2\pi)^3}\left|\mathcal{V}_{0\mathbf{k}}\right|^2\Omega_{\mathbf{k}} \\ &- \frac{1}{2}t^2\int \frac{d^3k}{(2\pi)^3}\left|\mathcal{V}_{0\mathbf{k}}\right|^2\Omega_{\mathbf{k}}^2 + ... \end{aligned} \tag{10.101}$$

By substituting (10.100) and (10.101) in (10.99) and equating equal powers of t we find the coefficients of expansion (10.100) to be

$$\mathcal{A} = \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\left|\mathcal{V}_{0\mathbf{k}}\right|^2, \tag{10.102}$$

$$\mathcal{B} = \frac{i}{6}\int \frac{d^3k}{(2\pi)^3}\left|\mathcal{V}_{0\mathbf{k}}\right|^2\Omega_{\mathbf{k}}, \tag{10.103}$$

and

$$\mathcal{C} = -\frac{1}{8}\int \frac{d^3k}{(2\pi)^3}\left|\mathcal{V}_{0\mathbf{k}}\right|^2\Omega_{\mathbf{k}}^2 + \frac{1}{12}\mathcal{A}^2. \tag{10.104}$$

Thus for early stages of decay $P(t) = |a_0(t)|^2$ has the form

$$\begin{aligned} P(t) &= |a_0(t)|^2 \approx \left[1 - \frac{1}{2}\left(\sqrt{\mathcal{A}}t\right)^2 + \frac{1}{24}\left(\sqrt{\mathcal{A}}t\right)^4 + ...\right] \\ &\times \exp\left[-\left(\mathcal{A}^2 - \mathcal{C}\right)\frac{t^4}{4}\right], \end{aligned} \tag{10.105}$$

or

$$P(t) \approx \cos^2(\sqrt{\mathcal{A}}t)\exp\left[-\left(\mathcal{A}^2 - \mathcal{C}\right)\frac{t^4}{4}\right]. \tag{10.106}$$

(See also the related discussion in Chapter 2) [5].

10.5 An Alternative Way of Calculating the Decay Width Using the Second Order Perturbation Theory

A simpler approach to the problem of exponential decay law is the direct application of the second order perturbation theory for calculating the decay width Γ and the shift in the bound state energy ΔE. Here we start with the total Hamiltonian of the particle H and write it as the sum of two terms

$$H = H_0 + H', \tag{10.107}$$

where

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2 + V_0(r) - V(R), \tag{10.108}$$

with

$$V_0(r) = \begin{cases} V(r) & \text{for } r < R \\ V(R) & \text{for } r > R \end{cases}, \tag{10.109}$$

and

$$H' = W_1(r) + V(R) = \begin{cases} V(R) & \text{for } r < R \\ V(r) & \text{for } r > R \end{cases}. \tag{10.110}$$

where $W_1(r)$ is given by Eq.(10.56).

Furthermore we assume that the unperturbed Hamiltonian H_0 has a bound state which we denote by $|0\rangle$,

$$H_0|0\rangle = E_0|0\rangle, \tag{10.111}$$

and that the particle is initially in this bound state.

The time-dependent Schrödinger equation for the total Hamiltonian is

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \left(H_0 + H'\right)|\Psi(t)\rangle, \tag{10.112}$$

which can also be written as

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H'(t)|\psi(t)\rangle, \tag{10.113}$$

where $|\psi(t)\rangle$ is defined by

$$|\Psi(t)\rangle = \exp\left(-\frac{iH_0 t}{\hbar}\right)|\psi(t)\rangle, \tag{10.114}$$

and

$$H^{'}(t) = \exp\left(\frac{iH_0 t}{\hbar}\right) H^{'} \exp\left(-\frac{iH_0 t}{\hbar}\right). \qquad (10.115)$$

Next let us define the decay amplitude of the initial state by $\langle 0|\psi(t)\rangle$, then from (10.113) we find [9]

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\langle 0|\psi(t)\rangle &= \left\langle 0|H^{'}(t)|\psi(t)\right\rangle \\ &= \left\langle 0|H^{'}(t)|0\right\rangle + \int \frac{d^3k}{(2\pi)^3}\left\langle 0|H^{'}(t)|\mathbf{k}\right\rangle \langle \mathbf{k}|\psi(t)\rangle, \end{aligned} \qquad (10.116)$$

where we have used the complete set of states

$$\int \frac{d^3k}{(2\pi)^3}|\mathbf{k}\rangle\langle\mathbf{k}| + |0\rangle\langle 0| = I, \qquad (10.117)$$

and I is the unit operator in Eq. (10.117). We divide both sides of (10.116) by $\langle 0|\psi(t)\rangle$ and write it as

$$i\hbar\frac{\partial}{\partial t}\ln\langle 0|\psi(t)\rangle = \left\langle 0|H^{'}(t)|0\right\rangle + \int \frac{d^3k}{(2\pi)^3}\left\langle 0|H^{'}(t)|\mathbf{k}\right\rangle \frac{\langle \mathbf{k}|\psi(t)\rangle}{\langle 0|\psi(t)\rangle}. \qquad (10.118)$$

By integrating (10.113) we find

$$|\psi(t)\rangle = |0\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t} H^{'}(t^{'})|0\rangle dt^{'}, \qquad (10.119)$$

and from this we calculate $\langle 0|\psi(t)\rangle$,

$$\langle 0|\psi(t)\rangle = 1 + \frac{1}{i\hbar}\int_{-\infty}^{t}\langle 0|H^{'}(t^{'})|0\rangle dt^{'}. \qquad (10.120)$$

Equation (10.120) shows that to the first order perturbation we have

$$\langle 0|\psi(t)\rangle \approx 1, \quad \text{and} \quad \langle \mathbf{k}|\psi(t)\rangle \approx \frac{1}{i\hbar}\int_{-\infty}^{t}\left\langle \mathbf{k}|H^{'}(t^{'})|0\right\rangle dt^{'}. \qquad (10.121)$$

Substituting these in (10.118) we have $\langle 0|\psi(t)\rangle$ to the second order in $H^{'}$,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\ln\langle 0|\psi(t)\rangle &\approx \left\langle 0|H^{'}(t)|0\right\rangle \\ &+ \frac{1}{i\hbar}\int_{-\infty}^{t}dt^{'}\int\frac{d^3k}{(2\pi)^3}\left\langle 0|H^{'}(t)|\mathbf{k}\right\rangle\left\langle \mathbf{k}|H^{'}(t^{'})|0\right\rangle. \end{aligned} \qquad (10.122)$$

Now using (10.115) we write $\left\langle 0|H'(t')|\mathbf{k}\right\rangle$ in terms of the matrix elements of $H'(r)$;

$$\left\langle 0|H'(t')|\mathbf{k}\right\rangle = \exp\left[\frac{i}{\hbar}(E_0 - E_{\mathbf{k}})t\right]\left\langle 0|H'|\mathbf{k}\right\rangle, \tag{10.123}$$

and a similar relation for $\left\langle \mathbf{k}|H'(t')|0\right\rangle$. Substituting these in (10.122) and assuming that H' is switched on slowly, i.e.

$$H'(t') \to H'(t') \exp\left(\frac{\mu t}{\hbar}\right), \quad \mu \to 0, \tag{10.124}$$

we find the last term in (10.122) to be equal to

$$\int \frac{d^3k}{(2\pi)^3} \frac{\left|\left\langle 0|H'(r)|\mathbf{k}\right\rangle\right|^2}{E_0 - E_{\mathbf{k}} + i\mu}. \tag{10.125}$$

From the well known relation [10]

$$\frac{1}{E_0 - E_{\mathbf{k}} + i\mu} \to \mathcal{P}\frac{1}{E_0 - E_{\mathbf{k}}} - i\pi(E_0 - E_{\mathbf{k}}), \tag{10.126}$$

where $\mathcal{P}$ represents the principal value of the integral, we can calculate the real and the imaginary parts of (10.125)

$$\int \frac{d^3k}{(2\pi)^3} \frac{\left|\left\langle 0|H'(r)|\mathbf{k}\right\rangle\right|^2}{E_0 - E_{\mathbf{k}} + i\mu} = \mathcal{P}\int \frac{d^3k}{(2\pi)^3} \frac{\left|\left\langle 0|H'(r)|\mathbf{k}\right\rangle\right|^2}{E_0 - E_{\mathbf{k}}} - \frac{i}{2}\Gamma,. \tag{10.127}$$

where

$$\Gamma = 2\pi \int \frac{d^3k}{(2\pi)^3} \left|\left\langle 0|H'(r)|\mathbf{k}\right\rangle\right|^2 \delta\left(E_{\mathbf{k}} - E_0\right), \tag{10.128}$$

is the decay width. The shift of the energy of the ground state is given by

$$E_0 + \Delta E_0 = E_0 + \left\langle 0|H'(r)|0\right\rangle + \mathcal{P}\int \frac{d^3k}{(2\pi)^3} \frac{\left|\left\langle 0|H'(r)|\mathbf{k}\right\rangle\right|^2}{E_0 - E_{\mathbf{k}}}. \tag{10.129}$$

10.6 Tunneling Through Two Barriers

The method outlined in Section (10.3) can be used to solve a number of different problems. For instance let us assume that there are two barriers

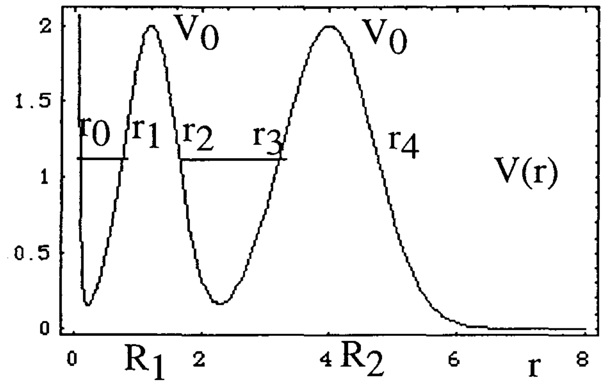

Figure 10.4: Tunneling through two barriers with the same maxima V_0. The points $r_0, r_1, ... r_4$ are the classical turning points.

given by $V(r)$, (see Fig. (10.4)), and the particle is initially localized in one of them [11]. The maximum height of the barriers are at the points $r = R_1$ and $r = R_2$, and for the sake of simplicity we assume that $V(R_1) = V(R_2) = V_0$. Furthermore we choose the wells such that each well separately can bind the particle and that $|E_0^{(1)} - E_0^{(2)}|$ is much smaller than the energy differences among the higher levels in each of the wells. The particle can be in one of the wells initially. Let us consider the case where at $t = 0$ the particle is in the second well and its eigenfunction is given by $\Phi_0^{(2)}$, where

$$H_0^{(2)}\Phi_0^{(2)} = \left[-\frac{\hbar^2}{2m}\nabla^2 + U_2(r)\right]\Phi_0^{(2)} = E_0^{(2)}\Phi_0^{(2)}. \tag{10.130}$$

In this relation $U_2(r)$ (see Fig (10.5)) is related to $V(r)$ by

$$U_2(r) = \begin{cases} V(r) & \text{for } R_1 < r < R_2 \\ V_0 & \text{for } r < R_1 \text{ or } r > R_2 \end{cases}. \tag{10.131}$$

Similarly we define $U_1(r)$ by

$$U_1(r) = \begin{cases} V(r) & \text{for } r \le R_1 \\ V_0 & \text{for } r > R_1 \end{cases}, \tag{10.132}$$

(see Fig. (10.6)). The difference between $V(r)$ and $U_2(r)$ is the perturbation

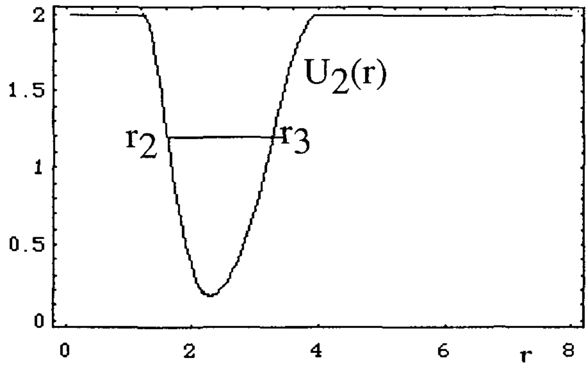

Figure 10.5: The potential $U_2(r)$ defined by Eq. (10.131) with a bound state of energy $E_0^{(2)}$.

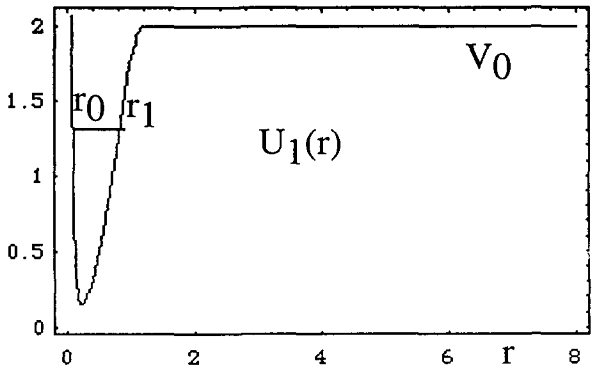

Figure 10.6: The potential $U_1(r)$ defined by Eq. (10.132) with a bound state of energy $E_0^{(1)}$.

$W_{10}(r)$;

$$W_{10}(r) = V(r) - U_2(r). \tag{10.133}$$

Thus the initial wave function $\Phi_0^{(2)}(\mathbf{r})$ is not an eigenfunction of the total Hamiltonian $H = H_0^{(2)} + W_{10}(r)$, but as before we find a wave packet $\Psi_0(\mathbf{r}, t)$ which describes the time evolution of $\Phi_0^{(2)}$;

$$\begin{aligned} \Psi_0(\mathbf{r}, t) &= b_0^{(2)}(t) \exp\left(-i\frac{E_0^{(2)}t}{\hbar}\right) \Phi_0^{(2)}(\mathbf{r}) \\ &+ \int \frac{d^3k}{(2\pi)^3} b_{\mathbf{k}}^{(2)}(t) \exp\left(-i\frac{E_{\mathbf{k}}^{(2)}t}{\hbar}\right) \Phi_{\mathbf{k}}^{(2)}(\mathbf{r}), \end{aligned} \tag{10.134}$$

where we have assumed that $H_0^{(2)}$ has only one bound state. The initial conditions for the coefficients $b_0^{(2)}(t)$ and $b_{\mathbf{k}}^{(2)}(t)$ are (see also Eq. (10.61))

$$b_0^{(2)}(0) = 1 \quad b_{\mathbf{k}}^{(2)}(0) = 0. \tag{10.135}$$

The method of Laplace transform that we used earlier in this chapter can be applied to this problem also with the result that

$$b_0^{(2)}(\varepsilon) = \frac{i}{\varepsilon - \left\langle \Phi_0^{(2)} | W_{10} + W_{10}\tilde{G}\left(E_0^{(2)} + \varepsilon\right) W_{10} | \Phi_0^{(2)} \right\rangle}, \tag{10.136}$$

where the Green function $\tilde{G}$ is a solution of

$$\tilde{G}(E) = \left(1 - \left|\Phi_0^{(2)}\right\rangle\left\langle\Phi_0^{(2)}\right|\right) \frac{1}{E + V_0 - H_0} \left[1 + (W_{10} + V_0)\tilde{G}\right]. \tag{10.137}$$

Just as the case that we discussed earlier, $b_0^{(2)}(\varepsilon)$ has a pole in the lower-half of the ε-plane, and $b_0^{(2)}(t)$ decays exponentially, $b_0^{(2)}(t) \sim \exp(-\frac{\Gamma t}{2\hbar})$, and as before Γ is related to the position of the pole $\Gamma = -2\,\mathrm{Im}\ \varepsilon_0$. The position of the pole can be found from the equation

$$\varepsilon_0 = \left\langle \Phi_0^{(2)} \left| W_{10} + W_{10}\tilde{G}\left(E_0^{(2)} + \varepsilon_0\right) W_{10} \right| \Phi_0^{(2)} \right\rangle. \tag{10.138}$$

To simplify this relation we define $G_{\tilde{W}}$ by

$$G_{\tilde{W}} = \frac{1}{E + \frac{\hbar^2\nabla^2}{2m} - \tilde{W}_{10}(r)}, \tag{10.139}$$

where $\tilde{W}_{10}(r)$ is given by

$$\tilde{W}_{10}(r) = W_{10}(r) + V_0. \tag{10.140}$$

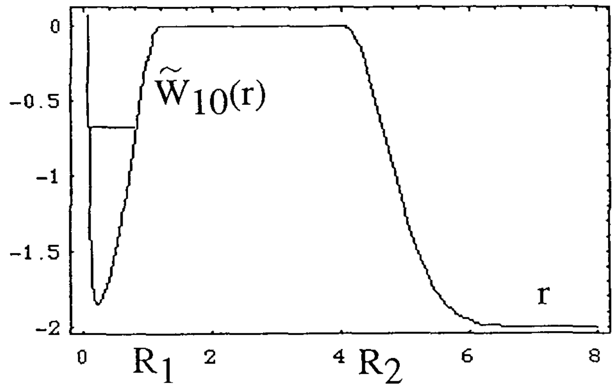

Figure 10.7: The potential $\tilde{W}_{10}(r)$ defined by Eq. (10.140) and is used for calculating $G_{\tilde{W}}$.

This potential is shown in Fig. (10.7). With the help of Eq. (10.137) we can write $\tilde{G}$ in terms of $G_{\tilde{W}}$;

$$\tilde{G} = G_{\tilde{W}} + G_{\tilde{W}}(U_2 - V_0)\tilde{G} - G_{\tilde{W}}\left(\left|\Phi_0^{(2)}\right\rangle\left\langle\Phi_0^{(2)}\right|\right)(1 + \tilde{W}_{10}\tilde{G}). \tag{10.141}$$

If the potential is wide enough, then the state corresponding to $E_0^{(1)}$ is stable, and when the condition $E \sim E_0^{(1)} \sim E_0^{(2)}$ is satisfied, then the Green function $G_{\tilde{W}}(E)$ can be written as

$$G_{\tilde{W}}(E) \approx G_{U_1}(E) + G_{\tilde{W}_0}(E), \tag{10.142}$$

where $G_{U_1}(E)$ is the Green function for the potential U_1 and $G_{\tilde{W}_0}(E)$ is the Green function for

$$\tilde{W}_0(r) = \tilde{W}_{10}(r) - U_1(r) + V_0. \tag{10.143}$$

Now if we substitute (10.142) in (10.141) and simplify the result, for the energy level $E = E_0^{(2)}$ we find the following expression;

$$\begin{aligned} E &= E_0^{(2)} + \left\langle\Phi_0^{(2)}\left|W_1\right|\Phi_0^{(2)}\right\rangle + \frac{\left|\left\langle\Phi_0^{(2)}|W_1|\Phi_0^{(1)}\right\rangle\right|^2}{E - E_0^{(1)} - \left\langle\Phi_0^{(1)}|W_2|\Phi_0^{(1)}\right\rangle} \\ &+ \left\langle\Phi_0^{(2)}\left|W_0 + W_0 G_{\tilde{W}_0} W_0\right|\Phi_0^{(2)}\right\rangle. \end{aligned} \tag{10.144}$$

In this equation W_1 and W_2 are given by

$$W_1 = U_1 - V_0, \quad W_2 = U_2 - V_0. \tag{10.145}$$

Next let us define the following symbols

$$d_{1,2} = \left\langle \Phi_0^{(1,2)} \left| W_{2,1} \right| \Phi_0^{(1,2)} \right\rangle, \tag{10.146}$$

$$\delta = 2\left\langle \Phi_0^{(2)} \left| W_1 \right| \Phi_0^{(1)} \right\rangle = 2\left\langle \Phi_0^{(2)} \left| W_2 \right| \Phi_0^{(1)} \right\rangle, \tag{10.147}$$

and

$$\Delta_0 - \frac{1}{2} i\Gamma_0 = \left\langle \Phi_0^{(2)} \left| W_0 + W_0 G_{\tilde{W}_0} W_0 \right| \Phi_0^{(2)} \right\rangle, \tag{10.148}$$

then we can write the eigenvalue equation (10.144) as the determinant

$$\begin{vmatrix} E - E_0^{(1)} - d_1 & -\frac{1}{2}\delta \\ -\frac{1}{2}\delta & E - \left(E_0^{(2)} + d_2 + \Delta_0 - \frac{i}{2}\Gamma_0\right) \end{vmatrix} = 0. \tag{10.149}$$

The roots of Eq. (10.149) are given by

$$\begin{aligned} E_{\pm} &= \frac{1}{2}\left(E_0^{(1)} + E_0^{(2)} + d_1 + d_2 + \Delta_0 - \frac{i}{2}\Gamma_0\right) \\ &\pm \frac{1}{2}\left[\left(E_0^{(1)} - E_0^{(2)} + d_1 - d_2 - \Delta_0 + \frac{i}{2}\Gamma_0\right)^2 + \delta^2\right]^{\frac{1}{2}}, \end{aligned} \tag{10.150}$$

and from it we can find $\varepsilon = E - E_0^{(2)}$. With the assumption that $|E_0^{(1)} - E_0^{(2)}|$ is less than δ and Γ_0, and using the inverse Laplace transform of $b_0^{(2)}(\varepsilon)$, we find $b_0^{(2)}(t)$ to be

$$b_0^{(2)}(t) = \frac{1}{\Gamma_+ - \Gamma_-}\left\{\Gamma_+ \exp\left(-\frac{\Gamma_+ t}{\hbar}\right) - \Gamma_- \exp\left(-\frac{\Gamma_- t}{\hbar}\right)\right\}, \tag{10.151}$$

where in this relation

$$\Gamma_{\pm} = \frac{1}{2}\left(\Gamma_0 \pm \sqrt{\Gamma_0^2 - 4\delta^2}\right). \tag{10.152}$$

10.7 Escape from a Potential Well by Tunneling Through both Sides

In most of the problems that we have studied so far, the trapped particle could have escaped from one side, and usually in this case the decay width is small and the lifetime is long. If in one-dimensional motion the particle can escape by tunneling through the barrier on both sides of the well where it is confined initially, then in general, the decay width is large and lifetime is short [13].

In this section we apply the one-dimensional scattering theory to calculate the decay width of such a system. Again we start with the Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi = 0, \tag{10.153}$$

where now because of the Gamow boundary conditions E is a complex eigenvalue. Let us denote the asymptotic values of $V(x)$ as $x \to -\infty$ and $x \to \infty$ by V_- and V_+ respectively. If the energy of the particle is greater than V_- and V_+ then the particle can approach the barrier from either $x < 0$ or $x > 0$, and therefore in this case the most general asymptotic conditions are

$$\psi \to \frac{N_-}{\sqrt{k_-}}\left[C\exp(-ik_-x) + D\exp(ik_-x)\right] \quad \text{as} \quad x \to -\infty, \tag{10.154}$$

and

$$\psi \to \frac{N_+}{\sqrt{k_+}}\left[A\exp(-ik_+x) + B\exp(ik_+x)\right] \quad \text{as} \quad x \to \infty. \tag{10.155}$$

In these relations k_+ and k_- are defined by

$$\hbar k_\pm = \sqrt{2m(E - V_\pm)}. \tag{10.156}$$

If E is positive in (10.156) we choose the positive sign for $k_\pm$, and if E is in the fourth quadrant of the complex E-plane $(0 < \arg E < \frac{\pi}{2})$, then we choose $k_\pm$ also in the fourth quadrant $(0 < \arg k_\pm < \frac{\pi}{2})$. The scattering matrix S by definition relates C and B of the outgoing wave to the coefficients A and D of the incoming wave

$$\begin{bmatrix} C \\ B \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} D \\ A \end{bmatrix}. \tag{10.157}$$

Once S is known then the coefficients of the reflection and transmission can be found from its matrix elements:

$$|T_{21}|^2 = \left|\frac{C}{A}\right|^2 = |S_{12}|^2, \tag{10.158}$$

$$|T_{12}|^2 = \left|\frac{B}{D}\right|^2 = |S_{21}|^2, \tag{10.159}$$

$$|R_{11}|^2 = \left|\frac{C}{D}\right|^2 = |S_{11}|^2, \tag{10.160}$$

and

$$|R_{22}|^2 = \left|\frac{B}{A}\right|^2 = |S_{22}|^2. \tag{10.161}$$

We can solve the Schrödinger equation (10.153) directly for the real or complex eigenvalues E and thus find the poles of the scattering matrix for the complex energies

$$\bar{E}_n = E_n - \frac{i}{2}\Gamma_n, \quad n = 0, 1, 2\ldots.. \tag{10.162}$$

These poles correspond to the resonant states where E_n's are the real part of the resonant energies and the positive quantities Γ_n are the resonant widths. Note that all the matrix elements S_{ij} have the common pole at $\bar{E}_n$.

As a first case we assume that there are two barriers one extending from $-\infty$ to 0 and the other from a to ∞, and in both directions the barriers tend to zero faster than x^{-2} as $x \to \pm\infty$. The solution of the Schrödinger equation in these three parts can be written as

$$\psi_1 = Cf_1(x) + Dg_1(x), \quad -\infty < x < 0, \tag{10.163}$$

$$\psi_2 = Fe^{ikx} + Ge^{-ikx}, \quad 0 < x < a, \tag{10.164}$$

and

$$\psi_3 = Ag_3(x) + Bf_3(x), \quad a < x < \infty, \tag{10.165}$$

where

$$\lim_{x\to-\infty} f_1(x) \to e^{-ikx}, \quad \lim_{x\to-\infty} g_1(x) \to e^{ikx}, \tag{10.166}$$

and

$$\lim_{x\to\infty} g_3(x) \to e^{-ikx}, \quad \lim_{x\to\infty} f_3(x) \to e^{ikx}. \tag{10.167}$$

By matching these solutions at the boundaries $x = 0$ and $x = a$, we obtain four linear equations for A, B, C, D, M and N. Solving for C, D, M and N in terms of A and B we find the matrix elements S_{ij} of (10.157). All these elements have a common denominator $\mathcal{D}$ which is given by

$$\begin{aligned} \mathcal{D} &= -k(1+e^{2ika})\left[f_1'(0)f_3(a) - f_1(0)f_3'(a)\right] \\ &- i(1-e^{2ika})\left[f_1'(0)f_3'(a) - k^2 f_1(0)f_3(a)\right], \end{aligned} \tag{10.168}$$

where

$$f_1'(0) = \left(\frac{df_1(x)}{dx}\right)_{x=0} \quad \text{and} \quad f_3'(a) = \left(\frac{df_3(x)}{dx}\right)_{x=a}. \tag{10.169}$$

The complex roots of $\mathcal{D}$ with the condition that Im $k^2 < 0$ gives us the poles of the scattering matrix for this case. As specific examples we discuss two problems.
(1) - Let the two barriers be represented by the potential

$$V(x) = \frac{\hbar^2}{2m}\begin{cases} v_0 e^{\mu x} & \text{for } -\infty < x < 0 \\ 0 & \text{for } 0 < x < a \\ v_1 e^{-\nu(x-a)} & \text{for } a < x < \infty \end{cases} . \tag{10.170}$$

The Schrödinger equation for the first part $-\infty < x < 0$ is given by

$$\frac{d^2\psi_1(x)}{dx^2} + \left[k^2 - v_0 e^{\mu x}\right]\psi_1(x) = 0. \tag{10.171}$$

This equation can be solved in terms of the Bessel function of imaginary index and argument [12]

$$\psi_1(x) = C J_{-\frac{2ik}{\mu}}\left(\frac{-i\sqrt{2v_0}}{\mu} e^{\frac{\mu x}{2}}\right) + D J_{\frac{2ik}{\mu}}\left(\frac{i\sqrt{2v_0}}{\mu} e^{\frac{\mu x}{2}}\right). \tag{10.172}$$

From the asymptotic form of $\psi_1(x)$ as $x \to \infty$, we find that

$$\begin{aligned} \psi_1(x) \quad \to \quad & \frac{C}{2^{-\frac{2ik}{\mu}}\Gamma(1 - \frac{2ik}{\mu})}\left(\frac{-i\sqrt{2v_0}}{\mu}\right)^{-\frac{2ik}{\mu}} e^{-ikx} \\ + \quad & \frac{D}{2^{\frac{2ik}{\mu}}\Gamma(1 + \frac{2ik}{\mu})}\left(\frac{i\sqrt{2v_0}}{\mu}\right)^{\frac{2ik}{\mu}} e^{ikx}. \end{aligned} \tag{10.173}$$

Thus $f_1(x)$ and $g_1(x)$ are given by $J_{-\frac{2ik}{\mu}}$ and $J_{\frac{2ik}{\mu}}$ respectively.
Similarly for $\psi_3(x)$ we find

$$\psi_3(x) = C J_{\frac{2ik}{\nu}}\left(\frac{-i\sqrt{2v_1}}{\nu} e^{\frac{-\nu(x-a)}{2}}\right) + D J_{-\frac{2ik}{\nu}}\left(\frac{i\sqrt{2v_1}}{\nu} e^{\frac{-\nu(x-a)}{2}}\right). \tag{10.174}$$

By substituting for $f_1(x)$ and $f_3(x)$ from Eqs. (10.172) and (10.174) in (10.168) we have an analytic expression for $\mathcal{D}(k)$ from which the pole in the complex k-plane can be determined.
(2)- As a second example of this approach to quantum tunneling let us consider the simple and solvable potential

$$V(x) = \left(\frac{\hbar^2}{2m}\right)\left(s_1\delta(x) + s_2\delta(x-a)\right) \tag{10.175}$$

for which the Schrödinger equation can be solved exactly (Chap.6). The matrix equation (10.157) for this problem is given by

$$\begin{bmatrix} C \\ B \end{bmatrix} = \begin{bmatrix} \frac{-Z_{12}}{Z_{22}} & \frac{Z_{11}Z_{22}-Z_{12}Z_{21}}{Z_{22}} \\ \frac{1}{Z_{22}} & \frac{-Z_{21}}{Z_{22}} \end{bmatrix} \begin{bmatrix} D \\ A \end{bmatrix}. \tag{10.176}$$

where

$$Z_{11}^* = Z_{22} = \left(1 - \frac{s_1}{2ik}\right)\left(1 - \frac{s_2}{2ik}\right) + \frac{s_1 s_2}{4k^4}\exp(2ika), \tag{10.177}$$

and

$$Z_{12} = Z_{21}^* = \left(1 + \frac{s_1}{2ik}\right)\frac{s_2}{2ik}\exp(2ika) + \left(1 - \frac{s_2}{2ik}\right)\frac{s_1}{2ik}. \tag{10.178}$$

We observe that all of the elements of the 2×2 matrix in (10.176) have poles for the same values of k. The location of these poles are given by the roots of $Z_{22} = 0$, and in order to satisfy the positivity requirement of Γ_0, Eq. (10.162), we have to choose those roots where Im $k^2 < 0$. For the numerical example let us choose $s_1 = 200L^{-1}, s_2 = 100L^{-1}$ and $a = 1L$, then $k^2 = (9.580 - 0.0073i)L^{-2}$. But for smaller values of s_1 and s_2 , e.g. $s_1 = 80L^{-1}, s_2 = 40L^{-1}$ the imaginary part of k^2 is larger $k^2 = (9.172 - 0.0415i)L^{-2}$. Using this formulation we can also calculate the transmission coefficient. Thus from (10.159) we have

$$|T_{12}|^2 = |S_{21}|^2 = \left|\frac{1}{Z_{22}}\right|^2 \tag{10.179}$$

and this is the same result that we found earlier, Eq. (6.49).
For the problem of a particle trapped between two rectangular wells see [14].

Now let us consider the case where the barrier extends from $-a_1$ to a_2. In this case $k_+ = k_- = k$, and we choose the normalization constant $N_\pm$ to be $N_\pm = \frac{1}{\sqrt{k}}$. For determining the poles of the S-matrix we can transform Eq. (10.153) to the nonlinear first order equation [3],

$$\frac{dS}{dx} = 2ikS + \left(\frac{mV(x)}{ik\hbar^2}\right)(1 + S(x))^2. \tag{10.180}$$

(Note that in [3] $S_0(x)$ is defined as $S_0(x) = -S(x)\exp(2ikx)$). Since the barrier outside the interval $-a_1 < x < a_2$ is zero, the boundary condition for solving (10.180) is

$$S(-a_1) = 0. \tag{10.181}$$

In Eq. (10.180) both S and k are complex quantities and we write them as

$$S = S_R + iS_I, \quad \text{and} \quad k = k_R + ik_I. \tag{10.182}$$

Next we decompose (10.180) into two real equations for S_R and S_I with the boundary condition (10.181) imposed on both of these functions. By integrating (10.180) and finding $S(a_2)$ we can determine the poles of S and also find the matrix elements of S. For instance the elements S_{22} and S_{12} are found to be:

$$S_{22} = S(a_2)\exp(-2ika_2), \tag{10.183}$$

and

$$S_{12} = \exp\left[\frac{1}{ik}\int_{-a_1}^{a_2}\left(\frac{m}{\hbar^2}V(x)\right)(1+S(x))^2\,dx\right]. \tag{10.184}$$

In order to find the position of the poles of the S-matrix it is easier to find the points in the complex k-plane where $\frac{1}{S_{ij}}$ is zero [13].

10.8 Decay of the Initial State and the Jost Function

As we have seen in Chapter 5, the Jost function plays an important role in the calculation of the wave function for a decaying state, and in particular its analytic properties in the complex k-plane ($k = \frac{\sqrt{2mE}}{\hbar}$) gives us important information about scattering. In this section we want to expand on the connection between the Jost function and the time dependence of the wave packet associated with a decaying state.

For simplicity we just consider the S wave (or $l = 0$ partial wave). The Jost function is defined as the solution of the Schrödinger equation [15] [16]

$$\left(-\frac{d^2}{dr^2} + v(r) - k^2\right) f(k,r) = 0, \quad k^2 = \frac{2mE}{\hbar^2}, \quad v(r) = \frac{2mV(r)}{\hbar^2}, \tag{10.185}$$

with the boundary condition

$$f(k,r) \to \exp(-ikr), \quad r > a, \tag{10.186}$$

where we have assumed that the barrier becomes negligible for $r > a$. If we denote $f(k, r = 0)$ by $f(k)$, then the phase shift $\delta(k)$ is related to $f(k)$ by

$$\exp[2i\delta(k)] = \frac{f(k)}{f(-k)}. \tag{10.187}$$

In cases where $v(r)$ does not bind the particle, $f(k)$ will have two important properties [15] [16]:
(i) - In the absence of bound states the Jost function is analytic for all finite values of k.
(ii) - The Jost function $f(k)$ cannot be zero in the half-plane Im $k < 0$.

If we denote the wave function which is regular at $r = 0$ by $u(k,r)$, then

$$u(k,r) = \frac{f(k)f(-k,r) - f(-k)f(k,r)}{i\sqrt{\pi}|f(k)|}. \tag{10.188}$$

where we have used a different normalization from that given in Eq. (5.43). The limit of $u(k,r)$ as r becomes larger than the range of the barrier a is

$$u(k,r) \to \sqrt{\frac{2}{\pi}} \sin\left[kr + \delta(k)\right], \quad r > a. \tag{10.189}$$

For real values of k this wave function is real. However here we want to consider the decay of an initial state which is localized in the region $0 < r < a$, and for such a system k would be complex. Let $K = k_R + ik_I$ be this complex number then $f(k)$ will be zero in the upper-half of the k-plane. The zeros of $f(k)$ are complex conjugate of each other, thus we can take both k_R and k_I as negative quantities. Let us next consider the function

$$B_0(r) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{\exp\left[i\delta(k)\right]}{k - K} u(k,r) dk, \tag{10.190}$$

which we will show is a wave packet concentrated in the region $r < a$. To this end we study the function $B(r)$ defined by the integral

$$B(r) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \frac{\exp\left[i(ka + \delta(k))\right]}{k - K} u(k,r) dk, \tag{10.191}$$

and note that for $r \ge a$, we can write $B(r)$ as

$$\begin{aligned} B(r) &= -\frac{1}{2\pi i} \int_{-\infty}^\infty \frac{\exp\left[ik(a-r)\right]}{k - K} dk \\ &+ \frac{1}{2\pi i} \int_{-\infty}^\infty \frac{\exp\left[i(ka + 2\delta(k) + kr)\right]}{k - K} dk. \end{aligned} \tag{10.192}$$

The first integral in (10.192) is zero since we can choose the contour in the lower-half of the k-plane. The second integral can be written as

$$-\frac{1}{2\pi i} \int_{-\infty}^\infty \frac{\exp\left[ik(r+a)\right]}{k - K} \left(\frac{f(k)}{f(-k)}\right) dk. \tag{10.193}$$

For this integral we choose a contour in the upper-half of the k-plane, and again we observe that this integral is zero. Since both integrals in (10.192) vanish, therefore

$$B(r) = 0, \quad r \geq a. \tag{10.194}$$

Now let us denote the difference between $B(r)$ and $B_0(r)$ by $B_1(r)$;

$$B_1(r) = B(r) - B_0(r), \tag{10.195}$$

and also define the absolute value $|B_0|^2$ and $|B_1|^2$ by

$$|B_i|^2 = \int_0^\infty |B_i(r)|^2 dr, \quad i = 0, 1. \tag{10.196}$$

Using the fact that the set $\{u(k,r)\}$ forms an orthonormal set,

$$\int_0^\infty u(k,r)u^*(k',r)dr = \delta(k-k'), \tag{10.197}$$

we can calculate $|B_0|^2$ from Eqs.(10.190) and (10.195)

$$\begin{aligned} |B_0|^2 &= \frac{1}{2\pi}\int_0^\infty \frac{dk}{|k-K|^2} = \frac{1}{2\pi}\int_0^\infty \frac{dk}{(k-k_R)^2 + k_I^2} \\ &= \frac{1}{2\pi k_I}\left(\frac{\pi}{2} + \tan^{-1}\frac{k_R}{k_I}\right). \end{aligned} \tag{10.198}$$

Furthermore from Eqs. (10.197) and (10.195) we can calculate $|B_1|^2$,

$$|B_1|^2 = \frac{1}{2\pi}\int_0^\infty \frac{dk}{|k+K|^2} = \frac{1}{2\pi k_I}\left(\frac{\pi}{2} - \tan^{-1}\frac{k_R}{k_I}\right). \tag{10.199}$$

From $|B_1|^2$ and $|B_0|^2$ we find that for the decays where the lifetime is long

$$\left|\frac{B_1}{B_0}\right|^2 \approx \frac{k_I}{\pi k_R}\left[1 + O\left(\frac{k_I}{\pi k_R}\right)\right]. \tag{10.200}$$

On the other hand as we have shown earlier that $B(r)$ for $r > a$ is zero, therefore

$$B_0(r) = -B_1(r), \quad r > a, \tag{10.201}$$

and from (10.201) we find that

$$|B_1|^2 = \int_0^\infty |B_1(r)|^2 dr \geq \int_a^\infty |B_1(r)|^2 dr = \int_a^\infty |B_0(r)|^2 dr. \tag{10.202}$$

By combining the two relations (10.200) and (10.202) we have

$$\int_0^\infty |B_0(r)|^2\, dr >> \int_a^\infty |B_0(r)|^2\, dr. \tag{10.203}$$

This last relation shows that B_0 is large only for $r < a$, i.e. it represents a wave packet at the time $t = 0$,

$$\Psi(r,0) = B_0(r). \tag{10.204}$$

In order to study the motion of this wave packet in time, we calculate the probability of finding this wave packet at time t in the interval $r < a$ from the expression

$$C_0 = \frac{1}{|B_0|^2}\int_0^\infty \Psi_0^*(r,0)\Psi_0(r,t)dr. \tag{10.205}$$

But from Eqs. (10.190) and (10.198) and from

$$u(r,t) = u(r,k)\exp\left(-\frac{i\hbar k^2 t}{2m}\right), \tag{10.206}$$

it follows that

$$C_0 = \frac{1}{2\pi|B_0|^2}\int_0^\infty \frac{\exp(-\frac{i\hbar k^2 t}{2m})}{(k-k_R)^2 + k_I^2}dk. \tag{10.207}$$

and this is similar to the result that we found in Chapter 2, Eq. (2.52) [4].

Let us consider the following simple example when the potential for the partial wave $l = 0$ is $v(r)$, where

$$v(r) = \begin{cases} -v_0 & \text{for } r < a \\ s\delta(r-a) & \text{for } r \ge a \end{cases}, \tag{10.208}$$

A simple calculation shows that the wave function in this case has the following form

$$u_I(r) = \sqrt{\frac{2}{\pi}}A(k)\sin\left(\sqrt{k^2+v_0}\,r\right), \quad r < a, \tag{10.209}$$

and

$$u_{II}(r) = \sqrt{\frac{2}{\pi}}\sin\left[kr + \delta(k)\right], \quad r > a, \tag{10.210}$$

where

$$A(k) = \frac{\sin[ka + \delta(k)]}{\sin(\sqrt{k^2+v_0}\,a)}, \tag{10.211}$$

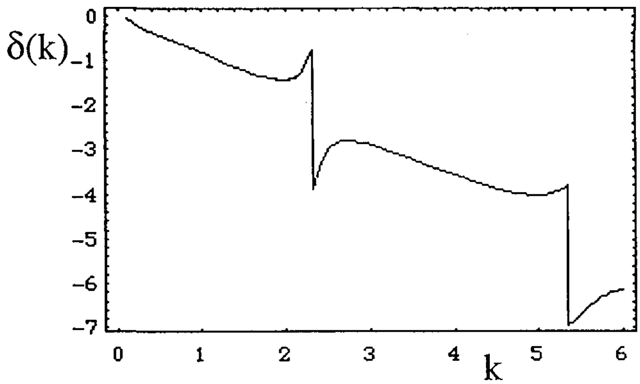

Figure 10.8: The wave number dependence of the phase shift $\delta(k)$ given by Eq. (10.212). The phase shift at $k = 2.3193L^{-1}$ is discontinuous.

is the amplitude of $u_I(r)$ and $\delta(k)$ is the phase shift

$$\delta(k) = -ka + \cot^{-1}\left[\frac{s}{k} + \frac{\sqrt{k^2+v_0}}{k}\cot\left(\sqrt{k^2+v_0}\,a\right)\right]. \tag{10.212}$$

In Fig. (10.8) the variation of $\delta(k)$ as a function of k is shown. For this plot we have used the parameters $a = 1L$, $v_0 = 2L^{-2}$ and $s = 6L^{-1}$. As we can see in this figure, $\delta(k)$ is discontinuous for $k_0 = 2.3193L^{-1}$ and the discontinuity of $\delta(k)$ is given by [5]

$$\delta(k_0 - \epsilon) - \delta(k_0 + \epsilon) = \pi, \quad \text{as} \quad \epsilon \to 0. \tag{10.213}$$

This state of the of the system is called an antibound state, and in addition to the discontinuity of the phase shift it has the following characteristics: As it is seen in Fig. (10.9), the amplitude $A(k)$ of the interior wave function $u_I(r)$ has a maximum about $k = k_0$ (or more accurately at $k = k_R = 2.3605L^{-1}$). If we expand $A(k)$ about this maximum we find

$$A(k) = A_0\frac{1}{(k-k_R)^2 + k_I^2}, \tag{10.214}$$

where for the this example $k_I = 0.1935L^{-1}$. The values of k_R and k_I show the validity of the inequality (10.200).

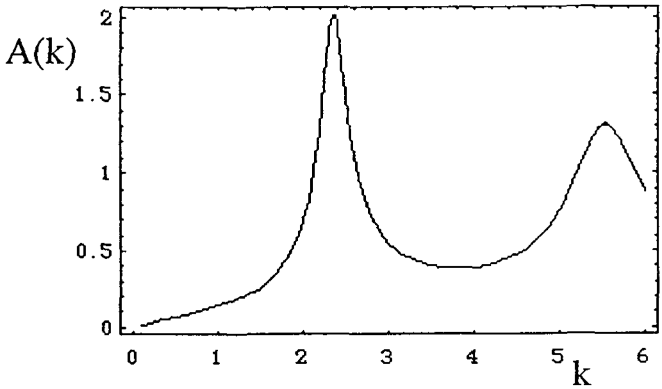

Figure 10.9: The amplitude of the wave function $A(k)$ inside the barrier, i.e. $r < a$ shown as a function of k.

Finally in Fig. (10.10) the time-delay which is proportional to $\frac{d\delta(k)}{dk}$ (Chapter 17) is shown as a function of k. Again we observe that this time-delay is large for $k = k_R$.

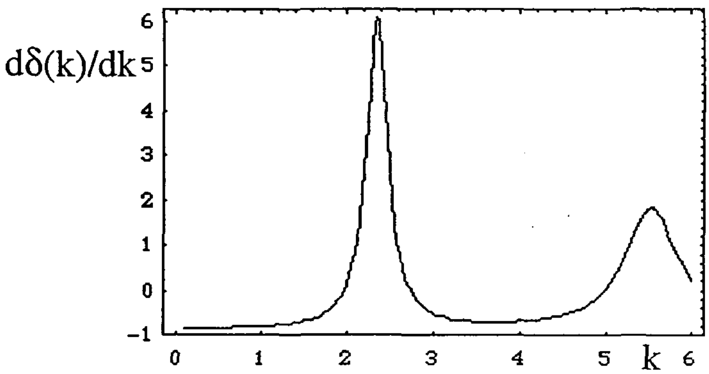

Figure 10.10: The rate of change of the phase shift with respect to the wave number k which is proportional to the time-delay.

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Chapter 11

The Method of Variable Reflection Amplitude Applied to Solve Multichannel Tunneling Problems

We have already seen that in the case of time-dependent potentials the wave equation can be written as an infinite set of coupled differential equations, Eq. (9.10). Similar set of equations results from the problem of tunneling of a composite system, e.g. tunneling of a bound molecule in one dimension (Chapter 20). Even in the simple case of one-dimensional tunneling from a nonsymmetric potential, we have a coupled channel problem [1].

In this chapter we present a method for solving this system with boundary conditions appropriate for tunneling. We note that here we have a situation where the boundary conditions for both $x \to -\infty$ and $x \to \infty$ contain the reflection and the transmission amplitudes but these are the quantities that we want to determine. Thus the standard methods of solving the Schrödinger equation numerically is not very helpful in solving these problems.

Here we first discuss a very simple and efficient way of the numerical integration which is suitable for tunneling problems [2] [3]. Then we consider a semi-classical approximation which may be regarded as an extension of the WKB method to multi-channel tunneling .

11.1 Mathematical Formulation

Let us consider a system of coupled equations:

$$\frac{d^2\psi_n}{dx^2} + k_n^2 - \sum_{m=0}^{\infty} v_{nm}(x)\psi_m(x) = 0, \quad n = 0, 1, 2, ... \tag{11.1}$$

If a plane wave from the left of the barrier approaches in the i-th channel, then we can write the formal solution of (11.1) as

$$\begin{aligned} \psi_{ni}(x) &= \exp(ik_n x)\delta_{ni} \\ &+ \frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_{-\infty}^{\infty} \exp(ik_n|x-x'|)v_{nm}(x')\psi_{mi}(x')dx'. \end{aligned} \tag{11.2}$$

Next we define the reflection and the transmission amplitudes by (see Eqs. (9.14) and (9.15))

$$R_{ni} = \frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_{-\infty}^{\infty} \exp(ik_n x')v_{nm}(x')\psi_{mi}(x')dx', \tag{11.3}$$

and

$$T_{ni} = \delta_{ni} + \frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_{-\infty}^{\infty} \exp(-ik_n x')v_{nm}(x')\psi_{mi}(x')dx'. \tag{11.4}$$

The direct but lengthy way of solving this problem is to solve the integral equation (11.2) numerically for $\psi_{ni}(x)$ for all significant n values and then substitute the result in Eqs, (11.3) and (11.4) to find the reflection and the transmission amplitudes. While this is possible, there is a simpler way for the direct calculation of R and T that we will discuss in this chapter. We begin our formulation by introducing a formal solution for the wave function of the cut-off potential $v_{nm}(y, x)$, where

$$v_{nm}(y, x) = v_{nm}(x)\theta(x - y), \tag{11.5}$$

and $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x > 0 \end{cases}. \tag{11.6}$$

The wave function for this cut-off potential is the solution of the integral equation [2]

$$\begin{aligned}\psi_{ni}(y,x) &= \exp(ik_n x)\delta_{ni}\\ &+ \frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_y^{\infty}\exp(ik_n|x-x'|)v_{nm}(x')\psi_{mi}(y,x')dx', \quad x \geq y.\end{aligned} \tag{11.7}$$

Next we define the variable reflection amplitude $R_{ni}(y)$ by

$$R_{ni}(y) = \frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_y^{\infty}\exp(ik_n x')v_{nm}(x')\psi_{mi}(y,x')dx'. \tag{11.8}$$

From Eqs. (11.7) and (11.8) it follows that

$$\psi_{ni}(y,y) = \exp(ik_n y)\delta_{ni} + R_{ni}(y)\exp(-ik_n y). \tag{11.9}$$

Now we find the derivative $\frac{\partial\psi_{ni}(y,x)}{\partial y}$ from (11.7) and we write it as

$$\begin{aligned}&\sum_{j=0}^{\infty}\frac{\partial}{\partial y}[\psi_{nj}(y,x)]B_{jn'}(y) = \exp(ik_n x)\delta_{n,n'}\\ &+ \sum_{j=0}^{\infty}\frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_y^{\infty}\exp(ik_n|x-x'|)v_{nm}(x')\\ &\times \left[\frac{\partial}{\partial y}\psi_{mj}(y,x')\right]B_{jn'}(y)dx', \quad x \geq y,\end{aligned} \tag{11.10}$$

where $B_{jn'}(y)$ in (11.10) is defined by the equation

$$-\sum_{j=0}^{\infty}\frac{1}{2ik_n}\exp(-ik_n y)\sum_{m=0}^{\infty}v_{nm}(y)\psi_{mj}(y,y)B_{jn'}(y) = \delta_{n,n'}. \tag{11.11}$$

Also from Eq. (11.10) we find that

$$\sum_{j=0}^{\infty}\frac{\partial}{\partial y}[\psi_{nj}(y,x)]B_{jn'}(y) = \psi_{nn'}(y,x). \tag{11.12}$$

This follows from the fact that the left hand side of (11.12) satisfies Eq. (11.7), i.e. the integral equation for $\psi_{nn'}(y,x)$.

Next we observe that we can write (11.8) for $R_{ni}(y)$ as

$$\sum_{n'=0}^{\infty} R_{nn'}(y)\left[B^{-1}(y)\right]_{n'j} = \frac{1}{2ik_n}\int_y^{\infty}\exp(ik_n x) \times \sum_{m=0}^{\infty}\left\{v_{nm}(x)\frac{\partial}{\partial y}\psi_{mj}(y,x)\right\}dx, \tag{11.13}$$

where $B^{-1}(y)$ is the inverse of the matrix which we have defined by (11.11).

By differentiating $R_{ni}(y)$ in Eq. (11.9) with respect to y and eliminating the integral which depends on $\frac{\partial}{\partial y}\psi_{mi}(y,x)$, we obtain the following equation for $R_{ni}(y)$;

$$\frac{d}{dy}R_{ni}(y) = -\frac{1}{2ik_n}\exp(ik_n y)\sum_{m=0}^{\infty}v_{nm}(x) \times \left\{\exp\left(ik_m y\right)\delta_{mi} + R_{mi}(y)\exp\left(-ik_m y\right)\right\} + \sum_{k=0}^{\infty}R_{nk}(y)\left[B^{-1}\right]_{ki}. \tag{11.14}$$

We find $[B^{-1}]_{n'i}$ from Eq. (11.11) to be;

$$\left[B^{-1}\right]_{n'j} = -\frac{1}{2ik_{n'}}\exp(-ik_{n'}y)\sum_{m=0}^{\infty}v_{n'm}\psi_{mj}(y,y). \tag{11.15}$$

By substituting the matrix $B^{-1}(y)$ from (11.15) in Eq. (11.14) and eliminating $\psi_{mj}(y,y)$ between (11.15) and (11.9) we find a set of first order nonlinear equations for $R_{nj}(y)$'s

$$\frac{d}{dy}R_{ni}(y) = -\sum_{j=0}^{\infty}\frac{1}{2ik_j}\left\{\exp(ik_j y)\delta_{nj} + R_{nj}(y)\exp(-ik_j y)\right\} \times \sum_{m=0}^{\infty}v_{jm}(y)\left\{\exp(ik_m y)\delta_{mi} + R_{mi}(y)\exp(-ik_m y)\right\}. \tag{11.16}$$

In a similar fashion we find a differential equation for the variable transmission amplitude $T_{ni}(y)$. Thus we first define $T_{ni}(y)$ by

$$T_{ni}(y) = \delta_{ni} + \frac{1}{2ik_n}\sum_{m=0}^{\infty}\int_y^{\infty}\exp(-ik_n x')v_{nm}(x')\psi_{mi}(y,x')dx', \tag{11.17}$$

and then by differentiating $T_{ni}(y)$ with respect to y and eliminating $\frac{\partial}{\partial y}\psi_{mi}(y,x)$ exactly as before, after some simplifications, we find the following set of differential equations:

$$\frac{d}{dy}T_{ni}(y) = -\sum_{j=0}^{\infty}\frac{1}{2ik_j}\exp(ik_jy)T_{nj}(y)$$
$$\times \sum_{m=0}^{\infty} v_{jm}(y)\left\{\exp(ik_my)\delta_{mi} + R_{mi}(y)\exp(-ik_my)\right\}. \quad (11.18)$$

Having obtained Eqs. (11.16) and (11.18) we need to determine the boundary conditions for these differential equations. They are found by comparing these equations with (11.3) and (11.4) and in this way we get

$$R_{ni}(y \to \infty) \to 0, \quad R_{ni}(y \to -\infty) = R_{ni}, \quad (11.19)$$

and

$$T_{ni}(y \to \infty) \to \delta_{ni}, \quad T_{in}(y \to -\infty) = T_{ni}. \quad (11.20)$$

By solving these equations for R_{ni} and T_{ni} we can find the transition probability $P_{i\to n}$ from the initial channel i to the final channel n in terms of $R(-\infty)$ and $T(-\infty)$,

$$P_{i\to n} = \left(\frac{k_n}{k_i}\right)\left\{|R_{ni}(-\infty)|^2 + |T_{ni}(-\infty)|^2\right\}. \quad (11.21)$$

For the numerical calculation of these nonlinear coupled differential equations, it is convenient to introduce new matrices $U_{ni}(y)$ and $Q_{ni}(y)$ in terms of $R_{ni}(y)$ and $T_{ni}(y)$ by the following relations:

$$R_{ni}(y) = \exp(ik_ny)\left[2ik_iU_{ni}(y) - \delta_{ni}\right]\exp(ik_iy), \quad (11.22)$$

and

$$T_{ni}(y) = 2ik_i\exp(ik_ny)Q_{ni}(y)\exp(ik_iy). \quad (11.23)$$

By substituting these in Eqs. (11.16) and (11.18) we find

$$\frac{d}{dy}U_{ni}(y) = \delta_{ni} - i(k_n + k_i)U_{ni}(y) - \sum_{j,m=0}^{\infty} U_{nj}(y)v_{jm}(y)U_{mi}(y), \quad (11.24)$$

and

$$\frac{d}{dy}Q_{ni}(y) = -i(k_n + k_i)Q_{ni}(y) - \sum_{j,m=0}^{\infty} Q_{nj}(y)v_{jm}(y)U_{mi}(y). \quad (11.25)$$

The boundary conditions for these equations are determined from Eqs. (11.19) and (11.20);

$$U_{ni}(+\infty) = \frac{1}{2ik_i}\delta_{ni}, \tag{11.26}$$

and

$$Q_{ni}(+\infty) = \frac{1}{2ik_i}\delta_{ni}\exp(-2ik_i y). \tag{11.27}$$

The great advantage of Eq. (11.24) over Eq. (11.16) is that U is a symmetric matrix - this follows from the symmetric nature of the matrix v_{jm}, whereas R is not symmetric. Thus instead of calculating N^2 elements of R_{ni} , we need to calculate $\frac{1}{2}N(N+1)$ elements of U_{ni}.

As an example let us calculate the reflection amplitude for the barrier given by

$$v(x) = 10\left\{\exp[-2(x-1)^2] + \exp[-2(x+1)^2]\right\}. \tag{11.28}$$

Here we have a single channel and Eq. (11.24) reduces to [4]

$$\frac{dU(y)}{dy} = 1 - 2ikU(y) - v(y)U^2(u), \tag{11.29}$$

with the boundary condition

$$U(+\infty) = \frac{1}{2ik}. \tag{11.30}$$

By integrating (11.29) from $y = \infty$ to $y = -\infty$, we calculate $U(-\infty)$, and then from Eq. (11.22) we have

$$R(-\infty) = \lim\left\{\exp(2iky)[2ikU(+\infty) - 1]\right\}, \quad \text{as} \quad y \to -\infty. \tag{11.31}$$

In Fig. (11.1) the potential (11.28) is shown. For this potential we have integrated Eq. (11.29) numerically for two values of the wave number $k = 2L^{-1}$ and $k = 2.48L^{-1}$. These are shown in Fig. (11.2).

For the wave number $k = 2.48L^{-1}$ the reflection amplitude suddenly becomes very small, i.e. a particle with the energy corresponding to this wave number can tunnel through the barrier easily, whereas for other energies of the particle less than the maximum height of the barrier $\sim 10L^{-2}$ the reflection amplitude is large (Fig. 11.3).

For a computational technique for studying the motion of a wave packet see [5].

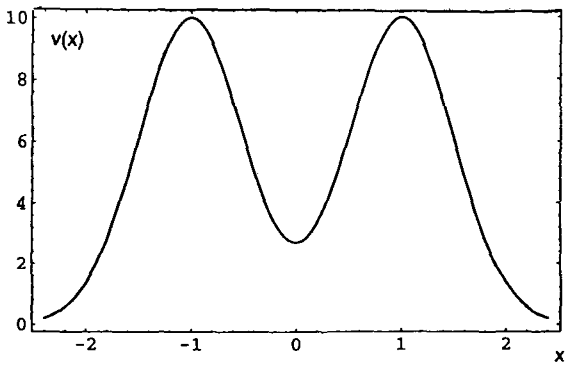

Figure 11.1: Single channel potential given by Eq. (11.28) is plotted as a function of x.

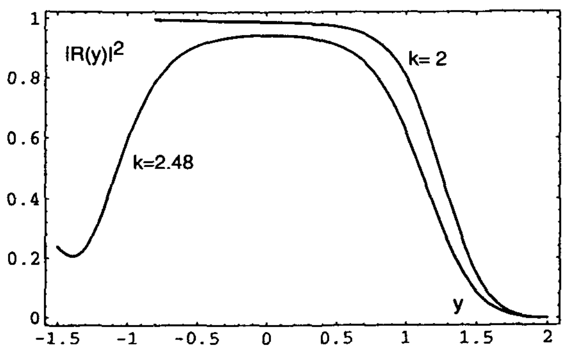

Figure 11.2: The single channel variable reflection amplitude for the potential shown in Fig. (11.1). For the wave number $k = 2.48L^{-1}$ there is resonant tunneling.

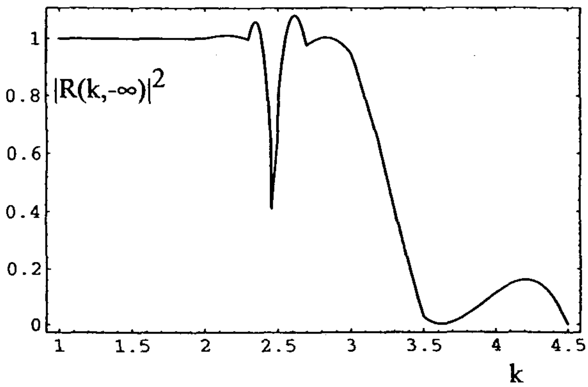

Figure 11.3: The reflection amplitude as a function of the wave number of the incoming particle.

11.2 Matrix Equations and Semi-classical Approximation for Many-Channel Problems

We can develop a matrix version of the WKB approximation for the many-channel tunneling problem that we discussed earlier [6] [7] [8]. For this we try to write the wave equation as well as the equations for R and T as matrix differential equations. Starting with Eq. (11.1), we write it as

$$\frac{d^2\psi(x)}{dx^2} + K_0^2\psi(x) = v(x)\psi(x). \tag{11.32}$$

We want to solve this equation subject to the boundary conditions

$$\psi(x) \to \exp(iK_0x)(1 + T_1), \quad \text{as} \quad x \to \infty, \tag{11.33}$$

and

$$\psi(x) \to \exp(iK_0x) + \exp(-iK_0x)R_1 \quad \text{as} \quad x \to -\infty, \tag{11.34}$$

where

$$K_0^2 = \begin{pmatrix} k_0^2 & 0 & 0 & 0 \\ 0 & k_1^2 & 0 & 0 \\ 0 & 0 & k_2^2 & \vdots \\ 0 & 0 & \cdots & \end{pmatrix}. \tag{11.35}$$

The quantities ψ, v, T_1 and R_1 are all matrices. Starting with Eq. (11.32) we can find nonlinear first order matrix equations for T_1 and R_1 as we did earlier in this chapter. To this end we again introduce the cut-off potential $v(y,x)$ by Eq. (11.5). For this potential we find matrices $R_1(y)$ and $T_1(y)$ from Eqs. (11.8) and (11.17). Then to simplify the resulting equations further we define two new matrices $R(y)$ and $T(y)$;

$$R(y) = \exp(-iK_0 y) R_1(y) \exp(-iK_0 y), \tag{11.36}$$

and

$$T(y) = [1 + T_1(y)] \exp(-iK_0 y), \tag{11.37}$$

then

$$\frac{dR(y)}{dy} = -i\left(R(y)K_0 + K_0 R(y)\right) - \frac{1}{2}(1 + R(y))\left(iK_0\right)^{-1} v(y)(1 + R(y)), \tag{11.38}$$

and

$$\frac{dT(y)}{dy} = -iT(y)K_0 - \frac{1}{2}T(y)(iK_0)^{-1} v(y)(1 + R(y)). \tag{11.39}$$

These equations are subject to the boundary conditions

$$R(\infty) = 0, \tag{11.40}$$

and

$$T(y) \to \exp(-iK_0 y), \quad \text{as } y \to \infty. \tag{11.41}$$

These are in a way the generalized forms of the matrices R_{ni} and T_{ni} introduced before, and $R_1(-\infty)$ and $T(-\infty)$ are the reflection and transmission amplitudes for the potential $v_{nm}(x)$. Note the difference between $T_1(-\infty)$ and $T(-\infty)$. These matrix equations are exact, but we can use the approximation which replaces them with linear matrix equation (see below).

Another way of finding the reflection and transmission amplitudes is to write the matrix Schrödinger equation as

$$\frac{d^2\psi(x)}{dx^2} + K^2(x)\psi(x) = 0, \tag{11.42}$$

where K^2 is the matrix

$$K^2(x) = K_0^2 - v(x). \tag{11.43}$$

Now we define the potential $v_2(x)$ by

$$v_2(x,y) = v(x)\theta(x-y) + v(y)\theta(y-x), \qquad (11.44)$$

and we set the following boundary conditions for the solution of (11.42)

$$\psi_2(y,x) \to \exp(iK_0x) + \exp(iK_0x)T_2(y), \qquad (11.45)$$

$$\psi_2(y,x) \to \exp[iK(y)x] + \exp[-iK(y)x]R_2(y), \quad x \le y, \qquad (11.46)$$

$$R_2(\infty) = T_2(\infty) = 0, \qquad (11.47)$$

$$R_2 = R_2(-\infty), \qquad (11.48)$$

and

$$T_2 = T_2(-\infty). \qquad (11.49)$$

In a way similar to the definitions (11.36) and (11.37) we introduce two matrices R_3 and T_3 by

$$R_3(y) = \exp[-iK(y)y]R_2(y)\exp[-iK(y)y, \qquad (11.50)$$

and

$$T_3(y) = [1 + T_2(y)]\exp[-iK(y)y]. \qquad (11.51)$$

Exactly as we derived the earlier nonlinear differential equations, here also we find the following equations for R_3 and T_3;

$$\begin{aligned} \frac{dR_3(y)}{dy} &= -i\left(R_3(y)K(y) + K(y)R_3(y)\right) \\ &+ \frac{1}{2}[1 + R_3(y)]K^{-1}(y)\frac{dK(y)}{dy}[1 - R_3(y)], \end{aligned} \qquad (11.52)$$

and

$$\frac{dT_3(y)}{dy} = -iT_3(y)K(y) + \frac{1}{2}T_3(y)K^{-1}(y)\frac{dK(y)}{dy}[1 - R_3(y)]. \qquad (11.53)$$

From these equations we can find the WKB approximation for the multichannel tunneling. In this approximation we assume that $R_3(y)$, the reflection amplitude is small, $R_3(y) \approx 0$, and therefore (11.53) reduces to

$$\frac{dT_3(y)}{dy} = -iT_3(y)K(y) + \frac{1}{2}T_3(y)K^{-1}(y)\frac{dK(y)}{dy}, \qquad (11.54)$$

which is a linear matrix differential equation and can be integrated for $T_3(y)$. If we use this approximation for a single channel, the solution of (11.54) with the boundary condition (11.47) gives us

$$T_3(x) = \sqrt{\frac{K(x)}{K_0}} \exp\left\{i \int_x^{\infty} [K(y) - K_0] dy\right\}, \tag{11.55}$$

or as $x \to -\infty$ we find the transmission amplitude to be

$$T_3(-\infty) = \exp\left\{i \int_{-\infty}^{\infty} [K(y) - K_0] dy\right\}, \tag{11.56}$$

which is a generalization of the WKB approximation to the many-channel problems.

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Chapter 12

Path Integral and Its Semi-Classical Approximation in Quantum Tunneling

In the preceding chapters we have studied certain aspects of the one- and three-dimensional tunneling using the Schrödinger equation as the starting point of our investigation. In this and the next two chapters we examine other methods of formulating and solving tunneling problems. First we consider the path integral approach to one-dimensional tunneling. In this approach we formulate the tunneling problem with the help of the Feynman propagator $D_F(x_f, x_i; T, 0)$ [1] [2] [3] [4] [5]. The square of the absolute value of this propagator is a measure of the probability of finding the particle which is initially at $x = x_i$ to be at $x = x_f$ at the time T.

According to Feynman, we can determine this propagator by summing over the classical paths , i.e. [5]

$$D_F \sim \int [\mathcal{D}(x)] \exp\left[\frac{i}{\hbar} S(x)\right], \tag{12.1}$$

a point which will be discussed later in detail. For the problem of tunneling that we want to study, it is more convenient to replace $D_F(x_f; x_i, T, 0)$ by its energy Fourier transform,

$$D_F(x_f, x_i; E) = \int_0^\infty \exp\left(\frac{iET}{\hbar}\right) D_F(x_f; x_i, T, 0) dT. \tag{12.2}$$

In the classical limit $\hbar \to 0$, in Eq. (12.1) $\frac{iS}{\hbar}$ becomes large, and we find an approximate value for the integral using the method of stationary phase [6] [7]. In this limit we get an expression which is similar to the WKB approximation, i.e.

$$D_F(x_f, x_i; T, 0) = f(x_f, x_i) \exp\left(\frac{i}{\hbar} S[x_{cl}]\right), \tag{12.3}$$

where in this equation $f(x_f, x_i)$ is given by [4]

$$f(x_f, x_i) = \frac{1}{\left[2\pi k(x_f) k(x_i) \int_{x_i}^{x_f} \frac{dx}{(k(x))^3}\right]^{\frac{1}{2}}}, \tag{12.4}$$

and $S[x_{cl}]$ is the classical action for a path joining the space time point (x_f, T) to $(x_i, 0)$. This action is expressible as

$$S[x_{cl}] = \int_{x_i}^{x_f} k_{cl}(x) dx - E_{cl} T' = \int_{x_i}^{x_f} \sqrt{2m[E_{cl} - V(x)]}\, dx - E_{cl} T'. \tag{12.5}$$

Here the constant E_{cl} is the classical energy of this path and is related to T' by the following relation

$$T' = \int_{x_i}^{x_f} \sqrt{\frac{m}{2[E_{cl} - V(x)]}} dx. \tag{12.6}$$

With the help of the stationary phase method, we can carry out the time integration in (12.2)

$$D_F(x_f, x_i; E) \approx \frac{m}{\sqrt{k(x_f) k(x_i)}} \exp\left[i \int_{x_i}^{x_f} k_{cl}(x) dx\right]. \tag{12.7}$$

So far we have assumed that a real path exists for the motion of the particle, but we can generalize this method and apply it to the cases where tunneling occurs.

For a constant energy E, we can write $D_F(x_f, x_i; E)$ as a sum over these extended paths, x_n, which connects x_i to x_f;

$$D_F(x_f, x_i; E) = \frac{m}{\sqrt{k(x_f) k(x_i)}} \sum_n K_n, \tag{12.8}$$

where this D_F is a semi-classical approximate form of the propagator, and the coefficients K_n are determined by the following set of rules [4] [8] [9]:
(1) - In the classically allowed region we use the factor

$$\exp\left[i\int_{x_1}^{x_2} k(x)dx\right], \quad \text{where} \quad k(x)=\sqrt{k^2-v(x)}, \tag{12.9}$$

whereas for the classically forbidden region, i.e. under the barrier the factor is

$$\exp\left[-\int_{x_1}^{x_2} q(x)dx\right], \tag{12.10}$$

where

$$q(x)=\sqrt{v(x)-k^2}. \tag{12.11}$$

The way that we use these factors will be shown by studying a specific example below.
(2) - If the reflection from a classical turning point is from a part where the classical motion is allowed, we use a factor $(-i)$. If the reflection is from the side where the classical motion is forbidden the factor that we use is $(-\frac{i}{2})$.

Let us consider the method of construction of $D_F(x_f, x_i; E)$ when there is a single barrier with turning points at $a(E)$ and $b(E)$, $b(E) > a(E)$ (see Fig. (12.1)).

The trajectory of the particle starts at $x = x_i$ to the left of $a(E)$ and ends at $x = x_f$ to the right of $b(E)$. In the wave picture the simplest path consists of a wave emanating from x_i, reaching the turning point $x = a(E)$, and propagating under the barrier from $a(E)$ to $b(E)$, and finally moving from $b(E)$ to x_f. For this case we can write the total amplitude as

$$D_F(x_f,x_i;E) = \frac{m}{\sqrt{k(x_f)k(x_i)}}\exp\left[i\int_{x_i}^{a} k(x)dx\right]$$
$$\times \left\{Z+\left(\frac{i}{2}\right)^2 Z^3+\left(\frac{i}{2}\right)^4 Z^5+\dots\dots\right\}\exp\left[i\int_{b}^{x_f} k(x)dx\right], \tag{12.12}$$

where Z which is given by

$$Z=\exp\left[-\int_a^b q(x)dx\right], \tag{12.13}$$

is the penetration factor in the WKB approximation. The infinite series in the curly bracket in (12.12) form a geometric series and thus can be summed to yield

$$\frac{Z}{1+\frac{1}{4}Z^2}. \tag{12.14}$$

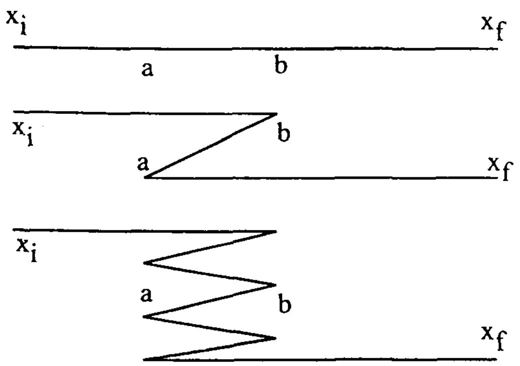

Figure 12.1: Possible extended classical paths connecting the initial point x_i to the final point x_f, with a number of reflections inside the barrier.

From (12.12) we find the coefficient of transmission to be equal to

$$|T(E)|^2 = \left|\frac{Z}{1+\frac{1}{4}Z^2}\right|^2, \tag{12.15}$$

where Z is a function of the energy E. Compare this result for an arbitrary barrier with Eq. (3.89) of the Miller-Good method and with Eq. (3.61) of the WKB approximation, and when the barrier is rectangular, compare it with the exact solution of the wave equation (6.71) for a rectangular barrier.

12.1 Application to the S-Wave Tunneling of a Particle Through a Central Barrier

Another problem which can be approximately solved by this method is the S-wave tunneling in a central potential. Here we have a case similar to the one that we discussed earlier, but with an additional boundary condition that the reduced wave function must be zero at $r = 0$. For the constant energy, E, of the particle there are two turning points a and b both dependent on

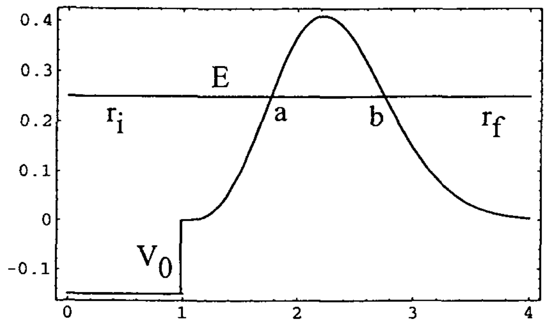

Figure 12.2: The particle is initially trapped in the attractive potential V_0 and by tunneling it can escape to $r \to \infty$. The points a and b are the classical turning points.

E, and we want to consider the extended paths joining the initial point r_i to the final point r_f of the trajectory where

$$r_i < a < b < r_f. \tag{12.16}$$

Here we have suppressed the dependence of a and b on E. Again we will study the tunneling situation where E is less than the height of the barrier (see Fig. 12.2). The extended paths are composed of a number of back and forth reflections in the region $r_i < r < a$, where the motion is allowed according to the laws of classical dynamics. After a number of reflections between these two points finally the wave travels to b and from there to r_f. The amplitude $A_2(b, a)$ of the motion between b and a which is forbidden by the laws of classical mechanics, as we have seen earlier, is given by the sum

$$A_2(b,a) = Z + \left(\frac{i}{2}\right)^2 Z^3 + \left(\frac{i}{2}\right)^4 Z^5 + \dots = \frac{Z}{1+\frac{1}{4}Z^2}, \tag{12.17}$$

where again

$$Z = \exp\left[-\int_a^b q(r)dr\right]. \tag{12.18}$$

There are other ways that the motion between these points can take place [1]:
(i) - From a the wave moves to b in all possible ways and then returns to a, we denote this amplitude by $A_2(a,a)$.
(ii) - From a the wave enters the region $0 < r < a$ and oscillates between the two turning points $r = a$ and $r = 0$ a number of times and finally returns to a. This amplitude will be denoted by $A_1(a,a)$.
(iii) - The wave returns to b in the forbidden region with an amplitude $A_2(b,a)$, where at b it may be reflected. The total amplitude for all these paths is

$$A(b,a) = A_2(b,a)\left\{1 + A_2(a,a)A_1(a,a) + [A_2(a,a)A_1(a,a)]^2 + ...\right\}. \tag{12.19}$$

This is also a geometrical series with the sum

$$A(b,a) = \frac{A_2(b,a)}{1 - A_1(a,a)A_2(a,a)}. \tag{12.20}$$

Thus to find the total amplitude, we have to find the partial amplitudes $A_1(a,a)$, $A_2(a,a)$..... For calculating $A_1(a,a)$, we observe that the simplest path starts from $r = a$, goes to the origin $r = 0$, and gets reflected there and comes back to $r = a$. The amplitude of this path according to the mentioned rule is

$$\exp(iKa)(-1)\exp(iKa), \tag{12.21}$$

where $K = \sqrt{k^2 + v_0}$ and v_0 is the depth of the potential well to the left of the barrier. The particle upon reflection with an amplitude $(-i)$ from the turning point $r = a$ can move to $r = a$, and again be reflected there. The total amplitude for this motion is

$$\begin{aligned} A_1(a,a) &= -e^{2iKa}\left\{1 + (-i)\left(-e^{2iKa}\right) + \left[(-i)\left(-e^{2iKa}\right)\right]^2 + ...\right\} \\ &= \frac{-\exp(2iKa)}{1 - i\exp(2iKa)}. \end{aligned} \tag{12.22}$$

The amplitude A_{22} is composed of the paths which start at $r = a$, pass through the classically forbidden region, are reflected at $r = b$ before returning to $r = a$. Since there are infinite reflections between these points, the resulting amplitude is the sum of the series

$$A_{22}(a,a) = \frac{i}{2}Z^2\left[1 + \frac{i^2}{4}Z^2 + \left(\frac{i^2}{4}Z^2\right)^2 + ...\right] = \frac{i}{2}\frac{Z^2}{1 + \frac{1}{4}Z^2}. \tag{12.23}$$

The last amplitude that we need is $B_1(r_1)$ which describes the motion from r_i inside the well to the point a without leaving the well. The first term of this sum is $\exp[iK(a-r_i)]$, which is the amplitude of the propagation from r_i to a with no reflection. To this we add the amplitude of of propagation from r_i to the origin and the reflection at the origin and its subsequent arrival at a, i.e. $e^{iKr_i}(-1)e^{iKa}$. But there can be multiple reflections between $r = 0$ and $r = a$, therefore the total amplitude for all these are given by

$$\begin{aligned} B_1(r_i) &= \left[e^{iK(a-r_i)} - e^{iK(a+r_i)}\right]\left[1 + ie^{2iKa} + \left(ie^{2iKa}\right)^2 + \ldots\ldots\right] \\ &= \frac{\exp[iK(a-r_i)] - \exp[iK(a+r_i)]}{1 - i\exp(2iKa)}. \end{aligned} \tag{12.24}$$

Thus in this semi-classical approximation the propagator turns out to be

$$\begin{aligned} D_F(r_f, r_i; E) &= \frac{m}{\sqrt{K_0 k(r_f)}} B_1(r_i) \exp\left[\int_b^{r_f} k(r)dr\right] A(b,a) \\ &= \left(\frac{-2im}{\sqrt{K_0 k(r_f)}}\right) \frac{\sin(Kr_i)\exp(iKa) Z \exp[i\int_b^{r_f} k(r)dr]}{\left(1+\frac{1}{4}Z^2\right)\left[1 - i\exp(2iKb)\right] + \frac{i}{2}Z^2\exp(2iKa)}. \end{aligned} \tag{12.25}$$

We can also write this propagator as

$$D_F(r_f, r_i; E) = \frac{m}{\sqrt{K_0 k(r_f)}}\left[\frac{\sin(Kr_i) Z \exp[i\int_b^{r_f} k(r)dr] e^{-i\frac{\pi}{4}}}{\sin(Ka + \frac{\pi}{4}) + \frac{i}{4}Z^2\cos(Ka + \frac{\pi}{4})}\right]. \tag{12.26}$$

The denominator in (12.26) is a complex quantity, and for the energy $E = E_0$ for which $\sin(K_0 a + \frac{\pi}{4})$ is zero, this denominator becomes imaginary. This is the case when the particle is trapped in the well. For this situation we have

$$K_0 = \left(n - \frac{1}{4}\right)\frac{\pi}{a}, \quad E_0 = \frac{1}{2m}K_0^2. \quad n = 0, 1, 2.... \tag{12.27}$$

For the energies close to E_0, we use the following expansion

$$\sin\left(Ka + \frac{\pi}{4}\right) \approx a(K - K_0)\cos\left(Ka + \frac{\pi}{4}\right) \approx \frac{ma}{K_0}(E - E_0)\cos\left(Ka + \frac{\pi}{4}\right), \tag{12.28}$$

and then by substituting (12.28) in (12.26) we obtain an approximate form of D_F for energies close to E_0

$$D_F(r_f, r_i; E) = \frac{(-1)^n}{a\sqrt{K_0 k(r_f)}} \frac{\sin(K_0 r_i) K_0 Z \exp\left[i\int_b^{r_f} k(r)dr\right] e^{-i\frac{\pi}{4}}}{E - E_0 + \frac{iK_0}{4ma} Z^2}. \tag{12.29}$$

The denominator in (12.29) has the Breit-Wigner form (see also Chapter 5). From the inverse Fourier transform of D_F we find the decay width. Thus if we make use of the integral

$$\frac{\hbar}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{E_0 - \hbar\omega - \frac{i}{2}\Gamma} d\omega = \begin{cases} \exp(-\frac{\Gamma t}{2\hbar})\exp(-i\frac{E_0 t}{\hbar}) & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}, \tag{12.30}$$

we find from (12.29) that

$$\Gamma = \frac{K_0}{2ma} Z^2 = \frac{\omega_0}{2\pi} \exp\left[-\int_a^b |p(r)| dr\right], \tag{12.31}$$

where in this relation $\frac{\omega_0}{2\pi}$ is the frequency of the oscillation of the particle between $r = 0$ and $r = a$

$$\frac{\omega_0}{2\pi} = \frac{K_0}{2ma} = \frac{1}{T_0}. \tag{12.32}$$

and $|p(r)| = \sqrt{v(r) - K_0^2}$. This is similar to the result that we found in Chapters 5 and 10.

12.2 Method of Euclidean Path Integral

In the part of space where tunneling takes place, the momentum of the particle is imaginary, but if we choose the time variable as an imaginary variable, then the momentum becomes real and the motion is possible in the sense of classical dynamics. We write this motion as an integral over the path [10] [11]

$$\left\langle x_f \left| \exp\left(-\frac{H\mathcal{T}}{\hbar}\right) \right| x_i \right\rangle = \mathcal{N} \int [\mathcal{D}(x)] \exp\left(-\frac{S}{\hbar}\right), \tag{12.33}$$

where we have used $t = -i\mathcal{T}$ ($\mathcal{T}$ is a positive number).

Here H is the Hamiltonian operator of the particle and $|x_i\rangle$ and $|x_f\rangle$

are the initial and final states of the particle. Now we expand $|x_i\rangle$ and $|x_f\rangle$ in terms of the energy eigenfunctions $|n\rangle$ of H which is defined by

$$H|n\rangle = E_n|n\rangle. \tag{12.34}$$

That is

$$|x_i\rangle = \sum_n |n\rangle\langle n|x_i\rangle. \tag{12.35}$$

With the help of this expansion we can write the left hand side of (12.33) as

$$\left\langle x_f \left| \exp\left(-\frac{H\mathcal{T}}{\hbar}\right)\right| x_i \right\rangle = \sum_n \exp\left(-\frac{E_n\mathcal{T}}{\hbar}\right)\langle x_f|n\rangle\langle n|x_i\rangle. \tag{12.36}$$

We observe that for large $\mathcal{T}$ in the right hand side of (12.36) only the lowest energy state and its corresponding wave function will make the major contribution. Now let us study the integral in Eq. (12.33) in which $\mathcal{N}$ is the normalization constant and S is the Euclidean action

$$S = \int_{-\frac{\mathcal{T}}{2}}^{\frac{\mathcal{T}}{2}} \left[\frac{1}{2}\left(\frac{dx}{dt}\right)^2 + V(x)\right] dt, \tag{12.37}$$

where we have assumed that the particle has a unit mass. In Eq. (12.33), $[\mathcal{D}(x)]$ shows that the integral is over all paths $x(t)$ which satisfy the initial and final conditions

$$x\left(-\frac{\mathcal{T}}{2}\right) = x_i, \quad \text{and} \quad x\left(\frac{\mathcal{T}}{2}\right) = x_f. \tag{12.38}$$

To make this idea clearer, we can define the paths in the following way: Let us assume that $\bar{x}$ is a function of t which satisfies the conditions (12.38), then a general set of functions which satisfies (12.38) can be written as

$$x(t) = \bar{x}(t) + \sum_n c_n x_n(t) \tag{12.39}$$

where $\{x_n\}$'s form a complete set of orthonormal states which vanish at the initial and final times, $t = -\frac{\mathcal{T}}{2}$ and $t = \frac{\mathcal{T}}{2}$,

$$\int_{-\frac{\mathcal{T}}{2}}^{\frac{\mathcal{T}}{2}} x_m(t)x_n(t)dt = \delta_{nm}, \tag{12.40}$$

and

$$x_n\left(\pm\frac{\mathcal{T}}{2}\right) = 0. \tag{12.41}$$

Now we define $[\mathcal{D}(x)]$ in the following way

$$[\mathcal{D}(x)] = \prod_n \frac{1}{\sqrt{2\pi\hbar}} dc_n. \tag{12.42}$$

Again we observe that we can calculate the right hand side of (12.33) in the semi-classical limit of $\hbar \to 0$. In this case, as we have seen earlier, the major contribution to the path integral comes from the path(s) for which S is minimum. For simplicity we assume that there is a single path and we denote it by $\bar{x}$. The minimum of S with respect to the variation of path is found from

$$\frac{\delta S}{\delta \bar{x}} = -\frac{d^2\bar{x}}{dt^2} + V'(\bar{x}) = 0, \tag{12.43}$$

in which $V'(x) = \frac{dV(x)}{dx}$. In addition we take $\{x_n\}$'s to be the eigenfunctions of the second derivative of S with respect to path, i.e. $\frac{\delta^2 S}{\delta x^2}$ for $x = \bar{x}$,

$$-\frac{d^2 x_n}{dt^2} + V''(\bar{x})x_n = \lambda_n x_n. \tag{12.44}$$

With these assumptions in the limit of $\hbar \to 0$, the path integral is expressible as a product of Gaussian integrals

$$\left\langle x_f \left| \exp\left(-\frac{HT}{\hbar}\right) \right| x_i \right\rangle = \mathcal{N} \exp\left[-\frac{S(\bar{x})}{\hbar}\right] \prod_n \frac{1}{\sqrt{\lambda_n}} (1 + O(\hbar))$$

$$= \mathcal{N} \exp\left[-\frac{S(\bar{x})}{\hbar}\right] \left\{\det\left[-\frac{\partial^2}{\partial t^2} + V''(\bar{x})\right]\right\}^{-\frac{1}{2}} (1 + O(\hbar)). \tag{12.45}$$

Here we have chosen all the eigenstates to be positive. Those cases where some of the eigenvalues are negative can be dealt with in a similar manner [11]. If there are a number of roots (or paths) for the equation $\frac{\delta S}{\delta x} = 0$ then we have to sum S over all of these paths.

Equation (12.44) is the equation of motion of a particle of unit mass in the potential $-V(x)$ for which the first integral is

$$E = \frac{1}{2}\left(\frac{d\bar{x}}{dt}\right)^2 - V(\bar{x}), \tag{12.46}$$

where E is a constant.

As an example consider the potential shown in Fig. (12.3), and let us take $x_i = x_f = d$. Then $\bar{x} = 0$ is the only solution which satisfies the

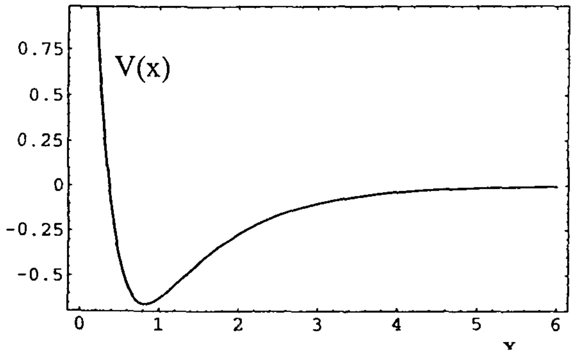

Figure 12.3: A potential with a single minimum at $x = d$.

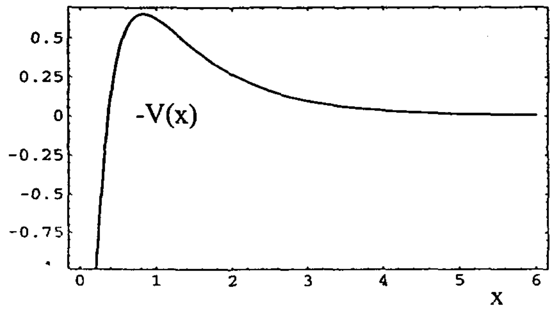

Figure 12.4: The negative of the potential shown in the previous figure.

initial and the final conditions and for this solution $S = 0$. If we denote $V''(d) = \omega^2$, we want to show that

$$\mathcal{N}\left[\det\left(-\frac{\partial^2}{\partial t^2}+\omega^2\right)\right]^{-\frac{1}{2}} = \sqrt{\frac{\omega}{\pi\hbar}}\exp\left(-\frac{\omega\mathcal{T}}{2}\right). \tag{12.47}$$

To prove this relation we write Eq. (12.44) in the following way:

$$\left(-\frac{d^2}{dt^2}+\omega^2\right)x_n = \lambda_n x_n, \tag{12.48}$$

where λ_n's are the characteristic values. The initial and final conditions for x_n's are given by (12.41). From Eqs. (12.48) and (12.41) we conclude that

$$x_n = A_n \sin\left(\sqrt{\lambda_n - \omega^2}\, t\right), \tag{12.49}$$

in which

$$\lambda_n = \omega^2 + \left(\frac{n\pi}{\mathcal{T}}\right)^2. \tag{12.50}$$

Next we consider the product [5]

$$\mathcal{N}\lim_{N\to\infty}\prod_{n=1}^{N}\frac{1}{\sqrt{\omega^2+\left(\frac{n\pi}{\mathcal{T}}\right)^2}}, \tag{12.51}$$

and write it as

$$\mathcal{N}\lim_{N\to\infty}\prod_{n=1}^{N}\frac{1}{\sqrt{\left(\frac{n\pi}{\mathcal{T}}\right)^2}}\prod_{n=1}^{N}\frac{1}{\sqrt{1+\left(\frac{\omega\mathcal{T}}{n\pi}\right)^2}}. \tag{12.52}$$

But the first product is independent of ω, therefore we choose $\mathcal{N}$ in such a way that

$$\mathcal{N}\lim_{N\to\infty}\prod_{n=1}^{N}\frac{1}{\sqrt{\left(\frac{n\pi}{\mathcal{T}}\right)^2}} = \frac{1}{\sqrt{2\pi\hbar\mathcal{T}}}, \tag{12.53}$$

hence

$$\mathcal{N}\lim_{N\to\infty}\prod_{n=1}^{N}\frac{1}{\sqrt{\omega^2+\left(\frac{n\pi}{\mathcal{T}}\right)^2}} = \left(\frac{\omega}{2\pi\hbar}\right)^{\frac{1}{2}}\frac{1}{\sqrt{\sinh\omega\mathcal{T}}}. \tag{12.54}$$

For $\omega\mathcal{T} >> 1$, this relation reduces to (12.47). The normalization constant $\mathcal{N}$ in (12.54) in the limit of $\omega \to 0$ is the same as the normalization constant for the motion of a free particle [5]. From Eqs. (12.45) and (12.47) it is clear that the lowest energy eigenvalue is

$$E_0 = \frac{1}{2}\hbar\omega\left(1 + O(\hbar)\right). \tag{12.55}$$

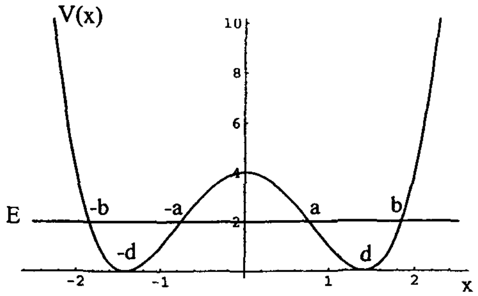

Figure 12.5: A symmetric double-well potential with minima at $x = -d$ and at $x = d$. For the energy E lower than $V(0)$, there are four turning points $-b$, $-a$, a and b.

12.3 An Example of Application of the Path Integral Method in Tunneling

In an earlier chapter, (7), we studied tunneling in a symmetric double-well potential. Now we apply the method of path integration to find the energy splitting between the two lowest states [11] [12].

Let us consider a symmetric double well $V(x)$ shown in Fig. (12.5). The potential $V(x)$ is an even function of x, i.e. $V(x) = V(-x)$, and has a minimum at $x = \pm d$, and we choose $V(x)$ so that $V(\pm d) = 0$. Here also we denote $V''(\pm d)$ by ω^2. First we want to calculate the two expectation values

$$\left\langle -d \left| \exp\left(-\frac{HT}{\hbar}\right) \right| -d \right\rangle = \left\langle d \left| \exp\left(-\frac{HT}{\hbar}\right) \right| d \right\rangle, \tag{12.56}$$

and

$$\left\langle d \left| \exp\left(-\frac{HT}{\hbar}\right) \right| -d \right\rangle = \left\langle -d \left| \exp\left(-\frac{HT}{\hbar}\right) \right| d \right\rangle. \tag{12.57}$$

To this end we find these path integrals in their semi-classical limit of $\hbar \to 0$, exactly as we found Eq. (12.43). For this we need to solve Eq.

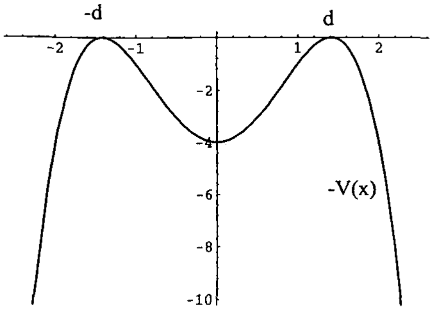

Figure 12.6: The negative of the double-well potential of Fig.(12.5).

(12.43) with proper initial and final conditions. The two solutions of this problem are obtained by placing the particle on one of the two maxima in the potential $-V(x)$ of Fig.(12.6). But there is another interesting solution for this problem, and that is when the particle starts its motion at the time $t = -\frac{1}{2}\mathcal{T}$ at $x = -d$ and reaches $x = d$ at $t = \frac{1}{2}\mathcal{T}$. Since at the end we want to consider the limit of $\mathcal{T} \to \infty$, therefore let us study the solution for this limit, i.e. the motion of the particle from $x = -d$ at $t = -\infty$ and its arrival at $x = d$ at $t = \infty$. In this situation the energy of the particle has to be infinitesimal. Thus

$$\frac{dx}{dt} = \sqrt{2V(x)}, \tag{12.58}$$

or its integral

$$t = t_1 + \int_0^x \frac{d\xi}{\sqrt{2V(\xi)}}. \tag{12.59}$$

In this relation t_1 is the constant of integration and it is the time when $x = 0$. This solution which is called instanton is shown in Fig. (12.7). In the same way we find another solution for the problem where the particle moves from d to $-d$. For this we replace t in Eq. (12.59) by $(-t)$ and we call this "anti-instanton".

From Eq. (12.59) we arrive at the following conclusions:

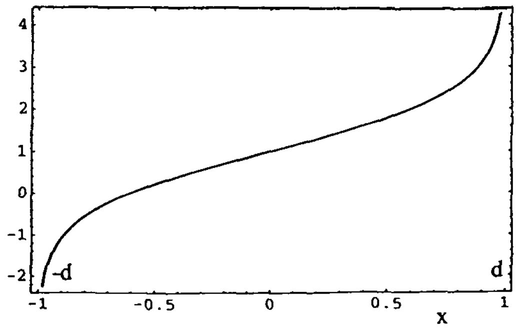

Figure 12.7: Plot of t as a function of x for the instanton solution, Eq. (12.59). The double-well potential $V(x) = -\frac{1}{2}x^2 + \frac{1}{4}(x^4 + 1)$ has been used here.

(i) - For the action of an instanton we find the simple expression

$$S_0 = \int \left[\frac{1}{2}\left(\frac{dx}{dt}\right)^2 + V(x)\right] dt = \int \left(\frac{dx}{dt}\right)^2 dt = \int_{-d}^{d} \sqrt{2V(x)}dx, \quad (12.60)$$

which is the same integral that we found for the penetration under the barrier using WKB approximation (when the energy E is zero).
(ii) - When t becomes large then x approaches d and we can write Eq. (12.58) approximately as

$$\frac{dx}{dt} = \omega(d - x). \quad (12.61)$$

By integrating (12.61), we find that for large t

$$d - x = Ce^{-\omega t}, \quad (12.62)$$

where C is the integration constant. Thus the "temporal" size of an instanton is about $\frac{1}{\omega}$. In the limit of $\mathcal{T} \to \infty$ of the motion from $-d$ to d is called a "bounce", and the center of this bounce is the point where $\frac{dx}{dt} = 0$.

Since this motion is independent of the origin of time, i.e. it is invariant under time translation, therefore the center of bounce can be any point on the t-axis.

For $\mathcal{T}$ large, each instanton or bounce whose center lies in the range of integration is a point where S becomes extremum. Similarly for n instantons we can evaluate the functional integral by summing over all bounces separated from each other with centers at $t_1, t_2, \dots\dots t_n$

$$\frac{\mathcal{T}}{2} > t_1 > t_2 \dots\dots > t_n > -\frac{\mathcal{T}}{2}, \tag{12.63}$$

provided that the path integral includes all of them. For this case we observe that :

(i) - For n instantons, $S = nS_0$, and S will be in the exponent in the integrand.

(ii) - To calculate the determinant, we observe that these instantons are separated from each other by long times and for all of them $x = 0$. Therefore here the determinant is a product of the contributions of temporal intervals about each instanton, remembering that these instantons are separated from each other by much longer times. Thus instead of (12.47) we find

$$\sqrt{\frac{\omega}{\pi\hbar}} \exp\left(-\frac{1}{2}\omega\mathcal{T}\right) K^n, \tag{12.64}$$

and we choose K in such a way that for one instanton we get the correct result.

(iii) - Now we can integrate over the coordinate of the centers of all instantons

$$\int_{-\frac{\mathcal{T}}{2}}^{\frac{\mathcal{T}}{2}} dt_1 \int_{-\frac{\mathcal{T}}{2}}^{t_1} dt_2 \dots \int_{-\frac{\mathcal{T}}{2}}^{t_{n-1}} dt_n = \frac{\mathcal{T}^n}{n!}. \tag{12.65}$$

(iv) - The order of integration over instantons and anti-instantons is not arbitrary. For instance if we start at $-d$, first we encounter an instanton, then an anti-instanton, etc. In addition if at the end we want to reach $-d$, then n must be even, and if we want to reach d, then n must be odd.

Using the aforementioned conditions, we calculate the sum

$$\begin{aligned} &\left\langle -d \left| \exp\left(-\frac{H\mathcal{T}}{\hbar}\right) \right| -d \right\rangle \\ &= \sqrt{\frac{\omega}{\pi\hbar}} \exp\left(-\frac{1}{2}\omega\mathcal{T}\right) \sum_{\text{even } n} \frac{[K\exp(\frac{-S_0}{\hbar})\mathcal{T}]^n}{n!} [1 + O(\hbar)]. \end{aligned} \tag{12.66}$$

In a similar way we calculate $\left\langle d \left| \exp(-\frac{H\mathcal{T}}{\hbar}) \right| -d \right\rangle$. Then the final result is

$$\left\langle \pm d \left| \exp(-\frac{H\mathcal{T}}{\hbar}) \right| -d \right\rangle$$

$$= \left(\frac{1}{2}\right)\sqrt{\frac{\omega}{\pi\hbar}}\exp\left(-\frac{1}{2}\omega\mathcal{T}\right)\left[\exp\left\{K\mathcal{T}e^{-\frac{S_0}{\hbar}}\right\}\mp\exp\left\{-K\mathcal{T}e^{-\frac{S_0}{\hbar}}\right\}\right]. \tag{12.67}$$

Comparing this equation with (12.36) we observe that these are the ground and the first excited states of the system with the energies

$$E_\pm = \frac{1}{2}\hbar\omega \pm \hbar K \exp\left(-\frac{S_0}{\hbar}\right). \tag{12.68}$$

The second term in Eq. (12.68) is much smaller than the first, but the splitting between these two energy levels caused by tunneling is of special interest;

$$E_+ - E_- = 2\hbar K \exp\left(-\frac{S_0}{\hbar}\right). \tag{12.69}$$

We have to determine K in Eq. (12.69) to complete our calculation. For this we observe that for one instanton, $\bar{x}$ can be obtained from (12.44), but since (12.44) is invariant under time translation, there will be an eigenfunction corresponding to the zero eigenvalue $\lambda_1 = 0$. Hence from (12.58) and (12.60) we find

$$x_1 = \frac{1}{\sqrt{S_0}}\frac{d\bar{x}}{dt}. \tag{12.70}$$

If we had to integrate over the coefficient c_1 in Eq. (12.39), we would have found infinity (since $\lambda_1 = 0$). But we can carry the integration in the following way: The change in $x(t)$ because of the change in t_1 is

$$dx = \frac{d\bar{x}}{dt}dt_1, \tag{12.71}$$

and the change induced in the coefficient c_1 is

$$dx = x_1 dc_1. \tag{12.72}$$

Therefore

$$\frac{1}{\sqrt{2\pi\hbar}}dc_1 = \left(\frac{S_0}{2\pi\hbar}\right)^{\frac{1}{2}} dt_1, \tag{12.73}$$

and in the calculation of the determinant, we should not include the contribution of λ_1. For a single instanton we find

$$\left\langle d\left|\exp\left(-\frac{H\mathcal{T}}{\hbar}\right)\right|-d\right\rangle$$

$$= N\mathcal{T}\sqrt{\frac{S_0}{2\pi\hbar}}\exp\left(-\frac{S_0}{\hbar}\right)\left({\det}'\left[-\frac{\partial^2}{\partial t^2}+V''(\bar{x})\right]\right)^{-\frac{1}{2}}, \tag{12.74}$$

where prime on the determinant denotes that the zero eigenvalue should be omitted in the calculation. By comparing (12.74) with one instanton term in Eq. (12.66) we find

$$K=\sqrt{\frac{S_0}{2\pi\hbar}}\left|\frac{\det\left[-\frac{\partial^2}{\partial t^2}+\omega^2\right]}{\det'\left[-\frac{\partial^2}{\partial t^2}+V''(\bar{x})\right]}\right|^{\frac{1}{2}}. \tag{12.75}$$

If A is a constant which is defined by the expansion

$$t=\int_0^{\bar{x}}\frac{dx}{\sqrt{2V(x)}}=-\ln\left[\frac{1}{\sqrt{S_0}}e^{-A}(d-\bar{x})\right]+O(d-\bar{x}), \tag{12.76}$$

then the constant K, Eq. (12.75), can be written as

$$K=\frac{S_0}{\hbar}e^A=\sqrt{2\omega}\beta, \tag{12.77}$$

where β will be defined shortly. This result turns out to be close to the result of WKB approximation (in the limit of zero energy). If we subtract the divergent part of t, Eq. (12.59), using (12.76), we find

$$t=\int_0^{\bar{x}}\left[\frac{1}{\sqrt{2V(x)}}-\frac{1}{\omega(d-x)}\right]dx+\frac{1}{\omega}\ln\frac{d}{d-\bar{x}}. \tag{12.78}$$

But as $\bar{x}\to d$, (12.78) approaches the limit of

$$t=\frac{1}{\omega}\ln\frac{d}{d-\bar{x}}+\frac{A}{\omega}. \tag{12.79}$$

Integrating (12.79), we can find the asymptotic form of $\bar{x}$ for large t;

$$\bar{x}\approx d-de^Ae^{-\omega t}, \tag{12.80}$$

or

$$x_1=\frac{1}{\sqrt{S_0}}\frac{d\bar{x}}{dt}\approx\frac{\omega d}{\sqrt{S_0}}e^Ae^{-\omega t}=\beta e^{-\omega t}. \tag{12.81}$$

Thus from Eqs. (12.77) and (12.81) we find

$$\beta=\frac{\omega de^A}{\sqrt{S_0}}\quad\text{and}\quad K=\omega d\sqrt{\frac{2\omega}{S_0}}e^A, \tag{12.82}$$

and therefore the splitting between the levels according to (12.69) is

$$E_+-E_-=2\hbar\omega d\sqrt{\frac{2\omega}{S_0}}e^Ae^{\frac{-S_0}{\hbar}} \tag{12.83}$$

As an example consider the double-well potential [13]

$$V(x) = \frac{V_0}{d^4}\left(x^2 - d^2\right)^2. \tag{12.84}$$

We have already seen that $\omega^2 = V''(d)$, hence

$$\omega^2 = \frac{8V_0}{d^2}. \tag{12.85}$$

From (12.60) and (12.76) we find S_0 and A to be

$$S_0 = \frac{16V_0}{3\omega} \quad \text{and} \quad A = \ln 2, \tag{12.86}$$

respectively. Substituting these in (12.83) we obtain the splitting between the lowest energy levels to be [13]

$$E_+ - E_- = 4\sqrt{3}\hbar\omega\left(\frac{16V_0}{6\pi\hbar\omega}\right)^{\frac{1}{2}} \exp\left[-\frac{16V_0}{3\hbar\omega}\right]. \tag{12.87}$$

For the application of the bounce method to asymmetric double-wells see [14]. The interesting case of tunneling through periodic potential by this method is discussed by Holstein [15].

12.4 Complex Time, Path Integrals and Quantum Tunneling

We have already seen that by introducing the idea of imaginary time, we can apply the technique of path integration to determine the eigenvalues of the ground and the first excited states of a double-well potential. Now we want to discuss further applications of the complex time formulation [4] [9] [16] [18].

Let us consider a one-dimensional barrier localized in a part of the x-coordinate, and let x_i and x_f be two arbitrary points one to the left and the other to the right of this barrier. In order to define the classical path between these two points according to the Newton's second law of motion

$$m\frac{d^2x_{cl}}{dt^2} = -\left(\frac{dV(x)}{dx}\right)_{x=x_{cl}}, \tag{12.88}$$

where x_{cl} is the classical path, we have to generalize the concept of time and assume that it is a complex variable. Then we can find the path for the part of the x-axis where $E < V(x)$. Next we consider all the paths which are defined in terms of $t^{(n)}$[4];

$$\begin{aligned} t^{(n)} &= \int_{x_i}^{a}\sqrt{\frac{m}{2(E-V(x))}}dx + \int_{b}^{x_f}\sqrt{\frac{m}{2(E-V(x))}}dx \\ &- i(2n+1)\int_{a}^{b}\sqrt{\frac{m}{2(V(x)-E)}}dx, \end{aligned} \tag{12.89}$$

which describes the propagation from x_i to x_f. This time consists of three parts: First the particle moves from x_i to a $(x_i < a)$, and the real time of arrival of the particle at a is given by

$$\Delta t_a = \int_{x_i}^{a}\sqrt{\frac{m}{2(E-V(x))}}dx. \tag{12.90}$$

The second is the propagation between a and b that takes place in the (imaginary) time $\Delta t_i^{(n)}$

$$\Delta t_i^{(n)} = -i(2n+1)\int_{a}^{b}\sqrt{\frac{m}{2(V(x)-E)}}dx. \tag{12.91}$$

Finally in the right side of the barrier the motion from b to x_f which is given by the (real) time Δt_b;

$$\Delta t_b = \int_{b}^{x_f}\sqrt{\frac{m}{2(E-V(x))}}dx. \tag{12.92}$$

The total time is the sum of these three terms which is given by (12.89). In Eq. (12.91), different $t^{(n)}$'s $(n = 0, 1, 2, ...)$ are for different reflections inside the barrier. Using this time $t^{(n)}$ we try to determine the propagator $D_F(x_f, x_i, t, 0)$ and its Fourier transform which is given by Eq. (12.2). To this end we write D_F in terms of an amplitude ρ and a phase ϕ;

$$D_F(x_f, x_i; t, 0) = \rho(t)\exp\left[\phi(t)\right], \tag{12.93}$$

where we have suppressed the dependence of ρ and ϕ on x_i and x_f. The Fourier transform of this propagator is expressible as

$$D_F(x_f, x_i; E) = \int_{0}^{\infty}\exp\left[i(Et+\phi(t))\right]\rho(t)dt. \tag{12.94}$$

We can calculate the integral in (12.94) using the method of stationary phase [6]. The point $\bar{t}$ where the exponential term in (12.94) is stationary can be obtained from

$$\begin{aligned}\frac{\partial}{\partial t}[tE(t)+\phi(t)] &= \frac{\partial}{\partial t}\left(Et+\int_{x_i}^{x_f}k(x)dx - t\bar{E}\right)\\ &= E-\bar{E}(t)-t\frac{\partial\bar{E}}{\partial t}+\int_{x_i}^{x_f}\frac{\partial k(x)}{\partial\bar{E}}\frac{\partial\bar{E}}{\partial t}dx=0,\end{aligned} \tag{12.95}$$

where in Eq. (12.95) $\int_{x_i}^{x_f}k(x)dx$ and $\bar{E}$ are given by the equations:

$$\begin{aligned}\int_{x_i}^{x_f}k(x)dx &= \int_{x_i}^{a}k(x)dx+\int_{b}^{x_f}k(x)dx\\ &+ i(2n+1)\int_a^b q(x)dx - 2in\ln(\frac{i}{2}),\end{aligned} \tag{12.96}$$

and

$$\int_{x_i}^{x_f}\frac{\partial k(x)}{\partial\bar{E}}dx = t. \tag{12.97}$$

This last expression defines $\bar{E}$. The calculation of the second derivative of the phase in the integrand of (12.94), i.e.

$$\begin{aligned}\frac{\partial^2}{\partial t^2}\left[Et+\phi(t)\right]_{t=\bar{t}} &= -\left[\frac{\partial\bar{E}}{\partial t}\right]_{t=\bar{t}} = -\left(\int_{x_i}^{x_f}\frac{\partial^2 k(x)}{\partial\bar{E}^2}dx\right)^{-1}\\ &= \left[m^2\int_{x_i}^{x_f}\frac{dx}{k^3(x)}\right]^{-1},\end{aligned} \tag{12.98}$$

enables us to write $D_F(x_f,x_i;E)$ in the following form

$$D_F(x_f,x_i;E)=\left[\frac{m^2}{k(x_f)k(x_i)}\right]^{\frac{1}{2}}\exp\left(i\int_{x_i}^{x_f}k(x)dx\right), \tag{12.99}$$

where the integral $\int_{x_i}^{x_f}k(x)dx$ is given by Eq. (12.96). Since $\bar{t}^{(n)}$'s are complex quantities, in the stationary phase method, we deform the path from $t=0$ to $t=\infty$ in such a way that it passes through each of $\bar{t}^{(n)}$'s, $n=0,1,2.....$ Thus D_F can be determined from the sum over all paths $\bar{t}^{(n)}$'s

$$\begin{aligned}D_F(x_f,x_i;E) &= \sum_{n=0}^{\infty}D^n(x_f,x_i;E)=\left[\frac{m^2}{k(x_f)k(x_i)}\right]^{\frac{1}{2}}\\ \times\ &\exp\left(i\int_{x_i}^{a}+i\int_b^{x_f}k(x)dx\right)\sum_{n=0}^{\infty}\left(\frac{i}{2}\right)^{2n}\exp\left[-(2n+1)\int_a^b q(x)dx\right].\end{aligned} \tag{12.100}$$

By carrying out the last sum we find the following expression for the propagator ;

$$D_F(x_f, x_i; E) = \sum_{n=0}^{\infty} D^n(x_f, x_i; E) = \left[\frac{m^2}{k(x_f)k(x_i)}\right]^{\frac{1}{2}}$$

$$\times \quad \exp\left(i\int_{x_i}^{a} + i\int_{b}^{x_f} k(x)dx\right) \frac{\exp[-\int_a^b q(x)dx]}{1 + \frac{1}{4}\exp[-2\int_a^b q(x)dx]}, \quad (12.101)$$

and this is the same relation that we found earlier (Eq. (12.12)).

As we have already seen, we can formulate the path integral for quantum tunneling using imaginary time variable (Euclidean formulation) or complex time as we have seen in this section. Now we want to show that in general we have to assume complex time variable for the path integral solution of tunneling problems [19] [20] [21]. Let us consider the one-dimensional tunneling where the barrier is located between the points x_i and x_f. If E is less than the maximum height of the potential, then a complex path joining these two points together is the solution of the differential equation;

$$\frac{dz}{dt} = \sqrt{2m[E - V(z)]} \quad z(0) = x_i, \quad z(\mathcal{T}) = x_f. \quad (12.102)$$

This equation gives us a curve in the complex z-plane which we denote by C. The time of arrival at x_f, is $\mathcal{T}(C)$ which can be determined from (12.102);

$$\mathcal{T}(C) = \int_C \frac{dz}{\sqrt{2m[E - V(z)]}}. \quad (12.103)$$

Since the potential is real there is a second solution for (12.103), $z^*(\mathcal{T})$, so that

$$\mathcal{T}^*(C) = \mathcal{T}(C^*). \quad (12.104)$$

The imaginary part of $\mathcal{T}$ is obtained by subtracting the two integrals, i.e.

$$\mathrm{Im}\,\mathcal{T} = \int_c \frac{dz}{\sqrt{2m[E - V(z)]}}, \quad (12.105)$$

where c is the closed contour which contains the branch points of the integrand, i.e. those defined by $E = V(z)$. Hence Im $\mathcal{T}$ cannot vanish and we need complex time for solving tunneling problems.

For one dimensional tunneling we can choose the complex time so that the path is real, but in higher dimensions we cannot have all of the coordinates of the tunneling particles real (see Chapter 15).

12.5 Path Integral and the Hamilton-Jacobi Coordinates

In the phase space the path integral is defined by the kernel $K(x_f, x_i; t_f, t_i)$, where this kernel is expressible as the integral [22]

$$\begin{aligned} &K(x_f, x_i; t_f, t_i) \\ &= \int \mathcal{D}[p]\mathcal{D}[x] \exp\left[\pm i \int_{t_a}^{t_b} \left(p\frac{dx}{dt} - \frac{1}{2m}p^2 - V(x)\right)\right], \quad \hbar = 1. \end{aligned} \tag{12.106}$$

This kernel can also be defined in terms of the following limit:

$$\begin{aligned} &K(x_f, x_i; t_f, t_i) \\ &= \lim_{n\to\infty} \prod_{j=1}^{n} dx_j \lim_{\epsilon\to 0} \prod_{j=1}^{n+1} \left(\frac{dp_j}{2\pi}\right) \exp\left\{ i \left[p_j(x_j - x_{j-1}) - \epsilon\frac{p_j^2}{2m} - \epsilon V(x_j)\right]\right\}. \end{aligned} \tag{12.107}$$

Once K is determined, we can find the wave function and solve the tunneling problem. For calculating K we use the method of classical transformation and the Hamilton-Jacobi coordinates. In the specific transformation that we will use, the potential barrier is included in the new canonical momentum P, the latter being defined as the square root of the old Hamiltonian :

$$P = \sqrt{\frac{p^2}{2m} + V(x)}. \tag{12.108}$$

The generator of this transformation $F_2(x, P, t)$ is [23] [24]

$$F_2(x, P, t) = \int^x \left[2m\left(P^2 - V(x)\right)\right]^{\frac{1}{2}} dx - P^2 t. \tag{12.109}$$

From this function, $F_2(x, P, t)$, we find that the new Hamiltonian is identically zero [23]

$$K \equiv H + \frac{\partial F_2}{\partial t} = 0. \tag{12.110}$$

Furthermore we can find the old momentum and the new coordinate from F_2;

$$p = \frac{\partial F_2}{\partial x} = \left[2m\left(P^2 - V(x)\right)\right]^{\frac{1}{2}}, \tag{12.111}$$

and

$$Q = \frac{\partial F_2}{\partial P} = \int^x \frac{4mPdx}{\sqrt{2m\left[P^2 - V(x)\right]}} - 2Pt. \tag{12.112}$$

Next we determine the action S in terms of the new canonical coordinates Q and P;

$$\begin{aligned} S &= \int \left(p\frac{dx}{dt} - H\right) dt = \int \left[-Q\frac{dP}{dt} - K + \frac{\partial F_2}{\partial t}\right] dt \\ &= \int \left[-Q\frac{dP}{dt} + \frac{\partial F_2}{\partial t}\right] dt. \end{aligned} \tag{12.113}$$

Now we return to Eq. (12.107) and replace all of the old canonical variables with the new ones except in the last integral $\int dp_{n+1}$, which we write as $\int dp$,

$$K(x_f, x_i; t_f, t_i) = \int \frac{dp}{2\pi} \prod_{j=1}^{n} \left(dQ_j \frac{dP_j}{2\pi}\right) \exp\left[-iQ_j\left(P_j - P_{j+1}\right)\right] \exp\left[iF_2\right]_i^f . \tag{12.114}$$

The integral over Q_j results in the delta function $\delta(P_j - P_{j+1})$ and the subsequent integral over P_j gives us

$$P_1 = P_2 = \ldots\ldots = P_n. \tag{12.115}$$

Thus we are left with a single integral

$$K(x_f, x_i; t_f, t_i) = \frac{1}{2\pi} \int \exp\left[i\left(F_2(f) - F_2(i)\right)\right] dp, \tag{12.116}$$

where p and dp are given by (12.111) and its differential. Here the path integral has been reduced to an ordinary integral and the dynamics of the system is contained in the variation of F_2 between x_i and x_f.
The kernel (12.116) satisfies the Schrödinger equation, and to demonstrate this we can substitute K in the Schrödinger equation and use the relation $\frac{\partial F_2}{\partial t} = P$ and Eq. (12.116). Furthermore if F_2 is continuous, K is also continuous and has the important property that it connects the wave function at one space-time point to the integral of the wave function over the whole space, but at a different time, i.e.

$$\psi(x_f, t_f) = \int_{-\infty}^{\infty} K(x_f, x_i; t_f, t_i)\psi(x_i, t_i)dx_i. \tag{12.117}$$

Let us apply this method to the problem of tunneling through a rectangular barrier. For a barrier of width a and height V_0 we write

$$V(x) = V_0\left[\theta(x + a) - \theta(x)\right] = V_0\tilde{\theta}_1(x), \tag{12.118}$$

and then from Eq. (12.109), we calculate F_2;

$$F_2(x,P,t) = -P^2 t + \sqrt{2m}Px\tilde{\theta}_2(x) + \sqrt{2m(P^2-V_0)}x\tilde{\theta}_1(x) + C, \quad (12.119)$$

where C is the constant of integration and in the calculation of K we set it equal to zero. From Eq. (12.111) we find dp;

$$dp = \sqrt{2m}\tilde{\theta}_2(x)dP + \frac{2mP\tilde{\theta}_1(x)}{\sqrt{2m(P^2-V_0)}}dP, \quad (12.120)$$

where in Eqs. (12.119) and (12.120) $\tilde{\theta}_2(x)$ is defined by

$$\tilde{\theta}_2(x) = \theta(-x-a) + \theta(x). \quad (12.121)$$

By substituting (12.119) and (12.121) in (12.116), we find that $K(x_f, x_i; t_f, t_i)$ is composed of the following terms depending on the locations of x_i and x_f,

$$\begin{aligned} K(x_f, x_i; \mathcal{T}) &= \left[\tilde{\theta}_2(x_f)\tilde{\theta}_2(x_i) + \tilde{\theta}_1(x_f)\tilde{\theta}_1(x_i)\exp(-iV_0\mathcal{T})\right] \\ \times &\left(\frac{\sqrt{2m}}{2\pi}\right)\int \exp\left[i\sqrt{2m}(x_f - x_i)P - i\mathcal{T}P^2\right]dP \\ + &\tilde{\theta}_2(x_f)\tilde{\theta}_1(x_i)\left(\frac{\sqrt{2m}}{2\pi}\right)\int \exp\left(i\sqrt{2m}x_f P - ix_i\sqrt{2m(P^2-V_0)}\right. \\ - &\left. i\mathcal{T}P^2\right)dP + \tilde{\theta}_1(x_f)\tilde{\theta}_2(x_i)\left(\frac{\sqrt{2m}}{2\pi}\right)\exp(-iV_0\mathcal{T}) \\ \times &\int \exp\left[i\sqrt{2m}x_f P - ix_i\sqrt{2m(P^2+V_0)} - i\mathcal{T}P^2\right]dP, \end{aligned} \quad (12.122)$$

where in this relation we have chosen t_i and t_f to be zero and $\mathcal{T}$ respectively.

12.6 Remarks About the Semi-Classical Propagator and Tunneling Problem

Let us consider a barrier like the one shown in Fig. (12.8) and take the two points x_i and x_f on the two sides of this barrier. Since we have specified both the position x_i and the time t_i of the particle, therefore according to

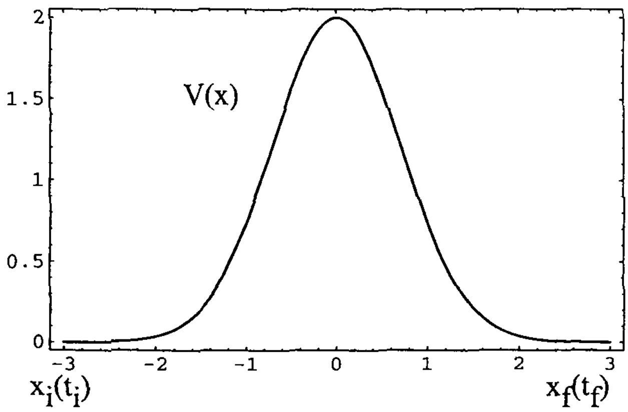

Figure 12.8: A typical finite barrier in the path of the particle. The particle is assumed to be at x_i at t_i and at x_f at the later time $t_f = \mathcal{T} + t_i$.

the uncertainty principle its momentum and energy are completely undetermined. Therefore there are classically allowed paths (over the barrier) which can be the path of the particle connecting x_i to x_f with the time of arrival of $\mathcal{T}$ at x_f after departing from x_i.

If $\mathcal{T}$ is very long, the energy associated with the paths will be very close to the top of the barrier, since the velocity of the particle for these energies would be very small. Thus it may seem that in the determination of $D_F(x_f, x_i; \mathcal{T})$, there is no need to include paths which connect x_i to x_f by tunneling, or that the semi-classical propagator Eq. (12.7) can be constructed only by the paths with energies higher than the barrier. Now if we want to find this kernel in the energy representation, we get Eq. (12.2). But for the energies lower than the maximum height of the barrier, the stationary phase method cannot be used for real times. That is the integral through the complex stationary point is not an approximation to the Fourier integral of (12.2).

Because of the presence of a non-rotatable branch cut singularity, we cannot view the evaluation of complex stationary point as arising from a deformation of the real time contour, and we have to search for a saddle point in the complex time-plane. In the semi-classical approximation we need only the real trajectories connecting x_i to x_f in the time of passage $\mathcal{T}$. We can inquire whether the classically forbidden tunneling paths indirectly affect the nature of the allowed paths, which in turn makes the semi-classical approximation a valid one. In other words is the Fourier transform of the allowed paths in (12.2) is a good approximation for calculating D_F?

In the case of an inverted harmonic potential $V(x) = V_0 - \frac{1}{2}m\omega^2 x^2$, $V_0 > 0$, from the classically allowed paths (over the barrier), one can find the classically forbidden paths (under the barrier). But as Mitra and Heller have shown [25], for other potentials which in the limit of $x \to \pm\infty$ tend to zero (such as the Eckart potential of Chapter 6) the above statement is not valid.

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Chapter 13

Heisenberg's Equations of Motion for Tunneling

In addition to the formulations of quantum tunneling in terms of the wave equation and by the path integral method, a third method, that of the Heisenberg equations can also be used to investigate the motion of the particle under a barrier. The similarity between the Heisenberg and the classical equations of motion in some cases helps us to a better understanding of the problem, specially when the Hamiltonian (or Lagrangian) of the corresponding classical system is difficult to find or is not unique [1] [2]. At the same time we have an alternative method of solving tunneling problem which is particularly useful in the formulation and the solution of the dissipative quantum tunneling problem [1]. Also a semi-classical method of approximation based on the Heisenberg equations can be formulated in which these equations are combined with the classical equations of motion [3]. This method has been applied to the quantum tunneling in cubic and quartic potentials [3] [4].

We begin this chapter by writing down the equations of motion for symmetric or asymmetric double-wells when the confining potential is given as a quartic function of x [5]. Later in this chapter we will investigate the time evolution of a wave packet describing the motion of a particle which is initially trapped behind the barrier, and by tunneling escapes to infinity [6].

13.1 The Heisenberg Equations of Motion for Tunneling in Symmetric and Asymmetric Double-Wells

This technique, in general, can be applied to any potential which is a polynomial in the coordinate x of the particle. The simplest example of such a potential which allows for tunneling has a cubic dependence on x , i.e.

$$V(x) = \frac{1}{2}\nu^2 x^2 - \frac{1}{3}\mu^3 x^3, \quad -\infty < x < +\infty. \tag{13.1}$$

This potential tends to $-\infty$ as $x \to +\infty$. The Hamiltonian operator for such a potential is not self-adjoint, but has a self-adjoint extension with deficiency indices $(1,1)$, and all the one parameter family of self-adjoint extensions have discrete spectrum [7] [8]. In a typical tunneling problem a Gaussian wave packet confined to the left of the central barrier, i.e. to the left of $x = \frac{\nu^2}{\mu^3}$ tunnels through the barrier and moves to the right [2]. A similar problem where the potential is the sum of inverse powers of the radial distance will be studied later.

The next case that we want to investigate in detail is the quartic potential $V(x)$ [9]

$$V(x) = \frac{1}{2}m\omega^2 x^2 \left[\left(\frac{x}{a}\right)^2 - A\left(\frac{x}{a}\right) + B\right], \tag{13.2}$$

where in (13.2), A and B are dimensionless coefficients and ω and a have the dimensions of $(\text{time})^{-1}$ and length respectively.
This potential has two minima at the points

$$x_0 = 0 \quad \text{and} \quad x_2 = \frac{a}{8}\left[3A + \sqrt{9A^2 - 32B}\right], \tag{13.3}$$

and these two are separated from each other by a barrier with maximum at x_1 where

$$x_1 = \frac{a}{8}\left[3A - \sqrt{9A^2 - 32B}\right]. \tag{13.4}$$

In Fig. (13.1) this potential is shown for the parameters $A = 14$, $B = 45$ and $a = 1L$. The Hamiltonian operator for this system is

$$H = \frac{1}{2m}p_x^2 + V(x), \tag{13.5}$$

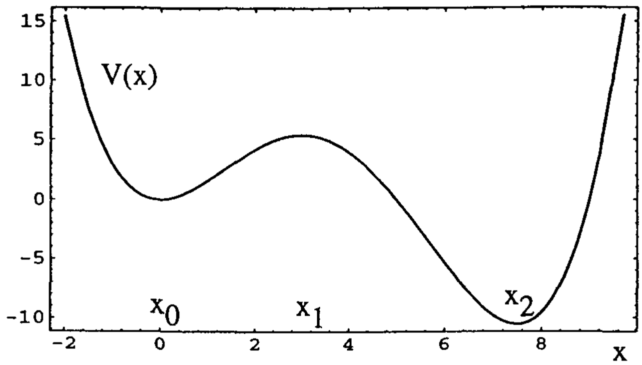

Figure 13.1: An asymmetric potential given by Eq. (13.2).

where p_x is the momentum conjugate to x, and hence satisfies the commutation relation

$$[x, p_x] = i\hbar. \tag{13.6}$$

In order to simplify our equations we introduce the conjugate variables ξ and p_ξ, where ξ is the dimensionless coordinate, and p_ξ is its conjugate momentum,

$$\xi = \frac{x}{a} \quad p_\xi = a p_x. \tag{13.7}$$

We also replace p_ξ by the dimensionless momentum p;

$$p = \frac{p_\xi}{m\omega a^2}. \tag{13.8}$$

With these changes the commutation relation becomes

$$[\xi, p] = \frac{i}{\beta^2}, \quad \beta^2 = \frac{m\omega a^2}{\hbar}, \tag{13.9}$$

where β is also a dimensionless constant. In terms of these variables the Hamiltonian operator takes the form

$$H = \frac{m\omega^2 a^2}{2}\left[p^2 + \xi^2\left(\xi^2 - A\xi + B\right)\right]. \tag{13.10}$$

We can also write H as a dimensionless Hamiltonian K,

$$K = \frac{\beta^2}{2}\left[p^2 + \xi^2\left(\xi^2 - A\xi + B\right)\right], \tag{13.11}$$

provided that instead of time, we use the dimensionless variable $\theta = \omega t$ as the conjugate of K.

The Heisenberg equations resulting from (13.11) are :

$$i\frac{d\xi}{d\theta} = [\xi, K] = \left[\xi, \beta^2 p\right] = ip, \tag{13.12}$$

and

$$i\frac{dp}{d\theta} = [p, K] = \left[p, -\beta^2\xi^2\left(\xi^2 - A\xi + B\right)\right] = -i\left(2\xi^3 - \frac{3}{2}A\xi^2 + B\xi\right). \tag{13.13}$$

Now we study the motion of a Gaussian wave packet which at the time $t = \frac{\theta}{\omega} = 0$ is located in the left well in such a way that its maximum is at the origin, $\xi = 0$. This wave packet by tunneling can pass through the barrier maximum at $\xi_1 = \frac{x_1}{a}$ and move to the other well. Since around the origin $\xi = 0$, we can expand (13.2) and approximate the potential with the harmonic potential

$$V(\xi) \approx \frac{1}{2}\beta^2 B\xi^2, \tag{13.14}$$

we can therefore choose as the wave packet the normalized wave function for the ground state of $V(\xi)$, i.e.

$$\psi(\xi) = \left(\frac{\nu}{\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{1}{2}\nu\xi^2\right], \tag{13.15}$$

where ν in this equation is given by

$$\nu = \sqrt{B}\beta^2. \tag{13.16}$$

Also noting that from (13.9) we have

$$p = -\frac{i}{\beta^2}\frac{d}{d\xi}, \tag{13.17}$$

therefore we can write the operator K as

$$K = \frac{\beta^2}{2}\left[-\frac{1}{\beta^4}\frac{d^2}{d\xi^2} + \xi^2\left(\xi^2 - A\xi + B\right)\right]. \tag{13.18}$$

The expectation value of K with the wave function (13.15) is

$$\langle 0|K|0\rangle = \frac{1}{2}\sqrt{B} + \frac{3}{8\beta^2 B}, \tag{13.19}$$

where we have denoted the ground state of the potential (13.14) by the ket $|0\rangle$.

If we displace the center of the wave packet (13.15) by a distance ξ_0, i.e. if instead of (13.15) we use $\psi(\xi - \xi_0)$, then the expectation value of K will become

$$\begin{aligned}\langle 0|K|0\rangle_{\xi_0} &= \frac{1}{2}\sqrt{B} + \frac{3}{8\beta^2 B} \\ &+ \xi_0\left[\frac{1}{2}\beta^2\xi_0\left(\xi_0^2 - \xi_0 A + B\right) + \frac{3}{2\sqrt{B}}\left(\xi_0 - \frac{1}{2}A\right)\right].\end{aligned} \tag{13.20}$$

Since we are interested in the tunneling of the wave packet, the energy of the wave packet has to be less than the maximum height of the barrier, i.e.

$$\langle 0|K|0\rangle_{\xi_0} < V(\xi_1), \quad \text{or} \quad \langle 0|K|0\rangle < V(\xi_1). \tag{13.21}$$

Let us consider two specific cases of quantum coherence for symmetric and quantum hopping for asymmetric double-wells:

(i) - If we choose $A = 2$ and $B = 1$, we have the symmetric double-well

$$V(\xi) = \frac{1}{2}\beta^2\xi^2(\xi - 1)^2. \tag{13.22}$$

The maximum height of this potential is at $\xi = \frac{1}{2}$ and is equal to $V_{max} = \frac{1}{32}\beta^2$. Then from Eq. (13.19) and the inequality (13.21) we find $\beta^2 > 16.72$ as the condition for tunneling.

(ii) - By choosing $A = 14$ and $B = 45$ we find an asymmetric double-well with a maximum at $\xi = 3$, and $V_{max} = 45\beta^2$. Again from (13.19) and (13.21) we obtain the condition $\beta^2 > 0.0645$ for tunneling. When ξ_0 is not zero we can find similar relations in the same way as we found these inequalities.

If the particle at the time $t = \frac{\theta}{\omega} = 0$ is around the origin $\xi = 0$, and its momentum is less than p_c, where

$$p_c = \xi_1\sqrt{\xi_1^2 - A\xi_1 + B}, \tag{13.23}$$

then the classical motion of the particle is simple oscillations about $\xi = 0$. On the other hand for momentum greater than p_c, the particle can pass over the barrier and reach the second well. Thus Eq. (13.23) determines the separatrix of the motion [13]. In the case of the symmetric well (13.22), with $\beta^2 = 20$, p_c is $\frac{1}{4}$ and the corresponding energy is $K_c = 0.5187$.

Having obtained the Hamiltonian and the commutation relations in dimensionless forms and knowing the condition for quantum tunneling, we can proceed and find the solution of the operator equations (13.12) and (13.13). For simplicity we choose the initial conditions in such a way that the expectation values of the coordinate as well as momentum of the particle vanish;

$$\langle 0|\xi(0)|0\rangle = 0, \tag{13.24}$$

and

$$\langle 0|p(0)|0\rangle = 0. \tag{13.25}$$

In order to find the time dependence of $\xi(t)$ and $p(t)$, i.e. to integrate the operator equations (13.12) and (13.13) we first consider the basis set $\{S_{m,n}\}$ of the Weyl-ordered products of powers of p and ξ [9] [10]

$$S_{m,n}(\theta) = \left(\frac{1}{2}\right)^m \sum_{j=0}^{\infty} \frac{m!}{(m-j)!j!} p^j(\theta)\xi^n(\theta)p^{m-j}(\theta). \tag{13.26}$$

The elements of this set satisfy an algebra (Bender-Dunn algebra) which is closed under the multiplication of the elements, viz, the product of two or more of $\{S_{m,n}\}$'s can be written as a linear combination of other $S_{m,n}$'s. The rule of multiplication is [9] [10] [11]

$$S_{m,n}(\theta)S_{r,s}(\theta) = \sum_{j=0}^{\infty}\left(\frac{i}{2}\right)^j \sum_{k=0}^{j} \frac{(-1)^{j-k}}{(j-k)!k!}\frac{1}{\beta^{2j}} S_{m+r-j,n+s-j}(\theta)$$
$$\times \frac{\Gamma(n+1)\Gamma(m+1)\Gamma(r+1)\Gamma(s+1)}{\Gamma(n-k+1)\Gamma(m+k-j+1)\Gamma(r-k+1)\Gamma(s+k-j+1)}. \tag{13.27}$$

A very useful relation which can be deduced from (13.27) is the commutation relation for $S_{m,n}$ and $S_{r,s}$;

$$[S_{m,n}(\theta), S_{r,s}(\theta)] = 2\sum_{j=0}^{\infty}\left(\frac{i}{2}\right)^{2j+1}$$
$$\times \sum_{k=0}^{2j+1} \frac{(-1)^k}{(2j+1-k)!k!}\frac{1}{\beta^{2j}} S_{m+r-2j-1,n+s-2j-1}(\theta)$$
$$\times \frac{\Gamma(n+1)\Gamma(m+1)\Gamma(r+1)\Gamma(s+1)}{\Gamma(m-k+1)\Gamma(n+k-2j)\Gamma(r+k-2j)\Gamma(s-k+1)}. \tag{13.28}$$

From the definition of $S_{m,n}$, Eq. (13.26) it is evident that

$$\xi(\theta) = S_{0,1}(\theta), \quad \text{and} \quad p(\theta) = S_{1,0}(\theta). \tag{13.29}$$

Using the above definitions and the commutation relation (13.28), we can calculate $\xi(\Delta\theta)$ in terms of the elements of $S_{m,n}$ at $\theta = 0$. For this we expand $\xi(\Delta\theta)$ as a power series in $\Delta\theta$

$$\xi(\Delta\theta) = \xi(0) + \frac{(\Delta\theta)}{1!}\left(\frac{d\xi}{d\theta}\right)_{\theta=0} + \frac{(\Delta\theta)^2}{2!}\left(\frac{d^2\xi}{d\theta^2}\right)_{\theta=0} + ... \tag{13.30}$$

Similarly we expand $p(\Delta\theta)$ as a power series in $(\Delta\theta)$. We note that the Hamiltonian operator K can also be written in terms of the basis set $\{S_{m,n}\}$;

$$K = \frac{\beta^2}{2}\left[S_{2,0} + S_{0,4} - AS_{0,3} + BS_{0,2}\right], \tag{13.31}$$

and thus the expansion (13.30) and its counterpart for $p(\Delta\theta)$ are special cases of the expression

$$\frac{dS_{m,n}}{d\theta} = \left[S_{m,n}, K\right]. \tag{13.32}$$

By substituting (13.31) in (13.32) and using (13.28) we obtain

$$\begin{aligned}\frac{dS_{m,n}}{d\theta} &= nS_{m+1,n-1} - 2mS_{m-1,n+3} + \frac{1}{2\beta^2}\frac{m!}{(m-3)!} \\ &\times \left(S_{m-3,n+1} - \frac{1}{4}AS_{m-3,n}\right) + \frac{3}{2}mAS_{m-1,n+2} - mBS_{m-1,n+1}.\end{aligned} \tag{13.33}$$

From the definitions (13.29), we can write the Heisenberg equations (13.12) and (13.13) as

$$\frac{dS_{0,1}}{d\theta} = S_{1,0}, \tag{13.34}$$

and

$$\frac{dS_{1,0}}{d\theta} = \frac{1}{2}\left(-4S_{0,3} + 3AS_{0,2} - 2BS_{0,1}\right). \tag{13.35}$$

Furthermore by knowing the derivatives $\frac{d^2S_{1,0}}{d\theta^2}, \frac{d^2S_{0,1}}{d\theta^2}, \frac{d^3S_{1,0}}{d\theta^3}$...... we can calculate $S_{0,1}(\Delta\theta) = \xi(\Delta\theta)$ in terms of $S_{m,n}(0)$. By continuing this process and calculating $S_{0,1}(2\Delta\theta)$......$S_{0,1}(N\Delta\theta)$ each as an infinite sum with terms $\{S_{m,n}(0)\}$, we find the series

$$S_{0,1}(\theta) = \sum_{r,s} C_{rs}(\theta)S_{r,s}(0), \tag{13.36}$$

where $C_{rs}(\theta)$'s are c-number functions of time.

In a similar way for $S_{1,0}(\theta)$ we find

$$S_{1,0}(\theta) = \sum_{r,s} D_{rs}(\theta) S_{r,s}(0). \tag{13.37}$$

Thus in general from the known Hamiltonian, e.g. (13.31) we can find the time dependence of any member of the basis set $S_{r,s}$ in the form

$$S_{r,s}(\theta) = \sum_{m,n} F_{rs;mn}(\theta) S_{m,n}(0). \tag{13.38}$$

Once the dependence of $S_{r,s}(\theta)$ on θ is known, then we can find its expectation value as a function of time from the equation

$$\langle 0|S_{r,s}(\theta)|0\rangle = \sum_{m,n} F_{rs;mn}(\theta) \langle 0|S_{m,n}(0)|0\rangle . \tag{13.39}$$

Using the Gaussian wave packet (13.15), we can calculate the expectation value of $\langle 0|S_{r,s}(\theta)|0\rangle$;

$$\begin{aligned} \langle 0|S_{r,s}(\theta)|0\rangle &= \frac{a^{r-s} B^{\frac{(r-s)}{4}} (r-1)!!(s-1)!!}{\beta^{(r+s)} 2^{\frac{(r+s)}{2}}}, \quad r \text{ and } s \text{ even}, \\ &= 0 \quad \text{otherwise}. \end{aligned} \tag{13.40}$$

13.2 Tunneling in a Symmetric Double-Well

The results of calculation of the expectation values $\langle 0|\xi(\theta)|0\rangle$ and $\langle 0|p(\theta)|0\rangle$ for the potential $V(\xi) = 10\xi^2(1-\xi)^2$ are shown in Fig. (13.2).

An important result of this calculation is that unlike the case of the Schrödinger equation, here the integration can be carried out for a relatively short time (compared to the period of the oscillation of the wave packet), of the order $\theta \approx 1.8$ (dimensionless units). Up to this time the explicit calculations of $\langle 0|K|0\rangle$ and $\langle 0|[\xi(\theta), p(\theta)]|0\rangle$, show that both of these expectation values remain constant. This indicates that the error in the numerical integration for times less than 1.8 is negligible. But for $\theta > 1.8$ both of these quantities oscillate and the oscillations become more chaotic and with larger amplitude as θ increases. In the integration of these operator equations we have used the expansion (13.30), and its analogue for $p(\Delta\theta)$ up to $(\Delta\theta)^6$. For the integration over longer times we have to include higher powers of

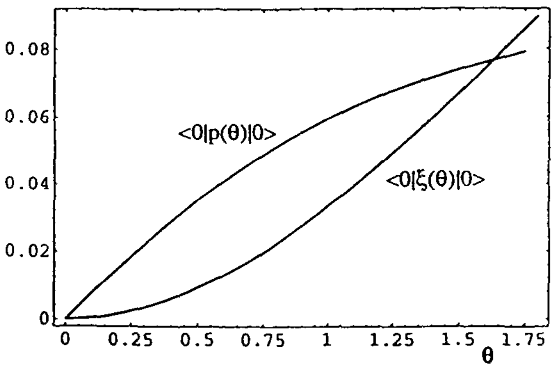

Figure 13.2: The time dependence of the ground state expectation values of $\xi(\theta)$ and $p(\theta)$ for the symmetric quartic potential $V(\xi) = 10\xi^2(1-\xi)^2$.

$(\Delta\theta)$ in the calculation and make the step size $\Delta\theta$ smaller.

We observe, (Fig. 13.2), that knowing the expectation values $\langle 0|\xi(\theta)|0\rangle$ and $\langle 0|p(\theta)|0\rangle$ will not be sufficient for determining the time of oscillation between the two wells. However by indirect way, e.g. using Prony's technique [5] (see also Chapter 23) we can find the period of oscillations by first calculating the two lowest energy eigenvalues, and then finding the period from Eq. (7.11). Alternatively we can keep higher order terms in the expansion (13.30) and /or use a smaller step size (we have used $\Delta\theta = 0.05$ in this calculation).

13.3 Tunneling in an Asymmetric Double-Well

For this case we consider a particle tunneling in the potential

$$V(\xi) = 0.05\xi^2\left(\xi^2 - 14\xi + 45\right), \tag{13.41}$$

which is shown in Fig. (13.1). As the initial condition we choose the same ones as we did before, i.e. (13.24) and (13.25). Here we note that for the numerical integration we need smaller step size $(\Delta\theta = 0.01)$ than the one

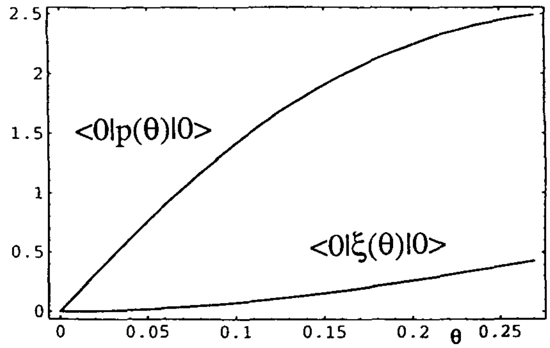

Figure 13.3: Expectation values of the position and momentum for the motion of a Gaussian wave packet in an asymmetrical double-well plotted as a function of dimensionless time θ. The asymmetric double-well is given by Eq. (13.41).

that we have used for the symmetric case. Even with this smaller step size, the maximum time for which the numerical integration is reliable is only $\theta \approx 0.28$. The plots of $\langle 0|\xi(\theta)|0\rangle$ and $\langle 0|p(\theta)|0\rangle$ as functions of θ are shown in Fig. (13.3).

As in the previous example we can use Prony's method [5] to determine the lowest energy levels of the system. However as we have seen from the solution of the wave equation that in general, the center of the wave packet $\langle 0|\xi(\theta)|0\rangle$ does not pass the point $\xi_1 = \frac{x_1}{a}$, i.e. the point where the potential has its central maximum. Thus the motion of $\langle 0|\xi(\theta)|0\rangle$ is limited to oscillations in one of the wells (here in the well to the left of V_{max}) unless resonant conditions are met. A limited part of the motion of the center of the wave packet in phase space, i.e. the parametric plot of $\langle 0|\xi(\theta)|0\rangle$ and $\langle 0|p(\theta)|0\rangle$ is shown in Fig. (13.4).

Another point which is worth mentioning is that the motion of $\langle 0|\xi(\theta)|0\rangle$, $\langle 0|p(\theta)|0\rangle$ in phase space is not given by a closed curve, since the Gaussian wave packet (13.15) contains an infinite number of components corresponding to noncommesurable energy levels .

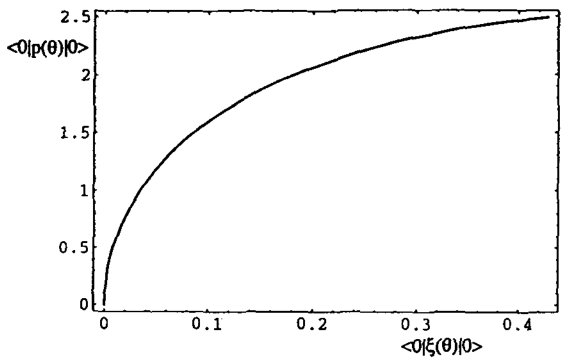

Figure 13.4: Phase space trajectory of the motion of a wave packet in the asymmetric double-well Eq. (13.41).

13.4 Tunneling in a Potential Which Is the Sum of Inverse Powers of the Radial Distance

So far we have dealt with the one-dimensional quantum coherence and hopping in confining potentials. Now we want to study the Heisenberg equations of motion for the three-dimensional problems with spherical symmetry, i.e. when the potential is a function of the inverse powers of the radial distance alone;

$$V(r) = \sum_{k=1}^{J} \frac{A_k}{r^k}. \tag{13.42}$$

For this problem we replace the basis set $\{S_{m,n}(p, \xi)\}$, Eq. (13.26) by $\{S_{m,n}(p_r, r)\}$;

$$S_{m,n} = \left(\frac{1}{2}\right)^n \sum_{k=0}^{n} \frac{n!}{(n-k)!k!} r^k \left(\frac{-i}{r}\frac{\partial}{\partial r}\right)^m r^{n-k}. \tag{13.43}$$

Then instead of the commutation relation (13.28) we have

$$[S_{m,n}(t), S_{r,s}(t)] = 2\sum_{j=0}^{\infty} \left(\frac{i}{2}\right)^{2j+1}$$

$$\times \quad \sum_{k=0}^{2j+1} \frac{(-1)^k}{(2j+1)!} \frac{(2j+1)!}{k!(2j+1-k)!} S_{m+r-2j-1,n+s-2j-1}(t)$$

$$\times \quad \frac{\Gamma(n+1)\Gamma(m+1)\Gamma(r+1)\Gamma(s+1)}{\Gamma(m-k+1)\Gamma(n+k-2j)\Gamma(r+k-2j)\Gamma(s-k+1)}. \quad (13.44)$$

As in the first problem we write the Hamiltonian in terms of the elements of the basis set $\{S_{m,n}\}$

$$H = \frac{1}{2} S_{2,0} + \sum_{k=1}^{J} A_k S_{0,-k}, \tag{13.45}$$

where we have assumed that the particle has a unit mass. Now from Eq. (13.44) and (13.45) we can find the time derivative of $S_{m,n}$

$$i\frac{dS_{m,n}}{dt} = [S_{m,n},\ H] = inS_{m+1,n-1} + 2\sum_{j=0}^{\infty}\left(\frac{i}{2}\right)^{2j+1} \times$$

$$\times \quad \frac{m!}{(m-2j-1)!(2j+1)!}\left[\sum_{k=1}^{J} A_k \frac{(k+2j)!}{(k-1)!} S_{m-2j-1,n-k-2j-1}\right]. \tag{13.46}$$

We can also write (13.46) as an operator equation with real coefficients;

$$\frac{dS_{m,n}}{dt} = nS_{m+1,n-1} + \sum_{j=0}^{\infty}\left(\frac{-1}{2}\right)^{j}$$

$$\times \quad \frac{m!}{(m-2j-1)!(2j+1)!}\left[\sum_{k=1}^{J} A_k \frac{(k+2j)!}{(k-1)!} S_{m-2j-1,n-k-2j-1}\right]. \tag{13.47}$$

For the integration of the equations of motion we start with the Taylor series for $S_{m,n}(\Delta t)$

$$S_{m,n}(\Delta t) = S_{m,n}(0) + \frac{\Delta t}{1!}\left(\frac{dS_{m,n}}{dt}\right)_{t=0} + \frac{(\Delta t)^2}{2!}\left(\frac{d^2 S_{m,n}}{dt^2}\right)_{t=0} + \dots\dots\dots \tag{13.48}$$

We can find the second term of this expansion, i.e. $\left(\frac{dS_{m,n}}{dt}\right)_{t=0}$ in terms of $S_{r,s}(0)$ directly from (13.47). Furthermore by differentiating (13.47) with respect to t and then eliminating $\frac{dS_{r,s}}{dt}$ from the resulting equation using again (13.47) we can calculate $\left(\frac{d^2 S_{r,s}}{dt^2}\right)_{t=0}$ in terms of $S_{r,s}(0)$ and so on.

In this way we find $S_{m,n}(\Delta t)$ as a linear combination of various $S_{r,s}$'s at $t=0$. By repeating this process we can calculate $S_{m,n}(2\Delta t)$, $S_{m,n}(3\Delta t)$.... $S_{m,n}(N\Delta t)$ all in terms of $S_{r,s}$ at $t=0$;

$$S_{m,n}(N\Delta t) = \sum_{j,k} C_{j,k}(N,\Delta t) S_{m-j+1,n-k}(0), \tag{13.49}$$

where $C_{j,k}(N,\Delta t)$'s are found as numerical coefficients for a given N and Δt.

As a very simple example let us consider the following Hamiltonian

$$H = \frac{1}{2}p_r^2 + \frac{A_2}{r^2} = \frac{1}{2}S_{2,0} + A_2 S_{0,-2}. \tag{13.50}$$

For this problem we write $S_{0,2}(t)$ as a Taylor series

$$S_{0,2}(t) = S_{0,2}(0) + \frac{t}{1!}\left(\frac{dS_{0,2}}{dt}\right)_{t=0} + \frac{t^2}{2!}\left(\frac{d^2S_{0,2}}{dt^2}\right)_{t=0} + ..., \tag{13.51}$$

and we determine the operators $\left(\frac{dS_{0,2}}{dt}\right), \left(\frac{d^2S_{0,2}}{dt^2}\right)$, ... from (13.47);

$$\frac{dS_{0,2}}{dt} = -i\left[S_{0,2}, H\right] = 2S_{1,1}, \tag{13.52}$$

$$\frac{d^2S_{0,2}}{dt^2} = -i\left[S_{1,1}, H\right] = 2S_{2,0} + 4A_2S_{0,-2}, \tag{13.53}$$

and

$$\frac{d^3S_{0,2}}{dt^3} = \frac{d}{dt}\left(2S_{2,0} + 4A_2S_{0,-2}\right) = 4\frac{dH}{dt} = 0. \tag{13.54}$$

This last equation shows that (13.51) terminates after only three terms

$$S_{0,2}(t) = S_{0,2}(0) + \frac{2t}{1!}S_{1,1}(0) + \frac{t^2}{2!}\left\{2S_{2,0}(0) + 4A_2S_{0,-2}(0)\right\}. \tag{13.55}$$

Equation (13.55) is the complete solution of the operator $r^2(t)$ as a function of time.

Now let us apply this method to the case of quantum tunneling. We choose the potential (13.42) to be the sum of three terms, including the centrifugal potential

$$V_{eff}(r) = \sum_{k=1}^{3} \frac{A_k}{r^k}, \tag{13.56}$$

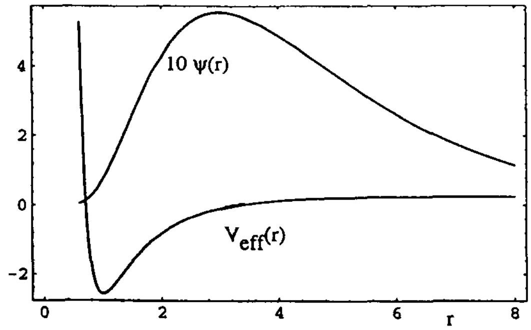

Figure 13.5: The effective radial potential given by Eq. (13.56). The initial wave packet is also shown in this figure.

and therefore $V_{eff}(r)$ is the effective radial potential . For A_1 and A_3 positive and A_2 negative (13.56) has a minimum followed by a maximum (see Fig. (13.5)). For the parameters $A_1 = 3.872L^{-1}$, $A_2 = -15.488L^0$ and $A_3 = 9.0349L$ (L is a unit of length) this potential is plotted in Fig. (13.6). With these parameters $V_{eff}(r)$ has a minimum at $r = 1L$, and has a maximum at $r = 7L$, where $V_{eff}(r = 7) = 0.2634$.
For calculating the probability of tunneling of a wave packet which is localized to the left of this maximum, we need to find the expectation value

$$\langle\psi|S_{m+j,n-k}|\psi\rangle = \int_0^\infty [\psi^* S_{m+j,n-k}(r\psi)]\, r dr, \tag{13.57}$$

for large values of the integer k. Thus here instead of a Gaussian wave packet we have to choose a wave packet with the property that the limit

$$\lim_{r\to 0}\left[\frac{1}{r^n}\left(r\psi(r)\right)\right] \to 0, \tag{13.58}$$

exists and that this relation should be true for any integer n. Since Eq. (13.43) is equivalent to

$$S_{m,-n} = \frac{1}{2^m}\sum_{j=0}^{m}\frac{m!}{j!(m-j)!r}p_r^j\left(\frac{1}{r^n}\right)p_r^{m-j}r, \quad n > 0, \tag{13.59}$$

therefore from Eqs. (13.58) and (13.59) it follows that

$$\langle\psi|S_{2m+1,-n}|\psi\rangle = 0, \tag{13.60}$$

and

$$\langle\psi|S_{2m,-n}|\psi\rangle = \frac{(-1)^m}{2^{2m}}\sum_{j=0}^{2m}\frac{(2m)!(-1)^j}{(2m-j)!j!}\int_0^\infty\left[\frac{\partial^j(r\psi)}{\partial r^j}\frac{1}{r^n}\frac{\partial^{2m-j}(r\psi)}{\partial r^{2m-j}}\right]dr. \tag{13.61}$$

These relations show that all of the matrix elements of $S_{m,-n}$ are real. For the wave packet we have to choose a function which satisfies the asymptotic condition (13.58). In the following calculation we will use the wave packet

$$r\psi(r) = \mathcal{N}\exp\left[-\frac{1}{2}\left(\frac{a}{r}+br\right)\right], \tag{13.62}$$

which is displayed in Fig. (13.6). In Eq. (13.62) $\mathcal{N}$ is the normalization constant and is given by

$$\mathcal{N} = \frac{1}{\sqrt{2}}\left(\frac{b}{a}\right)^{\frac{1}{4}}\left[K_1(2\sqrt{ab})\right]^{-\frac{1}{2}}, \tag{13.63}$$

where K_1 is the Bessel function of the imaginary argument [14]. This wave packet is the lowest eigenfunction for the potential

$$V(r) = \frac{1}{8r^4}\left(a^2 - 4ar - 2abr^2\right), \tag{13.64}$$

with the eigenvalue

$$\varepsilon = -\frac{b^2}{8}. \tag{13.65}$$

The center of this wave packet at the time $t = 0$ is at r_0, where

$$r_0 = \langle\psi|r|\psi\rangle = \sqrt{\frac{a}{b}}\frac{K_2(2\sqrt{ab})}{K_1(2\sqrt{ab})}. \tag{13.66}$$

In the following calculation the parameters $a = 9$ and $b = 1$ have been used, and for these values $r_0 = 3.7769$. Also for the A_k's given above

$$\langle\psi|H|\psi\rangle = 0. \tag{13.67}$$

Since the maximum height of the barrier is $V_{max} = 0.2674$, therefore the energy of the particle is less than this maximum height, and we are dealing with quantum tunneling.

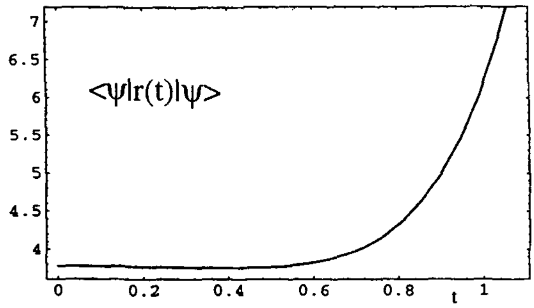

Figure 13.6: The motion of the center of the wave packet for tunneling through the potential (13.56). The initial position of the center of the wave packet is at $r_0 = 3.7769$, and the maximum height of the barrier is at $r = 7$.

By finding the expectation value $\langle\psi|S_{0,1}|\psi\rangle$ we can determine the motion of this center as a function of time t. The result of this calculation is shown in Fig. (13.6). In this approach we can set a limit for the accuracy of the result by calculating $\langle\psi|H|\psi\rangle$ and $\langle\psi|[r,p_r]|\psi\rangle$ and determining the maximum time for which the fractional change in these quantities is less than a given small number ϵ. For the above calculation this number is chosen to be $\epsilon = 10^{-4}$.

An interesting result of this calculation is that at the beginning the center of the wave packet moves toward the minimum of the potential, but when it reaches the point $r_1 = 3.755$, then it changes direction and by moving away from the minimum it tunnels through the barrier.

In Fig. (13.7) the plot of $\langle\psi|p_r(t)|\psi\rangle$ versus $\langle\psi|r(t)|\psi\rangle$ which is similar to the classical description of the motion in phase space is shown. In this formulation the probability of finding the particle (or wave packet) at time t behind the barrier, $P(t)$ can be calculated from

$$P(t) = \left|\langle\psi|\exp\left(iHt\right)|\psi\rangle\right|^2, \tag{13.68}$$

where $|\psi\rangle$ is the initial wave packet.

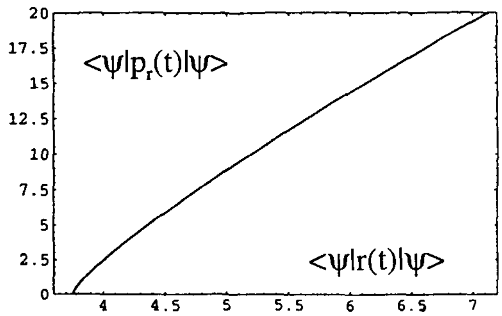

Figure 13.7: Parametric plot of $\langle\psi|p_r(t)|\psi\rangle$ versus $\langle\psi|r(t)|\psi\rangle$ for the wave packet (13.62).

13.5 Klein's Method for the Calculation of the Eigenvalues of a Confining Double-Well Potential

We have seen how, using the Heisenberg equations of motion, we can determine whether an initially localized wave packet in one of the wells of a double-well potential can tunnel through the barrier and appear in the other well. Just as the case of the Schrödinger equation, we can use the time-independent version of the Heisenberg equations to determine the eigenvalues of a symmetric (and possibly asymmetric) double-well potential.

The following method which was developed by Klein and collaborators [15] [16] [17] can be used when the potential is a polynomial function of the coordinate x. As a specific example let us consider the Hamiltonian [18]

$$H = \frac{1}{2}\left(p^2 - x^2\right) + \frac{1}{4}\lambda x^4, \tag{13.69}$$

where now p and x are $\infty \times \infty$ matrices.

The Heisenberg equations of motion are

$$[p, H] = ix - i\lambda x^3, \tag{13.70}$$

and

$$[x, H] = ip. \tag{13.71}$$

These relations together with the canonical commutation relation

$$[x, p] = i, \tag{13.72}$$

are needed for the determination of the eigenvalues. Since we are dealing with a one-dimensional problem, the energy levels will be non-degenerate. Let us denote the eigenstates of H by $|n\rangle$, i.e.

$$H|n\rangle = E_n|n\rangle, \tag{13.73}$$

and

$$\langle n|H|n'\rangle = 0. \quad \text{if} \quad n \neq n'. \tag{13.74}$$

By calculating the matrix elements of Eqs. (13.69)-(13.72) we find the following equations

$$(E_{n'} - E_n)\left\langle n|p|n'\right\rangle = i\left\langle n|x|n'\right\rangle - i\lambda\sum_{m'}\sum_{l'}\left\langle n|x|m'\right\rangle\left\langle m'|x|l'\right\rangle\left\langle l'|x|n'\right\rangle, \tag{13.75}$$

$$(E_{n'} - E_n)\left\langle n|x|n'\right\rangle = i\left\langle n|p|n'\right\rangle, \tag{13.76}$$

and

$$\sum_{j'}\left(\left\langle n|x|j'\right\rangle\left\langle j'|p|n'\right\rangle - \left\langle n|p|j'\right\rangle\left\langle j'|x|n'\right\rangle\right) = i\delta_{nn'}. \tag{13.77}$$

By eliminating $(E_{n'} - E_n)$ between Eqs. (13.75) and (13.76) we have

$$\begin{aligned}\left(\left\langle n|p|n'\right\rangle\right)^2 &= \left(\left\langle n|x|n'\right\rangle\right)^2 \\ &- \lambda\left\langle n|x|n'\right\rangle\sum_{m'}\sum_{l'}\left\langle n|x|m'\right\rangle\left\langle m'|x|l'\right\rangle\left\langle l'|x|n'\right\rangle.\end{aligned} \tag{13.78}$$

The symmetric potential in the Hamiltonian (13.69) implies that the energy eigenstates have a definite parity and this in turn means that

$$\left\langle n|x|n'\right\rangle = \left\langle n|p|n'\right\rangle = 0, \quad \text{when} \quad |n - n'| = \text{even}. \tag{13.79}$$

Furthermore the time reversal transformation does not affect the Hamiltonian, therefore

$$\left\langle n|x|n'\right\rangle = \left\langle n'|x|n\right\rangle = 0, \tag{13.80}$$

and

$$\left\langle n|p|n' \right\rangle = - \left\langle n'|p|n \right\rangle = 0. \tag{13.81}$$

For the numerical solution of the nonlinear algebraic equations (13.77) and (13.78) we find it convenient to write the matrix elements in terms of I and J rather than n and n', where [16]

$$n = 2I - 2, \quad n' = 2J - 1. \quad I, J = 1, 2, 3.... \tag{13.82}$$

In addition we replace $\left\langle n|x|n' \right\rangle$ and $\left\langle n|p|n' \right\rangle$ by $X(I,J)$ and $Y(I,J)$ defined by the following relations

$$X(I,J) = \left\langle n|x|n' \right\rangle = \left\langle n'|x|n \right\rangle, \tag{13.83}$$

and

$$Y(I,J) = -i \left\langle n|p|n' \right\rangle = i \left\langle n'|p|n \right\rangle. \tag{13.84}$$

Thus the indices I and J refer to the even and odd states respectively. Using these matrix elements we can write (13.77) and (13.78) as

$$\begin{aligned} &(Y(I,J))^2 + (X(I,J))^2 \\ - \quad &\lambda X(I,J) \sum_{I'=1}^{\nu+1} \sum_{J'=1}^{\nu} \left[X(I,J')X(I',J')X(I',J) \right] = E_M(I,I') = 0, \end{aligned} \tag{13.85}$$

$$\sum_{J=1}^{\nu} \left[X(I,J)Y(I',J) + Y(I,J)X(I',J) \right] + \delta(I,I') = C_E(I,I') = 0, \tag{13.86}$$

$$\sum_{I=1}^{\nu+1} \left[X(I,J)Y(I,J') + Y(I,J)X(I,J') \right] - \delta(J,J') = C_O(J,J') = 0. \tag{13.87}$$

The last two equations (13.86) and (13.87) have been obtained from (13.77) for even and odd states respectively. The sums over I, J, I' and J' are all from one to infinity and since these sums are convergent, therefore we can truncate them and reduce the number of equations to a finite number. To be more specific, in the ν-th order of approximation we have $2\nu+1$ states, $\nu+1$ of which have even and ν have odd parities. If we solve these equations for $2\nu(\nu+1)$ unknowns, i.e.

$$X(I,J), \quad Y(I,J), \quad 1 \le J \le \nu, \quad 1 \le I \le \nu + 1, \tag{13.88}$$

then we can find $2\nu + 1$ low-lying eigenvalues. Let us emphasize that the number of equations is more than the number of unknowns.

Klein and collaborators have investigated the numerical stability of the problem of anharmonic oscillator [15] [16] [17] and they have concluded that the "best" choice is to omit all those even commutators equations $C_E(I, I')$ (13.86) which involve the boundary terms $I = \nu+1$, $I' = 1, 2, \ldots.\nu+1$. This according to Klein *et al* is sensible since the main truncation errors come from the matrix elements involving boundary states. This omission makes the number of equations equal to the number of unknowns. For the $2\nu(\nu+1)$ unknowns we have the following $2\nu(\nu+1)$ equations

$$E_M(I, J) = 0, \quad 1 \le J \le \nu, \quad 1 \le I \le \nu+1, \tag{13.89}$$

$$C_E(I, I') = 0, \quad 1 \le I' \le I \le \nu, \tag{13.90}$$

and

$$C_O(J, J') = 0, \quad 1 \le J' \le J \le \nu. \tag{13.91}$$

From these equations the matrix elements $X(I, J)$ and $Y(I, J)$ can be determined. Once these quantities are known then from the Hamiltonian (13.69) we can calculate the ground state energy which we denote by $E(0)$,

$$\begin{aligned} E(0) &= \langle 0|H|0\rangle = \frac{1}{2}\sum_{J=1}^{\nu}\left[(Y(1,J))^2 - (X(1,J))^2\right] \\ &+ \frac{\lambda}{4}\sum_{J=1}^{\nu}\sum_{I=1}^{\nu+1}\sum_{J'=1}^{\nu} X(1,J)X(I,J)X(I,J')X(1,J'). \end{aligned} \tag{13.92}$$

The energies of the first few excited states can be calculated directly from $\langle n|H|n\rangle$ or simply from the following relations:
The energies of the odd states are given by

$$E(2J-1) = E(0) - \frac{Y(1,J)}{X(1,J)}, \quad J = 1, 2, \ldots.\nu, \tag{13.93}$$

and for the even states are determined from

$$E(2I-2) = E(1) + \frac{Y(I,1)}{X(I,1)}, \quad I = 2, .3 \ldots.\nu+1. \tag{13.94}$$

If we choose $\nu = 1$, then we have four unknowns, $X(1,1), Y(1,1), X(2,1)$ and $Y(2,1)$, and four equations $E_M(1,1), E_M(2,1), C_E(1,1)$ and $C_O(1,1)$. The last two equations are linear and can be solved for $Y(1,1)$ and $Y(2,1)$ in terms of $X(1,1)$ and $X(2,1)$. Substituting these in either $E_M(2,1)$ or in $E_M(1,1)$ and eliminating $X(2,1)$ between the two, gives us a nonlinear equation for $X(1,1)$;

$$\begin{aligned} &\left[1+4\left(X(1,1)\right)^4-12\lambda\left(X(1,1)\right)^6\right] \\ \times\ &\left[1+4\left(X(1,1)\right)^4+4\lambda\left(X(1,1)\right)^6\right]=0. \end{aligned} \tag{13.95}$$

From this first order approximation we can calculate the three lowest energy levels, but the answers are not very close to the exact result. In the next order, i.e. for $\nu=2$ we have to solve the resulting algebraic equation numerically. But the solution of the truncated set of equations (13.89)-(13.91) in any order, ν, is not unique. For instance for $\nu=2$ and $\lambda=1$ we have different sets of roots.

In Table I these roots are given and for comparison the results for $\nu=1$ are also shown. From these roots we can find other sets. In the case of $\nu=1$ we can change the sign of all $X(I,J)$'s and $Y(I,J)$'s and find a new set of roots. When $\nu=2$, we have shown only two sets of roots in Table I, the second set obtained from the first by a certain permutation of different roots. But we can find many more sets by changing the sign of $X(I,J)$'s and $Y(I,J)$'s. However only those solutions for which the results in successive approximations are close to each other are acceptable. For instance in Table I, the results $\nu=2A$ and $\nu=1$ are close to each other and therefore for $\nu=2$ we choose the numbers given in the third column.

In Table II the results obtained from the first and the second order approximation are compared with the exact eigenvalues found from the solution of the Schrödinger equation. In this calculation the value of $\lambda=1$ has been used. In Table III, the eigenvalues for $\lambda=0.5$ in the second order of approximation is tabulated.

A systematic approach proposed for solving Eqs. (13.89)-(13.91) is the following [17]: Suppose that we have a set of nonlinear equations

$$F_i(x_j,\lambda)=0,\quad i,j=1,2,....N. \tag{13.96}$$

These equations are dependent on the parameter λ. Let us assume that for $\lambda=\lambda_0$ the solution x_j^0 is known,

$$F_i(x_j^{(0)},\lambda_0)=0,\quad i,j=1,2,....N, \tag{13.97}$$

then by a small change in λ_0 say to $\lambda_0+\delta\lambda$, we have

$$F_i(x_j^{(0)},\lambda_0+\delta\lambda)=-B_i,\quad i,j=1,2,....N. \tag{13.98}$$

By expanding (13.98) and using (13.97) we obtain the following equations

$$\sum_j \left(\frac{\partial F_i}{\partial x_j^{(0)}}\right) \delta x_j^{(0)} = \sum_j A_{ij} \delta x_j^{(0)} \cong B_i, \tag{13.99}$$

Here

$$\delta x_j^{(0)} = x_j - x_j^{(0)}, \tag{13.100}$$

and thus

$$x_j^{(1)} = x_j^{(0)} + \delta x_j^{(0)}. \tag{13.101}$$

which gives us $x_j^{(1)}$, the solution to the first order. This process can be repeated to yield $x_j^{(2)}, x_j^{(3)}$... to the desired accuracy.

TABLE I - Matrix elements of the coordinate and momentum (for momentum, times (-i)), in the first and in second order approximation $\nu = 1$ and $\nu = 2$. Here the value of $\lambda = 1$ has been used in the calculation. Among the possible sets of solutions only two, ν=2 A and ν=2 B are shown in this table.

	ν =1	ν=2 A	ν=2 B
X(1,1)	0.7619	0.8129	0.0749
Y(1,1)	-0.6562	-0.5907	-0.2642
X(2,1)	1.0776	0.8764	-0.9665
Y(2,1)	0.9280	1.0896	1.5054
X(1,2)		0.0749	-0.8129
Y(1,2)		-0.2642	0.5907
X(2,2)		0.9665	0.8764
Y(2,2)		-1.5054	1.0896
X(3,1)		0.0788	1.2542
Y(3,1)		0.3198	1.5745
X(3,2)		1.2542	-0.0788
Y(3,2)		1.5745	-0.3198

TABLE II - The energies of the low-lying states of the double-well potential $(-\frac{1}{2}x^2 + \frac{1}{4}x^4)$ calculated from the Heisenberg equations are shown in this table for three orders of approximation. In the last column the same energies are calculated accurately using finite difference approximation and are shown for comparison.

	ν=1	ν=2 A	ν=2 B	ν=3	$E(n)$
n=0	0.1776	0.1474	0.2126	0.1474	0.1465
1	1.0389	0.8741	3.7400	0.8741	0.8672
2	1.9001	2.1173	2.1825	2.1173	2.0197
3		3.6748	0.9393	3.5316	3.5456
4		4.9303	4.9954	5.1777	5.1544
5				6.8729	6.8964
6				8.5001	8.7472

TABLE III - Same as TABLE II except for smaller λ (λ=0.5).

	$\nu = 1$	ν=2 A	$E(n)$
n=0	-0.0076	-0.0636	-0.0657
1	0.5598	0.3353	0.3281
2	1.1272	1.2582	1.2626
3		2.4252	2.3084

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Chapter 14

Wigner Distribution Function in Quantum Tunneling

We have already seen that a classical description of tunneling is possible at the expense of introducing an artificial system with infinite degrees of freedom (Chapter 8). Another approach which is also helpful in establishing a connection between quantum mechanical and semi-classical formulations of tunneling is based on the distribution function.

In quantum theory, starting from the wave function of a system one can define different distribution functions [1] [2] [3], but among these the one introduced by Wigner [4] [5] [6] has been studied more extensively, and this is the distribution function which we will be mainly interested in this chapter.

In quantum theory the density of the particles is related to the wave function of the system by

$$n(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2. \tag{14.1}$$

If we write $\psi(\mathbf{r}, t)$ in terms of its Fourier transform, i.e.

$$\psi(\mathbf{r}, t) = \int \frac{d^3p}{(2\pi)^3} \phi(\mathbf{p}, t) \exp(i\mathbf{p}.\mathbf{r}), \quad \hbar = 1, \tag{14.2}$$

then its density in momentum space, $n(\mathbf{p}, t)$, is given by

$$n(\mathbf{p}, t) = |\phi(\mathbf{p}, t)|^2. \tag{14.3}$$

In statistical mechanics the Boltzmann function $f_c(\mathbf{p}, \mathbf{r}, t)$ is a function with the property that $f_c(\mathbf{p}, \mathbf{r}, t)d^3r d^3p$ is the probability of finding a particle with momentum $\mathbf{p}$ and coordinate $\mathbf{r}$ in the volume $d^3r d^3p$ of the phase space at the time t [7]. Therefore the number of the particles per unit volume, and in a unit volume of momentum space are given by the relations

$$n(\mathbf{r}, t) = \int f_c(\mathbf{p}, \mathbf{r}, t) d^3p, \tag{14.4}$$

and

$$n(\mathbf{p}, t) = \int f_c(\mathbf{p}, \mathbf{r}, t) d^3r, \tag{14.5}$$

respectively. For instance in the case of a single particle whose classical trajectory and momentum are given by $\mathbf{r}$ and $\mathbf{p} = m\frac{d\mathbf{r}}{dt}$ the Boltzmann function is the product of two delta functions

$$f_c(\mathbf{p}, \mathbf{r}, t) = \delta\left[\mathbf{r} - \mathbf{r}(t)\right]\delta\left[\mathbf{p} - \mathbf{p}(t)\right]. \tag{14.6}$$

The Wigner distribution function $f(\mathbf{p}, \mathbf{r}, t)$ is the quantum analogue of the classical Boltzmann function [7]. This distribution function is defined in terms of the wave function of the system under consideration by

$$f(\mathbf{p}, \mathbf{r}, t) = \frac{1}{(2\pi)^3}\int \exp\left(-i\mathbf{p}.\mathbf{R}\right)\psi^*\left(\mathbf{r} - \frac{1}{2}\mathbf{R}, t\right)\psi\left(\mathbf{r} + \frac{1}{2}\mathbf{R}, t\right) d^3R, \tag{14.7}$$

where we have set $\hbar = 1$. It should be emphasized that in (14.7) $\mathbf{p}$ is not an operator but is an ordinary vector. We write the same distribution function in momentum space as

$$f(\mathbf{p}, \mathbf{r}, t) = \frac{1}{(2\pi)^3}\int \exp\left(i\mathbf{q}.\mathbf{r}\right)\phi^*\left(\mathbf{p} - \frac{1}{2}\mathbf{q}, t\right)\phi\left(\mathbf{p} + \frac{1}{2}\mathbf{q}, t\right) d^3q. \tag{14.8}$$

From these relations it follows that

$$\int f(\mathbf{p}, \mathbf{r}, t) d^3p = |\psi(\mathbf{r}, t)|^2, \tag{14.9}$$

and

$$\int f(\mathbf{p}, \mathbf{r}, t) d^3r = |\phi(\mathbf{p}, t)|^2, \tag{14.10}$$

and these correspond to the classical definitions (14.4) and (14.5). The function $f(\mathbf{p}, \mathbf{r}, t)$ is always real, but can be negative. However it is essential that (14.9) and (14.10) be positive quantities.

A novel derivation of the Wigner distribution function from an extension of the Lagrangian formulation to the phase space is given by Sobouti and Nasiri [8], but here we find the equation of motion for $f(\mathbf{p}, \mathbf{r}, t)$ directly from the time-dependent Schrödinger equation

$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{1}{2m}\nabla^2 + V(r)\right]\psi(\mathbf{r},t). \tag{14.11}$$

First from the integral form of $f(\mathbf{p}, \mathbf{r}, t)$ in momentum space we calculate the kinetic energy

$$\begin{aligned}&\int \frac{d^3q}{(2\pi)^3}\exp(i\mathbf{q}.\mathbf{r})\left(\frac{1}{2m}\right)\left[\left(\mathbf{p}+\frac{1}{2}\mathbf{q}\right)^2 - \left(\mathbf{p}-\frac{1}{2}\mathbf{q}\right)^2\right] \\ \times\ &\phi^*\left(\mathbf{p}-\frac{1}{2}\mathbf{q},t\right)\phi\left(\mathbf{p}+\frac{1}{2}\mathbf{q},t\right) = -\frac{i}{m}\mathbf{p}.\nabla_r f(\mathbf{p},\mathbf{r},t).\end{aligned} \tag{14.12}$$

With the help of this equation we find the equation of motion from the relation

$$\begin{aligned}&\frac{Df}{Dt} = \left(\frac{\partial}{\partial t} + \frac{1}{m}\mathbf{p}.\nabla_r\right) f(\mathbf{p},\mathbf{r},t) \\ =\ &\left(\frac{1}{i}\right)\int \frac{d^3R}{(2\pi)^3}\exp(-i\mathbf{p}.\mathbf{R})\left[V\left(\mathbf{r}+\frac{1}{2}\mathbf{R}\right) - V\left(\mathbf{r}-\frac{1}{2}\mathbf{R}\right)\right] \\ \times\ &\psi^*\left(\mathbf{r}-\frac{1}{2}\mathbf{R},t\right)\psi\left(\mathbf{r}+\frac{1}{2}\mathbf{R},t\right).\end{aligned} \tag{14.13}$$

In order to eliminate $\psi^*\psi$ in (14.13) we find the inverse Fourier transform of (14.7)

$$\int f(\mathbf{p},\mathbf{r},t)\exp(i\mathbf{p}.\mathbf{R})\,d^3p = \psi^*\left(\mathbf{r}-\frac{1}{2}\mathbf{R}\right)\psi\left(\mathbf{r}+\frac{1}{2}\mathbf{R}\right), \tag{14.14}$$

and substitute it in (14.13). After simplifying the result we get [9]

$$\begin{aligned}&\left(\frac{\partial}{\partial t} + \frac{1}{m}\mathbf{p}.\nabla_r\right) f(\mathbf{p},\mathbf{r},t) = \frac{1}{i}\int d^3K \int \frac{d^3R}{(2\pi)^3}\left[V\left(\mathbf{r}+\frac{1}{2}\mathbf{R}\right)\right. \\ -\ &\left.V\left(\mathbf{r}-\frac{1}{2}\mathbf{R}\right)\right] f(\mathbf{K}+\mathbf{p},\mathbf{r},t)\exp(i\mathbf{K}.\mathbf{r}).\end{aligned} \tag{14.15}$$

For one-dimensional tunneling (14.15) takes the simpler form of

$$\left(\frac{\partial}{\partial t} + \frac{p}{m}\frac{\partial}{\partial x}\right) f(p,x,t) = \int_{-\infty}^{\infty} f(p+K,x,t)J(x,K)dK, \tag{14.16}$$

where $J(x,K)$ is defined by

$$J(x,K) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty}[V(x+y) - V(x-y)]\exp\left(\frac{2iyK}{\hbar}\right)dy. \tag{14.17}$$

In this relation we have written the Planck constant explicitly. Now we can write an expansion of (14.16) as a power series in $\hbar$;

$$\frac{\partial f}{\partial t} = -\frac{p}{m}\frac{\partial f}{\partial x} + \sum_{n=0}^{\infty}\left(\frac{\hbar}{2i}\right)^{2n}\frac{1}{(2n+1)!}\left(\frac{\partial^{2n+1}V(x)}{\partial x^{2n+1}}\right)\left(\frac{\partial^{2n+1}f}{\partial p^{2n+1}}\right). \tag{14.18}$$

If the potential depends only on x and x^2, then (14.18) reduces to a linear first order partial differential equation;

$$\frac{\partial f}{\partial t} = -\frac{p}{m}\frac{\partial f}{\partial x} + \frac{\partial V(x)}{\partial x}\frac{\partial f}{\partial p}, \tag{14.19}$$

from which, using the method of characteristics [13], we find the Hamilton canonical equation

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial V(x)}{\partial x}. \tag{14.20}$$

If $V(x) = 0$, then the solution of (14.19) can be written as

$$f(x,p,t) = f\left(x - \frac{1}{m}pt, p, t\right), \tag{14.21}$$

and this shows that each point (x,p) of the phase space, the Wigner distribution function has a trajectory which is identical to the classical trajectory.

Another important example is the motion of a Gaussian wave packet with the center at x_0 and width Δx, i.e.

$$\psi(x) = \frac{1}{[2\pi(\Delta x)^2]^{\frac{1}{4}}}\exp\left[-\frac{(x-x_0)^2}{4(\Delta x)^2}\right]\exp\left(\frac{ip_0 x}{\hbar}\right). \tag{14.22}$$

Substituting this expression in the definition of $f(p,x,t)$,

$$f(p,x,t) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty}\exp\left(\frac{2ip\xi}{\hbar}\right)\psi^*(x-\xi,t)\psi(x+\xi,t)d\xi, \tag{14.23}$$

we find

$$\begin{aligned} f(p,x,t) &= \frac{1}{\pi\hbar}\exp\left[-\frac{1}{2(\Delta x)^2}\left(x - \frac{pt}{m} - x_0\right)^2\right] \\ &\times \exp\left[-\frac{1}{2(\Delta p)^2}(p-p_0)^2\right], \end{aligned} \tag{14.24}$$

where $\Delta p = \frac{\hbar}{2\Delta x}$.

Some of the important properties of the Wigner distribution function

(14.7) are the followings [10]:
(1) - The function $f(\mathbf{p}, \mathbf{r}, t)$ is Hermitian, and therefore it is a real function of $\mathbf{p}$ and $\mathbf{r}$.
(2) - If f is integrated over $\mathbf{r}$ it gives the correct probability for different $\mathbf{p}$'s and we have similar result when $\mathbf{p}$ and $\mathbf{r}$ are interchanged.
(3) - The correspondence between $f(\mathbf{p}, \mathbf{r}, t)$ and the wave function ψ is Galilean invariant.
(4) - The time-dependent distribution function is invariant under time reversal.
(5) - The transition probability between two states ψ_1 and ψ_2 is given in terms of the corresponding distribution functions by

$$\left|\int \psi_1(\mathbf{r})\,\psi_2(\mathbf{r})\,d^3r\right| = (2\pi)^3 \int\int f_1(\mathbf{r}, \mathbf{p})\, f_2(\mathbf{r}, \mathbf{p})\, d^3r d^3p. \tag{14.25}$$

(6) - Finally as Eq. (14.20) shows for the case of force-free motion the equations of motion are the same as the classical equations.

14.1 Wigner Distribution Function and Quantum Tunneling

The Wigner distribution function enables us to define a "trajectory" in phase space for a particle which tunnels through a barrier. For this purpose instead of the special case of (14.19) which is only valid when $V(x)$ depends on x and/or on x^2, we can use the general form which we can write as

$$\frac{\partial f}{\partial t} = -\frac{p}{m}\frac{\partial f}{\partial x} + \frac{\partial V_e(x,p)}{\partial x}\frac{\partial f}{\partial p}, \tag{14.26}$$

where $V_e(x,p)$ is defined by

$$\begin{aligned} \frac{\partial V_e(x,p)}{\partial x}\frac{\partial f}{\partial p} &= \frac{\partial V(x)}{\partial x}\frac{\partial f}{\partial p} + \frac{1}{3!}\left(\frac{\hbar}{2i}\right)^2 \frac{\partial^3 V(x)}{\partial x^3}\frac{\partial^3 f}{\partial p^3} \\ &+ \frac{1}{5!}\left(\frac{\hbar}{2i}\right)^4 \frac{\partial^5 V(x)}{\partial x^5}\frac{\partial^5 f}{\partial p^5} + \cdots. \end{aligned} \tag{14.27}$$

In this case the solution of Eq. (14.26) can be obtained from a generalization of the Hamilton canonical equation [11] [12]

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial V_e(x,p)}{\partial x}. \tag{14.28}$$

Now we want to discuss two examples of the application of the Wigner distribution function in quantum mechanical tunneling. The first case is that of tunneling through two rectangular barriers of height V_1 and width $b-a$ [12];

$$V(x) = \begin{cases} 0 & \text{for } x < a \\ V_1 & \text{for } a < x < b, \quad c < x < c+b-a \\ 0 & \text{for } b < x < c, \quad x > c+b-a \end{cases} . \tag{14.29}$$

If at the time $t = 0$ a Gaussian wave packet is located to the right of the barrier, i.e. when x_0 in (14.22) is positive, we can find the motion of the wave packet from Eqs. (14.16) and (14.17). In Fig. (14.1) the two dimensional plot of $f(x,p,t)$ at the initial time $t = 0$ and later times $t = 30$ and $t = 60$ are shown. The wave packet moves from the right to the left, and the tunneling changes the shape and the width of the packet.

From the motion of the wave packet we can find the tunneling time (Chapters 17 and 18) as a function of the energy associated with the wave packet. Fig. (14.2 left) shows the time of passage of a Gaussian wave packet from a single well, and the figure on the right shows the time of passage for the two barriers. The tunneling time for two barriers shows a peak at the resonant energy of the incident wave packet (see Chapter 19). Different curves in each figure correspond to different thicknesses $(b-a)$ of the barrier(s).

The important problem of ionization of a bound electron in the presence of a uniform electric field (Section 24.3) can also be formulated and solved with the help of the Wigner distribution function. For this problem the function $f(\mathbf{p}, \mathbf{r}, t)$, Eq. (14.7), is determined from the wave equation $\psi(\mathbf{r}, t)$, where $\psi(\mathbf{r}, t)$ is the solution of the Schrödinger equation [14],

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{2\pi\hbar^2}{m\kappa}\delta(\mathbf{r})\frac{\partial}{\partial r}r - e\mathbf{r}.\mathcal{E}\right]\psi(\mathbf{r},t). \tag{14.30}$$

In this equation $\mathcal{E}$ is the external electric field and κ is related to the binding energy of the electron, E_0, by

$$\kappa = \sqrt{\frac{2mE_0}{\hbar^2}}, \tag{14.31}$$

where it is assumed that the zero-range potential $\left(\frac{2\pi\hbar^2}{m\kappa}\delta(\mathbf{r})\frac{\partial}{\partial r}r\right)$ binds the electron. For the solution of this problem see the paper by Czirjak *et al* [14].

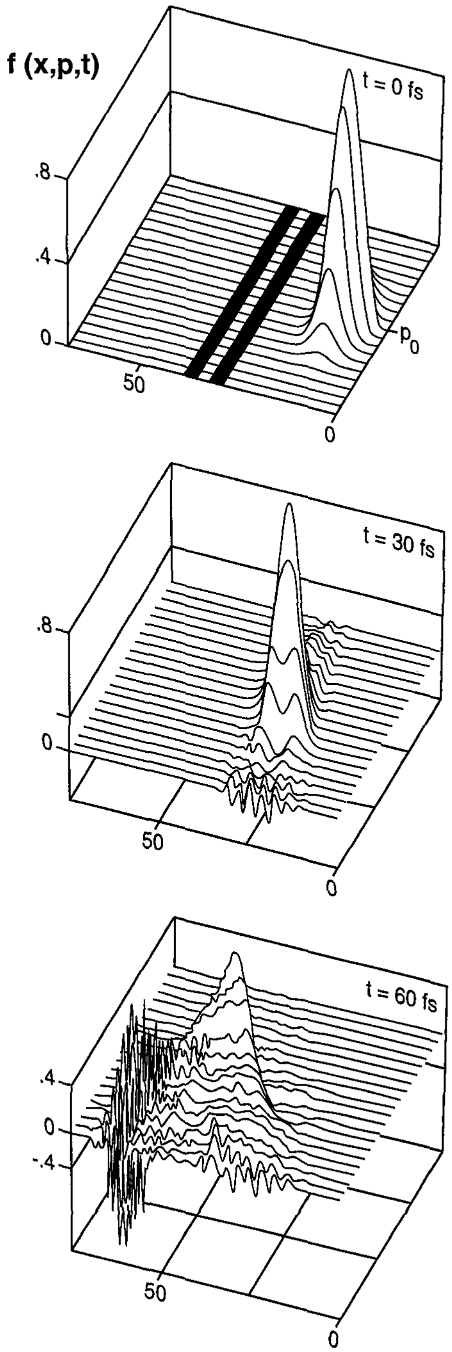

Figure 14.1: The Wigner distribution function for the tunneling of a Gaussian wave packet, Eq. (14.24), through two identical rectangular barriers. The two barriers are shown by two dark bands.

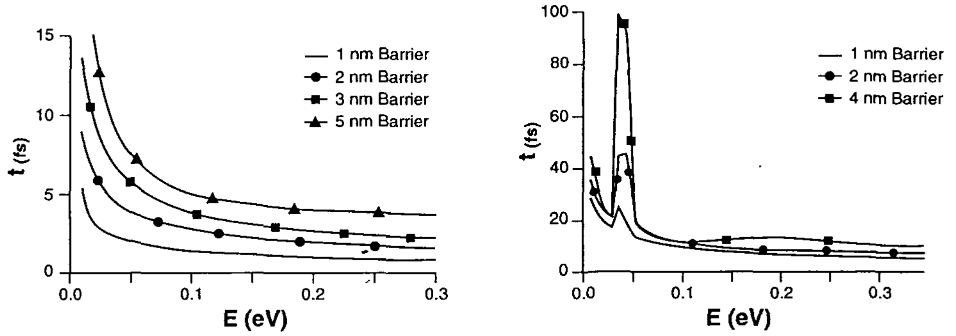

Figure 14.2: The time of passage of a Gaussian wave packet. The one on the left is for a single and on the right is for two identical barriers. The passage time is longer for thicker barriers.

14.2 Wigner Trajectory for Tunneling in Phase Space

In Chapter 8 we observed that quantum tunneling can be formulated as a classical motion of a particle coupled to a system with infinite number of degrees of freedom . An approximate solution of these equations shows that the motion of the particle is governed by the effective Hamiltonian $\mathcal{H}_{eff}(p, q, \pi_0, \xi_0)$, Eq. (8.21). From the canonical equations for the variables p and q we can define the trajectory in phase space for this tunneling.

A different way of formulating the concept of trajectory in phase space for the tunneling of a particle is by means of the Wigner distribution function. It should be emphasized that the concept of "trajectory" here is not the same as in classical dynamics, but it is a generalization of the classical concept. Thus in the limit of $\hbar \to 0$ the quantal trajectory tends to the classical trajectory, and for this reason it is a useful concept for relating quantum and classical theories. In the following discussion we use the units where $\hbar = 2m = 1$. First we observe that the Wigner distribution function allows us to define an effective force from Eqs. (14.26) and (14.27) or from

(14.16) and (14.17) [3];

$$F(p,x,t) = -\frac{\partial V_e(x,p)}{\partial x}$$
$$= \left(\frac{-i}{\pi(\frac{\partial f}{\partial p})}\right)\int_{-\infty}^{\infty}[V(x+y)-V(x-y)]\,G(p,x,y,t)dy, \quad (14.32)$$

where G is given by

$$G(p,x,y,t) = \int_{-\infty}^{\infty}\exp(-2iKy)f(p+K,x,t)dK. \quad (14.33)$$

We note that $F(p,x,t)$ is real, therefore we can use (14.32) or its complex conjugate. For a stationary state we consider the n-th eigenfunction for a particle moving in a double well potential, ψ_n. The Wigner distribution function for this problem is

$$f_n(p,x) = \frac{1}{\pi}\int_{-\infty}^{\infty}\exp(-2i\xi p)\psi_n^*(x+\xi)\psi_n(x-\xi)d\xi, \quad (14.34)$$

and for these stationary states f_n does not depend explicitly on t. Let us denote the force corresponding to the state n by $F_n(p,x)$. From Eq. (14.32) we can conclude that if the potential is symmetric, then $F_n(p,x)$ is an odd function of x and an even function of p. The argument is as follows: Because of the symmetry of the potential the eigenfunction $\psi_n(x)$ has a well-defined parity, i.e. $\psi_n(x) = \pm\psi_n(-x)$. Thus $f_n(p,x)$ is an even function of both p and x. Also $G_n(p,x,y) = G_n(p,-x,y)$ and $V(x) = V(-x)$, therefore from (14.32) we have $F_n(p,x) = F_n(-p,x)$ and the force $F_n(p,x)$ does not change under time-reversal transformation .

The problem of calculating the Wigner phase space trajectory cannot be done analytically even for very simple potentials, and the final answer can only be given numerically. In the following we try to find the Wigner trajectory for the quasi-solvable potential which we studied in Chapter 7. The potential is a special case of (7.75) for $n = 2$ and when the particle has a unit mass $m = 1$ [15];

$$V(x) = \frac{1}{2}\left[\frac{1}{8}\xi^2\cosh(4x) - 3\xi\cosh(2x) - \frac{1}{8}\xi^2\right]. \quad (14.35)$$

In Eq. (14.35) the parameter ξ determines the shape of the potential. From what we have seen in Chapter 7, we know that the three lowest energy levels and their eigenfunctions are known analytically, and that the ground state eigenfunction is

$$\psi_0(x) = \mathcal{N}_0 \left[\xi + a\cosh(2x)\right] \exp\left(-\frac{1}{4}\xi\cosh(2x)\right), \tag{14.36}$$

where a is related to the ground state energy E_0 by

$$E_0 = -a = -\left(1 + \sqrt{1+\xi^2}\right), \tag{14.37}$$

and $\mathcal{N}_0$ is the normalization constant.

Substituting $\psi_0(x)$ in (14.34) we find $f_0(p,x)$ [16];

$$\begin{aligned} f_0(p,x) &= \frac{1}{\pi}\mathcal{N}_0^2\left[\xi^2 + \left(\frac{2az}{\xi}\right)^2 - a^2\right] K_{ip}(z) \\ &+ \frac{1}{\pi}\mathcal{N}_0^2\left[a^2\left(\frac{d^2K_{ip}(z)}{dz^2}\right) - 4az\left(\frac{dK_{ip}(z)}{dz}\right)\right], \end{aligned} \tag{14.38}$$

where

$$z = \frac{1}{2}\xi\cosh(2x). \tag{14.39}$$

Using the properties of the Bessel function of complex index, ip, [17] we can write (14.38) as

$$\begin{aligned} f_0(p,x) &= \frac{1}{\pi}\mathcal{N}_0^2\left\{\left[\xi^2\left(\frac{2az}{\xi}\right)^2 - \frac{1}{2}a^2\right] K_{ip}(z) + \right. \\ &+ \left(\frac{a^2}{4\pi}\right)\left[K_{(ip+2)}(z) + K_{(ip-2)}(z)\right] \\ &+ \left.\left(\frac{2az}{\pi}\right)\left[K_{(ip+1)}(z) + K_{(ip-1)}(z)\right]\right\}, \end{aligned} \tag{14.40}$$

As we have pointed out earlier $f_0(p,x)$ is real. In Fig. (14.3) the contour plot of $f_0(p,x)$ is shown for $\xi = \frac{4}{3}$. Now we want to investigate some of the properties of the force $F_0(p,x)$. To begin with we want to know whether there are parts in phase space where $F_0(p,x)$ tends to infinity. After reaching these points the phase space trajectory changes its direction. From the definition of F_0, Eq. (14.32) it is evident that at the points where $\frac{\partial f_0}{\partial p} = 0$, $F_0(p,x)$ becomes infinity provided that at these points the integral is not zero.

By differentiating (14.40) we find the following equation;

$$\frac{\partial f_0}{\partial p} = \frac{\mathcal{N}_0^2}{\pi}\left[\xi^2 + \left(\frac{2az}{\xi}\right)^2 - a^2 - 4az\frac{\partial}{\partial z} + a^2\frac{\partial^2}{\partial z^2}\right]\frac{\partial K_{ip}(z)}{\partial p}. \tag{14.41}$$

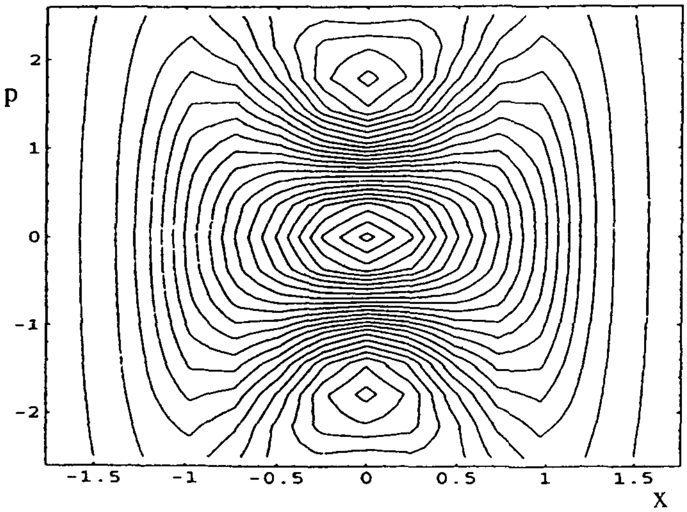

Figure 14.3: The contour plot of the Wigner distribution function for the ground state of the double-well potential given by (14.35). The parameter $\xi = \frac{4}{3}$ has been used in this calculation.

For calculating G_0, we substitute f_0 from (14.40) in (14.33);

$$\begin{aligned} G_0(p,x,y) &= \frac{\mathcal{N}_0^2}{\pi}\left[\xi^2 + \left(\frac{2az}{\xi}\right)^2 - a^2 - 4az\frac{\partial}{\partial z} + a^2\frac{\partial^2}{\partial z^2}\right] \\ &\times \int_{-\infty}^{\infty} e^{-2iky} K_{i(p+k)}(z)dk. \end{aligned} \tag{14.42}$$

The last integral can be evaluated analytically with the result that

$$\begin{aligned} G_0(p,x,y) &= \mathcal{N}_0^2\left[\xi^2 + \left(\frac{2az}{\xi}\right)^2 - a^2 - 4az\frac{\partial}{\partial z} + a^2\frac{\partial^2}{\partial z^2}\right] \times \\ &\times \exp[-z\cosh(2y)]\exp(2ipy). \end{aligned} \tag{14.43}$$

The last integral, i.e. the right hand side of (14.32) can be evaluated by using Eqs. (14.35) and (14.43). After some simplification we find the following expression:

$$\begin{aligned} F_0(p,x) &= -\left(\frac{\partial f_0(p,x)}{\partial p}\right)^{-1}\left\{\left[\xi^2 + a^2\sinh^2(2x)\right]S(p,x)\right. \\ &- \left. 2a\coth(2x)\frac{\partial S}{\partial x} + \left(\frac{a}{\xi\sinh(2x)}\right)^2\left[\frac{\partial^2 S}{\partial x^2} - 2\coth(2x)\frac{\partial S}{\partial x}\right]\right\}, \end{aligned} \tag{14.44}$$

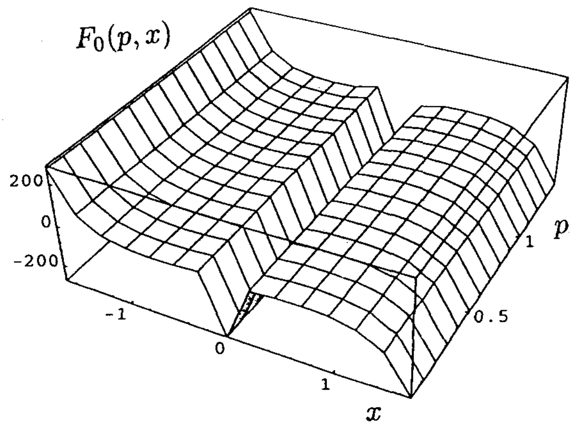

Figure 14.4: The state dependent "force" as defined by the Wigner trajectory. This force is given for the ground state of double-well potential Eq. (14.36).

in which $S(p,x)$ is given by

$$\begin{aligned} S(p,x) &= \frac{i\mathcal{N}_0^2}{2}\left\{\frac{1}{16}\xi^2\sinh^2(4x)\left[K_{(ip+2)}(z) - K_{(-ip+2)}(z)\right]\right\} \\ &- \frac{3i\mathcal{N}_0^2}{4}\left\{\xi\sinh(2x)\left[K_{(ip+1)}(z) - K_{(-ip+1)}(z)\right]\right\}. \end{aligned} \tag{14.45}$$

In Fig. (14.4) the two-dimensional plot of $F_0(p,x)$ as a function of x and p is shown. This force has a simple pole at $x = 0$ and tends to infinity at the boundaries. Once $F_0(p,x)$ is known, we can determine the Wigner trajectory from the equations of motion (see Eq. (14.26));

$$\frac{dx}{dt} = p, \quad \frac{dp}{dt} = F_0(p,x). \tag{14.46}$$

This trajectory is shown in Fig. (14.5) for the initial values $x(0) = -1.343$ and $p(0) = \pm 10^{-4}$. For comparison we have also shown the classical trajectory which is found from the solution of

$$\frac{dx}{dt} = p, \quad \frac{dp}{dt} = -\frac{\partial V(x)}{\partial x}, \tag{14.47}$$

using the same initial values that we have used for the Wigner trajectory [16].

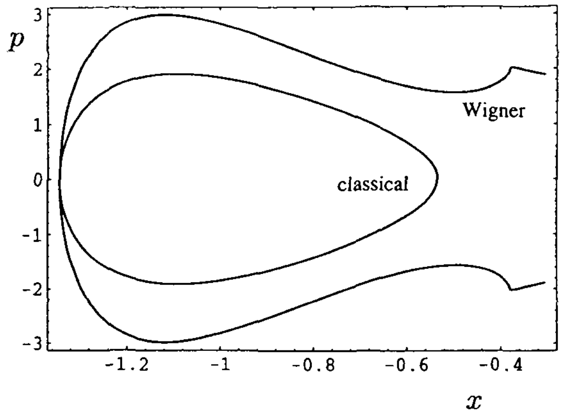

Figure 14.5: The Wigner trajectory is compared to the classical trajectory for the double-well potential $V(x)$, Eq. (14.35).

In Chapter 8 we studied a particular classical description of the tunneling process in detail. A different way of simulating quantum tunneling as a classical problem is by using an ensemble of trajectories where each trajectory is defined by the solution of the Hamilton's canonical equations (14.27) and (14.28). For instance in the case of cubic potential

$$V(x) = \frac{1}{2}m\omega^2 x^2 - \frac{1}{3}bx^3, \quad (b > 0), \tag{14.48}$$

the equation for the trajectories (14.28) simplifies to

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial V(x)}{\partial x} + \frac{\hbar^2}{24}\frac{\frac{\partial^3 f}{\partial p^3}}{\frac{\partial f}{\partial p}}\frac{\partial^3 V(x)}{\partial x^3}. \tag{14.49}$$

Due to the presence of the last term in (14.49) the classical force is state-dependent, but as Donoso and Martens [18] have pointed out, the ensemble averages of $\frac{dp}{dt}$ and $-\frac{\partial V(x)}{\partial x}$ are equal, i.e. the Ehrenfest theorem is satisfied and the ensemble average of the energy E is independent of time. These authors have studied the tunneling of a Gaussian wave packet through the barrier defined by (14.48) by replacing $f(x, p, t)$ by a finite ensemble of trajectories.

$$f_A(x, p, t) = \frac{1}{N}\sum_{j=1}^{N} \delta[x - x_j(t)]\delta[p - p_j(t)]. \tag{14.50}$$

Thus the force law assumes the form

$$\frac{dp_j}{dt} = -\left(\frac{\partial V(x)}{\partial x}\right)_j + \frac{\hbar^2 b}{12}\left(\frac{\frac{\partial^3 f}{\partial p^3}}{\frac{\partial f}{\partial p}}\right)_{x_j, p_j}, \tag{14.51}$$

where the value of the last term in (14.51) at each phase space point (x_j, p_j) is calculated by assuming a local Gaussian approximation of $f(x,p,t)$ around each point (x_j, p_j) [18]. Among other examples of the applications of the Wigner distribution function the problem of penetration in a potential step has been studied by Lee and Scully [19] and the distribution function for the Morse potential has been used by Henriksen *et al* [20].

14.3 Wigner Distribution Function for an Asymmetric Double-Well

In order to compare the distribution function for symmetric and asymmetric double-wells, again we choose a solvable model discussed in Section 7.7, where the double-well is given by Eq. (7.119). For this potential the ground state wave function is given by

$$\psi_0(x) = \begin{cases} N_0 \sin\left[\sqrt{\varepsilon_0}\,(x+1)\right] & \text{for } -1 \le x \le 0 \\ -N_0 \frac{\sin\sqrt{\varepsilon_0}}{\sin\sqrt{\varepsilon_0 - v_0}} \sin\left[\sqrt{\varepsilon_0 - v_0}\,(x-1)\right] & \text{for } 0 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}, \tag{14.52}$$

where ε_0 is the smallest root of

$$\sqrt{\varepsilon - v_0}\cot\sqrt{\varepsilon - v_0} + \sqrt{\varepsilon}\cot\sqrt{\varepsilon} + s_1 = 0. \tag{14.53}$$

By substituting $\psi_0(x)$ in Eq. (14.34) we calculate $f_0(p,x)$. The contour plot of $f_0(p,x)$ is shown in Fig.(14.6). The distribution function is a symmetric function of p but an asymmetric function of x.

14.4 Wigner Trajectory for an Oscillating Wave Packet

In Chapter 7 we observed that in a symmetric double well potential a linear combination of the ground and the first excited state forms a wave packet,

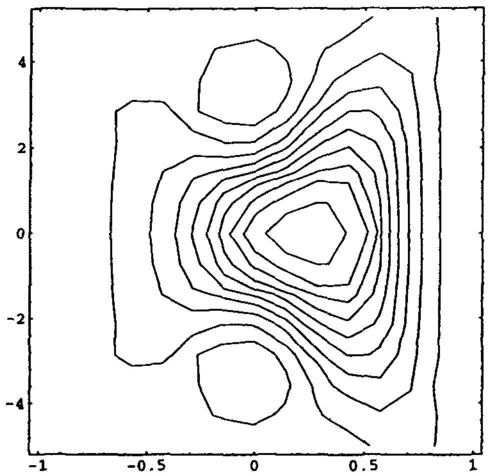

Figure 14.6: The contour plot of the Wigner distribution function for the ground state of the asymmetric double-well potential given by (7.119). The parameters $s_1 = 4L^{-1}$ and $v_0 = -4L^{-2}$ have been used in this calculation.

and this wave packet oscillates without changing its shape and with a fixed period between the two wells (see Eqs. (7.10) and (7.11)). The center of this wave packet and its momentum are given by

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)x\Psi(x,t)dx, \tag{14.54}$$

and

$$\langle p(t)\rangle = -i\int_{-\infty}^{\infty} \Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}dx. \tag{14.55}$$

respectively.

The parametric equation for $\langle p(t)\rangle$ and $\langle x(t)\rangle$ shows a closed curve, since $\Psi(x,t) = \Psi(x,t+T)$.

Now let us consider the Wigner trajectory in phase space for this wave packet. Here the distribution function is

$$f(p,x,t) = \frac{1}{\pi}\int_{-\infty}^{\infty} e^{-2i\xi p}\Psi^*(x+\xi,t)\Psi(x-\xi,t)d\xi. \tag{14.56}$$

This distribution function is also periodic, $f(p,x,t+T) = f(p,x,t)$. From Eq. (14.33) it follows that $G(p,x,y,t)$ is also periodic, and the periodicity of G and $\frac{\partial f}{\partial p}$ imply that $F(p,x,t)$ defined by (14.32) is periodic. But the periodicity in phase space does not follow from the periodicity of the applied forces in time.

14.5 Margenau-Hill Distribution Function for a Double-Well Potential

We have seen some of the applications of the Wigner distribution function for quantum tunneling. However as we mentioned at the beginning of this chapter there are other distribution functions, some simpler and others more complicated than Wigner's.

Margenau and Hill [1] [2] proposed a simple distribution function $f^M(x,p,t)$ defined by the relation

$$f^M(x,p,t) = \frac{1}{2\pi}\mathrm{Re}\left\{\psi(x,t)\int_{-\infty}^{\infty} e^{-ipz}\psi^*(x-z,t)\,dz\right\}, \quad \hbar = 1. \quad (14.57)$$

Again this distribution function satisfies the basic relations (14.9) and (14.10). In order to compare the results of (14.57) with (14.40) we use the same wave function (14.36) in Eq. (14.57) and find $f_0^M(x,p)$ to be

$$\begin{aligned} f_0^M(x,p) &= \frac{\mathcal{N}_0^2}{2\pi}\mathrm{Re}\left\{[\xi + a\cosh(2x)]\exp\left[-\frac{1}{4}\xi\cosh(2x)\right]\exp(-ixp)\right. \\ &\times \left.\left[\frac{\xi}{2}K_{\frac{ip}{2}}\left(\frac{\xi}{4}\right) - 2a\frac{d}{d\xi}K_{\frac{ip}{2}}\left(\frac{\xi}{4}\right)\right]\right\}. \end{aligned} \quad (14.58)$$

The contour plot of this distribution function for $\xi = \frac{4}{3}$ is shown in Fig. 14.7. Here unlike the Wigner distribution function the contour follows the contour lines of the double-well potential closely.

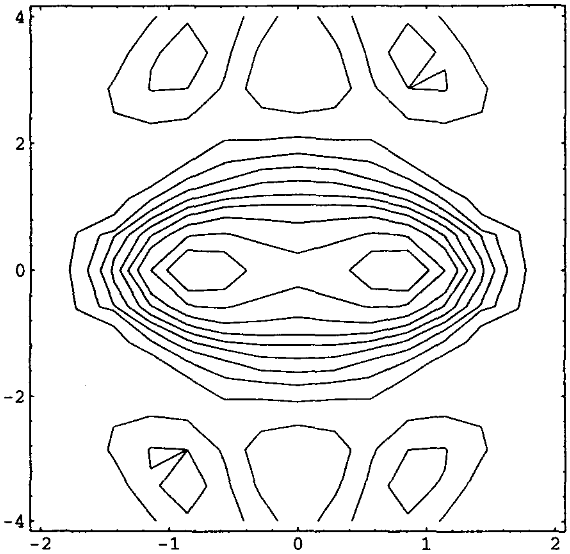

Figure 14.7: The contour plot of the Margenau-Hill distribution function for the ground state of the symmetric double-well potential given by (14.35).

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Chapter 15

Complex Scaling and Dilatation Transformation Applied to the Calculation of the Decay Width

In Chapter 10 we studied the connection between the properties of the scattering matrix and the tunneling problem. For the scattering of a particle from a center of force, the S-matrix has simple poles in the complex E-plane and the position of these poles on the negative real E-axis are the bound state eigenvalues. For the continuum spectrum, the S-matrix has a cut along the Re $E > 0$ [1] [2] [3].

When the potential forms a barrier and the system is unstable, then the S-matrix can have one or several poles in the complex E-plane at points where

$$E = E_R - \frac{i}{2}\Gamma, \quad \Gamma > 0. \tag{15.1}$$

We have already seen the method of finding these poles through analytic continuation in Chapter 10. Now we want to study a different technique which is known as the complex scaling method.

First we note that for the analytic continuation in the complex E plane we can use the dilatation transformation, where $\mathbf{r}$, the position vector is replaced by [4] [5] [6]

$$\mathbf{r} \to \mathbf{r}e^{i\theta}. \tag{15.2}$$

In this relation θ, the parameter of the transformation can be real or complex. This θ should not be confused with the azimuthal coordinate θ. The transformation (15.2) forms a continuous group, with the infinitesimal generator given by

$$\mathbf{A}(\theta) = \mathbf{r}.\mathbf{p} + \mathbf{p}.\mathbf{r}. \tag{15.3}$$

Denoting the original Hamiltonian by H, the transformed Hamiltonian will depend on the parameter θ,

$$H \to H(\theta) = Te^{-2i\theta} + V(\mathbf{r}e^{i\theta}), \tag{15.4}$$

where T is the kinetic energy and V is the potential energy of the tunneling particle. Since $H(\theta)$ depends on θ, the eigenfunctions $\psi(\theta)$ will also be functions of θ, i.e.

$$H(\theta)\psi(\theta) = E(\theta)\psi(\theta), \tag{15.5}$$

and

$$H^\dagger(\theta)\bar{\psi}(\theta) = E^*(\theta)\bar{\psi}(\theta). \tag{15.6}$$

Here $H^\dagger(\theta)$ is the Hermitian adjoint of $H(\theta)$. After the transformation the expectation value of any operator, say, F is defined by

$$\langle|F(\theta)|\rangle = \langle\bar{\psi}(\theta)|F(\theta)|\psi(\theta)\rangle\,. \tag{15.7}$$

The condition for the invariance of the eigenvalues under this dilatation transformation is that

$$\langle\bar{\psi}(\theta)\,[A(\theta), H(\theta)]\,|\psi(\theta)\rangle = 0. \tag{15.8}$$

If we substitute Eqs. (15.3) and (15.4) in (15.8) we can write (15.8) as

$$2\,\langle\bar{\psi}(\theta)|T(\theta)|\psi(\theta)\rangle = \langle\bar{\psi}(\theta)|\mathbf{r}.\nabla V(\theta)|\psi(\theta)\rangle\,. \tag{15.9}$$

This is the complex extension of the virial theorem in quantum theory [7] [8]. By solving the Schrödinger equation for the transformed Hamiltonian $H(\theta)$ we find the following results [5]:

(i) - In the complex E-plane the bound state eigenvalues remain at their initial positions (i.e. before rotation). We know that the original bound states are L^2 integrable, and we require the same integrability for the transformed wave function. For instance if $\psi(r) = 2\exp(-r)$, then $\psi(r,\theta) = 2\exp(-2re^{i\theta})$. For the latter to be L^2 integrable we impose the condition that $|\theta| < \frac{\pi}{2}$. This condition guarantees that the square integrability is preserved under the transformation, and inversely the transformation $\mathbf{r} \to \mathbf{r}e^{i\theta}$,

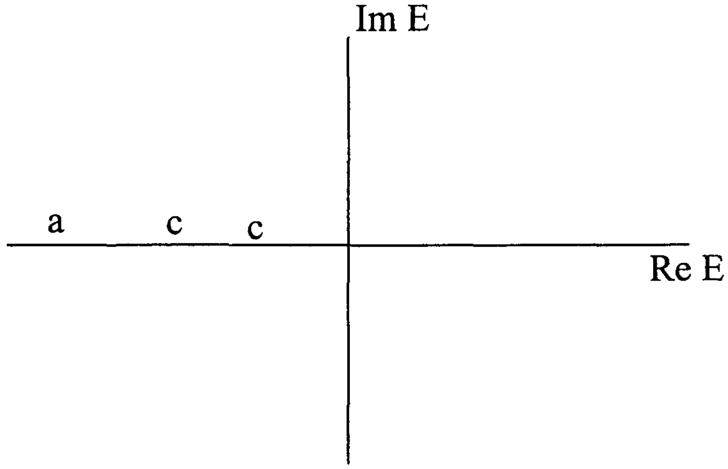

Figure 15.1: The poles and the cuts of the scattering matrix in the complex E-plane.

$H \to H(\theta)$ does not produce any new wave function which is L^2 integrable.
(ii) - All wave functions for the continuum will be rotated by an angle (-2θ) in the lower half of the complex E-plane. In Fig. (15.1) the discrete eigenvalue a and the continuum energy from the threshold c to infinity are shown before the transformation. After the transformation, taking θ to be a real number we have the singularities displayed in Fig. (15.2). The cuts at different thresholds are drawn as the lines cb, the position of the bound state a has not been affected and the point d, the resonant pole remains in the lower half plane (see Eq. (15.1)).
(iii) - The energies where the cuts start for a given H (shown by c) are the same as those of $H(\theta)$. But for $H(\theta)$ these cuts are rotated by an angle (-2θ).
(iv)- When θ is large enough, then the branch cuts will pass through the pole $E = E_R - \frac{i}{2}\Gamma$ (shown as d), and when this happens we find a new eigenvalue of $H(\theta)$ at this pole.
(v) - When a resonant pole appears in the E-plane, it will not be affected by increasing θ unless θ becomes so large that another branch cut passes through this pole. When this new value of θ is assumed, then the earlier pole disappears.

The properties outlined above were derived at first for the potentials of the form $gr^{-\beta}$ $(0 < \beta < \frac{3}{2})$, and then for a linear superposition of the

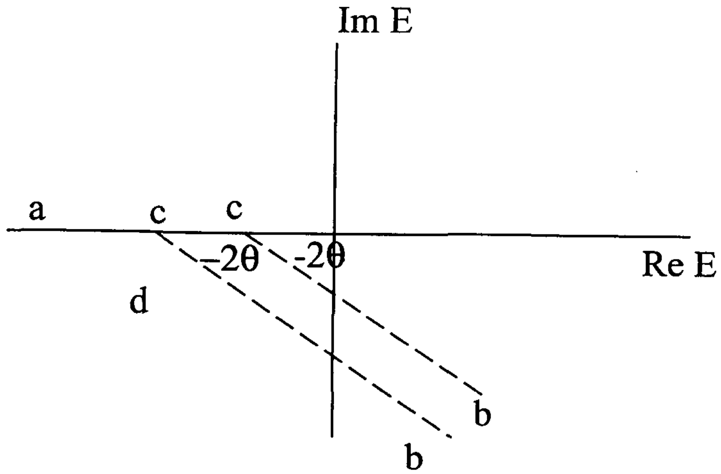

Figure 15.2: The eigenvalue spectrum of the transformed Hamiltonian $H(\theta)$ showing a bound state (a), and the branch cuts at different thresholds. These are shown after a rotation by an angle (-2θ). The point d in the lower half plane is the position of the complex energy pole.

Yukawa potentials $\sum_n \frac{a_n}{r}\exp(-\mu_n r)$. Later this method was applied to the potentials that do not have all of the properties (i)-(v) listed above, e.g. a polynomial in x of the form $\frac{1}{4}x^2 - \lambda x^3$, and the separable potentials. However when the method of dilatation transformation was applied to these interactions, accurate results were obtained for both E_R and Γ. Let us emphasize that the potential with the properties (i)-(v) must vanish in the limit of $r \to \infty$, therefore for the infinite number of continuum states the dominant term in the Hamiltonian is the kinetic energy $Te^{-2i\theta}$, and it is for this reason that we have the rotation of (-2θ) in the complex E-plane. But for a potential like $\frac{1}{4}x^2 - \lambda x^3$ which is divergent as x^3 when $x \to \infty$, the asymptotic form of the continuum states cannot be determined solely by the kinetic energy, but by a balance between the kinetic and the potential energies. Since under rotation these energies rotate in opposite directions (-2θ for kinetic and 3θ for potential) therefore after rotation, the imaginary part of some of the eigenvalues become negative while others become positive.

As a first example for the application of this method let us consider the S-wave scattering for a δ-function potential for which the Schrödinger equation for the radial $u = r\psi$ is

$$\frac{d^2u}{dr^2} + [E - \lambda\delta(r-b)]\,u = 0, \tag{15.10}$$

where we have set $\hbar = 2m = 1$. After rotation Eq. (15.10) becomes

$$e^{-2i\theta}\frac{d^2u}{dr^2} + \left[E - \lambda\delta(re^{i\theta} - b)\right]u = 0. \tag{15.11}$$

The asymptotic form of (15.10) and (15.11) as r tends to infinity, before and after rotation are:

$$u(r) \to C\left[S(E)\exp(i\sqrt{E}r) - \exp(-i\sqrt{E}r)\right], \tag{15.12}$$

and

$$u(r,\theta) \to C\left[S(E)\exp\left(i\sqrt{E}re^{i\theta}\right) - \exp\left(-i\sqrt{E}re^{i\theta}\right)\right]. \tag{15.13}$$

This last relation shows that $u(r,\theta)$ diverges as $r \to \infty$ unless $\sqrt{E}$ is replaced by

$$\sqrt{E} \to ke^{-i\theta}, \tag{15.14}$$

and when this is done then we can write Eq. (15.11) as

$$\frac{d^2u}{dr^2} + \left[k^2 - \lambda e^{i\theta}\delta\left(r - be^{-i\theta}\right)\right]u = 0, \tag{15.15}$$

This equation can be solved to yield

$$u(r) = \begin{cases} A\sin(kr) & \text{for } r < be^{-i\theta} \\ C\left[S(k)e^{ikr} - e^{-ikr}\right] & \text{for } r > be^{-i\theta} \end{cases}, \tag{15.16}$$

Imposing the condition for the continuity of the logarithmic derivative of u at $r = be^{-i\theta}$ we find

$$S(k,\theta) = \frac{N(k,\theta)}{D(k,\theta)} = \exp\left[-2ikbe^{-i\theta}\right]\left\{\frac{ke^{-i\theta}\left[\cot(kbe^{-i\theta}) + i\right] + \lambda}{ke^{-i\theta}\left[\cot(kbe^{-i\theta}) - i\right] + \lambda}\right\}. \tag{15.17}$$

The bound state energy in the E-plane is the point where $S(k,\theta)$ has a pole, i.e. where $D(k,\theta)$ which is the denominator of $S(k,\theta)$ is zero;

$$D(k,\theta) = ke^{-i\theta}\left[\cot\left(kbe^{-i\theta}\right) - i\right] + \lambda = 0. \tag{15.18}$$

To find the eigenvalue equation for the bound state we have to find the analytic continuation of $D(k)$ in the lower half of the k-plane ($k \to -i\gamma$, $\gamma > 0$) [1]. For this purpose we choose $\theta = -\frac{\pi}{2}$ and with this choice (15.18) reduces to [1] [4]

$$D(k, \theta = -\frac{\pi}{2}) = \gamma \coth(\gamma b) + \gamma + \lambda = 0. \tag{15.19}$$

This equation shows that for the presence of a bound state, λ in (15.19) must be negative and that $E = \gamma^2 e^{i\pi} = -\gamma^2$ is the bound state energy. For positive values of λ, we have to solve the two equations:

$$\mathrm{Im}\ \ D(k, \theta) = 0, \tag{15.20}$$

and

$$\mathrm{Re}\ \ D(k, \theta) = 0, \tag{15.21}$$

for k and θ. If we assume that

$$k = k_0 \quad \text{and} \quad \theta = \theta_0, \tag{15.22}$$

is one of the roots of Eqs. (15.20) and (15.21), then the complex number

$$E = k^2 = k_0^2 \exp(-2i\theta_0) = E_R - \frac{i}{2}\Gamma, \tag{15.23}$$

gives us the values of E_R and Γ.

For the second problem we want to determine the decay width for the tunneling of a particle when the Hamiltonian is given by

$$H = -\frac{d^2}{dx^2} + \frac{1}{4}x^2 - \lambda x^3, \quad \lambda > 0. \tag{15.24}$$

For very small λ we can assume that the system is a harmonic oscillator which is perturbed by a small term $-\lambda x^3$. For the positive values of λ the potential in (15.24) has a minimum at $x = 0$ and a maximum at $x = \frac{1}{6\lambda}$, and the height of this maximum is $V_{max} = \frac{5}{216\lambda^2}$. If we choose λ to be equal to 0.0481, then $V_{max} = 1.0005$. Noting that the energy eigenvalues for the unperturbed system is $E_n = n + \frac{1}{2}$ [7], therefore we have a resonance state with the energy $E = \frac{1}{2}$ which is below V_{max}. Because of the sign of λx^3 in the potential, the continuum energy states of the system starts at $E = -\infty$ (like Stark effect), therefore any angle of rotation will show resonant states.

Yaris and collaborators [5] have studied the unperturbed Hamiltonian

$$H_0 = -\frac{d^2}{dx^2} + \frac{1}{4}\Omega^2 x^2, \tag{15.25}$$

and by expanding the eigenfunctions of (15.24) in the basis of harmonic oscillator wave functions (15.25) [7] [8] and then by diagonalization have calculated E_R and Γ. Their results show that with relatively large variations in the values of Ω and θ, the corresponding changes in Γ and E_R are very small. For instance for the sets of parameters ($\Omega = 0.5, \theta = 0.2$), ($\Omega = 0.5, \theta = 0.5$) and ($\Omega = 1, \theta = 0.2$), θ in radians, they have obtained $E_R = 0.4659$ and $\Gamma = 2.28 \times 10^{-3}$.

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Chapter 16

Multidimensional Quantum Tunneling

Quantum tunneling problems in two and three dimensions can be divided into the special cases where the Schrödinger equation is separable in one of the orthogonal coordinate systems [1] and the general case where the wave equation is not separable. For the former groups, as we have seen earlier, the problem is reducible to an effective one-dimensional problem. The non-separable cases are the subject of discussion in this chapter.

We begin this chapter with a brief review of the pioneering approach of Kapur and Peierls [2] which can be regarded as a generalization of the semi-classical (WKB) method. There are other similar works on multi-dimensional tunneling all based on WKB approximation [3] [4] [5] [6] [7] [8]. There are also few exceptional cases where the Schrödinger equation can be solved analytically or numerically [9] [10] [11] [12] [13].

16.1 The Semi-classical Approach of Kapur and Peierls

Suppose a particle of mass m and energy E is moving in a potential $V(x, y, z)$. We want to determine the probability of finding this particle around the point P_1 with the coordinates (x, y, z) when around this point $V(x, y, z)$ is greater than E. In the neighborhood of P_1 we can write the wave function of the particle as

$$\psi = \exp\left(-\frac{S}{\hbar}\right), \tag{16.1}$$

and by substituting this in the Schrödinger equation we find the following equation for S

$$(\nabla S)^2 - \hbar \nabla^2 S = 2m(V - E). \tag{16.2}$$

In general the first term in the left hand side of (16.2) is greater than the second term. Now if $V - E$ is large and its variation with the changing of the coordinate of P_1 is small, then the same conditions will exist for the vector ∇S. Therefore except for those points where the direction of ∇S changes rapidly, the variation of each of the components of ∇S is small and consequently $\nabla^2 S$ will also be small.
If we ignore $\hbar\nabla^2 S$ in (16.2), in the zeroth order of approximation we have

$$(\nabla S)^2 = 2m(V - E), \tag{16.3}$$

which apart from the sign of the right hand side is the Hamilton-Jacobi equation [16] .

It should be noted that S is a complex function and in particular for a free particle with positive kinetic energy S is pure imaginary. If the potential changes discontinuously on the two sides of a given plane, and if the direction of motion of this particle makes an angle with this plane, then the real component of ∇S is perpendicular and its imaginary component is parallel to this plane.
Since $|\psi(x, y, z)|^2 dxdydz$ measures the probability of finding the particle in a volume $dxdydz$ at the point (x, y, z) therefore it is important to find the real part of S accurately.

If we write S as

$$S = \sigma + i\tau, \tag{16.4}$$

where both σ and τ are real function, then from (16.3) we find

$$(\nabla\sigma)^2 = 2m(V - E) + (\nabla\tau)^2, \tag{16.5}$$

and

$$(\nabla\sigma).(\nabla\tau) = 0. \tag{16.6}$$

Noting that in Eq. (16.5) $(\nabla\tau)^2 \geq 0$, hence

$$|\nabla\sigma| \geq \sqrt{2m(V - E)}. \tag{16.7}$$

The equality sign in (16.7) is true only if S is real.

We can determine the probability per unit volume at the point P_1 from Eqs. (16.1) and (16.2)

$$|\psi(P_1)|^2 = \exp\left(-\frac{2\sigma(P_1)}{\hbar}\right), \tag{16.8}$$

where $\sigma(P_1)$ is given by

$$\sigma(P_1) = \sigma(P_0) + \int_{P_0}^{P_1} |\nabla\sigma|\, ds. \tag{16.9}$$

In Eq. (16.9) ds is the line element and the path of integration is along the line of the steepest decent of $(\nabla\sigma)$. The point P_0 just like P_1 must be a point along this line of steepest decent [14] [15] of $\nabla\sigma$, otherwise it is arbitrary. In Eq. (16.9) we follow this line up to the point where the approximation (16.3) is no longer valid. In this part of space where $E > V$, the probability of finding the particle is large. Therefore as long as the point P_1 is not very close to the boundary of this region (i.e. $E = V$), the magnitude of $|\psi|^2$ depends on how σ decreases from P_1 to P_0 which is given by the integral (16.9). In order to calculate this integral and to find the point P_0 we need to know the lines of the steepest decent [14] for the vector $\nabla\sigma$, and this, in general, is not possible unless σ is known. But we can calculate a minimum for this integral. If we evaluate the integral in (16.9) from an arbitrary point P_1 to the end point P_0', where this P_0' is at the boundary of the classically allowed region, $(E > V)$, then there exist a particular path and a point P_0' which gives us the minimum of the integral. Therefore

$$\sigma(P_1) - \sigma(P_0) = \int_{P_0}^{P_1} |\nabla\sigma|\, ds \geq min \int_{P_0'}^{P_1} |\nabla\sigma|\, ds, \tag{16.10}$$

where *min* denotes the minimum of the integral, and is found by choosing the path and the end point. Using Eq. (16.7), we can write (16.10) as

$$\sigma(P_1) - \sigma(P_0) \geq min \int_{P_0'}^{P_1} \sqrt{2m(V-E)}\, ds. \tag{16.11}$$

We can find the path which minimizes the integral from the variational principle [16]

$$\delta \int_{P_0'}^{P_1} \sqrt{2m(V-E)} ds = 0, \tag{16.12}$$

where the upper limit of the integral, P_1, is fixed but P_0' should be varied along this boundary line. From Eq. (16.11) we can find the lower bound for

$\sigma(P_1) - \sigma(P_0)$. But for the general case the difference between this value and the actual minimum is not known. In the exceptional cases where S in the region of interest is real, or in most of the region is real, in Eq. (16.10) we can choose the equality sign. Furthermore in this case the line of the steepest decent for ∇S is found from Eq. (16.12) provided that we do not change the end point P_0'. The line(s) of steepest decent [15] are found from the relation

$$\frac{dx}{ds} = \frac{1}{\sqrt{(\nabla\sigma)^2}}\frac{\partial\sigma}{\partial x}, \tag{16.13}$$

and similar relations for y and z. If S is real then $\sigma = S$ and hence

$$\frac{dx}{ds} = \frac{1}{\sqrt{2m(V-E)}}\frac{\partial\sigma}{\partial x}, \tag{16.14}$$

and again similar equations for y and z. From this last relation it follows that

$$\frac{\partial\sigma}{\partial x} = \sqrt{2m(V-E)}\frac{dx}{ds}, \tag{16.15}$$

and

$$\frac{d}{ds}\left(\frac{\partial\sigma}{\partial x}\right) = \frac{d}{ds}\left\{\sqrt{2m(V-E)}\frac{dx}{ds}\right\}. \tag{16.16}$$

The left hand side of (16.16) can also be written as $\frac{\partial}{\partial x}\left(\frac{d\sigma}{ds}\right)$ which by using (16.7) can be written as

$$\frac{\partial}{\partial x}\sqrt{V-E} = \frac{d}{ds}\left\{\sqrt{(V-E)}\frac{dx}{ds}\right\}, \tag{16.17}$$

and additional equations for y and z. This equation can also be written as [2] [17] [18] [19]

$$2(V-E)\frac{d^2x_i}{ds^2} + \frac{dx_i}{ds}\left(\sum_i \frac{\partial V}{\partial x_i}\frac{dx_i}{ds}\right) = \frac{\partial V}{\partial x_i}, \tag{16.18}$$

where x_1, x_2 and x_3 denote the coordinates x, y and z respectively.

The following example serves to illustrate the role of the imaginary part of S. Let us assume that a particle of mass m moves in a three dimensional space and the potential barrier is only a function of the z coordinate. If the wave function is an eigenstate of the x and y components of the momentum of the particle, we can write it in the following way:

$$\psi(\mathbf{r}) = \phi(z)\exp\left[i(k_x x + k_y y)\right]. \tag{16.19}$$

Now if we replace $\phi(z)$ by its WKB approximate form, then $\psi(\mathbf{r})$ becomes

$$\psi(\mathbf{r}) \approx \exp\left[-\sigma(z) - i\tau\right], \tag{16.20}$$

where

$$\tau = -(k_x x + k_y y). \tag{16.21}$$

From Eq. (16.5) we find the only component of $\nabla\sigma$ to be;

$$\left(\frac{d\sigma}{dz}\right)^2 = 2m\left[V(z) + \frac{1}{2m}(k_x^2 + k_y^2) - E\right]. \tag{16.22}$$

This equation shows that the effective height of the barrier has increased by the amount $[\frac{1}{2m}(k_x^2+k_y^2)]$, therefore the probability of penetration of the particle is smaller than when both k_x and k_y are zero. This example also shows that when $\tau = 0$, the momentum of the particle has at least a nonzero component.

For a somewhat different generalization of the WKB approximation to multidimensional systems and its application in the calculation of lifetime see [20].

16.2 Wave Function for the Lowest Energy State

For the ground state of a particle we can simplify the method of Kapur and Peierls in the following way [21]:

Let us assume that the minimum of the potential $V(\mathbf{r})$ is at the origin $\mathbf{r} = 0$, and at this point $V(0) = 0$. Around this minimum we can expand the potential and write it as a quadratic function of the coordinates

$$V(\mathbf{r}) = \frac{1}{2}\sum_{i,j} V_{ij}x_i x_j, \tag{16.23}$$

where in this relation V_{ij} is a positive matrix [22] with real elements. Next we expand the action S and the energy E in powers of the Planck constant $\hbar$,

$$S = S_0 + \hbar S_1 + \hbar^2 S_2 + \ldots \tag{16.24}$$

and

$$E = E_0 + \hbar\epsilon_1 + \hbar^2\epsilon_2 + \ldots. \tag{16.25}$$

In the classical limit of $\hbar \to 0$, from the value of $V(0) = 0$, it follows that $E_0 = 0$ and thus for very small $\hbar$, the zero point energy is $\hbar\epsilon_1$. If in

Eq. (16.2) we equate the coefficients of $\hbar^0$ and $\hbar$ separately equal to zero we get

$$(\nabla S_0)^2 = 2mV(\mathbf{r}), \tag{16.26}$$

and

$$2(\nabla S_0).(\nabla S_1) = (\nabla S_0)^2 - 2m\epsilon_1. \tag{16.27}$$

By solving these equations and making use of Eq. (16.1) we find the approximate wave function:

$$\psi(\mathbf{r}) = \exp\left[-S_1(r)\right]\exp\left[-\frac{S_0(r)}{\hbar}\right]. \tag{16.28}$$

These equations can be solved for a multidimensional simple harmonic oscillator. In this case the solution of Eq. (16.26) is

$$S_0 = \frac{1}{2}\sum_{i,j} B_{ij}x_ix_j, \tag{16.29}$$

where B_{ij} is the positive root of the matrix mV_{ij}.

If S_1 is a constant and is a solution of Eq. (16.27) then ϵ_1 must satisfy the relation

$$E = \hbar\epsilon_1 = \frac{\hbar}{2m}\sum_i B_{ii}. \tag{16.30}$$

We note that since the matrix B_{ij} is a positive matrix [22], then from Eq. (16.28) the boundary condition $\psi(\mathbf{r} \to \infty) \to 0$ is automatically satisfied. Let us consider a potential which, around $\mathbf{r} = 0$, has the form of a simple harmonic potential but is arbitrary otherwise. We can use Kapur and Peierls formalism to find S, but this problem is simpler from the general case for the following reasons:

(i) - The wave function for the ground state is real, therefore S_0 is also real and in Eq. (16.7) the equality sign should be used.

(ii) - The point P_0' the lower limit of the integral in (16.11) can change in the boundary $V = E$, and as Eq. (16.23) shows this point is at the origin of the coordinate system.

These two simplifying conditions yield the following wave function in the WKB approximation

$$\psi(\mathbf{r}) = \mathcal{N}\exp\left[-S_1\right]\exp\left[-\frac{1}{\hbar}\int_C \sqrt{2mV}ds\right]. \tag{16.31}$$

The path of the line integral in (16.31) is along the line of the steepest decent of ∇S_0 from the origin to the point $\mathbf{r}$, i.e. at each point of C the direction of ∇S_0 is parallel to C.

As it was discussed earlier the equations for the trajectory which gives us the minimum for the integral in(16.12) are:

$$m\frac{d^2x_j}{dt^2} = \frac{\partial V}{\partial x_j} \tag{16.32}$$

and

$$\sum_j \frac{1}{2}m\left(\frac{dx_j}{dt}\right)^2 - V = 0. \tag{16.33}$$

These are the classical equations of motion for the inverted potential $(-V)$.

Once S_0 is determined from (16.26), we can calculate S_1 from the equation

$$S_1 = \int_C \left[\frac{\nabla^2 S_0 - 2m\epsilon_1}{2\sqrt{2mV}}\right] ds. \tag{16.34}$$

We note that the denominator of the integrand in (16.34) is zero at the origin, therefore for S_1 to be a well-defined function at $\mathbf{r} = 0$, the expression $\nabla^2 S_0 - 2m\epsilon_1$ must vanish.

For the harmonic oscillator that we studied earlier this condition is the same as (16.27). The normalization constant $\mathcal{N}$ in (16.31) can be found from the integral $\int |\psi|^2 d^3r = 1$. For some of the applications of the semi-classical theory of multi-dimensional tunneling to nuclear physics the reader is referred to the papers [23] [24] [25].

16.3 Calculation of the Low-Lying Wave Functions by Quadrature

A method very similar to what we have discussed in the previous section is formulated by Friedberg *et al* [26] [27] for determination of the eigenvalues and wave functions of the motion of a particle in N-dimensions. We start with the Hamiltonian

$$H = -\frac{1}{2m}\nabla^2 + g^2 v(\mathbf{r}), \tag{16.35}$$

where g^2 is the strength of the barrier (or scale factor). We assume that $v(\mathbf{r}) \geq 0$ for all $\mathbf{r}$ values. We write the wave function which now depends on the parameter g, for large g as

$$\psi(\mathbf{r}) = \exp\left[-gS(g,\mathbf{r})\right]. \tag{16.36}$$

Next we expand both $gS(g,\mathbf{r})$ and the eigenvalue $E(g)$ in powers of g;

$$gS(g,\mathbf{r}) = gS_0(\mathbf{r}) + S_1(\mathbf{r}) + \frac{1}{g}S_2(\mathbf{r}) + \frac{1}{g^2}S_3(\mathbf{r}) + \dots.. \tag{16.37}$$

and

$$E = gE_0 + E_1 + \frac{1}{g}E_2 + \frac{1}{g^2}E_3 + \dots... \tag{16.38}$$

Substituting (16.36) and (16.37) in the Schrödinger equation $H\psi(\mathbf{r}) = E\psi(\mathbf{r})$ and equating the coefficients of g^{-n} on both sides we find the following set of equations:

$$(\nabla S_0)^2 = 2v(\mathbf{r}), \tag{16.39}$$

$$\nabla S_0.\nabla S_1 = \frac{1}{2}\nabla^2 S_0 - E_0, \tag{16.40}$$

$$\nabla S_0.\nabla S_2 = \frac{1}{2}\left[\nabla^2 S_1 - (\nabla S_1)^2\right] - E_1, \tag{16.41}$$

and so on.

For a harmonic oscillator potential $v(\mathbf{r}) \approx \frac{1}{2}\mathbf{r}^2$ and the ground state wave function will be proportional to $\exp\left[-\frac{1}{2}gr^2\right]$. Thus the parameter g^{-1} indicates the anharmonicity of the potential.
We write Eq. (16.39) as

$$\frac{1}{2}(\nabla S_0)^2 - v(\mathbf{r}) = e = 0+. \tag{16.42}$$

In general the potential $v(\mathbf{r})$ can have several minima at the points

$$\mathbf{r} = \mathbf{0}, \mathbf{a}_1, \mathbf{a}_2 \dots\dots \mathbf{a}_n, \tag{16.43}$$

and we assume that at these points

$$v(\mathbf{0}) = v(\mathbf{a}_1) = v(\mathbf{a}_2) = \dots\dots.. = 0. \tag{16.44}$$

Consider the case where $v(\mathbf{r})$ has a minimum at $\mathbf{r} = 0$, and that $v(\mathbf{0}) = 0$. For the trajectory $\mathbf{r}(t)$ which begins at $\mathbf{r} = 0$ when $t = 0$ and ends at $\mathbf{r}_{\mathcal{T}}$ when $t = \mathcal{T}$

$$\mathbf{r}(0) = 0 \quad \text{and} \quad \mathbf{r}(\mathcal{T}) = \mathbf{r}_{\mathcal{T}}, \tag{16.45}$$

we have the action integral

$$S_0\left(\mathbf{r}_{\mathcal{T}}, e\right) = \int_0^{\mathcal{T}} \left[\frac{1}{2}\left(\frac{d\mathbf{r}}{dt}\right)^2 - (-v(\mathbf{r}))\right] dt + \mathcal{T}e. \tag{16.46}$$

Here

$$\mathcal{T} = \left(\frac{\partial S_0}{\partial e}\right)_{\mathbf{r}_{\mathcal{T}}}, \tag{16.47}$$

is the time that takes the classical particle to move from the origin to $\mathbf{r}_{\mathcal{T}}$.

Since $-v(\mathbf{r}) \le 0$, the integrand in (16.46) is positive everywhere. As e tends to zero, $\frac{d\mathbf{r}}{dt}$ goes to zero as $\sqrt{e}$, and the total time goes to infinity as $\frac{1}{\sqrt{e}}$, hence

$$\lim_{e\to 0} \mathcal{T}e \to 0, \tag{16.48}$$

and $S_0(\mathbf{r}_{\mathcal{T}}, 0)$ will be equal to the integral in (16.46) evaluated along the classical trajectory

$$\frac{d^2\mathbf{r}}{dt^2} = \nabla v(\mathbf{r}). \tag{16.49}$$

If we take the energy e along the trajectory to be positive then the velocity will continue in its original direction when the particle passes through other minima, $\mathbf{r} = \mathbf{a}_i$. Thus in the limit of $e \to 0$, ∇S_0 becomes zero at $\mathbf{r} = \mathbf{a}_i$, but the sign of $\frac{d\mathbf{r}}{dt}$ remains the same before and after leaving the point $\mathbf{a}_i$. This means that ∇S_0 will have kinks at $\mathbf{r} = \mathbf{a}_i$. At $\mathbf{r} = 0$, $v(0) = 0$ therefore $\nabla S_0 = 0$ as $e \to 0$, and $S_0(\mathbf{r})$ is analytic since trajectories emanating from $\mathbf{r} = 0$ move in different directions.

We note that for $\mathbf{r} \to \infty$ and $e \to 0$, $\mathcal{T} \to \infty$ and since the quantity in the square bracket in Eq. (16.46) can be zero only at a finite number of points, therefore $S_0(\mathbf{r} \to \infty)$ will go to infinity.

Having found $S_0(\mathbf{r})$, we introduce a new function $\zeta(\mathbf{r})$ by

$$\zeta(\mathbf{r}) = gS(\mathbf{r}) - gS_0(\mathbf{r}) = S_1(\mathbf{r}) + \frac{1}{g}S_2(\mathbf{r}) + \frac{1}{g^2}S_3(\mathbf{r}) + \ldots\ldots, \tag{16.50}$$

then we can write the ground state wave function $\psi(\mathbf{r})$ as

$$\psi(\mathbf{r}) = \exp\left[-gS_0(\mathbf{r}) - \zeta(\mathbf{r})\right]. \tag{16.51}$$

Substituting this in the Schrödinger equation, $H\psi = E\psi$, we find

$$g\nabla S_0.\nabla\zeta = \frac{1}{2}\left[g\nabla^2 S_0 + \nabla^2\zeta - (\nabla\zeta)^2\right] - E. \tag{16.52}$$

From Eq. (16.39) and the fact that $v(0) = 0$ it follows that at $\mathbf{r} = 0$ $\nabla S_0(0) = 0$, and the left hand side of (16.52) is zero.

Assuming $\nabla\zeta$ to be regular we have

$$E = \frac{1}{2}\left[g\nabla^2 S_0 + \nabla^2\zeta - (\nabla\zeta)^2\right]_{\mathbf{r}=0}. \tag{16.53}$$

If we expand both sides of (16.53) using (16.37) and (16.38) we find Eqs. (16.39)-(16.41) for $E_0, E_1 \dots$.

$$E_0 = \frac{1}{2}\left(\nabla^2 S_0\right)_{\mathbf{r}=0}, \tag{16.54}$$

$$E_1 = \frac{1}{2}\left[\nabla^2 S_1 - (\nabla S_1)^2\right]_{\mathbf{r}=0}, \tag{16.55}$$

etc.

For calculating $S_1(\mathbf{r})$ we observe that the general solution of the Hamilton-Jacobi equation (16.39) is of the form [16]

$$S_0 = S_0\left(r, \theta, \phi; \alpha_\theta, \alpha_\phi\right), \tag{16.56}$$

where the classical path is given by

$$\theta_0 = \frac{\partial S_0(\mathbf{r}, \alpha)}{\partial \alpha_\theta}, \quad \text{and} \quad \phi_0 = \frac{\partial S_0(\mathbf{r}, \alpha)}{\partial \alpha_\phi}. \tag{16.57}$$

In these equations we have written $S_0(\mathbf{r}, \alpha_\theta, \alpha_\phi)$ as $S_0(\mathbf{r}, \alpha)$. From (16.40) it follows that S_1 is a function of S_0 and α, i.e. $S_1(S_0, \alpha)$, and this S_1 is a solution of

$$(\nabla S_0)^2 \left(\frac{\partial S_1}{\partial S_0}\right)_\alpha = \frac{1}{2}\nabla^2 S_0 - E_0. \tag{16.58}$$

This equation can be integrated to yield

$$S_1(\mathbf{r}, \alpha) = S_1(S_0, \alpha) = \int_0^{S_0} \frac{\left[\frac{1}{2}\nabla^2 S_0 - E_0\right]}{(\nabla S_0)^2}\, dS_0, \tag{16.59}$$

where the integration is carried out along the classical trajectory of $\alpha =$ constant. Similarly from (16.41) we have

$$S_2(\mathbf{r}, \alpha) = S_2(S_0, \alpha) = \int_0^{S_0} \frac{\left[\frac{1}{2}\left(\nabla^2 S_1 - (\nabla S_1)^2\right) - E_1\right]}{(\nabla S_0)^2}\, dS_0. \tag{16.60}$$

The iterative solutions given by Eq. (16.52) can be continued to arbitrary order and the ground state energy E and the wave function

$\exp[-gS(\mathbf{r}, g)]$ can be calculated to desired accuracy. Friedberg *et al* have shown how this method can be used for the calculation of the wave function and the energy levels of the ground as well as the excited states [27]. As an example of this method let us consider the one-dimensional problem for the symmetric double-well potential where the Hamiltonian is given by

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}g^2\left(x^2 - a^2\right)^2. \tag{16.61}$$

Let us denote the two lowest eigenfunctions of (16.61) for even and odd states by $\psi_S(x)$ and $\psi_A(x)$ respectively with the corresponding eigenvalues E_S and E_A. Also let us define the left and right wave packets $\psi_+(x)$ and $\psi_-(x)$ by

$$\psi_\pm = \frac{1}{\sqrt{2}}\left[\psi_A(x) \pm \psi_S\right]. \tag{16.62}$$

Now if $\mathcal{E}$ and Δ are given by

$$\mathcal{E} = \frac{1}{2}\left(E_A + E_S\right), \quad \text{and} \quad \Delta = \frac{1}{2}\left(E_A - E_S\right), \tag{16.63}$$

then from the Hamiltonian (16.61) and Eqs. (16.62) and (16.63) we find the following relations:

$$(H - \mathcal{E})\,\psi_\pm(x) = -\Delta\psi_\mp(x), \tag{16.64}$$

and

$$\frac{d}{dx}\left[\psi_- \frac{d\psi_+}{dx} - \psi_+\frac{d\psi_-}{dx}\right] = 2\Delta(\psi_-^2 - \psi_+^2). \tag{16.65}$$

The wave function (16.36) for this case can be written as

$$\psi(x) = \exp\left[-gS(x, g)\right], \tag{16.66}$$

where $gS(x, g)$ can be expanded in powers of g^{-1}, Eq. (16.37). To the zeroth order from Eq. (16.39) we find

$$S_0(+) = \exp\left[-g\left(\frac{x^3}{3} + \frac{2a^3}{3} - a^2x\right)\right], \tag{16.67}$$

and

$$S_0(-) = \exp\left[-g\left(-\frac{x^3}{3} + \frac{2a^3}{3} + a^2x\right)\right]. \tag{16.68}$$

Higher order terms in the expansion can be calculated from Eqs. (16.40) and (16.41). To the zeroth order, we can set Δ in Eqs. (16.64) and (16.65) equal to zero and use (16.64) to find $\mathcal{E} = ga$. For calculating higher order terms we use the expansions [26]

$$\mathcal{E} = ga \sum_{m=0,n=0} C_{m,n} \left(ga^3\right)^{-m} \exp\left(-\frac{4}{3}nga^3\right), \tag{16.69}$$

and

$$\Delta = 4\left(\frac{2}{\pi}g^3a^5\right)^{\frac{1}{2}} \sum_{m=0,n=1} D_{mn} \left(ga^3\right)^{-m} \exp\left(-\frac{4}{3}nga^3\right). \tag{16.70}$$

These together with $S_1(\pm)$, $S_2(\pm)$.... and Eqs. (16.64) and (16.65) give us the coefficients C_{mn} and D_{mn} of the expansions (16.69) and (16.70). Thus

$$\mathcal{E} \approx ga - \frac{1}{4a^2} + \frac{9}{2^6}\frac{1}{ga^3} + \ldots., \tag{16.71}$$

and

$$\Delta \approx 4\left(\frac{2}{\pi}g^3a^5\right)^{\frac{1}{2}} \exp\left(-\frac{4}{3}ga^3\right). \tag{16.72}$$

If we choose $a = \frac{5}{\sqrt{2}}$ and $g = \frac{2\sqrt{2}}{25}$, then from Eqs. (16.71) and (16.72) we find $E_S = 0.381$ and $E_A = 0.388$. These should be compared to the exact results of $E_S = 0.374$ and $E_A = 0.380$.

16.4 Method of Quasilinearization Applied to the Problem of Multidimensional Tunneling

As an introduction to the method of quasilinearization [28] let us study the solution of the nonlinear classical Hamilton-Jacobi equation in one dimension.

We start with the equation [16]

$$\left(\frac{dS}{dx}\right)^2 = k^2 - v(x) - \varepsilon w(x) = q^2 - \varepsilon w(x), \tag{16.73}$$

where S is the Hamilton characteristic function [16], k^2 is the energy of the particle and $v(x) - \varepsilon w(x)$ is the potential acting on the particle. Here $v(x)$ is the major part of the potential and $\varepsilon w(x)$ is a small perturbation.

Instead of solving (16.73) directly, which we can do, we consider a set of linear differential equations:

$$2\left(\frac{dS_n}{dx}\right)\left(\frac{dS_{n-1}}{dx}\right)-\left(\frac{dS_{n-1}}{dx}\right)^2=q^2-\varepsilon w(x),\quad n=1,2,.... \tag{16.74}$$

so that in the limit of $n\to\infty$, the function $S_n(x)$ tends to $S(x)$ of Eq. (16.73) [28] [29]. In order to solve the set of equations (16.74), we start with the equation for S_0,

$$\left(\frac{dS_0}{dx}\right)^2=k^2-v(x), \tag{16.75}$$

then from Eq. (16.74) we calculate $\left(\frac{dS_1}{dx}\right),......\left(\frac{dS_n}{dx}\right)$:

$$\left(\frac{dS_1}{dx}\right)=\left(\frac{dS_0}{dx}\right)-\left(\frac{\varepsilon w(x)}{2q(x)}\right), \tag{16.76}$$

$$\left(\frac{dS_2}{dx}\right)=\left(\frac{dS_1}{dx}\right)-\left(\frac{\varepsilon^2 w^2(x)}{8q(x)[q^2(x)-\frac{1}{2}\varepsilon w(x)]}\right), \tag{16.77}$$

$$\begin{aligned}\left(\frac{dS_3}{dx}\right)&=\left(\frac{dS_2}{dx}\right)\\ &+\left(\frac{\varepsilon^4 w^4(x)}{128q(x)[q^2(x)-\frac{1}{2}\varepsilon w(x)][(q^2(x)-\frac{1}{2}\varepsilon w(x))^2-\frac{\varepsilon^2 w^2}{8}]}\right),\end{aligned} \tag{16.78}$$

and so on.

If we compare this expansion of $S_n(x)$ and the expansion of $\left(\frac{dS}{dx}\right)$ as a power series in ε we find that the expansion of S_n converges faster than the power series.

Now let us apply this method to the solution of the problem of tunneling in two dimensions. A similar technique can be used for a general three-dimensional tunneling.

We will use the units where the mass of the particle is $\frac{1}{2}$ and $\hbar=1$. If in the polar coordinates (r,ϕ) the potential barrier is just a function of r, then the Schrödinger equation for the radial part of the wave function is

$$\frac{d^2u}{dr^2}+\left[k^2-v_e(r)\right]u(r)=0,\quad v_e(r)=v(r)+\frac{m^2-\frac{1}{4}}{r^2}. \tag{16.79}$$

In Eq. (16.79) m is an integer which appears in the radial part by separating the ϕ coordinate. If the barrier has a range R so that $v(r>R)=$

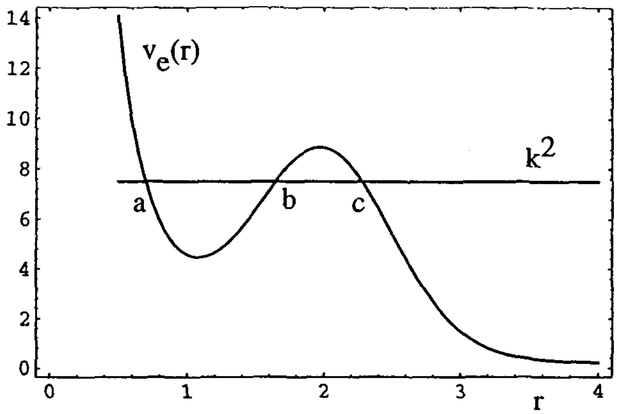

Figure 16.1: The effective radial potential $v_e(r) = v(r) + \frac{m^2 - \frac{1}{4}}{r^2}$, and the energy of the particle k^2. The turning points are a, b and c.

0, then $u(r)$ can be found from the solution of (16.79) with the boundary conditions

$$u(r=0) = 0, \tag{16.80}$$

and

$$\left(\frac{1}{u}\frac{du}{dr}\right)_{r=R} = \left(\frac{d}{dr}\ln\left[\sqrt{r}H_m^{(1)}(kr)\right]\right)_{r=R}. \tag{16.81}$$

The function $H_m^{(1)}(kr)$ is the Hankel function of order m [30]. For a simple barrier in two dimensions usually there are three turning points which we denote by a, b and c ($c > b > a$, (see Fig. 16.1)). As we have seen in Chapter 3 the semi-classical approximation can be applied to this problem, and we first solve the problem using the WKB approximation. There are four parts to the wave function in the four regions;

$$u_1(r) = \frac{C}{\sqrt{K_0(r)}}\sinh\left[\int_0^r K_0(r)dr\right], \quad r < a, \tag{16.82}$$

$$u_2(r) = \frac{2D}{i\sqrt{K_0(r)}}\left(e^L - \frac{1}{4}e^{-L}\right)\exp\left\{i\left(\int_r^b K_0(r)dr - \frac{\pi}{4}\right)\right\}$$

$$+ \frac{2D}{i\sqrt{K_0(r)}}\left(e^L + \frac{1}{4}e^{-L}\right)\exp\left\{-i\left(\int_r^b K_0(r)dr - \frac{\pi}{4}\right)\right\},$$
$$a < r < b, \tag{16.83}$$

$$\begin{aligned} u_3(r) &= \frac{D}{\sqrt{\mathcal{K}_0(r)}}\left[e^{-L}\exp\left\{\int_b^r \mathcal{K}_0(r)dr\right\}\right. \\ &- \left. 2ie^L \exp\left\{-\int_b^r \mathcal{K}_0(r)dr\right\}\right], \quad b < r < c, \end{aligned} \tag{16.84}$$

and

$$u_4(r) = \frac{2D}{\sqrt{K_0(r)}}\exp\left[i\left(\int_c^r K_0(r)dr - \frac{\pi}{4}\right)\right], \quad r > c, \tag{16.85}$$

where in these equations C and D are constants and the phase $\left(\frac{-i\pi}{4}\right)$ comes from the WKB connection formula of Chapter 3 . The functions $K_0(r)$, $\mathcal{K}_0(r)$ and the constant L are defined by the following relations;

$$K_0(r) = \left[k^2 - v(r) - \frac{m^2 - \frac{1}{4}}{r^2}\right]^{\frac{1}{2}}, \tag{16.86}$$

$$\mathcal{K}_0(r) = \left[v(r) + \frac{m^2 - \frac{1}{4}}{r^2} - k^2\right]^{\frac{1}{2}}, \tag{16.87}$$

and

$$L = \int_b^c \mathcal{K}_0(r)dr. \tag{16.88}$$

If k^2 is known, then Eqs. (16.82)-(16.85) which satisfy the WKB conditions for matching at b and c will determine the wave function for all radial distances $r > c$.
At the first turning point $r = a$ the logarithmic derivatives of u_1 and u_2 should be equal, viz,

$$\Lambda = \frac{1}{ku_1(a)}\left(\frac{du_1(r)}{dr}\right)_{r=a} = \frac{1}{ku_2(a)}\left(\frac{du_2(r)}{dr}\right)_{r=a}. \tag{16.89}$$

This equation will be the eigenvalue equation for the complex discrete k^2 values. We can also write it as

$$e^{2L} = \left(\frac{i}{4}\right)\frac{[(\beta^2 - \Lambda^2)\cos(2\delta) + 2\Lambda\beta\sin(2\delta)]}{[(\beta^2 + \Lambda^2) + (\Lambda^2 - \beta^2)\sin(2\delta) + 2\Lambda\beta\cos(2\delta)]}, \tag{16.90}$$

where δ, β and Λ are given by

$$\delta = \int_a^b K_0(r)dr, \tag{16.91}$$

$$\beta = \frac{1}{k}K_0(a), \tag{16.92}$$

and

$$\Lambda = \frac{1}{k}\mathcal{K}_0(a)\coth\left[\int_0^a \mathcal{K}_0(r)dr\right]. \tag{16.93}$$

Now we want to solve this problem using the method of quasilinearization assuming that the potential is discontinuous at a, b and c, and thus the turning points for tunneling are independent of the energy.

We write the wave function for $r > c$ as

$$u_4(r) = \frac{1}{\sqrt{K(r)}}\exp\left[i\left(\int K(r)dr - \frac{\pi}{4}\right)\right], \quad r > c, \tag{16.94}$$

and substitute it in the Schrödinger equation (16.79), and thus find the nonlinear equation for $K(r)$;

$$\frac{1}{2K}\left(\frac{d^2K}{dr^2}\right) - \frac{3}{4K^2}\left(\frac{dK}{dr}\right)^2 + K^2 - K_0^2(r) = 0. \tag{16.95}$$

If K changes vary slowly as a function of r, then from (16.95) we conclude that $K \approx K_0(r)$ and this is the same result that we found from WKB approximation. Using the method of quasilinearization we can write Eq. (16.95) in the approximate form

$$\begin{aligned}&\frac{1}{2K_{n-1}}\left(\frac{d^2K_{n-1}}{dr^2}\right) - \frac{3}{4K_{n-1}^2}\left(\frac{dK_{n-1}}{dr}\right)^2 \\ + \quad &2K_nK_{n-1} - K_{n-1}^2 - K_0^2(r) = 0,\end{aligned} \tag{16.96}$$

and then by choosing

$$K_{n=0} = K_0(r), \tag{16.97}$$

from (16.96) we can find $K_1(r)$;

$$K_1(r) = K_0(r) + \left(\frac{1}{8K_0^3}\right)\frac{d^2v_e}{dr^2} + \left(\frac{5}{32K_0^5}\right)\left(\frac{dv_e}{dr}\right)^2, \tag{16.98}$$

where $v_e(r)$ is the effective potential, Eq. (16.79). In the same way for the wave function under the barrier we find two functions $u_\pm(r)$, and from their linear combination we find $u_3(r)$,

$$u_\pm(r) = \frac{1}{\sqrt{\mathcal{K}(r)}} \exp\left[\pm \int \mathcal{K}(r)dr\right], \tag{16.99}$$

where $\mathcal{K}(r)$ is a solution of the equation

$$\frac{1}{2\mathcal{K}}\left(\frac{d^2\mathcal{K}}{dr^2}\right) - \frac{3}{4\mathcal{K}^2}\left(\frac{d\mathcal{K}}{dr}\right)^2 - \mathcal{K}^2 - \mathcal{K}_0^2(r) = 0. \tag{16.100}$$

We can use the method of quasilinearization to solve (16.100) as we did for (16.95).

16.5 Solution of the General Two-Dimensional Problems

We can apply the method of quasilinearization to the general case where the potential is noncentral and is a function of the radial as well as angular coordinates. Here we will consider the two-dimensional tunneling of a particle through a barrier given by $v(r,\phi)$. The Schrödinger equation for this case is written as

$$\nabla^2\psi + \left[k^2 - v(r,\phi)\right]\psi = 0. \tag{16.101}$$

Now if we replace ψ by S where

$$\psi = \exp(iS), \quad \hbar = 1, \tag{16.102}$$

and substitute in (16.101) we find the nonlinear equation

$$(\nabla S)^2 - \left[k^2 - v(r,\phi)\right] - i\nabla^2 S = 0. \tag{16.103}$$

Applying the technique of quasilinearization, we write for (16.103) the set of linear equations

$$2(\nabla S_n . \nabla S_{n-1}) = \left[k^2 - v(r,\phi)\right] + i\left(\nabla^2 S_{n-1}\right) + (\nabla S_{n-1})^2, \quad n = 1,2,3... \tag{16.104}$$

We observe that the function $S(r,\phi)$ is the limit of $S_n(r,\phi)$ when n tends to infinity. Equation (16.104) shows that in the classical limit when $\nabla^2 S_{n-1}$ can be ignored, we have a quasilinearized form of the Hamilton-Jacobi equation.

This equation, in general, is not separable and we cannot write it as the sum of two terms $S_n(r,\phi) = S_n^{(1)}(r) + S_n^{(2)}(\phi)$. In addition, in this limit, S_n is not a real function since k^2 is complex. For solving Eqs. (16.104) we first calculate the angular average of $v(r,\phi)$, and assume that it is not zero,

$$\bar{v}(r) = \frac{1}{2\pi}\int_0^{2\pi} v(r,\phi)d\phi. \tag{16.105}$$

We also note that for the potential $\bar{v}(r)$, S_0 which satisfies the equation

$$(\nabla S_0)^2 = k^2 - \bar{v}(r), \tag{16.106}$$

is separable and has a solution of the form

$$S_0(r,\phi) = \nu\phi \pm \int K_0(\nu, r)dr, \tag{16.107}$$

where ν is the separation constant and

$$K_0(\nu, r) = \left[k^2 - \bar{v}(r) - \left(\frac{\nu}{r}\right)^2\right]^{\frac{1}{2}}. \tag{16.108}$$

The classical path of the particle in this approximation is [16]

$$\frac{\partial S_0(r\phi)}{\partial \nu} = \phi_0 = \phi - (\pm)\int \frac{\nu dr}{r^2 K_0(\nu, r)}. \tag{16.109}$$

Here ϕ_0 is a constant. We need the two relations (16.107) and (16.109) as the starting solutions for this approximation. In the n-th order we assume that $S_{n-1}(r,\phi)$ is known and we want to find $S_n(r,\phi)$. Using the method of characteristics [31] [32] we find the solution of (16.104) to be given by

$$\frac{dr}{\left(\frac{\partial S_{n-1}}{\partial r}\right)} = \frac{r^2 d\phi}{\left(\frac{\partial S_{n-1}}{\partial \phi}\right)} = \frac{2dS_n}{[k^2 - v(r,\phi(r)) + (\nabla S_{n-1})^2 + i(\nabla^2 S_{n-1})]}. \tag{16.110}$$

From these equations we find $\phi(r)$ and $S_n(r,\phi)$. Thus in the n-th order of approximation the path of the particle is found from the solution of the differential equation

$$\frac{d\phi}{dr} = \frac{1}{r^2\left(\frac{\partial S_{n-1}}{\partial r}\right)}\left(\frac{\partial S_{n-1}}{\partial \phi}\right). \tag{16.111}$$

By integrating these equations we find $\phi(r)$ and then by substituting $\phi(r)$ in $v(r,\phi)$, we can determine $S_n(r)$ from (16.104)

$$S_n = \frac{1}{2}\int \left(\frac{\partial S_{n-1}}{\partial r}\right)^{-1} \left[k^2 - v(r,\phi(r)) + (\nabla S_{n-1})^2 + i\left(\nabla^2 S_{n-1}\right)\right] dr. \tag{16.112}$$

If we repeat this process we find S_{n+1}, $S_{n+2}\dots.$ successively.

As an example, let us consider the calculation of S in the first order for a problem with three turning points, and as before we denote these points by a, b and c. In the region where the energy of the particle is greater than the height of the barrier, i.e.

$$\mathrm{Re}\, k^2 \geq \bar{v}(r) + \left(\frac{\nu^2}{r^2}\right), \tag{16.113}$$

we use the symbol S_0^I, and for the range of r values where

$$\mathrm{Re}\, k^2 \leq \bar{v}(r) + \left(\frac{\nu^2}{r^2}\right), \tag{16.114}$$

we use the symbol S_0^{II}. In these regions we find the following expressions for S_0^I and S_0^{II};

$$S_0^I(r,\phi) = \nu\phi \pm \int K_0(\nu,r)dr, \tag{16.115}$$

and

$$S_0^{II}(r,\phi) = \nu\phi \pm i\int \mathcal{K}_0(\nu,r)dr. \tag{16.116}$$

Using these we calculate the Laplacian of S_0^I and S_0^{II},

$$\nabla^2 S_0^I = \pm\left(\frac{dK_0}{dr} + \frac{K_0}{r}\right), \tag{16.117}$$

and

$$\nabla^2 S_0^{II} = \pm\left(\frac{d\mathcal{K}_0}{dr} + \frac{\mathcal{K}_0}{r}\right). \tag{16.118}$$

From Eqs. (16.113)-(16.116) and Eq. (16.104) we find S_1^I and S_1^{II} to be

$$S_1^I(r,\phi) = \pm\int Q_0^I(\nu,r)dr + \nu\phi + \left(\frac{i}{2}\right)\ln(rK_0), \tag{16.119}$$

and

$$S_1^{II}(r,\phi) = \pm i\int Q_0^{II}(\nu,r)dr + \nu\phi + \left(\frac{i}{2}\right)\ln(r\mathcal{K}_0), \tag{16.120}$$

where $Q_0^I(\nu, r)$ and $Q_0^{II}(\nu, r)$ are defined by

$$Q_0^I(\nu, r) = K_0(\nu, r) + \frac{[\bar{v}(r) - v(r, \phi(r))]}{2K_0(\nu, r)}, \tag{16.121}$$

and

$$Q_0^{II}(\nu, r) = K_0(\nu, r) - \frac{[\bar{v}(r) - v(r, \phi(r))]}{2K_0(\nu, r)}. \tag{16.122}$$

Thus from Eqs. (16.119) and (16.120) we find $S_1^I(r, \phi)$ to be;

$$S_1^I(r, \phi) = \pm \int K_0(\nu, r) dr + \nu\phi$$
$$+ \left(\frac{1}{2\nu}\right) \int [\bar{v}(r(\phi)) - v(r(\phi), \phi)]\, r^2(\phi) d\phi + \left(\frac{i}{2}\right) \ln(rK_0), \tag{16.123}$$

and we find a similar relation for $S_1^{II}(r, \phi)$. Up to this point we have assumed ν to be an arbitrary parameter. Now we impose the condition of single-valuedness on $\psi(r, \phi)$ and hence on $S(r, t)$. Noting that $\psi = \exp(iS)$, and that S is given either by (16.119) or by (16.120), we conclude that

$$\nu = m, \quad \text{where } m \text{ is an integer or zero}, \tag{16.124}$$

and this is the case whether the motion is over or is under the barrier.

There is another way that we can impose this condition on $\psi(r, \phi)$. For this we express the angular dependence of ψ in terms of $\Phi(\phi)$ where

$$\Phi(\phi) = \exp\left\{ i\nu\phi + \left(\frac{i}{2\nu}\right) \int [\bar{v}(r(\phi)) - v(r(\phi), \phi)]\, r^2(\phi) d\phi \right\}. \tag{16.125}$$

Then the uniqueness of the wave function implies that

$$\Phi(\phi) = \Phi(\phi + 2n\pi), \quad n \text{ is an integer}. \tag{16.126}$$

The eigenvalues ν the roots of Eq. (16.126) are different from $\nu = m$, Eq. (16.124), since they belong to two different approximate forms of $\psi(r, \phi)$. If the potential $\bar{v}(r)$ in (16.105) changes very rapidly as a function of r, say like a δ-function, we can use Eq. (16.104) but with a small modification. In this case for the starting function we use S_0 which is the solution of

$$(\nabla S_0)^2 - \left[k^2 - \bar{v}(r)\right] - i\nabla^2 S_0 = 0, \tag{16.127}$$

where this S_0 is directly found from the solution of the Schrödinger equation (16.101) and (16.102)

$$S_0 = m\phi - i \ln\left\{\frac{u(m,r)}{\sqrt{r}}\right\}. \tag{16.128}$$

If we substitute (16.128) in (16.110), we find $\phi(r)$ and $S_1(r)$ as the following integrals

$$\phi(r) = i\int^r \frac{m}{r^2 \frac{d}{dr}\left\{\ln\left(\frac{u(m,r)}{\sqrt{r}}\right)\right\}} dr, \tag{16.129}$$

and

$$S_1(r) = i\int^r \frac{\left\{i\nabla^2 S_0 + k^2 - \bar{v}(r) + \frac{1}{2}[\bar{v}(r) - v(r,\phi(r))]\right\}}{\frac{d}{dr}\left\{\ln\left(\frac{u(m,r)}{\sqrt{r}}\right)\right\}} dr. \tag{16.130}$$

We can simplify (16.130) by eliminating $k^2 - \bar{v}(r)$ between (16.127) and (16.130) and thus find $S_1(r,\phi)$ as

$$S_1(r,\phi) = S_0(r,\phi) + \left(\frac{i}{2}\right)\int^r \frac{[\bar{v}(r) - v(r,\phi(r))]}{\frac{d}{dr}\left\{\ln\left(\frac{u(m,r)}{\sqrt{r}}\right)\right\}} dr. \tag{16.131}$$

16.6 The Most Probable Escape Path

In the method of Kapur and Peierls we imposed two conditions that now we want to relax. They were:
(i) - The action was expressed in Cartesian coordinates.
(ii) - The energy k^2 was assumed to be real. Now we want to use the complex values for k^2 and express the action in two (or three) dimensional polar (or spherical polar) coordinates.

In the first order of quasilinear approximation, from the potential $v(r,\phi(r))$ we can determine $S_1(r,\phi)$, but $\phi(r)$ depends on the constant ϕ_0 which enters in the definition of S_1 through the integration of (16.111). We can choose this constant so that $\phi(r)$ in the n-th order of approximation be the same function which is found from the contribution for the most probable escape path in the $(n-1)$-th order of approximation. Since the wave function under the barrier is of the form $\psi \sim \exp(-\mathrm{Im}\, S)$, therefore we can find the most probable escape path by calculating the minimum of

$\mathrm{Im}\,(S(\phi_0))$ with respect to the integration constant ϕ_0 for a given m value. Suppose that ϕ_0^M is a complex number which minimizes Im $S(m, \phi_0)$, then the equation

$$\mathrm{Im}\ S(m, \phi_0^M) = min\ \mathrm{Im}\ S(m, \phi_0), \tag{16.132}$$

can be used to find ϕ_0^M and thus the most probable escape path to the first order.

As we have already seen there are two approximate forms for S_1. If the potential is a smooth function of r we have S_1^{II}, Eq. (16.120), and when $\bar{v}(r)$ changes rapidly with r, we have S_1, Eq. (16.131). From these we find the imaginary part of S_1;

$$\mathrm{Im}\ S_1^{II} = \mathrm{Im}\ S_0^{II} \pm \frac{1}{2}\mathrm{Re}\int_b^c \frac{[v(r, \phi(r)) - \bar{v}(r)]}{\mathcal{K}_0(r)} dr + \frac{1}{2}\mathrm{Re}\,[\ln \mathcal{K}_0(r)], \tag{16.133}$$

and

$$\mathrm{Im}\ S_1 = \mathrm{Im}\ S_0 \pm \frac{1}{2}\mathrm{Re}\int_b^c \frac{[v(r, \phi(r)) - \bar{v}(r)]}{\frac{d}{dr}\left[\frac{\ln u(m,r)}{\sqrt{r}}\right]} dr. \tag{16.134}$$

The $\pm$ signs in these equations denote the incoming and the outgoing waves. Since in both of these expressions only the part under the integral sign depends on ϕ_0, therefore ϕ_0^M can be found from the minimum of the integral

$$\left|\mathrm{Re}\int_b^c [v(r, \phi(r)) - \bar{v}(r)] \frac{dr}{D(r)}\right|, \tag{16.135}$$

where $D(r)$ for S_1^{II} is $\mathcal{K}_0(r)$ and for S_1 is $-\frac{d}{dr}\left[\frac{\ln u(m,r)}{\sqrt{r}}\right]$. By determining ϕ_0^M we can find the most probable escape path for the outgoing waves from Eq. (16.109). For the approximate form (16.133) this path is given by [17] [18] [33]

$$\phi(r) = \phi_0^M - i\nu \int_b^r \frac{dr}{r^2 \mathcal{K}_0(r)}, \quad \nu = \sqrt{m^2 - \frac{1}{4}}. \tag{16.136}$$

However if the approximation (16.134) is used then we have

$$\phi(r) = \phi_0^M + im \int_b^r \frac{dr}{r^2 \frac{d}{dr}\left[\frac{\ln u(m,r)}{\sqrt{r}}\right]}. \tag{16.137}$$

As specific examples we consider the following two noncentral potentials

$$v_1(r, \phi) = v_0 \theta(r - b)\theta(c - r)(1 + \epsilon \cos \phi), \tag{16.138}$$

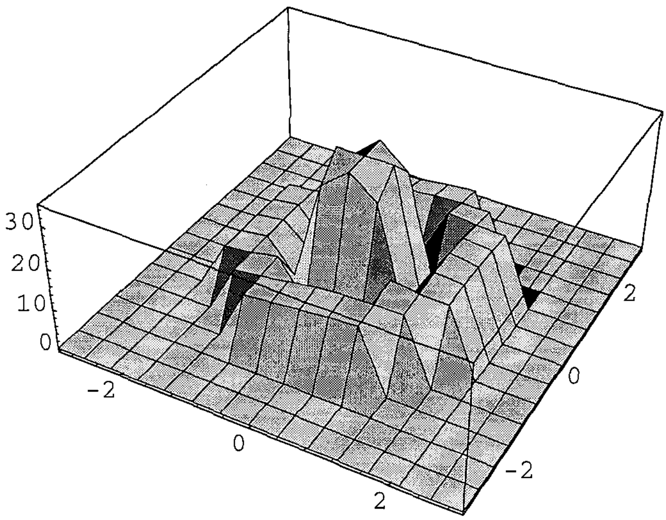

Figure 16.2: The three-dimensional plot of the potential $v_1(r,\phi)+\frac{m^2}{r^2}$ where v_1 is given by Eq. (16.138). The parameters of the potential are $v_0 = 14L^{-2}$, $c = 2, b = 1$, $\epsilon = 0.2$ and we have also used $m = 2$.

and

$$v_2(r,\phi) = \lambda\delta(r-b) + \epsilon v_0 \theta(r-b)\theta(c-r)\cos\phi, \tag{16.139}$$

where $\theta(x)$ is the step function. The contour plot of $v_1(r,\phi) + \left(\frac{m^2}{r^2}\right)$ is shown in Fig. (16.2). In the case of the first example we can use either of the two approximations whereas for the second example we can only use the approximation given by Eq. (16.134). In both cases we find the most probable escape path by minimizing Im S_1

$$min\ (\text{Im}\, S_1) = min\left[\frac{1}{2}\text{Re}\left|\int_b^c \frac{\epsilon v_0 \cos[\phi(r)]}{D(r)}dr\right|\right]. \tag{16.140}$$

For the two potentials (16.138) and (16.139), b and c are independent of ϕ_0, therefore (16.140) can be written as

$$min\ (\text{Im}\, S_1) = min\left|\text{Re}\ (A\cos\phi_0 + B\sin\phi_0)\right]. \tag{16.141}$$

In this relation A and B are complex numbers obtained from the integral (16.140). The complex eigenvalue k^2 in these equations can be found

(16.139), then k^2 must be calculated from the continuity of the wave function and its derivative at the turning points b and c. For potential $v_1(r,\phi)$ we observe that $\bar{v}(r)$ is nonzero only in the region $b < r < c$. Thus for the solution of the Schrödinger equation we find the following functions:

$$u_2(r) = A\sqrt{r}J_m(kr), \quad r < b, \tag{16.142}$$

$$\begin{aligned} u_3(r) &= \sqrt{r}\left\{B\exp\left[iS_n^{II}(r,b)\right] + C\exp\left[-iS_n^{II}(r,b)\right]\right\}, \\ & \quad n = 0,1,2\ldots \quad b < r < c, \end{aligned} \tag{16.143}$$

and

$$u_4(r) = 2D\sqrt{r}H_m(kr), \quad r > c. \tag{16.144}$$

In these equations A, B, C, and D are constants and $S_n^{II}(r,b)$ for $n = 0$ and $n = 1$ are defined by (16.116) and (16.120) respectively provided that we take ϕ to be zero. Now by equating the logarithmic derivatives of u at the points $r = b$ and $r = c$ we find

$$\begin{aligned} &\exp[2iS_n^{II}(c,b)] \\ &= \frac{\left[\frac{d}{dr}\left(iS_n^{II} - \ln J_m(kr)\right)\right]_{r=b}\left[\frac{d}{dr}\left(iS_n^{II} + \ln H_m(kr)\right)\right]_{r=c}}{\left[\frac{d}{dr}\left(iS_n^{II} + \ln J_m(kr)\right)\right]_{r=b}\left[\frac{d}{dr}\left(iS_n^{II} - \ln H_m(kr)\right)\right]_{r=c}}, \end{aligned} \tag{16.145}$$

where in this relation

$$S_n(c,b) = S_n(r = c, \phi = 0) - S_n(r = b, \phi = 0), \tag{16.146}$$

and $S_n(r,\phi)$ is found from

$$\begin{aligned} S_n(r,\phi) &= S_{n-1}(r,\phi) \\ &+ \frac{1}{2}\int\left(\frac{\partial S_{n-1}}{\partial r}\right)^{-1}\left[k^2 - v(r,\phi_{n-1}(r)) - \left(\frac{\nu}{r}\right)^2 - \left(\frac{\partial S_{n-1}}{\partial r}\right)^2\right]dr \\ &+ \left(\frac{i}{2}\right)\ln\left(r\frac{\partial S_{n-1}}{\partial r}\right). \end{aligned} \tag{16.147}$$

This equation is the simplified form of (16.112).

We can calculate the complex eigenvalues directly from (16.145). But if want to determine the root with the smallest imaginary part Δk_i, which gives us the lifetime

$$k = k_r - i\Delta k_i, \tag{16.148}$$

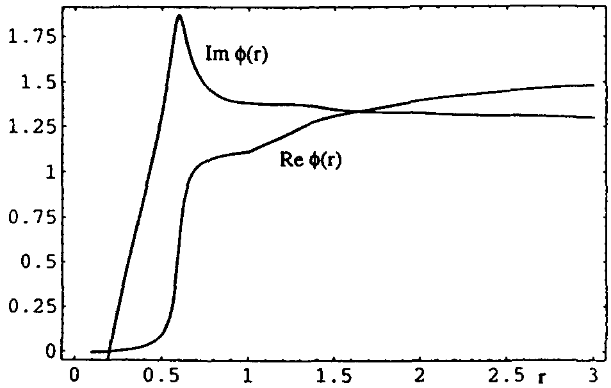

Figure 16.3: The real and imaginary parts of $\phi(r)$ shown as a function of r. These functions are calculated for the potential $v_2(r, \phi)$, Eq. (16.139).

we can use the following approximation:
For this particular root, $\exp\left[2iS_n^{II}(c, b)\right]$ will be very large (for bound state it is infinity), and this means that the probability of finding the particle in the range $0 \leq r \leq b$ is large. This condition means that the denominator in (16.145) is very small and thus the real part of k is the root of

$$\frac{d}{dr}\left[iS_0^{II} + \ln J_m(kr)\right]_{r=b} = 0. \tag{16.149}$$

By substituting (16.148) and (16.149) in (16.145) we can find Δk_i. For the potential (16.138) if we choose the parameters $\epsilon = 0$, and $v_0 = 24L^{-2}$ and also take $m = 2$, for the smallest Δk_i we obtain the eigenvalue $k = (4.999 - 0.0385i)L^{-1}$.
Once k is found from Eqs. (16.142)-(16.144) we can determine a wave function which has a real and an imaginary part (due to the fact that k is complex). Since S_n is a complex function, from Eq. (16.111) it follows that the concept of the "path" of the particle, $\phi(r)$, must be generalized to include an imaginary part as well as the real part.
In Fig. (16.3) the real and imaginary parts of $\phi(r)$ are shown for the potential $v_2(r, \phi)$, Eq. (16.139). The parameters used are $\lambda = 5L^{-1}$, $\epsilon = 0$ and $m = 2$. Similarly for the potential $v_1(r, \phi)$ with the constants $v_0 = 24L^{-1}$, $\epsilon = 0$ and for the state $m = 2$ we find curves of Re $\phi(r)$ and Im $\phi(r)$ shown

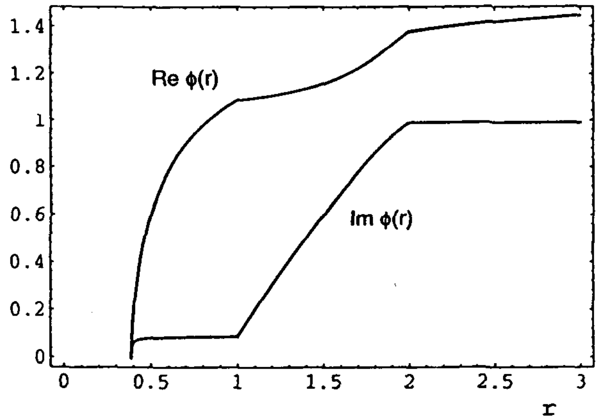

Figure 16.4: Same as in Fig. (16.3), but for the potential $v_1(r, \phi(r))$.

in Fig. (16.4).

The concept of the complex "paths" and the idea of complex time which we studied earlier in connection with the instantons in Chapter (12) are closely related. As we have seen in Chapter (12), the motion of a particle under the barrier can be found from the Schrödinger equation provided that we replace the time t with the imaginary time $-i\mathcal{T}$.

Let us again consider the two-dimensional motion of a particle of mass M which moves in a potential field $V(r)$. The Lagrangian for this motion is

$$L = \frac{1}{2}M\left[\left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\theta}{dt}\right)^2\right] - V(r). \tag{16.150}$$

Now we replace t by $-i\tau$ and we find the new Lagrangian,

$$L = -\frac{1}{2}M\left[\left(\frac{dr}{d\tau}\right)^2 + r^2\left(\frac{d\theta}{d\tau}\right)^2\right] - V(r). \tag{16.151}$$

Since $\frac{\partial L}{\partial \tau} = 0$, therefore we have a conserved quantity

$$E = V(r) - \frac{1}{2}M\left(\frac{dr}{d\tau}\right)^2 - \frac{p_\theta^2}{2Mr^2}. \tag{16.152}$$

where p_θ is the momentum conjugate to the coordinate θ,

$$p_\theta = -Mr^2\left(\frac{d\theta}{d\tau}\right). \tag{16.153}$$

From Eqs. (16.152) and (16.153) we find

$$d\theta = \frac{\mp i p_\theta dr}{M r^2 \sqrt{\left(\frac{2}{M}\right)\left(V - E - \frac{p_\theta^2}{2Mr^2}\right)}}. \tag{16.154}$$

Now if we replace θ by $i\phi$ and p_θ by $-ip_\phi = -i\nu$, we observe that (16.154) and (16.136) are identical.

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Chapter 17

Group and Signal Velocities

In this and the next two chapters we will discuss various attempts to answer the question of "How long does it take a particle or a wave packet to move from one side of a barrier and appear on the other side if the energy of the particle is less than the maximum height of the potential barrier?" Recent progress in fabrication of semiconductor structures in the nanometer range has brought this problem to the forefront of research. But as we will see, no satisfactory answer has so far been found.

As an introduction to the theory of tunneling time we first observe that we can associate different velocities for the propagation of a wave in a dispersive medium [1] [2]:

(1) - The phase velocity which is the velocity of propagation of a pure sinusoidal wave of infinite extent.

(2) - The group velocity which is defined as the velocity of a group of waves forming a wave packet and is given by $\frac{d\omega}{dk}$ [3]. For the wave packet

$$\Psi(x,t) = \int A(k)\exp[-i(\omega t - kx)]dk, \tag{17.1}$$

this velocity is the velocity of a point where the wave packet has its maximum value.

(3) - Front velocity is the velocity that discontinuous foreunner of the wave moves in the medium.

(4) - To define the signal velocity we first observe that when a wave train or a pulse with a given amplitude and wavelength propagates in a dispersive medium, then the forerunner part of the pulse has a small amplitude.

This forerunner is followed by the main part of the pulse with a well-defined frequency and amplitude. Finally the tail of the pulse arrives, again with a small amplitude. The signal velocity is the velocity with which the main part of the pulse propagates. An accurate definition of this velocity will be given later.

Let us consider a pulse which is initially confined to the segment (x_1, x_2). The initial shape of the pulse is given by [4] [5]

$$\Psi(x,t) = \begin{cases} A\exp(ik_0x) & \text{for } x_1 \geq x \geq x_2 \\ 0 & \text{for } x < x_2,\ x > x_1 \end{cases}. \tag{17.2}$$

This wave packet can be found from the superposition of two waves:

$$\psi_1 = \begin{cases} 0 & \text{for } x > x_1 \\ A\exp(ik_0x) & \text{for } x \leq x_1 \end{cases}, \tag{17.3}$$

and

$$\psi_2 = \begin{cases} 0 & \text{for } x > x_2 \\ A\exp(ik_0x) & \text{for } x \leq x_2,\quad x_1 > x_2 \end{cases}. \tag{17.4}$$

In the absence of any external potential, the solution of the Schrödinger equation for the plane wave is given by

$$\psi(x,t) = A\exp[i(kx - \omega t)],\quad \omega = \frac{\hbar k^2}{2m}. \tag{17.5}$$

Using this we can write the time evolution of the waves (17.3) and (17.4) in free space as contour integrals

$$\psi_1(x,t) = \frac{1}{2\pi i}\oint \frac{B}{(k-k_0)}\exp\left[ik(x-x_1) - \frac{i\hbar k^2 t}{2m}\right] dk, \tag{17.6}$$

and

$$\psi_2(x,t) = \frac{1}{2\pi i}\oint \frac{C}{(k-k_0)}\exp\left[ik(x-x_2) - \frac{i\hbar k^2 t}{2m}\right] dk. \tag{17.7}$$

In both of these expressions the closed contour extends from $(-\infty + i\epsilon)$ to $(\infty + i\epsilon)$. For $t = 0$ if we choose the contour as a semi-circle in the upper-half of the complex k-plane, then the integrand in (17.6) tends to zero for $(x - x_1) > 0$ as the radius of the circle tends to infinity. However if $(x - x_1) < 0$, then for $\psi_1(x, 0)$ we have to close the contour in the lower half of the k-plane. Here because of the presence of the pole at $k = k_0$, the integrals for $\psi_1(x, 0)$ and $\psi_2(x, 0)$ become equal to $B\exp[ik_0(x - x_1)]$ and

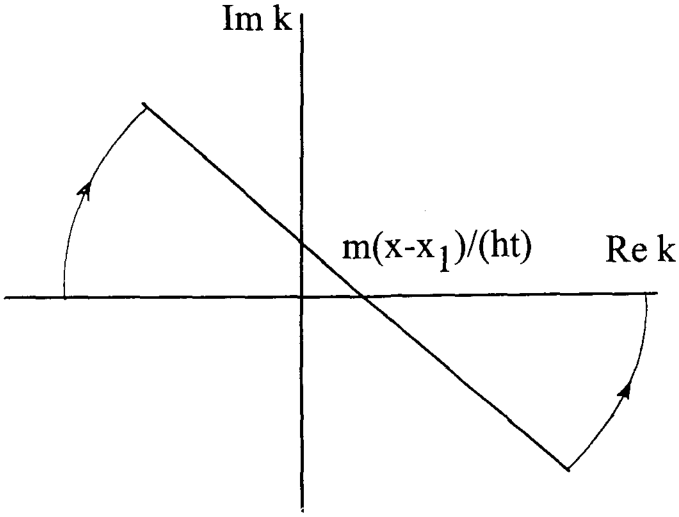

Figure 17.1: Contour for integration of $\psi_1(x,t)$ and $\psi_2(x,t)$, Eqs. (17.6) and (17.7).

$C\exp[ik_0(x-x_2)]$ respectively.
Comparing these to the initial form of the wave packet, we find

$$B\exp(-ik_0x_1) = A = C\exp(-ik_0x_2). \tag{17.8}$$

For negative values of t with $(x-x_1) > 0$, and a contour in the upper half of the k-plane, $\psi_1(x,t)$ is zero and so is $\psi_2(x,t)$ for $(x-x_1) > 0$, and $t < 0$. Thus for $t < 0$ if there is a wave, it will exist only in the region $x \le x_1$. For $t = 0$ we know that there is a wave train between x_1 and x_2 and nowhere else.

Now let us consider what happens when t is greater than zero. First we examine $\psi_1(x,t)$, Eq. (17.6), for $t > 0$. If for a moment we ignore the pole at $k = k_0$, and choose a contour which is composed of a part of great circle and a line with an angle α which passes through the point $k = K$, where K is a real number (Fig. (17.1)), then we can evaluate (17.6) in the following way: The integral along the line $k = K + re^{i\alpha}$, where r is the distance along the line and this integral is given by

$$\exp\left[-r\sin\alpha\,(x-x_1) + \frac{\hbar}{m}Kr\sin\alpha + \frac{\hbar}{2m}tr^2\sin 2\alpha\right]. \tag{17.9}$$

Now if we choose K and α to be

$$K = m\frac{(x-x_1)}{\hbar t},\quad \alpha = \frac{3\pi}{4}, \tag{17.10}$$

respectively, then (17.9) becomes

$$\exp\left(-\frac{\hbar t r^2}{2m}\right). \tag{17.11}$$

Thus with this choice of K and α the integral along the line becomes very small. Now we can complete the contour with two arcs of the great circle from $\theta = \pi$ to $\theta = \frac{3\pi}{4}$ and from $\theta = \frac{-3\pi}{4}$ to $\theta = 0$. From these parts nothing will be added to the integral. Next we include the effect of the pole at $k = k_0$. If $K = \frac{m(x-x_1)}{\hbar t}$ is greater than k_0, then by deforming the contour we can close it without crossing the pole, and this is possible if t is small enough. But as t increases we reach a time where $K = k_0$ and at this time the inclusion of this pole adds the term

$$B\exp\left[ik_0(x-x_1) - \frac{i\hbar}{2m}t{k_0}^2\right], \tag{17.12}$$

to the integral and this is exactly the sinusoidal term that we had at $t = 0$. Thus following Sommerfeld (and Brillouin) [1] we can state that the contribution of the line integral is the forerunner wave, but the main part of the wave comes from the contribution of the pole at $k = k_0$. This main part of the wave packet which is a sinusoidal moves with the velocity $\frac{\hbar k_0}{m}$, as is evident from (17.12). But for $\psi_1(x,t)$ there is no tail of the wave since it continues to be sinusoidal for all later times. In the same way we can write an integral representation for $\psi_2(x,t)$ which is identical with $\psi_1(x,t)$ except for a displacement in space. Ignoring the contribution of the integral along the line, the main part of the wave is the same as the one we assumed at $t = 0$. Also we observe that for this special case the signal velocity which is the velocity of the wave front is equal to the group velocity. Since the time development of the wave function $\Psi(x,t)$ is governed by the Schrödinger equation and is zero outside the region $x_2 \le x \le x_1$, therefore the integral

$$I = \int_{x_2}^{x_1} |\Psi(x,t)|^2 dx, \tag{17.13}$$

is conserved.

As Stevens has observed [5], we can use this procedure to construct a many-electron wave function. To this end we note that at $t = 0$, any function of x which is zero in the segment (x_2, x_1) will be orthogonal to $\Psi(x,0)$, therefore we can divide the x-axis into an infinite number of segments each of length $(x_1 - x_2)$, and for each construct a wave packet. All these wave packets represent identical pulses except for the relative displacement. These pulses remain orthogonal to each other for all times (ignoring the fore- and after-runners), and they all move with the same signal velocity. According to the exclusion principle we can associate two electrons (one spin up and one spin down) with each pulse.

Now let us apply this method to study the one-dimensional quantum tunneling. In the following discussion we use the units $\hbar = 2m = 1$, and assume a barrier of the form $V\theta(x)$, where $\theta(x)$ is the step function. The Schrödinger equation for this problem is given by

$$i\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V\theta(x)\psi. \tag{17.14}$$

Here we assume that initially the pulse is located near the edge of the potential, $x = 0$, and we further assume that at $t = 0$, there is no wave inside the barrier, but for $t > 0$, the wave will start moving into the barrier with a frequency ω_0. We want to investigate the propagation of the wave inside the barrier, i.e. in the direction of positive x. Here for simplicity we write the time dependence of the wave function as

$$\psi(0,t) = \begin{cases} 0 & \text{for } t < 0 \\ \exp(-i\omega_0 t) & \text{for } t > 0 \end{cases} \tag{17.15}$$

We can also write this $\psi(0,t)$ as a contour integral

$$\psi(0,t) = \frac{1}{2\pi i}\oint \frac{\exp(-i\omega t)}{(\omega - \omega_0)} d\omega, \tag{17.16}$$

where the contour extends from $\omega = -\infty + i\epsilon$ to $\omega = \infty + i\epsilon$. Similar to the argument given for the motion of a free particle, we can write the general solution of the tunneling problem as

$$\psi(x,t) = \frac{1}{2\pi i}\oint \frac{\exp(-i\omega t)\exp\left(x\sqrt{V - \omega}\right)}{(\omega - \omega_0)} d\omega. \tag{17.17}$$

Since in taking the square root in the integrand we have the ambiguity of plus or minus signs, we change the variable from ω to Z, where

$$Z^2 = \omega - V. \tag{17.18}$$

Then we can write (17.17) as

$$\psi(x,t) = \frac{\exp(-iVt)}{\pi i}\oint \frac{\exp(-iZ^2 t)\exp(ixZ)}{(Z^2 + V - \omega_0)} Z dZ. \tag{17.19}$$

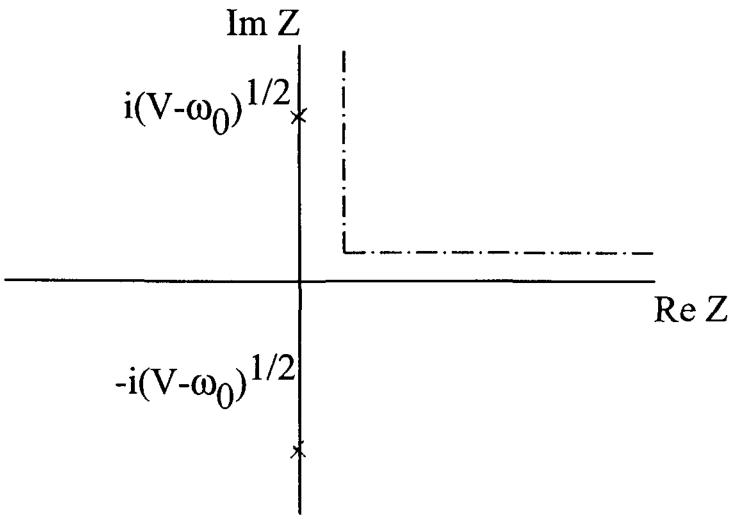

Figure 17.2: Contour for integration of Eq. (17.19).

For the case of tunneling where $V > \omega_0$, we choose the contour of integration for (17.19) in the following way: The contour starts at Re $Z = \infty$ and continues to $Z = 0$, then it goes up along the Im Z axis but it bypasses the pole at $i\sqrt{V-\omega_0}$ (Fig. (17.2)). The rest of the contour consists of a large circle from $\theta = \frac{\pi}{2}$ to $\theta = 0$. The main part of the integral is proportional to the absolute value of $\exp[-iZ^2t + ixZ]$ which can be written as

$$\left|\exp\left[-iZ^2t + ixZ\right]\right| = \exp\left[R^2 t\sin(2\theta) - xR\sin(\theta)\right]. \tag{17.20}$$

We observe that in limit $R \to \infty$ this expression becomes negligibly small for $t < 0$ and $x > 0$. But the derivative of $Z^2t - xZ$, i.e. $2Zt - x$ is zero when $Z = \frac{x}{2t}$. Thus we can use the method of steepest decent to calculate the integral on the line [6]

$$Z = \frac{x}{2t} + re^{i\alpha}. \tag{17.21}$$

Since the absolute value of $\exp[-iZ^2t + ixZ]$ on this line is equal to $\exp[r^2\sin(2\alpha)]$, therefore we choose α to be equal to $\frac{3\pi}{4}$, and with this choice we find the contribution to the integral along the line (17.21) to be

$$\frac{1}{\pi i}\exp(-iVt)\exp\left(\frac{ix^2}{4t}\right)\int_{-\infty}^{\infty}\frac{\exp(-r^2t)\left[\left(\frac{x}{2t}\right)\exp\left(\frac{3i\pi}{4}\right) - r\right]}{\left[\left(\frac{x}{2t}\right) + r\exp\left(\frac{3i\pi}{4}\right)\right]^2 + V - \omega_0}dr. \tag{17.22}$$

This integral is small for all positive values of x and t. Now we have to see whether by deforming the contour we have crossed the pole or not? The line (17.21) intersects the Im Z axis at $\frac{ix}{2t}$, therefore if $\sqrt{V-\omega_0} < \frac{x}{2t}$, we have not crossed the pole. However if

$$\sqrt{V-\omega_0} \geq \frac{x}{2t}, \tag{17.23}$$

then we have a contribution from the pole to the integral which is equal to

$$\exp(-i\omega_0 t)\exp(-\sqrt{V-\omega_0}\, x). \tag{17.24}$$

As we have seen for the case of a free particle this is the main part of the wave. The difference with the case of a free particle is that here the amplitude of the wave inside the barrier is smaller than that of the outside by a factor of $\exp(-\sqrt{V-\omega_0}x)$.

An interesting result of this approach is that we can find the time of arrival of the wave at the point x inside the barrier. This is obtained from the equality in Eq. (17.23), i.e.

$$t = \frac{x}{2\sqrt{V-\omega_0}}. \tag{17.25}$$

From this we conclude that the wave velocity under the barrier is constant and with the proper factors of $\hbar$ and $2m$ can be written as

$$v = 2\sqrt{\frac{\hbar}{2m}(V-\omega_0)}. \tag{17.26}$$

This result is similar to the one advocated by Büttiker and Landauer [7] [8], but it differs from what we know about the motion of a Gaussian wave packet as we will see at the end of this section.
If $\omega_0 > V$, then the pole would be at $\sqrt{\omega_0 - V}$ on the real Z axis. Using the same method, we observe that the main contribution to the integral is

$$\exp(-i\omega_0 t)\exp(i\sqrt{\omega_0 - V}\, x), \tag{17.27}$$

instead of (17.24), and this is exactly the result that we obtain from the motion of a particle above the barrier. We note also that the symmetry of the velocity about $\omega_0 = V$ which seems reasonable.

Another simple and interesting case is when in addition to $V\theta(x)$, we have a potential λx, so that the Schrödinger equation in units of $\hbar = 2m = 1$ is

$$-\frac{\partial^2\psi}{\partial x^2} + (V - \lambda x)\psi = i\frac{\partial\psi}{\partial t}. \tag{17.28}$$

With the help of WKB method we can find the wave function for the energy ω to be

$$\psi_\omega(x,t) = e^{-i\omega t}\exp\left(i\int i\sqrt{\omega - V + \lambda x}\,dx\right), \tag{17.29}$$

Now if we assume that the parameter λ is small, we can expand the integrand in (17.29) and obtain the approximate wave function. Using the WKB method we find the wave function to be

$$\psi_\omega(x,t) = e^{-i\omega t}\exp\left(ix\sqrt{\omega - V} + \frac{1}{4}\frac{i\lambda x^2}{\sqrt{\omega - V}}\right). \tag{17.30}$$

From this approximate wave function we obtain the wave packet

$$\psi(x,t) = \frac{1}{2\pi i}\int\frac{d\omega}{(\omega-\omega_0)}e^{-i\omega t}\exp\left[ix\sqrt{\omega - V} + \frac{1}{4}\frac{i\lambda x^2}{\sqrt{\omega - V}}\right], \tag{17.31}$$

where the contour in this case is parallel and is slightly above the real ω axis. In order to evaluate this integral we use the method of steepest decent. Writing the exponent in (17.31) as a function of Z, Eq. (17.18), we have

$$W(Z) = -Z^2 t + xZ + \frac{\lambda x^2}{4Z}, \tag{17.32}$$

from which we can calculate the principle turning point by finding the root of

$$\frac{dW}{dZ} = -2Zt + x - \frac{\lambda x^2}{4Z^2}. \tag{17.33}$$

Now we choose the contour to be composed partly of a line making an angle $\alpha = \frac{3\pi}{4}$ with the Re Z-axis and passing through the point given by the root of (17.33). The main part of the wave packet in Eq. (17.31) comes from the pole contribution when this line crosses the pole at $i\sqrt{V-\omega_0}$. As before (see Eq. (17.25)) the time of arrival of the wave to the point x is found from

$$-2\sqrt{V-\omega_0}\,t + x - \frac{\lambda x^2}{4(V-\omega_0)} = 0. \tag{17.34}$$

This is the classical expression for the position of a particle moving with a constant acceleration (to the order λ).

Now let us return to the question of the symmetry between the wave velocities under and over the barrier. If we accept this symmetry, then we have to conclude that the pulses with energies far from the maximum height of the barrier V move faster than those with energies close to V, Eq. (17.26).

But as we have seen in Chapter 7, Eq (7.16), the period of the wave packet in a symmetric double-well is

$$T_0 = \frac{\hbar}{E_{i+1} - E_i}, \tag{17.35}$$

whenever E_{i+1} and E_i are close to each other and are far from E_{i+2} and E_{i-1}. On the other hand from the inequalities

$$E_5 - E_4 > E_3 - E_2 > E_1 - E_0, \tag{17.36}$$

which exist between the energy levels (at least in one-dimensional tunneling) and Eq. (17.35), we observe that the periods for the wave packets associated with higher energy levels are shorter than those with lower energies. Thus the tunneling from one well to the other takes place in shorter time when the energy is higher. Is this related to the fact that the wave packets $\frac{1}{\sqrt{2}}(\psi_{i+1} \pm \psi_i)$ are not completely localized in the right or the left well or is it due to other factors? At this stage we do not know the correct answer.

The foregoing discussion advanced by Stevens [4] [5] can be criticized for a number of reasons including the followings [9]:

(i) - In what way one can associate the position of the particle to the location of the front of the wave packet?

(ii) - Collins *et al* have found that the terms neglected in this approach are as important as those that have been retained [10].

(iii) - The detailed numerical work of Jauho and Jonson [11] shows that while the initial wave front is sharp, once the wave has tunneled through the barrier, the front will not remain sharp or distinct.

Let us briefly discuss the argument of Collins *et al.* In the above formulation we note that as Eq. (17.24) shows the signal velocity (not the group velocity) of the wave packet inside the barrier is reduced by the factor $\exp(-\sqrt{V-\omega_0}x)$ [10]. Since we associate the motion of the particle with the group velocity, this result is open to question [10]. By using the integration over the wave number k, rather than the energy ω, we can write the initial wave function as

$$\psi(x, t=0) = \frac{1}{2\pi i}\int_{-\infty+i\epsilon}^{\infty+i\epsilon} \frac{\exp\left[ik_0x + ik(x - x_0)\right]}{k - k_0}dk, \tag{17.37}$$

where the line of integration is just above the real k-axis. This is a sinusoidal wave function extending over all space for $x < x_0$ and is zero for $x \geq$

x_0. When the particle tunnels into a step potential $V\theta(x)$, then the wave function at the time t is given by

$$\psi(x,t) = \frac{1}{\pi i}\int \frac{\exp\left[-i(kx_0+\omega t) - qx\right]}{(k-k_0)(k+q)} kdk. \tag{17.38}$$

where $q = \sqrt{V-\omega}$. The pole contributions to the integral comes from the pulse edge $k = k_0$ and also from the barrier $k = -q$. These poles do not produce significant changes in the integral as the contour crosses through $\sqrt{V-\omega_0}$. On the other hand, if following Stevens, we introduce a new variable Z according to Eq. (17.18), then there would be poles at $Z = \pm i\sqrt{V-\omega_0}$ which would change the wave function. But this change of variable from k to Z will cause problems with the integration limits (squaring operation). Thus we have different results depending on whether we write the contour integration over the wave number or over the energy [10].

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Chapter 18

Time-Delay, Reflection Time Operator and Minimum Tunneling Time

One of the controversial issues of modern quantum theory has been the question of tunneling time, i.e. the time that takes a particle to move from one side of the barrier to the other side. A related and interesting problem is that of the time-delay caused by tunneling. It is this latter question which we want to consider first. Like most of the problems of quantum theory our starting point is the familiar classical concept of travel time or time-delay. Thus with the help of classically well-defined idea of the motion of a particle in a potential field we can obtain expressions for the time-delay as well as reflection time, and then use these to formulate their quantum counterparts. The difficulty with this approach is the non-uniqueness of the quantal operators corresponding to the same classical observable.

We have already seen that the solution of the operator Heisenberg equation (Chapter 13) and the Wigner trajectory (Chapter 14) provide us with concepts closely related to the travel times of classical dynamics.

18.1 Time-Delay in Tunneling

Suppose that we have two particles both starting at the point $(-a)$ (see Fig. (18.1)) and both reaching the point a on the other side of the barrier $V(x)$, but one traveling the distance of $-a$ to a in free space and the other reaching a from $-a$ by tunneling. We assume that the barrier exists only for $-a < x < a$. Denoting the mass and the energy of each particle by m and E respectively, the travel time of the first (free) particle between the points $-a$ and a according to classical mechanics is equal to

$$t_1 = \frac{2a}{v_0} = \frac{2ma}{\sqrt{2mE}}, \tag{18.1}$$

where v_0 is the velocity of the particle. For the second particle if $E > V(x)$ the classical travel time is

$$t_2 = \int_{-a}^{a} \frac{mdx}{\sqrt{2m[E - V(x)]}}. \tag{18.2}$$

Therefore the time-delay due to the presence of the barrier is given by

$$\tau_c = t_2 - t_1 = \int_{-a}^{a} \left[\frac{m}{\sqrt{2m(E - V(x))}} - \frac{m}{\sqrt{2mE}}\right] dx. \tag{18.3}$$

Now we will study this problem in the semi-classical approximation. To this end we start with the Schrödinger equation with the potential $V(x)$,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + [E - V(x)]\psi = 0, \tag{18.4}$$

and use the WKB approximation to find the solution of Eq. (18.4),

$$\psi(x) \approx \mathcal{N} \exp\left[\frac{i}{\hbar}\int_{-a}^{x} \sqrt{2m(E - V(x))}\, dx\right], \quad -a \le x \le a, \tag{18.5}$$

where $\mathcal{N}$ is the normalization constant and again we have assumed that $E \ge V(x)$ in this interval. For $x > a$, we can write the wave function as

$$\psi(x) = \mathcal{N} \exp\left[\frac{i}{\hbar}\sqrt{2mE}\, x + i\eta(E)\right], \quad x > a, \tag{18.6}$$

which is the wave function for a free particle. The phase shift $\eta(E)$ which is dimensionless is caused by the presence of the potential $V(x)$, and is given by [1]

$$\eta(E) = \frac{1}{\hbar}\int_{-a}^{a} \left\{[2m(E - V(x))]^{\frac{1}{2}} - [2mE]^{\frac{1}{2}}\right\} dx. \tag{18.7}$$

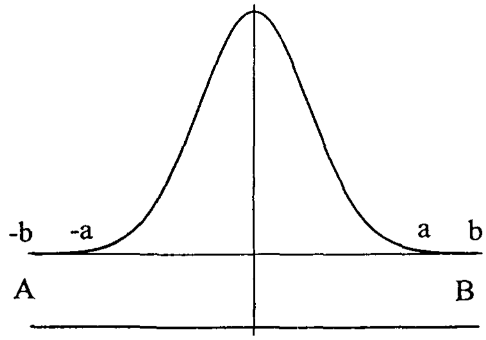

Figure 18.1: The time of arrival of two particles, both starting at $x = -a$, and arriving at $x = a$, one by means of tunneling and the other moving as a free particle.

This relation is obtained by matching the inside and the outside solutions, Eqs. (18.5) and (18.6) respectively. If we differentiate $\eta(E)$ with respect to E we have

$$\hbar\frac{d\eta(E)}{dE} = \int_{-a}^{a}\left\{\frac{1}{\sqrt{2m(E-V(x))}} - \frac{1}{\sqrt{2mE}}\right\} m dx. \tag{18.8}$$

By comparing Eqs. (18.3) and (18.8) we find that $\hbar\frac{d\eta(E)}{dE}$ corresponds to the time-delay in classical mechanics.

Next we want to derive the full quantum mechanical expression for the time-delay. We first observe that $\frac{mdx}{\sqrt{2mE}}$ and $\frac{mdx}{\sqrt{2m(E-V(x))}}$ are the classical probabilities of finding a free particle and a particle moving under the influence of the potential $V(x)$ in the range dx. In quantum mechanics these probabilities are given by $|\psi_0(x,E)|^2 dx$ and $|\psi(x,E)|^2 dx$ respectively, where $\psi_0(x,E)$ is the wave function for a free particle. This wave function is normalized according to the relation

$$|\psi_0(x,E)|^2 = \sqrt{\frac{m}{2E}}, \tag{18.9}$$

which agrees with the classical probability given above, and a similar normalization for $|\psi(x,E)|^2$ (see Eqs. (18.16) and (18.17) below). With the help of these wave functions we can write the quantum mechanical time-delay τ_q as

$$\tau_q = \int_{-a}^{a} \left[|\psi(x,E)|^2 - |\psi_0(x,E)|^2 \right] dx. \tag{18.10}$$

This expression is valid whether $E \geq V(x)$ or $E < V(x)$, as long as $V(x)$ asymptotically goes to zero,

$$\lim_{x\to\pm\infty} V(x) \to O\left(\frac{1}{x^{2+\epsilon}}\right), \quad \epsilon > 0. \tag{18.11}$$

Next we try to establish the connection between τ_q and the derivative of the phase shift, $\hbar\frac{d\eta(E)}{dE}$. First we note that for $x > |a|$, $\psi(x,E)$ and $\psi_0(x,E)$ differ from each other only by a phase factor. Then we write the Schrödinger equation (18.4) as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + [V(x) - E]\,\psi = (H - E)\psi = 0. \tag{18.12}$$

By differentiating (18.12) with respect to E we obtain

$$(H - E)\frac{\partial \psi}{\partial E} - \psi = 0. \tag{18.13}$$

Now from Eqs. (18.12) and (18.13) and their Hermitian conjugates we find $\psi^*\psi$;

$$\psi^*\psi = -\frac{\hbar^2}{2m}\mathrm{Re}\left\{\frac{\partial}{\partial x}\left[\psi^*\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial E}\right) - \frac{\partial\psi}{\partial E}\frac{\partial\psi^*}{\partial x}\right]\right\}, \tag{18.14}$$

therefore

$$\int_{-x}^{x}\psi^*\psi dx = -\frac{\hbar^2}{2m}\mathrm{Re}\left[\psi^*\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial E}\right) - \frac{\partial\psi}{\partial E}\frac{\partial\psi^*}{\partial x}\right]\Bigg|_{-x}^{x}. \tag{18.15}$$

With the normalization of $\psi(x,E)$ which for $|x| > a$ is identical to the normalization of $\psi_0(x,E)$, we can write the asymptotic form of $\psi(x,E)$ as

$$\psi(x,E) = \sqrt{\frac{m}{\hbar k}}\left[e^{ikx} + R(k)e^{-ikx}\right], \quad x < -a, \tag{18.16}$$

and

$$\psi(x,E) = \sqrt{\frac{m}{\hbar k}}T(k)e^{ikx}, \quad x > a, \tag{18.17}$$

where $k = \sqrt{\frac{2mE}{\hbar}}$. In these relations $|R(k)|^2$ and $|T(k)|^2$ are the reflection and transmission coefficients respectively. Now we go back to Eq. (18.9) and change the normalization of $\psi_0(x,E)$ so that it conforms to the asymptotic form of (18.16), i.e.

$$|\psi_0| = |T(k)|\sqrt{\frac{m}{\hbar k}}. \tag{18.18}$$

Next we substitute (18.16) - (18.18) in (18.10) to find τ_q

$$\tau_q = \hbar\left\{|R(k)|^2\left(\frac{d\delta}{dE}\right) + |T(k)|^2\left(\frac{d\eta}{dE}\right)\right\} + \hbar|R(k)|\left(\frac{\sin(2kx-\delta)}{2E}\right). \tag{18.19}$$

In this equation $\delta(E)$ and $\eta(E)$ are the phases of $R(k)$ and $T(k)$ respectively. The last term in Eq. (18.19) is sinusoidal and space-dependent and to eliminate it we calculate the average value of τ_q which we denote by $\langle\tau_q\rangle$,

$$\langle\tau_q\rangle = \lim_{x\to\infty}\int_x^{2x}\tau_q(x')dx'. \tag{18.20}$$

From this definition it follows that

$$\langle\tau_q\rangle = \hbar\left\{|R(k)|^2\left(\frac{d\delta}{dE}\right) + |T(k)|^2\left(\frac{d\eta}{dE}\right)\right\}, \tag{18.21}$$

and this is the quantal definition of the time-delay.

Now if the kinetic energy of the particle is large compared to the height of the barrier, or in the case of tunneling provided that $|R(k)|$ is very small, i.e.

$$|R(k)|^2 \approx 0, \quad |T(k)|^2 \approx 1, \tag{18.22}$$

then equation (18.21) reduces to

$$\langle\tau_q\rangle = \hbar\frac{d\eta}{dE}, \tag{18.23}$$

which is the result that we found from the WKB approximation.

In some exceptional cases τ_q, Eq. (18.10), is identical with $\langle\tau_q\rangle$ of Eq. (18.23). For instance consider the reflectionless potential

$$V(x) = -\left(\frac{\hbar^2}{2m}\right)\frac{2\beta^2}{\cosh^2(\beta x)}, \tag{18.24}$$

for which the wave function is

$$\psi(x) = \sqrt{\frac{m}{\hbar k}}\left[1 - \left(\frac{2\beta}{\beta+ik}\right)\frac{e^{2\beta x}}{(1+e^{2\beta x})}\right]e^{ikx}. \tag{18.25}$$

From this wave function we find that

$$R(k) \equiv 0, \quad T(k) = \frac{ik - \beta}{ik + \beta}. \tag{18.26}$$

Therefore,

$$\tan \eta(k) = \frac{\text{Im } T(k)}{\text{Re } T(k)} = \frac{2\beta k}{k^2 - \beta^2}, \tag{18.27}$$

and from (18.23), we have

$$\langle \tau_q \rangle = \frac{m}{\hbar k}\frac{d\eta(k)}{dk} = -\frac{2m\beta}{\hbar k(k^2 + \beta^2)^2}. \tag{18.28}$$

Note that in this case the potential is attractive, thus we have a time-advance rather than time-delay. By substituting (18.25) in (18.10) we find that

$$\tau_q = \int_{-\infty}^{+\infty} \left[|\psi(x)|^2 - \frac{m}{\hbar k}\right] dx = \langle \tau_q \rangle . \tag{18.29}$$

18.2 Time-Delay for Tunneling of a Wave Packet

In the preceding section we found the time-delay for tunneling of a particle with a definite energy E. Now we will study a similar problem, but instead of a plane wave we use a wave packet. For three-dimensional scattering this problem was formulated and solved by Wigner [2][3]. The following derivation is similar to the Wigner's work except that it is applied to one-dimensional tunneling.

Let us consider a wave packet incident from the left of a barrier. This wave packet is composed of two waves each with a fixed frequency (energy), but these two frequencies are close to each other. The incident wave packet is of the form

$$\begin{aligned} \psi_{in} &= \frac{1}{2}\sqrt{\frac{m}{\hbar k}}\{\exp[i(kx - \omega t)] + \exp[i(k + \Delta k)x - i(\omega + \Delta\omega)t]\} \\ &= \sqrt{\frac{m}{\hbar k}}\cos\left[\frac{1}{2}(\Delta k x - \Delta\omega t)\right]\exp\left[\frac{i}{2}(\Delta k x - \Delta\omega t)\right] \\ &\times \exp[i(kx - \omega t)]. \end{aligned} \tag{18.30}$$

The center of this wave packet at the time t is the point x and Eq. (18.30) shows that

$$t = \frac{\Delta k}{\Delta\omega}x. \tag{18.31}$$

The wave packet after tunneling through the barrier ψ_{tr}, acquires a phase, $\eta(\omega)$. That is the wave packet on the right side of the barrier has the form

$$\begin{aligned}\psi_{tr} &= \frac{1}{2}\sqrt{\frac{m}{\hbar k}}\{\exp[i(kx-\omega t+\eta(\omega))] \\ &+ \exp[i(k+\Delta k)x - i(\omega+\Delta\omega)t + i\eta(\omega+\Delta\omega)]\}. \end{aligned} \tag{18.32}$$

Since $\Delta\omega$ is small, therefore

$$\eta(\omega+\Delta\omega) = \eta(\omega) + \frac{d\eta(\omega)}{d\omega}\Delta\omega. \tag{18.33}$$

From Eqs. (18.32) and (18.33) we conclude that

$$\begin{aligned}\psi_{tr} &= \sqrt{\frac{m}{\hbar k}}\cos\left[\frac{1}{2}\left(\Delta k x - \Delta\omega t + \Delta\omega\frac{d\eta}{d\omega}\right)\right] \\ &\times \exp\left\{i(kx-\omega t+\eta(E)) + \frac{i}{2}\left(\Delta k x - \Delta\omega t + \Delta\omega\frac{d\eta}{d\omega}\right)\right\}. \end{aligned} \tag{18.34}$$

Thus the wave transmitted to the right of the barrier has a minimum at x at the time t' where

$$t' = \left(\frac{\Delta k}{\Delta\omega}\right)x + \left(\frac{d\eta}{d\omega}\right). \tag{18.35}$$

By comparing (18.31) and (18.35) we find the following expression for the time-delay

$$t' - t = \left(\frac{d\eta}{d\omega}\right) = \hbar\left(\frac{d\eta}{dE}\right). \tag{18.36}$$

For a derivation of this result using wave packet and semi-classical approximation see Bohm [3]. This time-delay is one-half of what Wigner [2] found for the three-dimensional problem, viz, $t' - t = 2\hbar\left(\frac{d\eta}{dE}\right)$.

In this formulation we assumed that the wave packet was incident on the barrier from $x = -\infty$ and after tunneling, has moved asymptotically to $x = +\infty$. We can formulate a discrete version of the problem of time-delay by assuming that the barrier exists in the segment $-a \le x \le a$, but the motion of the particle is confined to a box of length $2b$ (Fig. (18.1)) [4]. This means that the asymptotic condition (18.11) is replaced by

$$V(x) = +\infty, \quad |x| > b, \quad b > a. \tag{18.37}$$

In the following discussion we choose the units so that $\hbar = m = 1$.

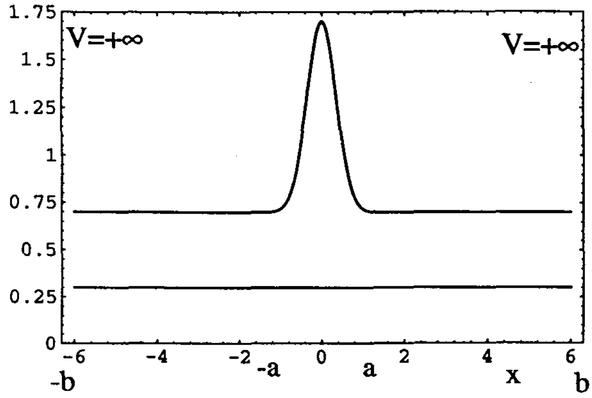

Figure 18.2: Particles confined to move in the region $-b \le x \le b$. The barrier is situated in the region $-a \le x \le a$ with $a < b$.

In the absence of the barrier the solution of the Schrödinger equation with the boundary condition (18.37) is given by

$$\phi_e(n,x) = \frac{1}{\sqrt{b}} \cos\left[\left(n - \frac{1}{2}\right)\frac{\pi x}{b}\right], \tag{18.38}$$

and

$$\phi_o(n,x) = \frac{1}{\sqrt{b}} \sin\left(\frac{n\pi x}{b}\right), \tag{18.39}$$

where in these equations n is a positive integer and the subscripts e and o refer to even and odd parity states. The eigenvalues corresponding to these wave functions are

$$E_e(n) = \left(n - \frac{1}{2}\right)^2 \frac{\pi^2}{2b^2} = \frac{{k_e}^2}{2}, \quad E_o(n) = \frac{n^2\pi^2}{2b^2} = \frac{{k_o}^2}{2}. \tag{18.40}$$

When b is large the eigenvalues for a given n are close to each other. The eigenfunctions ϕ_e and ϕ_o satisfy the orthogonality conditions

$$\int_{-b}^{b} \phi_e(n,x)\phi_e(j,x)dx = \int_{-b}^{b} \phi_o(n,x)\phi_o(j,x)dx = \delta_{n,j}, \tag{18.41}$$

and

$$\int_{-b}^{b} \phi_o(n,x)\phi_e(j,x)dx = 0. \tag{18.42}$$

Now we assume that the initial wave packet is localized to the left of the barrier, i.e.

$$\Phi(x,0)=\begin{cases} f(x) & \text{for } -b\le x\le 0 \\ 0 & \text{for } b\ge x\ge 0\end{cases}. \tag{18.43}$$

and that it is normalized;

$$\int_{-b}^{b}|\Phi(x,0)|^2dx=1. \tag{18.44}$$

In order to determine the evolution of this wave packet in time we expand it in terms of ϕ_e and ϕ_o;

$$\Phi(x,0)=\sum_1^\infty[A_n\phi_e(n,x)+B_n\phi_o(n,x)], \tag{18.45}$$

where A_n and B_n are the Fourier coefficients,

$$A_n=\int_{-b}^{0}\Phi(x,0)\phi_e(n,x)dx, \tag{18.46}$$

and

$$B_n=\int_{-b}^{0}\Phi(x,0)\phi_o(n,x)dx. \tag{18.47}$$

Using the expansion (18.45), we can write the time development of $\Phi(x,0)$ as

$$\Phi(x,t)=\sum_{n=1}^\infty\left\{A_n\phi_e(n,x)\exp[-iE_e(n)t]+B_n\phi_o(n,x)\exp[-iE_o(n)t]\right\}. \tag{18.48}$$

The probability of finding the particle on the left side of the barrier at time t can be calculated from $\Phi(x,t)$;

$$\begin{aligned}P^-(t)&=\int_{-b}^{0}|\Phi(x,t)|^2dx\\ &=\frac{1}{2}+\frac{8}{\pi}\sum_{n=1}^\infty\sum_{j=1}^\infty\frac{jA_nB_j}{(2n-1)^2-4j^2}\cos\left\{[E_e(n)-E_o(j)]\,t\right\},\end{aligned} \tag{18.49}$$

where we have used the normalization condition (18.44). For a wave packet which is completely confined to the left of the barrier usually one of the terms in the double sum (18.49) is large compared to other terms. As an example consider the wave packet $\Phi(x,0)$ given by

$$\Phi(x,0)=\begin{cases}\sqrt{\frac{2}{b}}\sin(\frac{\pi x}{b}) & \text{for } -b\le x\le 0\\ 0 & \text{for } b\ge x\ge 0\end{cases}. \tag{18.50}$$

In this case the coefficients A_n and B_n are given by

$$A_n = \frac{4\sqrt{2}}{\pi}\frac{1}{(2n-1)^2 - 4}, \tag{18.51}$$

and

$$B_n = \frac{1}{\sqrt{2}}\delta_{n,1}. \tag{18.52}$$

By substituting these values in (18.49) we find $P^-(t)$ to be

$$P^-(t) = \frac{1}{2} + \sum_{n=1}^{\infty}\left(\frac{32}{\pi^2}\right)\frac{1}{[(2n-1)^2-4]^2}\cos\{[E_e(n) - E_o(1)]t\}, \tag{18.53}$$

The maximum value of the sum in (18.53) is $\frac{1}{2}$. Now if we approximate the sum by its first term we have

$$P^-(t) = \frac{1}{2} + \frac{32}{9\pi^2}\cos\{[E_e(1) - E_o(1)]t\}. \tag{18.54}$$

The maximum value of the second term in Eq. (18.18) (at $t = 0$) is equal to 0.36, therefore just keeping the first term of the sum is a good approximation. If we accept this approximation for $P^-(t)$, we observe that this function of t oscillates with a period T_0, where

$$T_0 = \frac{2\pi}{E_e(1) - E_o(1)}. \tag{18.55}$$

Next let us assume that in the segment $(-b, b)$ there is a symmetric potential extending from $-a$ to a. We want to determine the time evolution of the wave packet $\Psi(x,t)$, which at the time $t = 0$ is located to the left of the barrier. Just as before we expand $\Psi(x, 0)$ in terms of $\psi_o(n,x)$ and $\psi_e(n,x)$. These two functions are the eigenfunctions of the Schrödinger equation with the boundary conditions

$$\psi_o(n, \pm b) = \psi_e(n, \pm b) = 0. \tag{18.56}$$

In this case the motion of the wave packet is given by

$$\Psi(x,t) = \sum_{n=1}^{\infty}\{\, a_n\psi_e(n,x)\exp[-i\mathcal{E}_e(n)t] + b_n\psi_o(n,x)\exp[-i\mathcal{E}_o(n)t]\} \tag{18.57}$$

where a_n and b_n are real coefficients defined like (18.46) and (18.47) but with $\psi(n,x)$'s replacing $\phi(n,x)$'s, and $\mathcal{E}_e(n)$ and $\mathcal{E}_o(n)$ are two consecutive eigenvalues. Since $\Psi(x,0)$ is located to the left of the barrier, therefore the probability of finding the particle at time t in the left side is $\mathcal{P}^-(t)$, where

$$\mathcal{P}^-(t) = \int_{-b}^{0} |\Psi(x,t)|^2 dx. \tag{18.58}$$

The initial conditions here implies that $\mathcal{P}^-(0) = 1$. For a potential which is symmetric about the origin, the normalized eigenfunctions satisfy the following conditions

$$\int_{-b}^{0} |\psi_e(x,t)|^2 dx. = \int_{-b}^{0} |\psi_o(x,t)|^2 dx = \frac{1}{2}. \tag{18.59}$$

Now by substituting (18.57) in (18.58) and making use of (18.59), we can write $\mathcal{P}^-(t)$ as

$$\mathcal{P}^-(t) = \frac{1}{2} + 2\sum_{n=1}^{\infty}\sum_{j=1}^{\infty} a_n b_j \Gamma(n,j) \cos\left\{[\mathcal{E}_e(n) - \mathcal{E}_o(j)]t\right\}, \tag{18.60}$$

where $\Gamma(n,j)$ is defined by

$$\Gamma(n,j) = \int_{-b}^{0} \psi_e(n,x)\psi_o(j,x) dx. \tag{18.61}$$

In this case we can also use the approximation that we used earlier and keep only the term with $n = j = 1$. Here because of the presence of the barrier this approximation works better than in the previous case. Hence

$$\mathcal{P}^-(t) \approx \frac{1}{2} + 2\Gamma(1,1) \cos\left\{[\mathcal{E}_e(1) - \mathcal{E}_o(1)]t\right\}. \tag{18.62}$$

This is the analogue of $P^-(t)$, Eq. (18.54). This approximate form of $\mathcal{P}^-(t)$ is sinusoidal and its period is given by

$$T_0' = \frac{2\pi}{\mathcal{E}_e(1) - \mathcal{E}_o(1)}. \tag{18.63}$$

If we denote the time-delay caused by the presence of the barrier by τ, then

$$\tau = \frac{1}{2}(T_0' - T_0) = \pi\left\{\frac{1}{\mathcal{E}_e(1) - \mathcal{E}_o(1)} - \frac{1}{E_e(1) - E_o(1)}\right\}. \tag{18.64}$$

This relation can be simplified when $\mathcal{E}_o - E_o$ and $\mathcal{E}_e - E_e$ are small compared to E_o and E_e, i.e.

$$\tau = \pi\left\{\frac{\mathcal{E}_o(1) - E_o(1) - \mathcal{E}_e(1) + E_e(1)}{[E_o(1) - E_e(1)]^2}\right\}. \tag{18.65}$$

Here we should emphasize two points regarding this formulation. First in our example the wave packet (18.50) was chosen so that the lowest state $n = 1$ contributed to the sum significantly.
If we choose $\Phi(x,t)$ as

$$\Phi(x,0) = \begin{cases} \sqrt{\frac{2}{b}} \sin\left(\frac{N\pi x}{b}\right) & \text{for } -b \le x \le 0 \\ 0 & \text{for } b \ge x \ge 0 \end{cases} , \tag{18.66}$$

we can find τ for two upper energy levels $E_o(N)$ and $E_e(N)$. The second point is that our result (18.64) is valid whether $V(x) \ge E$ or $V(x) \le E$, since in our derivation no assumptions were made regarding either of these inequalities.

We can also ask whether there is a connection between time-delays given by Eqs. (18.23) and (18.65). To show that these results are related to each other we consider Schwinger's method of relating the phase shift to the energy shift $(\mathcal{E}_e - E_e)$ [5].

Let us denote the phase shifts for different parity states by η_i, where $i = e$ denotes even and $i = o$ odd states. Then at the points outside the barrier $V(x)$, we have the following wave functions:

$$\psi_o(x < -a) = N_o \sin\left(\kappa_o x - \frac{1}{2}\eta_o\right), \tag{18.67}$$

$$\psi_o(x > a) = N_o \sin\left(\kappa_o x + \frac{1}{2}\eta_o\right), \tag{18.68}$$

$$\psi_e(x < -a) = N_e \cos\left(\kappa_e x - \frac{1}{2}\eta_e\right), \tag{18.69}$$

$$\psi_e(x > a) = N_e \cos\left(\kappa_e x + \frac{1}{2}\eta_e\right). \tag{18.70}$$

In these equations N_o and N_e are the normalization constants, and κ_o and κ_e are directly related to $\mathcal{E}_o$ and $\mathcal{E}_e$;

$$\mathcal{E}_{o,e} = \frac{1}{2}\kappa_{o,e}{}^2. \tag{18.71}$$

The constant quantities η_e and η_o are the phase shifts for even and odd states, and since we are dealing with a one-dimensional problem each of the wave functions are shifted by $\frac{1}{2}\eta_{e,o}$ (for two- or three-dimensional systems the reduced wave function is zero at the origin, hence the shift in the wave function will be $\eta_{e,o}$). By imposing the boundary conditions (18.56) at $x = \pm b$ on the wave functions we find that

$$\kappa_e b + \frac{\eta_e}{2} = \pm\left(N - \frac{1}{2}\right)\pi, \quad \kappa_o b + \frac{\eta_o}{2} = \pm N\pi, \tag{18.72}$$

where N is a positive integer. We choose the positive signs in these relations, so that Eqs. (18.67)-(18.70) in the limit of $\eta_{e,o} \to 0$, agree with $\phi_o(N,x)$ and $\phi_e(N,x)$, Eqs. (18.38)-(18.39). Now we write the time-delay τ, Eq. (18.65) as

$$\tau = 2\pi \frac{({k_o}^2 - {k_e}^2 + {\kappa_e}^2 - {\kappa_o}^2)}{({k_o}^2 - {k_e}^2)^2}. \tag{18.73}$$

Also from Eqs. (18.38) and (18.39) we conclude that

$$k_o - k_e = \frac{\pi}{2b}, \quad k_o + k_e = \left(2N - \frac{1}{2}\right)\frac{\pi}{b}, \tag{18.74}$$

$$\kappa_o - \kappa_e = \frac{1}{b}\left[\frac{\pi}{2} - \frac{1}{2}(\eta_o - \eta_e)\right], \tag{18.75}$$

and

$$\kappa_o + \kappa_e = \frac{1}{b}\left\{\left(2N - \frac{1}{2}\right)\pi - \frac{1}{2}(\eta_o + \eta_e)\right\}, \tag{18.76}$$

If we substitute these in (18.73), we can write τ in terms of η_o and η_e

$$\tau = \left\{\frac{\eta_o - \eta_e}{E_o - E_e} + \frac{\eta_o + \eta_e}{(4N-1)(E_o - E_e)} - \frac{{\eta_o}^2 - {\eta_e}^2}{(4N-1)\pi(E_o - E_e)}\right\}. \tag{18.77}$$

Next we try to find the limit of τ, Eq. (18.77), as b tends to infinity. When b becomes large, N also becomes large, so that both $E_o = \frac{N^2\pi^2}{2b^2}$, and $E_e = (N - \frac{1}{2})^2\frac{\pi^2}{2b^2}$ remain bounded. In this limit the last two terms in (18.77) become negligible compared to the first term, i.e. τ tends to

$$\tau = \frac{\eta_o - \eta_e}{E_o - E_e}. \tag{18.78}$$

The difference $E_o - E_e = \frac{N\pi^2}{2b^2}$ tends to zero as $b \to \infty$, and at the same time the difference $\eta_o - \eta_e$ becomes very small. Thus in this limit (18.78) goes over to $\tau = \frac{d\eta}{dE}$, which we found earlier by a different method.

The last problem of the time-delay that we want to study is a special case of one-dimensional tunneling, where an arbitrary potential acts on the particle between $-a$ and a but is infinity at the boundaries, i.e.

$$\begin{aligned} V(x) &= +\infty, \quad x < -b, \quad V(x) = +\infty, \quad x > c, \\ & V(x) \neq 0, \; -a < x < a, \end{aligned} \tag{18.79}$$

where $a < b < c$. If the potential $V(x)$ between $x = -a$ and $x = a$ is removed, then the eigenfunctions and the eigenvalues are

$$\phi(n,x) = \left(\frac{2}{b+c}\right)\sin\left[n\pi\left(\frac{c-x}{b+c}\right)\right], \tag{18.80}$$

and

$$E_n = \frac{1}{2}{k_n}^2 = \frac{n^2\pi^2}{2(c+b)^2}. \tag{18.81}$$

The presence of the potential in the range $-a < x < a$ modifies the wave function and the characteristic energies to the following forms:

$$\psi(x) = N\sin[\kappa(x+b)], \quad x \le -a, \tag{18.82}$$

$$\psi(x) = N\sin[\kappa(x+b)+\eta], \quad x \ge a, \tag{18.83}$$

and

$$\mathcal{E} = \frac{1}{2}\kappa^2. \tag{18.84}$$

The wave function (18.83) must vanish at $x = c$, hence

$$\kappa_n(c+b) + \eta_n = n\pi. \tag{18.85}$$

In the present case there is no symmetry, and we need to choose c so that the resonant condition is satisfied. For this case instead of (18.73) we define τ according to the relation

$$\tau = 2\pi\frac{\left({k_N}^2 - {k_{N-1}}^2 + {\kappa_{N-1}}^2 - {\kappa_N}^2\right)}{\left({k_N}^2 - {k_{N-1}}^2\right)^2}. \tag{18.86}$$

Just like the earlier case we find the limit of τ as c tends to infinity, keeping $\frac{N}{c}$ a fixed nonzero value. In this limit τ is given by

$$\tau = \frac{\eta_N - \eta_{N-1}}{E_N - E_{N-1}}, \tag{18.87}$$

which is similar to Eq. (18.78). However unlike the symmetric case, here if $\frac{c}{b}$ is large, then the wave packet which originally was localized in the segment $-b \le x \le 0$ tunnels away from this region and does not return to it for a very long time. This follows from the fact that in the limit $c \to \infty$ the difference $\mathcal{E}_N - \mathcal{E}_{N-1}$ is proportional to $\frac{2N-1}{(c+b)^2}$ and therefore $T_0' = \frac{2\pi}{\mathcal{E}_N - \mathcal{E}_{N-1}}$ goes to infinity.

18.3 Landauer and Martin Criticism of the Definition of the Time-Delay in Quantum Tunneling

In this section following the work of Landauer and Martin [6] and Leavens and Aers [7] we want to show that there is apparently no causal relationship between the peak (or the center) of the incident wave packet and the peak (or center) of the transmitted wave. We know that the velocity of the different components of the wave packet are not equal, and the components with higher energy travel faster through the barrier than the lower energy components. Therefore we can select these components so that the transmitted wave packet is mostly formed from the forerunner part of the incident wave packet. These can be chosen in such a way that the maximum of the transmitted wave appears on the other side of the potential before the maximum of the incident wave packet reaches the barrier. This is apparently a violation of the principle of causality (see also Chapter 22). Thus we need a better and more realistic definition of the tunneling time-delay. The argument of Landauer and Martin is as follows:

Consider a wave packet of width $\hbar\Delta k$ in momentum space which tunnels through a barrier where the transmission amplitude for the plane wave with momentum $\hbar k$ is given by $T(k)$. Let us assume that the wave packet is initially located at $x = x_0$ to the left of the barrier, and the barrier is zero outside the segment $a < x < b$, $(x_0 << a)$. A wave packet approaching this barrier is of the form

$$\psi_{in}(x,t) = \int_0^\infty A(k)\exp\left[i\left(kx - \frac{E(k)t}{\hbar}\right)\right]dk, \tag{18.88}$$

where $A(k)$ is the amplitude of the plane wave. For early times $t \approx 0$ this wave packet does not interact with the barrier if we choose $x_0 << a$. As $t \to \infty$, a part of the incident wave is reflected and a part is transmitted. The transmitted wave is expressible as

$$\psi_{tr}(x,t) = \int_0^\infty A(k)T(k)\exp\left[i\left(kx - \frac{E(k)t}{\hbar}\right)\right]dk. \tag{18.89}$$

In terms of the Fourier components, we can write $\psi_{in}(x,t)$ and $\psi_{tr}(x,t)$ as

$$\phi_{in}(k) = A(k)\exp\left[i\left(kx - \frac{E(k)t}{\hbar}\right)\right], \tag{18.90}$$

and

$$\phi_{tr}(k) = A(k)|T(k)| \exp\left[i\left(kx - \frac{E(k)t}{\hbar} + \eta(k)\right)\right], \tag{18.91}$$

where

$$T(k) = |T(k)|e^{i\eta(k)} = \exp[-\alpha(k) + i\eta(k)], \tag{18.92}$$

is the transmission amplitude.

Let us assume that $A(k)$ has a peak at $k = k_0$, then the position of the peak at the time t found from the incident wave $\phi_{in}(k)$ is

$$x_{in}(t) = x_0 + \frac{\hbar}{m}\langle k\rangle_{in}\, t, \tag{18.93}$$

and for the transmitted wave at the time t is

$$x_{tr} = x_0 + \frac{\hbar}{m}\langle k\rangle_{tr}\, t - \left\langle\frac{d\eta(k)}{dk}\right\rangle_{tr}. \tag{18.94}$$

Here $\langle f(k)\rangle_{in}$ and $\langle g(k)\rangle_{tr}$ are defined by

$$\langle f(k)\rangle_{in} = \frac{\int_{-\infty}^{\infty}|\phi_{in}(k)|^2 f(k)dk}{\int_{-\infty}^{\infty}|\phi_{in}(k)|^2 dk}, \tag{18.95}$$

and

$$\langle g(k)\rangle_{tr} = \frac{\int_{-\infty}^{\infty}|\phi_{tr}(k)|^2 g(k)dk}{\int_{-\infty}^{\infty}|\phi_{tr}(k)|^2 dk}, \tag{18.96}$$

respectively. In particular the incident wave arrives at $x = a$ at $t = t_a$, where from (18.93) we have

$$x_{in}(t_a) = a = x_0 + \frac{\hbar}{m}\langle k\rangle_{in}\, t_a. \tag{18.97}$$

The transmitted wave leaves the other side of the barrier at $x = b$ at $t = t_b$, where

$$x_{tr}(t_b) = b = x_0 + \frac{\hbar}{m}\langle k\rangle_{tr}\, t_b - \left\langle\frac{d\eta(k)}{dk}\right\rangle_{tr}. \tag{18.98}$$

If we choose $A(k)$ to be a Gaussian

$$A(k) = \exp\left[-\frac{(k-k_0)^2}{2(\Delta k)^2}\right], \tag{18.99}$$

then using the expansion

$$\begin{aligned} - \quad & \alpha(k) + i\eta(k) = -\alpha(k_0) + i\eta(k_0) \\ + \quad & (k - k_0)\left[-\left(\frac{d\alpha(k)}{dk}\right)_{k_0} + i\left(\frac{d\eta(k)}{dk}\right)_{k_0}\right], \end{aligned} \tag{18.100}$$

we get

$$b = x_0 + \frac{\hbar}{m}\left[k_0 - \left(\frac{d\alpha(k)}{dk}\right)_{k_0}(\Delta k)^2\right] t_b - \left(\frac{d\eta(k)}{dk}\right)_{k_0}. \tag{18.101}$$

Similarly using the wave packet (18.99) we can write (18.97) as

$$a = x_0 + \frac{\hbar}{m} k_0 t_a. \tag{18.102}$$

Equation (18.101) shows that the potential shifts the effective velocity with which the transmitted component has reached the barrier by an amount

$$-\frac{\hbar}{m}(\Delta k)^2\left(\frac{d\alpha(k)}{dk}\right)_{k_0}. \tag{18.103}$$

This change of velocity is positive, e.g. for a rectangular opaque barrier ($\alpha > 1$) of height V_0 , $\alpha(k)$ is given by

$$\alpha(k) = (b - a)\left(\frac{2mV_0}{\hbar^2} - k^2\right)^{\frac{1}{2}}, \tag{18.104}$$

and therefore $\left(\frac{d\alpha(k)}{dk}\right)_{k=k_0} < 0$. Now if $t_b < t_a$, then the center of the transmitted wave packet leaves the barrier before of the arrival of the incident wave on the other side. This inequality can be written as

$$\left(\frac{m}{\hbar}\right)\frac{\left[b - \left(\frac{d\eta(k)}{dk}\right)_{k_0}\right]}{\left[k_0 - (\Delta k)^2\left(\frac{d\alpha(k)}{dk}\right)_{k_0}\right]} < \frac{ma}{\hbar k_0}, \tag{18.105}$$

or

$$-\frac{a}{k_0}\left(\frac{d\alpha(k)}{dk}\right)_{k_0}(\Delta k)^2 > (b - a) + \left(\frac{d\eta(k)}{dk}\right)_{k_0}. \tag{18.106}$$

At this point Landauer and Martin [6] argue that if the wave packet is allowed to travel a large distance $a - x_0$ or if Δk is large, the inequality (18.106) is satisfied and thus the motion of the center of peak of the wave packet cannot be used to define a measure of the time-delay.

18.4 Time-Delay in Multi-Channel Tunneling

Let us consider the extension of the concept of time-delay to the cases where the barrier couples a number of channels similar to the coupled equations found for periodic potentials, Eq. (9.7) [9]. Here we assume that the incident wave enters in the n-th channel and after tunneling emerges from the j-th channel. If we denote the time-delay for this case by $\langle \Delta\tau_{nj}\rangle$, we can write (see Eq. (18.20))

$$\langle \Delta\tau_{nj}\rangle = \lim_{x\to\infty}\left[\frac{1}{x}\int_x^{2x}\Delta\tau_{nj}(x')dx'\right], \tag{18.107}$$

where

$$\Delta\tau_{nj}(x) = \frac{1}{2}\int_{-x}^{x}\sum_p\left[\psi^*_{np}(x')\psi_{pj}(x') - \phi^*_{np}(x')\phi_{pj}(x')\right]dx'$$
$$+ \quad \frac{1}{2}\int_{-x}^{x}\sum_p\left[\psi_{np}(x')\psi^*_{pj}(x') - \phi_{np}(x')\phi^*_{pj}(x')\right]dx'. \tag{18.108}$$

Here $\Delta\tau_{nj}(x)$ is the multi-channel generalization of τ_q, Eq. (18.10), and $\psi_{nj}(x')$ is the wave function for scattering or tunneling from the n-th to the p-th channel and $\phi_{nj}(x') = \psi_{nj}(x', V=0)$ is the same wave function but in the absence of the potential. The parameter E which is the energy of the particle in the incident channel is a continuous variable, $\frac{1}{2}k_n^2 = E - n\omega$, and the partial derivative $\frac{\partial\psi_{np}}{\partial E}$ is well-defined. Thus by differentiating the coupled differential equation

$$\frac{d^2\psi_{np}}{dx^2} + {k_n}^2\psi_{np} = \sum_q V_{nq}\psi_{qp}, \quad m = \hbar = 1, \tag{18.109}$$

with respect to E, and using the equation for the Hermitian conjugate of (18.109), we find

$$\sum_p \psi^*{}_{np}\psi_{pj} = -\frac{1}{2}\frac{\partial}{\partial x}\sum_p\left\{\psi^*{}_{np}\frac{\partial}{\partial x}\left(\frac{\partial\psi_{pj}}{\partial E}\right) - \left(\frac{\partial\psi^*{}_{np}}{\partial x}\right)\left(\frac{\partial\psi_{pj}}{\partial E}\right)\right\}. \tag{18.110}$$

Following the method that we described for a single channel we need the asymptotic form of the wave functions $\psi_{np}(x)$ in order to carry out the integration in (18.108). These asymptotic forms are given by

$$\psi_{np}(x\to-\infty) = \frac{1}{\sqrt{k_n}}\left[\exp(ik_nx)\delta_{np} + R_{np}\exp(-ik_nx)\right], \tag{18.111}$$

and

$$\psi_{np}(x \to \infty) = \frac{1}{\sqrt{k_n}} T_{np} \exp(ik_n x). \tag{18.112}$$

Now by integrating (18.110) from $-x$ to x and using the asymptotic expressions for ψ_{np} and ψ^*_{np}, we have

$$\begin{aligned}
&\int_{-x}^{x} dx \sum_p \psi^*{}_{np}\psi_{pj} \\
= &\left(\frac{x}{2k_n}\right)(2 + T^*{}_{nn}T_{nj} + T^*{}_{nj}T_{nn} + R^*{}_{nn}R_{nj} + R^*{}_{nj}R_{nn}) \\
- &i\left[\frac{1}{8(E - n\omega)}(T^*{}_{nn}T_{nj} - T^*{}_{nj}T_{nn} + R^*{}_{nn}R_{nj} - R^*{}_{nj}R_{nn})\right] \\
- &\frac{i}{2}\left[T^*_{nn}\left(\frac{\partial T_{nj}}{\partial E}\right) + T^*{}_{nj}\left(\frac{\partial T_{nn}}{\partial E}\right) + R^*{}_{nn}\left(\frac{\partial R_{nj}}{\partial E}\right) + R^*{}_{nj}\left(\frac{\partial R_{nn}}{\partial E}\right)\right] \\
- &\ c.c. + J,
\end{aligned} \tag{18.113}$$

where *c.c.* refers to the complex conjugate of the terms in the last square bracket, and J denote those terms which vanish upon averaging. Equations (18.111) and (18.112) show that only for open channels, i.e. those channels with real k_n we have these limits, otherwise $\psi_{np}(x \to \infty)$ will be zero. For the open channels it is simpler to write T_{np} and R_{np} in terms of the phases δ_{np} and η_{np};

$$T_{np} = \frac{1}{2}\left[\exp(2i\delta_{np}) + \exp(2i\eta_{np})\right], \tag{18.114}$$

and

$$R_{np} = \frac{1}{2}\left[\exp(2i\eta_{np}) - \exp(2i\delta_{np})\right]. \tag{18.115}$$

If we substitute these on the left side of (18.113), that part can be written as

$$\left(\frac{x}{2k_n}\right)\left\{\cos[2(\delta_{nj} - \delta_{nn})] + \cos[2(\eta_{nj} - \eta_{nn})] + 2\right\}. \tag{18.116}$$

This equation shows that the coefficient of x is nonnegative. Now let us examine the wave function ψ_{np} when $V = 0$. In this case the incident and the outgoing channels are the same. We choose the phase of this wave function to be

$$\begin{aligned}
\phi_{np}(x) \ = \ &\frac{1}{2\sqrt{k_n}}\left[\cos 2(\delta_{nj} - \delta_{nn}) + \cos 2(\eta_{nj} - \eta_{nn}) + 2\right]^{\frac{1}{2}} \\
\times \ &\exp(ik_n x)\delta(n, p),
\end{aligned} \tag{18.117}$$

where in this equation $\delta(n,p)$ is the Kronecker delta and should not be confused with the phases δ_{np} and δ_{nj}.

By substituting $\phi_{np}(x)$ in (18.108) and making use of (18.116) we observe that when we calculate all the terms which are proportional to x, according to Eq. (18.107), these terms cancel each other and the average $\langle\Delta\tau_{nj}\rangle$ simplifies;

$$\begin{aligned}\langle\Delta\tau_{nj}\rangle &= \frac{1}{8(E-n\omega)}\left[\sin 2(\delta_{nj}-\delta_{nn}) + \sin 2(\eta_{nj}-\eta_{nn})\right] \\ &- \frac{i}{2}\left[T^*_{nn}\left(\frac{\partial T_{nj}}{\partial E}\right) + T^*_{nj}\left(\frac{\partial T_{nn}}{\partial E}\right) + R^*_{nn}\left(\frac{\partial R_{nj}}{\partial E}\right) + R^*_{nj}\left(\frac{\partial R_{nn}}{\partial E}\right)\right] \\ &- c.c., \end{aligned} \tag{18.118}$$

where $c.c.$ denotes the complex conjugate of the last part (in square brackets) of Eq. (18.118). Now if we replace T_{nn} , T_{nj},... in terms of their phases we find

$$\begin{aligned}\langle\Delta\tau_{nj}\rangle &= \frac{1}{8(E-n\omega)}\left[\sin 2(\delta_{nj}-\delta_{nn}) + \sin 2(\eta_{nj}-\eta_{nn})\right] \\ &+ \frac{1}{2}\left[\left(\frac{d\delta_{nn}}{dE} + \frac{d\delta_{nj}}{dE}\right)\cos 2(\delta_{nj}-\delta_{nn})\right] \\ &+ \frac{1}{2}\left[\left(\frac{d\eta_{nn}}{dE} + \frac{d\eta_{nj}}{dE}\right)\cos 2(\eta_{nj}-\eta_{nn})\right]. \end{aligned} \tag{18.119}$$

This is a general expression for the time-delay for different incoming and outgoing channels. In particular when the incoming and the outgoing channels are the same, $\langle\Delta\tau_{nn}\rangle$ takes the form

$$\langle\Delta\tau_{nn}\rangle = \left(\frac{d\delta_{nn}}{dE} + \frac{d\eta_{nn}}{dE}\right). \tag{18.120}$$

We note that in the case of a single channel if we substitute T and R in Eq. (18.21) in terms of their phases, i.e. Eqs. (18.114) and (18.115) we obtain $\langle\tau_q\rangle$ to be of the form

$$\langle\tau_q\rangle = \hbar\left\{\left(\frac{d\delta}{dE} + \frac{d\eta}{dE}\right) + \cos 2(\delta-\eta)\left(\frac{d\delta}{dE} - \frac{d\eta}{dE}\right)\right\}. \tag{18.121}$$

Since the second term in this equation is oscillatory and its average is zero, we find $\langle\tau_q\rangle$ to be the same as $\langle\Delta\tau_{nn}\rangle$ given by Eq. (18.120). It is interesting to note that the first term of $\langle\tau_{nj}\rangle$ blows up when $E = n\omega$ which corresponds to resonance situation.

18.5 Reflection Time in Quantum Tunneling

In this section we want to study the question of the time that a particle spends under a divergent barrier, i.e. a barrier which tends to infinity on one side and is zero on the other side;

$$V(x) = \begin{cases} 0 & \text{for } x \leq 0 \\ \infty & \text{for } x \to \infty \end{cases} . \tag{18.122}$$

Apart from these conditions, the shape of $V(x)$ is arbitrary. The asymptotic form of the potential $V(x \to \infty) \to \infty$ means that a wave packet $\Psi(x,t)$ which is incident from the left is completely reflected.

Here we want to determine the time τ_R that such a wave packet has spent in the region of nonzero potential before returning to the part where $V(x) = 0$, i.e. $x < 0$.
According to classical mechanics this time is given by

$$\tau^{cl}{}_R = \int_{-\infty}^{\infty} \theta[x(t)]dt, \tag{18.123}$$

where $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x > 0 \end{cases} , \tag{18.124}$$

and $x(t)$ is the position of the particle at the time t.

Now let us consider a similar definition according to the laws of quantum mechanics. Since this time is measurable, by analogy with the classical equation (18.123), we examine the expectation value of $\theta(x)$ [9] [10]

$$\tau_R = \int_{-\infty}^{\infty} dt \int_0^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \langle \Psi|\theta(x)|\Psi\rangle \, dt = \left\langle \hat{T}_R \right\rangle, \tag{18.125}$$

where $\left\langle \hat{T}_R \right\rangle$ is the reflection time operator . The exact form of this operator is the subject of our inquiry. First we observe that

$$\psi_E(x) = \sqrt{\frac{m}{2\pi\hbar^2 k}} \left(e^{ikx} + R(E)e^{-ikx}\right), \tag{18.126}$$

is the eigenfunction of the Schrödinger equation for $x < 0$. Here we have chosen the amplitude of $\psi_E(x)$ so that it satisfies the δ-function normalization condition (see Eq. (18.130) below). Since we have complete reflection therefore

$$R(E) = [R^*(E)]^{-1}, \tag{18.127}$$

or we can write $R(E)$ in terms of a single phase shift $\delta(E)$ as

$$R(E) = e^{i\delta(E)}. \tag{18.128}$$

Inside the barrier and for large x, the wave function will be exponentially damped, therefore the complete solution of the Schrödinger equation will be of the form:

$$\Psi(E,x) = \begin{cases} \psi_E(x) & \text{for } x < 0 \\ O(e^{-\gamma x}) & \text{for } x \to \infty \end{cases}. \tag{18.129}$$

Thus the overall normalization of the wave function is expressible as

$$\int_{-\infty}^{\infty} \psi(E_1,x)^*\psi(E_2,x)dx = \delta(E_1 - E_2). \tag{18.130}$$

The set $\{\psi(E,x)\}$ forms a complete set and we can expand the wave packet $\Psi(x,t)$ in terms of $\psi(E,x)$;

$$\Psi(x,t) = \int_0^{\infty} f(E)\psi(E,x)\exp\left(\frac{-iEt}{\hbar}\right)dE, \tag{18.131}$$

where $f(E)$ is the coefficient of expansion. Now if we substitute (18.131) in (18.125), we find the expectation value of $\hat{T}_R$;

$$\left\langle \hat{T}_R \right\rangle = 2\pi\hbar \int_0^{\infty} |f(E)|^2 dE \int_0^{\infty} |\psi(E,x)|^2 dx. \tag{18.132}$$

The function $f(E)$ can be determined from the original shape of the wave packet, i.e.

$$f(E) = \int_{-\infty}^{\infty} \psi^*(E,x)\Psi(x,0)dx, \tag{18.133}$$

and if $\Psi(x,0)$ is properly normalized, then $f(E)$ also satisfies the normalization condition

$$\int_0^{\infty} |f(E)|^2 dE = 1. \tag{18.134}$$

Now following the same method that we used in obtaining (18.15), i.e.

$$\begin{aligned} &\int_0^{\infty} \psi^*(E,x)\psi(E,x)dx \\ &= -\frac{\hbar^2}{2m}\left[\psi^*(E,x)\frac{\partial}{\partial x}\left(\frac{\partial\psi(E,x)}{\partial E}\right) - \frac{\partial\psi(E,x)}{\partial E}\frac{\partial\psi^*(E,x)}{\partial x}\right]_0^{\infty}, \end{aligned} \tag{18.135}$$

and substituting Eqs. (18.126) and (18.128) in (18.129) we get

$$\int_0^\infty \psi^*(E,x)\psi(E,x)dx = \frac{1}{2\pi}\left(\frac{d\delta(E)}{dE} + \frac{\sin\delta(E)}{2E}\right). \tag{18.136}$$

By substituting this in (18.132) we obtain $\left\langle \hat{T}_R \right\rangle$;

$$\left\langle \hat{T}_R \right\rangle = \hbar \int_0^\infty |f(E)|^2 \left(\frac{d\delta(E)}{dE} + \frac{\sin\delta(E)}{2E}\right) dE. \tag{18.137}$$

Noting that (18.137) depends on $|f(E)|^2$, we can write $\left\langle \hat{T}_R \right\rangle$ as

$$\begin{aligned} \left\langle \hat{T}_R \right\rangle &= \left\langle \Psi|\hat{T}_R|\Psi \right\rangle = \int_0^\infty dE_1 \int_0^\infty dE_2 \left\langle \Psi|E_1\right\rangle \left\langle E_1|\hat{T}_R|E_2\right\rangle \left\langle E_2|\Psi\right\rangle \\ &= \int_0^\infty dE_1 \int_0^\infty f^*(E_1)T_R(E_1,E_2)f(E_2)\exp\left[-\frac{i(E_2-E_1)t}{\hbar}\right] dE_2. \end{aligned} \tag{18.138}$$

Comparing (18.137) and (18.138), we obtain the matrix elements of $\hat{T}_R$

$$\left\langle E_1|\hat{T}_R|E_2\right\rangle = T_R(E_1,E_2) = \tau_R(E_1)\left\langle E_2|E_1\right\rangle = \tau_R(E_1)\delta(E_1-E_2). \tag{18.139}$$

Thus the eigenvalues of $\hat{T}_R$ are

$$\tau_R(E) = \hbar\left(\frac{d\delta(E)}{dE} + \frac{\sin\delta(E)}{2E}\right), \tag{18.140}$$

and the Hermitian operator has a unique representation, Eqs. (18.139) and (18.140). Since this $\hat{T}_R$ is independent of the time and is also diagonal in the energy representation, therefore its commutator with the Hamiltonian operator is zero,

$$\left[\hat{H},\hat{T}_R\right] = 0. \tag{18.141}$$

The coordinate representation of $\hat{T}_R$ is given by

$$T_R(x_1,x_2) = T_R{}^*(x_2,x_1) = \int_0^\infty \left\langle x_1|E\right\rangle \tau_R(E)\left\langle E|x_2\right\rangle dE, \tag{18.142}$$

and this shows that $\hat{T}_R$ is nonlocal in the coordinate representation.

Let us now consider two simple examples of τ_R which can be calculated analytically.

(i) - For the linear potential

$$V(x) = \begin{cases} 0 & \text{for } x<0 \\ Fx & \text{for } x \ge 0 \end{cases}, \tag{18.143}$$

the solution of the Schrödinger equation is given in terms of the Airy function (see Chapter 6);

$$\psi(E, x \geq 0) = N A_i \left[\left(\frac{2mF}{\hbar^2}\right)^{\frac{1}{3}} \left(x - \frac{E}{F}\right)\right]. \tag{18.144}$$

From Eq. (18.123) we can calculate ${\tau^{cl}}_R(E)$, and from (18.140) we obtain $\tau_R(E)$;

$$ {\tau^{cl}}_R(E) = \tau_R(E) = \frac{2\hbar k}{F}, \quad \sqrt{2mE} = \hbar k. \tag{18.145}$$

It is interesting to note that for this barrier the reflection time in classical and quantum mechanics are the same and the latter is independent of $\hbar$.
(ii) - Quadratic potential - In this case

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ \frac{1}{2} m\omega^2 x^2 & \text{for } x \geq 0 \end{cases}, \tag{18.146}$$

and the wave function for $x \geq 0$ is the Whittaker function [13]. By using this solution in (18.140), we find $\tau_R(E)$ as

$$\tau_R(E) = \left[\psi\left(\frac{3}{4} - \varepsilon\right) - \psi\left(\frac{1}{4} - \varepsilon\right)\right] \frac{\sqrt{\varepsilon}}{\omega} \left\{ \frac{\Gamma(\frac{1}{4} - \varepsilon)\Gamma(\frac{3}{4} - \varepsilon)}{\varepsilon \Gamma\left(\frac{1}{4} - \varepsilon\right)^2 + \Gamma\left(\frac{3}{4} - \varepsilon\right)^2} \right\}, \tag{18.147}$$

where Γ and ψ are gamma and digamma functions and

$$\varepsilon = \frac{E}{2\hbar\omega}, \tag{18.148}$$

is a dimensionless number. For the values of E equal to $(j + \frac{1}{2})\hbar\omega$, the reflection time τ_R assumes a simpler form. For instance when $j = 2n$ we have

$$\tau_R\left[E = \left(2n + \frac{1}{2}\right)\hbar\omega\right] = \frac{\sqrt{\pi} 2^{n+1} n!}{\omega\sqrt{4n+1}(2n-1)!!}, \tag{18.149}$$

and for $j = 2n - 1$ the result is

$$\tau_R\left[E = \left(2n - \frac{1}{2}\right)\hbar\omega\right] = \frac{\sqrt{\pi} 2^{n-1}\sqrt{4n-1}(n-1)!}{\omega(2n-1)!!}. \tag{18.150}$$

In the limit of $n \to \infty$, Eqs. (18.149) and (18.150) tend to the classical time of reflection

$${\tau^{cl}}_R(E) = \frac{\pi}{\omega}. \tag{18.151}$$

18.6 Minimum Tunneling Time

Bracher and Kleber [11] have suggested the concept of the minimum tunneling time, which like the reflection time is well-defined in quantum theory. Starting with the Schrödinger equation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi, \tag{18.152}$$

we write the probability current $j[\psi(E)]$ as

$$j[\psi(E)] = \frac{\hbar}{m}\mathrm{Im}\left[\psi^*(E)\frac{d\psi(E)}{dx}\right]. \tag{18.153}$$

Now we define the time that a particle spends between the points $x = a$ and $x = b$ by

$$\tau_D[\psi(E)] = \frac{1}{j[\psi(E)]}\int_a^b |\psi(E,x)|^2\, dx. \tag{18.154}$$

This τ_D is the time that is necessary for the current $j[\psi(E)]$ to replace all of the particles in the segment $a < x < b$ with new ones.

From the definition of τ_D it is clear that this time is a ratio of two quadratic functionals of $\psi(E,x)$. Thus if we replace $\psi(E,x)$ by $\alpha\psi(E,x)$, where α is a nonzero constant τ_D will not change. In addition τ_D is always a positive quantity and is bounded below. Hence one can find a function (or functions) say $\psi_m(E,x)$, so that $\tau_D[\psi(E)]$ assumes its minimum value

$$\tau_{min}(E) = \min_{H\psi=E\psi}\left\{\frac{1}{j[\psi(E)]}\int_a^b |\psi(E,x)|^2 dx\right\}. \tag{18.155}$$

Also from the definition (18.154) it is clear that there is no maximum for τ_D, since $j[\psi(E)] = 0$ makes it infinite.
As an example consider a rectangular barrier of height V_0, and width d;

$$V(x) = V_0\theta\left(x - \frac{1}{2}d\right)\theta\left(\frac{1}{2}d - x\right), \tag{18.156}$$

where $\theta(x)$ is a step function. Let us denote the wave number of the particle under the barrier by κ, where

$$\kappa = \frac{1}{\hbar}\sqrt{2m|E - V(x)|}, \tag{18.157}$$

then under the barrier the wave function will be a superposition of the two functions

$$c(x) = \cosh(\kappa x), \quad s(x) = \sinh(\kappa x). \tag{18.158}$$

But if $E > V_0$, then we replace $\cosh(\kappa x)$ and $\sinh(\kappa x)$ by $\cos(\kappa x)$ and $\sin(\kappa x)$ respectively. Using these we can calculate τ_{min} from Eq. (18.155),

$$\tau_{min} = \begin{cases} \frac{m}{\hbar\kappa^2}\left[\sinh^2(\kappa d) - (\kappa d)^2\right]^{\frac{1}{2}} & \text{for } E < V_0 \\ \frac{1}{\sqrt{3}}\frac{md^2}{\hbar} & \text{for } E = V_0 \\ \frac{m}{\hbar\kappa^2}\left[(\kappa d)^2 - \sinh^2(\kappa d)\right]^{\frac{1}{2}} & \text{for } E > V_0 \end{cases} . \tag{18.159}$$

For this problem if we use the semi-classical approximation when $E \geq V_0$ we find

$$\tau_{min} = \frac{d}{v_{cl}(E)}, \tag{18.160}$$

where $v_{cl}(E)$ is the classical velocity of the particle. However if $E \leq V_0$ then we have

$$\tau_{min} = \tau_{min}{}^{WKB} = \frac{m}{2\hbar\kappa^2}e^{\kappa d}. \tag{18.161}$$

In Fig. (18.3) we see that $\tau_{min}(E)$ is a well-defined continuous function of $E - V_0$ which joins $\tau_{min}{}^{WKB}$ when $V_0 > E$ on one side and approaches $\tau^{cl}{}_{min}$ for $E > V_0$ on the other side.

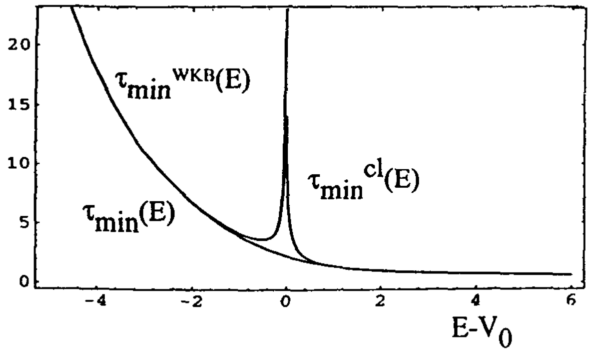

Figure 18.3: Minimum tunneling time for a rectangular barrier Eq. (18.159), and its semi-classical approximation.

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Chapter 19

More about Tunneling Time

We have already seen that a proper formulation of quantum mechanical reflection time is given by Bracher and Kleber [1]. This is achieved by constructing a Hermitian operator T_R defined by (18.125) and this operator commutes with the Hamiltonian and measures the reflection time. But for the problem of tunneling time no corresponding Hermitian operator is known. We have also discussed the problems associated with the measurement of delay time in tunneling using the motion of the center or the peak of the wave packet as an indicator of the travel time.

In this chapter we study some of the other possible ways of formulating tunneling time [2] [3] [4] [5] [6] [7] [8] [9]. But first let us consider a typical example and order of magnitude of the tunneling time in condensed matter physics. An electron with an effective mass of $m^* = 0.07m_e$, where m_e is the bare mass of the electron, tunnels through $GaAs/AlGaAs/GaAs$ structure [10]. If the height of the barrier is $V_0 = 0.23eV$ and the width of the barrier is $d = 60 \times 10^{-10}m$, then for the incident energy of $E = 0.115eV$, the tunneling time is about $6 \times 10^{-15}s$.

In the following sections whenever the wave packet description is used we assume the following conditions:

(i) - The kinetic energy of the wave packet in free space must be less than the height of the barrier (see also Chapter 13).

(ii) - The width of the barrier should not be large, since then only the high frequency components of the incident wave packet are transmitted.

(iii) - On account of the spreading of the wave packet the observation time must not be very long.

19.1 Dwell and Phase Tunneling Times

The dwell time (or sojourn time) [10] is the time spent by the particle in any finite region of space, averaged over all incoming particles. In one-dimensional tunneling as we have seen in Chapter 18 there are two phases, one for the reflection amplitude $\delta(E)$ and the other for the transmission amplitude $\eta(E)$. The dwell time is not only dependent on the phases but also on the magnitudes of $R(E)$ and $T(E)$. On the other hand we can define two phase times, i.e. one time associated with the reflection-, and the other associated with the transmission phase. These are given by $\hbar\frac{d\delta}{dE}$ and $\hbar\frac{d\eta}{dE}$ respectively.

As we have seen earlier (Chapter 18), in classical dynamics the probability of finding a particle of energy E in an interval (x_1, x_2) is proportional to the time that the particle spends in this interval

$$P_{cl} \propto \int_{x_1}^{x_2} \frac{dx}{v(x)} = \int_{x_1}^{x_2} \frac{dx}{\sqrt{2m(E-V(x))}}. \tag{19.1}$$

The same probability in quantum mechanics is expressible in terms of the wave function

$$P_Q = \int_{x_1}^{x_2} |\psi(x,E)|^2\, dx, \tag{19.2}$$

where $\psi(x,E)$ is properly normalized (see Eqs. (18.16) and (18.17)). This probability is also a measure of the time that the particle spends in this interval. Thus we define the dwell time by

$$\tau_D(x_1, x_2; E) = \int_{x_1}^{x_2} |\psi(x,E)|^2\, dx. \tag{19.3}$$

We can relate this dwell time to the phase times using the method outlined in Chapter 17, Eqs. (18.12)-(18.19). Thus we find

$$\begin{aligned}\tau_D(x_1, x_2; E) &= \hbar\left\{|R(E)|^2\left(\frac{d\delta}{dE}\right) + |T(E)|^2\left(\frac{d\eta}{dE}\right)\right\}\\ &+ \frac{\hbar}{2E}|R(k)|\sin(2kx_1-\delta) + \frac{\hbar k}{4E}(x_2-x_1)|T(k)|^2.\end{aligned} \tag{19.4}$$

As an example let us consider the rectangular barrier $v_2\theta(x)\theta(a-x)$, Eq. (6.68), for which the transmission amplitude is given by (6.69). Noting that $T(k)$ is complex and writing it as $|T(k)|\exp[i\eta(k)]$, where $k = \frac{\sqrt{2mE}}{\hbar}$, we find

$$\eta(k) = -\tan^{-1}\left[\frac{q^2-k^2}{2kq}\tanh(qa)\right]. \tag{19.5}$$

Thus the transmission phase time $\tau_{pT}(k)$ in this case is

$$\begin{aligned}\tau_{pT} &= \frac{m}{\hbar k}\frac{d\eta(k)}{dk} \\ &= \frac{m}{\hbar k q \mathcal{D}(k)}\left[2qak^2(q^2-k^2)+(q^2+k^2)^2\sinh(2qa)\right], \qquad (19.6)\end{aligned}$$

where

$$\mathcal{D}(k) = 4k^2q^2 + (q^2+k^2)^2\sinh^2(qa). \qquad (19.7)$$

In a similar way we can find the reflection phase time $\tau_{pR}(k)$. This is different from the reflection time that we discussed in Chapter 18. Both of these phase times tend to infinity as k goes to zero. However for the same rectangular well if we calculate $\tau_D(0,a,k)$, we find

$$\tau_D(0,a,k) = \frac{mk}{\hbar q D(k)}\left[2qa(q^2-k^2)+(q^2+k^2)\sinh(2qa)\right]. \qquad (19.8)$$

For an opaque barrier, i.e. when $qa >> 1$, the transmission is very small, and both τ_{pT} and τ_D will assume the simpler forms of

$$\tau_{pT} \to \frac{2m}{k\sqrt{2m(V-E)}} \quad \text{for} \quad qa >> 1, \qquad (19.9)$$

and

$$\tau_D \to \frac{\hbar k}{qV} = \frac{\hbar^2 k}{V\sqrt{2m(V-E)}} \quad \text{for} \quad qa >> 1, \qquad (19.10)$$

respectively. Thus both of these tunneling times for opaque barriers are independent of the widths of the barriers.

This independence of τ_{pT} and τ_D from the width of the barrier is sometimes referred to as the Hartman effect [11] [12]. For the second example let us consider the case of separable potential of Chapter 7 (Eq. (7.40)), where $T(k)$ and $R(k)$ are known analytically (Eqs. (7.45) and (7.46)). In this case the phase times are both given by

$$\tau_{pT} = \tau_{pR} = -\mathrm{Im}\,\frac{m}{\hbar k}\frac{d}{dk}\ln R(k). \qquad (19.11)$$

For this particular barrier τ_{pT} goes through zero at the local maximum of $|T(k)|^2$, (see Fig. (7.8)), and reaches a maximum before decreasing and then asymptotically going to zero as $k \to \infty$. For the parameters given in 7.2 the zero of $\tau_{pT}(k)$ is located at $k = 1.483L^{-1}$.

Finally it is interesting to determine the phase time for two δ-function

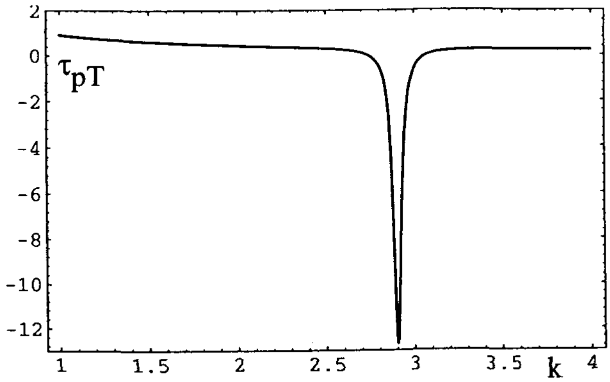

Figure 19.1: The transmission phase time for two δ-function potentials measured in units of $\frac{ma}{\hbar k}$. The resonant wave number is at $k = 2.906L^{-1}$.

barriers under the resonant condition. In Eq. (6.49) we obtained an analytic expression for $T(k)$ for the potential given by Eq. (6.48). Again we note that the transmission phase time is

$$\tau_{pT}(k) = -\frac{m}{\hbar k}\mathrm{Im}\,\frac{d}{dk}\ln T(k), \tag{19.12}$$

when $T(k)$ is given by (6.49). This phase time should be compared to the travel time of a free particle with the same energy and mass over the distance equal to the width of the potential a. Measured in the units of this travel time, $\frac{ma}{\hbar k}$, we have

$$\tau_{pT}(k) = -\frac{1}{a}\mathrm{Im}\,\frac{d}{dk}\ln T(k), \tag{19.13}$$

This phase time for $s_1 = s_2 = 24L^{-1}$ and $a = 1$ is plotted as a function of k in Fig. (19.1) and shows a very sharp minimum for the resonant energy corresponding to the value of $k = 2.906L^{-1}$. The same feature is seen in the variation of the dwell time $\tau_D(0, a, k)$ defined by (19.3). For the present example $\tau_D(0, a, k)$ can be determined analytically, and its dependence on k is shown for the above parameters in Fig. (19.2). This $\tau_D(0, a, k)$ is also measured in units of the travel time of a free particle, $\frac{ma}{\hbar k}$.

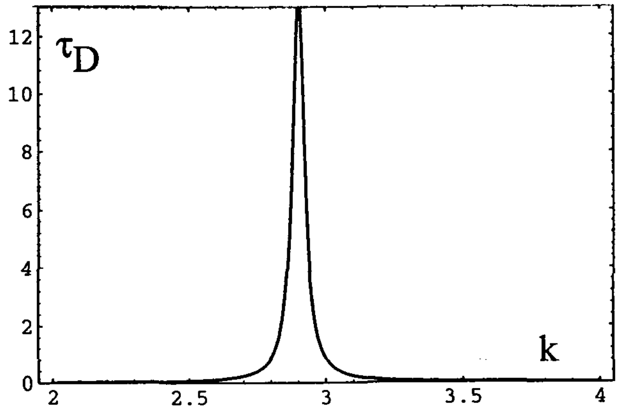

Figure 19.2: The dwell time for tunneling through two δ-function potentials measured in units of $\frac{ma}{\hbar k}$.

19.2 Büttiker and Landauer Time

The possibility of using the tunneling particle itself as a clock for measuring the tunneling time has been discussed by Büttiker and Landauer [13] [14]. These authors, in a series of papers, proposed two different forms of such a clock where in both the Hamiltonian of the tunneling particle contains a time-dependent term. In the first one Büttiker and Landauer [13] [14] considered the tunneling of a particle in a time-dependent potential of the form (see also [15] [17])

$$V(x) = V_0(x) + V_1(x)\cos(\omega t). \tag{19.14}$$

If the period $T_0 = \frac{2\pi}{\omega}$ in this potential is much longer than the tunneling time, the particle feels the effect of a time-independent potential. On the other hand for the frequencies much larger than the inverse of the tunneling time, the particle feels the effect of an oscillating field for which the average potential does not change. Since the particles can absorb or emit energies equal to $n\hbar\omega$, the time that the current takes to pass through the barrier will be changed.

The time that the particle spends under the barrier can be found from the relation

$$\mathcal{T} = \int_{x_1}^{x_2} \frac{m dx}{\hbar q(x)} = \int_{x_1}^{x_2} \frac{\sqrt{m} dx}{\sqrt{2(V_0(x) - E)}}, \tag{19.15}$$

where m is the mass of the particle, x_1 and x_2 are the classical turning points and

$$q(x) = \frac{1}{\hbar}\sqrt{2m\left[V_0(x) - E\right]}. \tag{19.16}$$

Eq. (19.15) is found from the WKB approximation where it is assumed that $E < V_0(x)$.

For the sake of simplicity let us assume that the potential V_0 is a rectangular barrier of height V_0 and width d, located between $x = \frac{-d}{2}$ and $x = \frac{d}{2}$. The transmission coefficient for this potential is (see Eq. (6.71))

$$|T|^2 = \left[1 + \frac{{k_0}^4}{4k^2q^2}\sinh^2(qd)\right]^{-1}, \tag{19.17}$$

where $\hbar k_0 = \sqrt{2mV_0}$ and $\kappa = \sqrt{{k_0}^2 - k^2}$. For a barrier which reflects most of the particles, $qd >> 1$, and the transmission coefficient for all the particles with $E < V_0$ is nearly equal to

$$|T|^2 = \frac{16k^2q^2}{{k_0}^4}e^{-2qd}. \tag{19.18}$$

Now let us assume that the potentials $V_0(x)$ and $V_1(x)$ are both similar square wells and both are located between $x = \frac{-d}{2}$ and $x = \frac{d}{2}$. If we denote the eigenfunctions of the Hamiltonian H_0 by $\varphi(E, x)$, i.e.

$$H_0\varphi(E, x) = E\varphi(E, x), \tag{19.19}$$

then

$$\psi_\pm(x, t; E) = \varphi(E, x)\exp\left(-\frac{iEt}{\hbar}\right)\exp\left[\frac{-iV_1}{\hbar\omega}\sin(\omega t)\right], \tag{19.20}$$

is the wave function for the time-dependent Schrödinger equation

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x, t)\right]\psi_\pm = i\hbar\frac{\partial\psi_\pm}{\partial t}. \tag{19.21}$$

The wave function inside the region $\frac{-d}{2} \le x \le \frac{d}{2}$ for H_0 is

$$\varphi(E, x) = \exp\left(\pm\kappa x\right), \tag{19.22}$$

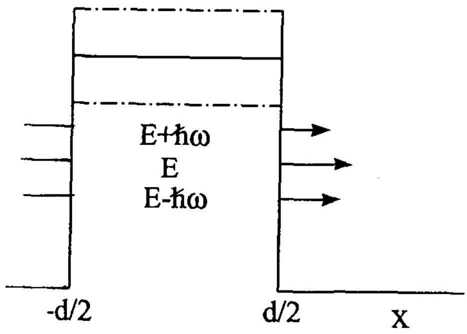

Figure 19.3: Tunneling through the time-dependent barrier given by Eq. (19.14).

and in this range we can decompose (19.20) into components whose energies are $E \pm n\hbar\omega$. To this end we write

$$\psi_{\pm}(x,t;E) = e^{\pm\kappa x}\exp\left(-\frac{iEt}{\hbar}\right)\left[\sum_{n=-\infty}^{\infty} J_n\left(\frac{V_1}{\hbar\omega}\right)e^{-in\omega t}\right]. \tag{19.23}$$

Now if the dimensionless number $\frac{V_1}{\hbar\omega}$ is small, we can expand the expression in the bracket in (19.23) and keep the terms with energies $E \pm \hbar\omega$ (see Fig. (19.3)). Thus we have three wave functions corresponding to the energies E and $E \pm \hbar\omega$, and we use the superposition principle to match the incident, the reflected and the transmitted waves inside and outside the barrier. In this way we find the following wave functions for E and $E \pm \hbar\omega$;

$$\psi_t = D\exp\left(-ikx - \frac{iEt}{\hbar}\right), \tag{19.24}$$

and

$$\psi_{t\pm} = D_{\pm}\exp\left[-ik_{\pm}x - i(E \pm \hbar\omega)t\right], \tag{19.25}$$

where

$$D = \left(\frac{4k\kappa}{k_0{}^2}\right)e^{-\kappa d}\exp\left[-i\arctan\left(\frac{\kappa^2 - k^2}{2k\kappa}\right)\right]e^{-ikd}, \tag{19.26}$$

and

$$D_{\pm} = \mp D \left(\frac{V_1}{2\hbar\omega}\right) \exp\left[\mp i \left(\frac{m\omega d}{2\hbar k}\right)\right] \left[\exp(\pm\omega\mathcal{T}) - 1\right], \tag{19.27}$$

and $\mathcal{T} = \frac{md}{\hbar\kappa}$ would be the travel time of the particle through the rectangular barrier of width d if the real velocity of the particle were $v = \frac{\hbar\kappa}{m}$. In arriving at Eq. (19.27), we have made two simplifying assumptions:
(i) - $\hbar\omega << E$, so that the wave number $k_{\pm}$ is nearly equal to

$$k_{\pm} = \frac{1}{\hbar}\sqrt{2m(E \pm \hbar\omega)} \approx k \pm \frac{m\omega}{\hbar k}, \tag{19.28}$$

and
(ii) - $\hbar\omega << V_0 - E$, therefore

$$\kappa_{\pm} \approx \kappa \mp \frac{m\omega}{\hbar\kappa}, \tag{19.29}$$

is a good approximation.

From Eq. (19.27) we can calculate the transmission probabilities for the energies $E \pm \hbar\omega$;

$$|T_{\pm}|^2 = |D_{\pm}|^2 = \left(\frac{V_1}{2\hbar\omega}\right)^2 \left[\exp(\pm\omega\mathcal{T}) - 1\right]^2 |T|^2, \tag{19.30}$$

where $|T|^2$ is given by Eq. (19.18). For high frequencies $\omega\mathcal{T} > 1$ and from Eq. (19.29) we conclude that $|T_+|^2$ for the energy $E+\hbar\omega$ grows exponentially large and $|T_-|^2$ becomes very small. Therefore for a barrier which is opaque (i.e. κd is large), we can use the difference between $|T_+|^2$ and $|T_-|^2$ to find $\mathcal{T}$ which is the tunneling time.
Thus from Eq. (19.30), we have

$$\tanh(\omega\mathcal{T}) = \frac{|T_+|^2 - |T_-|^2}{|T_+|^2 + |T_-|^2}, \tag{19.31}$$

which shows how $\mathcal{T}$ can be determined by measuring $|T_+|^2$ and $|T_-|^2$.

19.3 Larmor Precession

In the preceding discussion we showed how an oscillatory potential can be used to define the tunneling time of a particle [13] [14] [16]. If a spinning

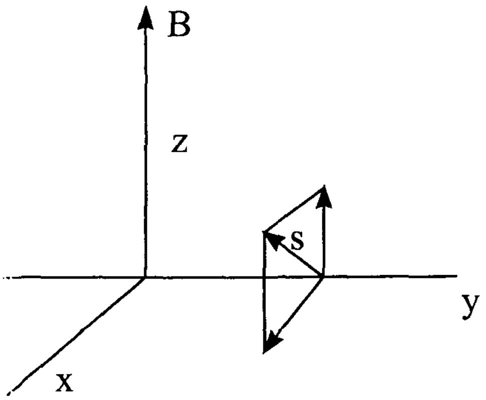

Figure 19.4: Larmor precession of a charged particle with spin **s** in the magnetic field **B**.

particle which is tunneling through a barrier has a charge e and a weak magnetic field B acts on it, then one can determine a tunneling time with the aid of the Larmor precession of the charged particle. For instance let us assume that we have a stream of charged particles all having spin $\frac{1}{2}$ and all polarized in the x direction and that these particles move in the direction of the positive y-axis. When a weak magnetic field B is applied along the z direction, then an additional term $(\frac{1}{2}\hbar\omega_L)\sigma_z$ will be added to the Hamiltonian ($\omega_L = -\frac{eB}{2mc}$ is the Larmor frequency [18]) . Thus while the particle is tunneling, the potential barrier, because of the action of the magnetic field, the spin axis of the particle will rotate (see Fig 19.4).

For this problem we can write the amplitudes for the transmission and reflection as

$$T = |T|e^{i\Delta\phi}, \tag{19.32}$$

$$R = -i|R|e^{i(\Delta\phi+\phi_a)}, \tag{19.33}$$

and

$$R' = -i|R|e^{i(\Delta\phi-\phi_a)}. \tag{19.34}$$

In these relations T and R are the transmission and reflection amplitudes of the particles reaching from the left and $T' = T$ and R' are the transmission and reflection amplitudes for the particles coming from the right. The phase $\Delta\phi$ is the phase acquired by the transmitted particle and right. The phase $\Delta\phi$ is the phase acquired by the transmitted particle and ϕ_a is the additional phase that the incident wave from the right of the barrier will have upon reflection.

The expectation value of S_y, the y component of spin is

$$\langle S_y \rangle = \frac{1}{2}\hbar^2\omega_L \left(\frac{\partial \Delta\phi}{\partial V_0}\right) = -\frac{1}{2}\hbar\omega_L \mathcal{T}_{T,y}, \tag{19.35}$$

where the time $\mathcal{T}_{T,y}$ characterizes the rotation in the xy-plane. For the z component the expectation value of the spin is

$$\langle S_z \rangle = \frac{1}{2}\hbar\omega_L \mathcal{T}_{T,z}, \tag{19.36}$$

where now $\mathcal{T}_{T,z}$ characterizes the rotation in the xz-plane,

$$\mathcal{T}_{T,z} = -\hbar\frac{\partial}{\partial V_0}\ln|T|. \tag{19.37}$$

If we consider the x component of spin, we have

$$\langle S_x \rangle = \frac{\hbar}{2}\left(1 - {\omega_L}^2{\mathcal{T}_T}^2\right). \tag{19.38}$$

This equation determines the total change in the direction of the spin-axis when the particle has tunneled through the barrier. The change is related to the traversal time $\mathcal{T}_T$ where

$$\mathcal{T}_T = \left[(\mathcal{T}_{T,y})^2 + (\mathcal{T}_{T,z})^2\right]^{\frac{1}{2}} = \hbar\left[\left(\frac{\partial \ln|T|}{\partial V_0}\right)^2 + \left(\frac{\partial \Delta\phi}{\partial V_0}\right)^2\right]^{\frac{1}{2}}. \tag{19.39}$$

Equation (19.39) shows that this traversal time is composed of two terms, one is related to the derivative of the transmission probability with respect to the height of the barrier V_0, and the other to the derivative of the change of the phase $\Delta\phi$ with respect to V_0. The reflection of the particles coming from the left defines the times

$$\mathcal{T}_{R,y} = -\hbar\frac{\partial(\Delta\phi + \phi_a)}{\partial V_0}, \tag{19.40}$$

and

$$\mathcal{T}_{R,z} = -\hbar\frac{\partial \ln|R|}{\partial V_0}, \tag{19.41}$$

In the same way if we consider the particles coming from right we have

$$\mathcal{T}'_{R,y} = -\hbar \frac{\partial(\Delta\phi - \phi_a)}{\partial V_0}, \tag{19.43}$$

$$\mathcal{T}'_{R,z} = -\hbar \frac{\partial \ln |R|}{\partial V_0}, \tag{19.44}$$

and

$$\mathcal{T}'_R = \left[\mathcal{T}'^2_{R,y} + \mathcal{T}'^2_{R,z}\right]^{\frac{1}{2}} = \hbar \left[\left(\frac{\partial \ln |R|}{\partial V_0}\right)^2 + \left(\frac{\partial(\Delta\phi - \phi_a)}{\partial V_0}\right)^2\right]^{\frac{1}{2}}. \tag{19.45}$$

For a symmetric barrier $\phi_a = 0$ and we have one reflection time. It should be noted that the transmission and reflection times are both real and positive.
Depending on whether $E > V_0$ or $E < V_0$ and under the conditions where WKB method is valid we have the following possibilities:
(i) - When $E < V_0$, i.e. for tunneling, T in this approximation is given by

$$T = \exp\left\{-\int \left[\left(\frac{2m}{\hbar^2}\right)(V_0(x) - E)\right]^{\frac{1}{2}} dx\right\}, \tag{19.46}$$

and $\Delta\phi$ is independent of V_0.
(ii) - For the flight over the barrier we have

$$T = e^{i\Delta\phi} = \exp\left\{i\int \left[\left(\frac{2m}{\hbar^2}\right)(E - V_0(x))\right]^{\frac{1}{2}} dx\right\}. \tag{19.47}$$

From Eqs. (19.46) , (19.47) and (19.39) we can calculate $\mathcal{T}_T$ in the semi-classical limit for the two cases of E large and E small. For instance if $E > V_0$, for $\mathcal{T}_T$ we find

$$\mathcal{T}_T = \int \frac{m dx}{\sqrt{2m(E - V_0)}} = \int \frac{dx}{v_P(x)}, \tag{19.48}$$

where $v_P(x)$ is the speed of the particle.

We have already mentioned that for an asymmetric barrier the reflection coefficient from the two sides have the same magnitude but different phases. For instance let us determine the reflection amplitudes for the potential

$$V(x) = V_1\theta(x)\theta(a - x) + V_2\theta(x - a)\theta(b + a - x)\theta(b - x). \tag{19.49}$$

phases. For instance let us determine the reflection amplitudes for the potential

$$V(x) = V_1\theta(x)\theta(a-x) + V_2\theta(x-a)\theta(b+a-x)\theta(b-x). \tag{19.49}$$

By solving the Schrödinger equation we find that the reflection amplitudes from the left and the right sides of the barrier are:

$$R_L = \frac{(q-ik)X(k) - (q+ik)}{(q+ik)X(k) - (q-ik)}, \tag{19.50}$$

and

$$R_R = e^{2ikb}\frac{(p+ik)F(k) - (p-ik)}{(p+ik) - (p-ik)F(k)}, \tag{19.51}$$

where

$$q = \sqrt{V_1 - k^2}, \quad p = \sqrt{V_2 - k^2}, \tag{19.52}$$

$$X(k) = e^{-2qa}\frac{(q+p)(p-ik) - (q-p)(p-ik)\exp[2p(b-a)]}{(q-p)(p+ik) + (q+p)(p-ik)\exp[2p(b-a)]}, \tag{19.53}$$

and

$$F(k) = -e^{2p(b-a)}\frac{(q+p)(q-ik) - (q-p)(q+ik)\exp[-2qa]}{(q-p)(q-ik) - (q+p)(q+ik)\exp[-2qa]}. \tag{19.54}$$

For those values of k^2 where both p and q are real quantities, the reflection coefficients $|R_R|^2$ and $|R_L|^2$ are the same but the phases of R_R and R_L are different.

19.4 Tunneling Time and its Determination Using the Internal Energy of a Simple Molecule

We have already seen that the rotation of the spin of a charged particle in a weak magnetic field can be used to define a tunneling time. From the motion of a simple one-dimensional molecule which has an internal degree of freedom we can define a tunneling time provided that the center of mass of a molecule does not coincide with its center of charge. Here we follow a formulation advanced by Jarvis and Bulte [19].

Before we start discussing this problem we should emphasize that various tunneling times that we have seen and we will see differ from each other, and in each case the measured time depends on the way that we measure it.

The system that we want to study is a diatomic molecule where the two atoms are held together by a spring force. This molecule approaches from the left towards a rectangular barrier of height V_0 and width d, and it may eventually pass the barrier. The Hamiltonian operator for this system is

$$H = \frac{{p_1}^2}{2m_1} + \frac{{p_2}^2}{2m_2} + \frac{1}{2}K\left(x_1 - x_2\right)^2 + V_0\theta\left(x^* + \frac{d}{2}\right)\theta\left(\frac{d}{2} - x^*\right). \quad (19.55)$$

where we have assumed that the barrier interacts with the charge of the molecule which is located at

$$x^* = \beta x_1 + (1-\beta)x_2, \quad (19.56)$$

Here β ($0 \leq \beta \leq 1$) is a constant. In Eq. (19.56) K is the spring constant and θ is the step function. We can write the Hamiltonian in the center of mass coordinates

$$H = \frac{1}{2M}P^2 + \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 + V_0\theta\left(x^* + \frac{d}{2}\right)\theta\left(\frac{d}{2} - x^*\right), \quad (19.57)$$

where $M = m_1 + m_2$ is the total and $m = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass of the molecule.

Now we assume that:

(i) - The spacing between the energy levels of the molecule, i.e. $\hbar\omega$ is small compared to the kinetic energy of the molecule.

(ii) - The effective distance, viz, the distance between the center of charge and the center of mass is small compared to the DeBroglie wavelength.

If $\frac{1}{\alpha} = \sqrt{\frac{\hbar}{m\omega}}$ is a measure of the length of the oscillator and k is the wavelength associated with the center of mass then the above assumptions can be stated as

$$\frac{\hbar^2 k^2}{2M} >> \frac{\hbar^2\alpha^2}{m}, \quad (19.58)$$

and

$$\frac{\hbar^2\alpha^2}{M\beta^2} >> \frac{\hbar^2 k^2}{M}. \quad (19.59)$$

For simplicity we can choose $\beta = 1$, therefore m and M can be regarded as adjustable parameters. Now let us express the state of the molecule in terms of the coherent phase $|k,\beta\rangle$ [20] in which each level n is associated

If we assume that the period $\frac{2\pi}{\omega}$ is small compared to the interaction time scale ($\hbar\omega << E$), so the the internal state of the molecule does not change, then the reflection and transmission amplitudes will depend only on E_n (i.e. the center of mass kinetic energy). When the barrier is opaque then the transmission amplitude is given by the WKB approximation

$$T = -\exp[-\kappa(E)a + i\eta(E)], \tag{19.61}$$

where $\eta(E)$ is the phase and $\kappa(E)$ is given by

$$\kappa(E) = \sqrt{2m(V_0 - E)}. \tag{19.62}$$

In the present problem for every state of the system $|k_n\rangle \otimes |n\rangle$ we have the corresponding T_n and R_n;

$$T_n = T(E_0 - n\hbar\omega) \approx T(E_0)\left[1 + \left(a\frac{d\kappa}{dE} - i\frac{d\eta}{dE}\right)n\hbar\omega\right], \tag{19.63}$$

where E_0 stands for $E - \frac{1}{2}\hbar\omega$. The overlap of the time dependent transmitted state with $|n\rangle$ is given by [20]

$$(\beta(t))^n T(E_n) \approx (\beta)^n T(E_0) \exp\left[-in\omega\left(t + \hbar\frac{d\eta}{dE}\right) - n\omega\hbar a\frac{d\kappa(E)}{dE}\right]. \tag{19.64}$$

From this discussion it is clear that the tunneling time, in general, can be a complex quantity.

19.5 Intrinsic Time

Let us consider the special case where (i) - the height of the barrier is infinite, and (ii) - the molecule is at its ground state and has a wave number k_0. For this case we want to determine the reflection amplitude for the quantum state n of the molecule. The energy conservation implies that

$$\frac{\hbar^2 k_n^2}{2M} + \left(n + \frac{1}{2}\right)\hbar\omega = \frac{\hbar^2 {k_0}^2}{2M} + \frac{1}{2}\hbar\omega = E. \tag{19.65}$$

If we denote the amplitude of the reflected wave by R_n, then we can write the complete solution of the Schrödinger equation as

$$|\psi\rangle = \beta_0|k_0\rangle \otimes |0\rangle + \sum_{n=0}^{\infty}\left(R_n[2^n n!\sqrt{\pi}]^{\frac{1}{2}}\right)\, |-k_n\rangle \otimes |n\rangle, \tag{19.66}$$

If we denote the amplitude of the reflected wave by R_n, then we can write the complete solution of the Schrödinger equation as

$$|\psi\rangle = \beta_0|k_0\rangle \otimes |0\rangle + \sum_{n=0}^{\infty} \left(R_n[2^n n!\sqrt{\pi}]^{\frac{1}{2}}\right) \, |-k_n\rangle \otimes |n\rangle, \tag{19.66}$$

with its corresponding wave function as

$$\langle x, u|\psi\rangle = \beta_0 \exp(ik_0 x) H_0(u) e^{-\frac{1}{2}u^2} + \sum_{n=0}^{\infty} R_n \exp(-ik_n x) H_n(u) e^{-\frac{1}{2}u^2}. \tag{19.67}$$

Here there are a finite number of real k_n's and an infinite number of imaginary k_n's, $k_n = -i\kappa_n$. For the cases where $m_1 = m_2$, the barrier will be located at $x_1 = x + \frac{u}{2\alpha} = 0$ and the wave function must vanish at this point

$$\beta_0 \exp\left(-ik_0\frac{u}{2\alpha}\right) H_0(u) e^{-\frac{1}{2}u^2} + \sum_{n=0}^{\infty} R_n \exp\left(ik_n\frac{u}{2\alpha}\right) H_n(u) e^{-\frac{1}{2}u^2} = 0. \tag{19.68}$$

Now if $\hbar\omega << E_0$, we can approximate k_n by k_0 and denote both of these by k and also $\frac{k}{\alpha}$ by Δ, then write (19.68) as

$$e^{-i\Delta u} \exp(-u^2) = \sum_{n=0}^{\infty} \left(-\frac{R_n}{\beta_0}\right) H_n(u) \exp\left(-u^2\right). \tag{19.69}$$

By expanding the generating function for the Hermite polynomial, viz,

$$\exp\left[u^2 + 2iux\right] = \sum_{n=0}^{\infty} \frac{1}{n!}(iu)^n H_n(u), \tag{19.70}$$

we find

$$-\frac{R_n}{\beta_0} = \left[\frac{(-i\Delta)^n}{2^n n!}\right]. \tag{19.71}$$

We can also express Eq. (19.69) in terms of the operator

$$\begin{aligned} &\exp\left[-\frac{i}{\sqrt{2}}\Delta(a + a^\dagger)\right] |0\rangle \\ = \;& e^{\frac{-1}{4}\Delta^2} \exp\left[-\frac{i}{\sqrt{2}}\Delta a^\dagger\right] \exp\left[-\frac{i}{\sqrt{2}}\Delta a\right] |0\rangle \\ = \;& e^{\frac{-1}{4}\Delta^2} \sum_{n=0}^{\infty} \left[\frac{(-i\Delta)^n}{2^{\frac{n}{2}}\sqrt{n!}}\right] |n\rangle, \end{aligned} \tag{19.72}$$

which operates on u. From this equation we conclude that the operator $1 - \frac{i\Delta}{\sqrt{2}(a+a^\dagger)}$ is the generator of reflection. With the help of this operator we can also define an intrinsic time for reflection, transmission or tunneling.

Now if we go back to a finite square barrier with the height V_0, we can define an effective Hamiltonian operator by

$$H_{eff} = \frac{1}{\sqrt{2}} V_0 \left(a + a^\dagger\right). \tag{19.73}$$

Due to the action of this Hamiltonian we have a change in the internal state of the oscillator, and assuming that this H_{eff} is a small perturbation we can define an interaction time as

$$\mathcal{T}_{IR} = \frac{2i\hbar}{V_0} \frac{R_1}{R_0}. \tag{19.74}$$

Similarly for the tunneling in the state n, i.e. $T_n \, |k_n\rangle \otimes |n\rangle$ we can have a tunneling time $\mathcal{T}_{IT}$, where

$$\mathcal{T}_{IT} = \frac{2i\hbar}{V_0} \frac{T_1}{T_0}. \tag{19.75}$$

In the limit when $V_0 \to \infty$, both $\mathcal{T}_{IT}$ and $\mathcal{T}_{IR}$ become zero. Clearly these times depend on R_1 and T_1. Also from Eqs. (19.71) and (19.74) we have

$$\mathcal{T}_{IR} = \frac{\hbar\Delta}{V_0}. \tag{19.76}$$

Our next task will be to show that for the case of a barrier of height V_0 and width a, $\left(-\frac{a}{2} < x < \frac{a}{2}\right)$, this result follows from the calculation of R and T. For this we write the wave function as an expansion in terms of R and T for the regions I, II and III defined as follows :

$$\begin{aligned} \psi_I &= \Big\{\beta_0 e^{ik_0x} H_0(u) + R_0 e^{-ik_0x} H_0(u) \\ &+ R_1 e^{-ik_1x} H_1(u) + R_2 e^{-ik_2x} H_2(u)\Big\} \exp\left(-\frac{1}{2}u^2\right) + O(3), \\ & x < -\frac{a}{2}, \end{aligned} \tag{19.77}$$

$$\begin{aligned} \psi_{II} &= \{\gamma_0 e^{\kappa_0 x} H_0(u) + \delta_0 e^{-\kappa_0 x} H_0(u) + \gamma_1 e^{\kappa_1 x} H_1(u) + \delta_1 e^{-\kappa_1 x} H_1(u) \\ &+ \gamma_2 e^{\kappa_2 x} H_2(u) + \delta_2 e^{-\kappa_2 x} H_2(u)\} \exp\left(-\frac{1}{2}u^2\right) + O(3), \\ & -\frac{a}{2} < x < \frac{a}{2}, \end{aligned} \tag{19.78}$$

and

$$\psi_{III} = \left\{T_0 e^{ik_0 x} H_0(u) + T_1 e^{ik_1 x} H_1(u) + T_2 e^{ik_2 x} H_2(u)\right\} \exp\left(-\frac{1}{2}u^2\right)$$
$$+ \quad O(3), \quad x > \frac{a}{2}, \tag{19.79}$$

where in (19.78) γ_i and δ_i are constants. Here we have also assumed that the incoming molecule approaches the barrier while it is in the ground state, and its amplitude in this state is β_0. The above expansion contains terms up to and including u^2. For this potential we have to impose the continuity of the wave equation at the boundaries $x = \pm\frac{a}{2}$. However the continuity of the derivatives are with respect to the variable x_1, where

$$\frac{\partial}{\partial x_1} = \frac{1}{2}\frac{\partial}{\partial x} + \alpha\frac{\partial}{\partial u}. \tag{19.80}$$

In this way we get six equations which we can expand up to the second order in u^2, and from the expansion determine R_i and T_i. Here it is important to separate the u and Δ variables.

For the first excitation the reflection and the transmission amplitudes after the matrix inversion are:

$$\begin{bmatrix} {R_1}^{(1)} \\ {T_1}^{(1)} \end{bmatrix} \approx J \begin{bmatrix} -(\kappa_1 - ik_1) & 2\kappa_1 e^{-\kappa_0 a} \\ -2\kappa_1 e^{-\kappa_0 a} & (\kappa_1 - ik_1) \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix}, \tag{19.81}$$

where

$$J = \left(\frac{2MV_0}{\hbar^2}\right)\frac{e^{-ik_0 a}}{4(\kappa_0 - ik_0)^2}, \tag{19.82}$$

and

$$\xi = \frac{-2ik_0}{(\kappa_0 - ik_0)}, \quad \eta = \frac{2\kappa_0 e^{-\kappa_0 a}}{(\kappa_0 - ik_0)}\xi. \tag{19.83}$$

In the limit of $\kappa a > 1$, we can ignore $\exp(-2\kappa_0 a)$, and moreover we have $k_i = k$, and $\kappa_i = \kappa$ for $i = 0, 1$, therefore from (19.81) we find

$${R_1}^{(1)} = \frac{i\Delta(\kappa + ik)}{2(\kappa - ik)} e^{-ika}. \tag{19.84}$$

But R_0 is given by

$$R_0 = -\frac{(\kappa + ik)}{(\kappa - ik)} e^{-ika}, \tag{19.85}$$

and therefore in this limit we have the following result

$$\frac{{R_1}^{(1)}}{{R_0}^{(0)}} = -\frac{i\Delta}{2}, \tag{19.86}$$

and the reflection time $\mathcal{T}_{IR}$ is obtained as a function of Δ and V_0, i.e. $\mathcal{T}_{IR} = \frac{\hbar\Delta}{V_0}$ (see Eq. (19.76)).

19.6 A Critical Study of the Tunneling Time Determination by a Quantum Clock

In this section we want to discuss the problem of measuring the tunneling time with a quantum clock [21] (see also [22] [23] [24] [25]). We will show that because of the interaction between the clock and the particle, the total Hamiltonian is not separable and thus the motion of the particle influences the reading of the clock. For this purpose we consider a clock that works between two distinct events, and if the clock is adjusted to read zero at $t = -\infty$, then at $t = \infty$ it will read a nonzero number. That is we assume that the clock stops working before and after the occurrence of these events. For instance we can take these two events to be the arrival of a particle at a point x_1, and again its arrival at x_2, $(x_1 < x_2)$.

One of the simplest clocks that we can imagine is a system with large spin S whose time evolution can be used to measure the time. The interaction of this system with the particle is given by the potential

$$H' = \frac{2\pi\hbar P(x) S_z}{(2S+1)\mathcal{T}}, \tag{19.87}$$

where $P(x)$ is zero outside the range $x_1 < x < x_2$ and $P(x) = 1$ inside. The Hamiltonian of the particle plus the clock is

$$H = \frac{1}{2m}p^2 + V(x) + \frac{2\pi\hbar P(x) S_z}{(2S+1)\mathcal{T}}, \tag{19.88}$$

in which $V(x)$ is the potential barrier, which we assume to be negligible as $x \to -\infty$, and $\mathcal{T}$ is a parameter. First let us study the working of this clock, and for this purpose we define the orthogonal states of the clock by

$$|N\mathcal{T}\rangle = \frac{1}{\sqrt{(2S+1)}} \sum_{M=-S}^{S} \exp\left[-\frac{2\pi i N M}{2S+1}\right] |M\rangle. \tag{19.89}$$

Now if in (19.88) the kinetic energy is negligible, we can commute the last two terms even when $P(x) = 1$. If we denote the state of the clock at $t = 0$ by $|0\rangle$, then its state at t is given by

$$|t\rangle = \exp\left[-\frac{2\pi i t S_z P(x)}{(2S+1)\mathcal{T}}\right] |0\rangle. \tag{19.90}$$

For discrete times $t_N = N\mathcal{T}$, we can read the clock by finding the expectation value of the operator

$$|N\mathcal{T}\rangle\langle N\mathcal{T}| = \frac{1}{2S+1}\sum_{M,M'} \exp\left[-\frac{2\pi i N(M-M')}{(2S+1)}\right]|M\rangle\langle M'|. \tag{19.91}$$

From this equation it is apparent that $\mathcal{T}$ is a measure of the accuracy (or resolving power) of the clock. When we include the kinetic energy in (19.88) then we observe that outside the range $x_1 < x < x_2$ there is no interference between the clock and the particle, and that it is only inside this range that we have interference. Therefore we have to choose $x_2 - x_1$ as small as possible. To solve the problem of interference first let us consider the special case where $V(x)$ in (19.88) is zero, and assume that at $t = 0$ the clock is in the state M. Thus the motion of the particle is subject to the interaction

$$\frac{2\pi\hbar M}{(2S+1)\mathcal{T}}\theta(x_2 - x)\theta(x - x_1) \tag{19.92}$$

and no other force.

Let us also assume that the energy of the particle is much larger than the height of this barrier. In this case a small part of the incoming wave from the left is reflected and most of it is transmitted over the barrier. The effect of the barrier to the order M, is to change the phase of the transmitted wave by a factor proportional to $M(x_2 - x_1)$. Now the initial state of the clock $|0\mathcal{T}\rangle$, is a superposition of states $|M\rangle$, where the phase of $|M\rangle$ shifts by an amount proportional to M. If the time of transmission through the length $x_2 - x_1$ is $n\mathcal{T}$, where n is an integer, then we can determine the transmission time exactly. Otherwise the expectation value of (19.89) determines the time, and this time is measured with an accuracy $\mathcal{T}$.

Next let us study the complete problem of a wave approaching the rectangular barrier from the left. First we formulate the problem for a plane wave and later for the case of a wave packet. To indicate different reflections, we enumerate different barriers from the left. For a wave incident from the left of the barrier in region I, the total wave is of the form

$$\phi(x,t:k) = \exp\left[i(kx - \omega t)\right] + R(k)\exp[-i(kx + \omega t)], \tag{19.93}$$

where ω and k are related by

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}. \tag{19.94}$$

Equation (19.93) shows that in addition to the incident wave with unit amplitude, there is also a reflected wave with amplitude $R(k)$ which depends not only on the wave number k but also on the barriers II, III,..... At different points along the x-axis, there are incident and reflected waves (for some of the parts, k can be imaginary), except for the last region where there is no reflected wave. For this problem the boundary conditions are expressible as the continuity of the logarithmic derivative of the wave function inside and outside the barriers, and these determine the reflection and transmission coefficients .

If we want to study the motion of a wave packet which is originally localized in part I, and has the waveform $\Phi(x)$, we first obtain its Fourier transform

$$\tilde{\Phi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(x) e^{-ikx} dx, \tag{19.95}$$

where this integral is only over the region I of the x coordinate. The inverse transform of (19.95) is

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\Phi}(k) e^{ikx} dk. \tag{19.96}$$

The time evolution of the wave packet in part I can be found from

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \oint \tilde{\Phi}(k) \left[e^{ikx} + R(k) e^{-ikx}\right] e^{-i\omega t} dk. \tag{19.97}$$

Noting that at $t = 0$, there should be no effect from the reflections from parts II, III,....we choose the contour for the complex integration in the k-plane which extends from $k = -R$ to $k = R$ on the real k-axis and joins a large semi-circle of radius R in the upper-half plane deformed in such a way that it avoids crossing the poles of $\tilde{\Phi}(k)$ and $R(k)$. Now if we couple the clock to one of the segments II, III,... or a part of these segments, we can determine the wave packet for the desired case. As before we denote the state of the clock at $t = 0$ by $|0\mathcal{T}\rangle$, and note that now $R(k)$ will depend on M, therefore

$$\Psi(x,t) = \frac{1}{\sqrt{2S+1}} \frac{1}{\sqrt{2\pi}} \oint \sum_{M} \tilde{\Phi}(k) \left[e^{ikx} + R(k) e^{-ikx}\right] e^{-i\omega t} \, |M\rangle dk. \tag{19.98}$$

The probability that the clock at time t will be in the state $|N\mathcal{T}\rangle$ consists of parts coming from different regions I, II,....... For instance for the region I this is given by

$$P = \frac{1}{2\pi(2S+1)^2} \int$$

$$\times \left|\sum_M \exp\left(-\frac{2i\pi NM}{2S+1}\right) \oint \tilde{\Phi}(k)\left[e^{ikx} + R(k)e^{-ikx}\right] e^{-i\omega t} dk\right|^2 dx, \tag{19.99}$$

where the integration over x is limited to region I. Since the integrand in (19.99) is a positive quantity, no matter where the clock is located it will read a nonzero value. It is also important to know where one should place such a clock so as to measure the time that the particle passes through a particular region.

For the general case we know that all of the waves arriving from different regions should be added together. But the interesting case is the one where most of the incident wave will be reflected, and therefore we need to consider only the wave arriving at I. This wave is composed of an incident wave packet and the reflected waves. After sufficient time one can ignore the incident wave and retain only the reflected wave and this is proportional to R_M. Now if R_M causes a phase shift of the form $\exp\left(\frac{i\lambda M}{\mathcal{T}}\right)$, then the expectation value (19.99) assumes a maximum when we have the equality

$$\frac{\lambda M}{\mathcal{T}} = \frac{2\pi NM}{2S+1}. \tag{19.100}$$

But an examination of different barriers indicates that R_M cannot have the indicated form. If we have a square barrier of the form $V_0\theta(x)\theta(a-x)$, and $P(x)$ is zero for $x < 0$ and $x > a$, then for the state M the height of the barrier will be increased by an amount $\frac{2\pi\hbar M}{(2S+1)\mathcal{T}}$ and the reflection amplitude will be

$$R_M(k) = -\frac{(K^2+k^2)(1-e^{-2Ka})}{(K-ik)^2 - e^{-2Ka}(K+ik)^2}, \tag{19.101}$$

where K satisfies the following relation

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2 K^2}{2m} + V_0 + \frac{2\pi M\hbar}{(2S+1)\mathcal{T}}. \tag{19.102}$$

Now if we expand $R_M(k)$ as a series in e^{-2Ka} we find

$$R_M(k) = -\frac{(K^2+k^2)}{(K-ik)^2}\left(1-e^{-2Ka}\right)\left[1 + e^{-2Ka}\frac{(K+ik)^2}{(K-ik)^2} + \dots\right]. \tag{19.103}$$

The first term of this expansion, i.e. $-\frac{K^2+k^2}{(K-ik)^2}$ is the reflection from the wall of the first barrier. The term with $\exp(-2Ka)$ shows a wave which has passed through a barrier once and is reflected from the second wall. Other terms show higher order reflections from the two walls . But the first term of this expansion depends on M (see Eq.(19.102)), even though this wave has not entered the barrier and should not have activated the clock. To interpret this result we observe that because of the coupling between the particle and the clock, the system which at $t = 0$ was uncoupled, is now perturbed, and this perturbation causes the clock to register a nonzero number.

The important conclusion is that in general, the atomic clock is unable to measure the tunneling time of the particle as it passes through the barrier.

19.7 Tunneling Time According to Low and Mende

Again we study the one-dimensional tunneling and use the system of units where $\hbar = m = 1$. We write the wave packet associated with the incident particle which is moving towards the barrier as [26] [27]

$$\Psi_0(x) = \int_{-\infty}^{\infty} a(k - k_0) \exp[ik(x - x_0)]dk. \tag{19.104}$$

Here x_0 and k_0 are the position and momentum of the particle at $t = 0$ respectively. If we change the variable to $p = k - k_0$, we can write $\Psi_0(x)$ in the simpler form of

$$\Psi_0(x) = \exp[ik_0(x - x_0)]f(x - x_0), \tag{19.105}$$

where $f(x)$ is the Fourier transform of $a(p)$,

$$f(x) = \int_{-\infty}^{\infty} a(p)e^{ipx}dp. \tag{19.106}$$

From Eqs. (19.104) and (19.105) it is clear that $f(x)$ has a minimum at $x = 0$ and $a(p)$ has a maximum at $p = 0$, and the widths Δx and Δp satisfy the uncertainty relation $\Delta x \Delta p \approx 1$. The time development of Ψ is found from the Schrödinger equation

$$\begin{aligned} \Psi(x,t) &= \int_{-\infty}^{\infty} a(k - k_0) \exp[ik(x - x_0) - iE(k)t]dk \\ &= \exp\{i[k_0(x - x_0) - E(k_0)t]\} \\ &\times \int_{-\infty}^{\infty} a(p) \exp\left\{i\left[p(x - x_0 - k_0 t) - \frac{i}{2}p^2 t\right]\right\} dp, \end{aligned} \tag{19.107}$$

where we have replaced E by $\frac{k^2}{2}$. Now let us study the implication of this relation. For very short times which satisfy the inequality

$$(\Delta p)^2 t << 1, \tag{19.108}$$

the wave packet moves without changing its shape;

$$\Psi_0(x,t) = \exp[ik_0(x-x_0) - iE(k_0)t] f(x - x_0 - k_0 t). \tag{19.109}$$

We can interpret the inequality (19.108) in another way: We know that the change in the width Δx of the wave packet is

$$\delta(\Delta x) = (\Delta p)t, \tag{19.110}$$

and from (19.108) and (19.110), we find that

$$\frac{\delta(\Delta x)}{\Delta x} << 1. \tag{19.111}$$

When a potential $V(x)$ is on the path of the wave packet we can obtain the time dependence of the wave packet by first expanding Ψ_0 in terms of the complete set $\left\{\psi_k{}^{(0)}\right\}$ the eigenfunctions of the complete Hamiltonian. For $k > 0$ these eigenfunctions have the asymptotic property

$$\psi_k{}^{(0)}(x) = \begin{cases} e^{ikx} + R(k)e^{-ikx} & \text{for } x \to -\infty \\ T(k)e^{ikx} & \text{for } x \to \infty \end{cases}, \tag{19.112}$$

where again $R(k)$ and $T(k)$ are the reflection and transmission amplitudes.

Next we use one of the basic assumptions of the scattering theory, viz, that the coefficients of the expansion of $\Psi_0(x)$ in terms of $\left\{\psi_k{}^{(0)}\right\}$ are the same as those of the expansion of $\Psi_0(x)$ in terms of $\left\{e^{ikx}\right\}$. Thus we have

$$\Psi_0(x) = \int_{-\infty}^{\infty} a(k-k_0)\exp(-ikx_0)\psi_k{}^{(0)}(x)dk. \tag{19.113}$$

This is true provided that the difference $\delta\Psi_0(x)$ defined by

$$\delta\Psi_0(x) = \int_{-\infty}^{\infty} a(k-k_0)\exp(-ikx_0)\left[\psi_k{}^{(0)}(x) - \exp(ikx)\right]dk, \tag{19.114}$$

is very small for all values of x. If this is satisfied then

$$\Psi_T(x,t) \approx \int_{-\infty}^{\infty} a(k-k_0)T(k)\exp[-ik(x-x_0)]\exp[-iE(k)t]dk. \tag{19.115}$$

will be the transmitted wave.

For a rectangular barrier of height V_0 and width a, if $k^2 > 2V_0$, the particle flies over the barrier and then the dependence of $T(k)$ on k is mainly due to the k-dependence of the phase of $T(k)$, and we can write the total transmission amplitude as the sum of $T(k)$'s for multiple reflections. Here we just need the first term $T^{(0)}(k)$ since it is a continuation from $k^2 < 2V_0$ of the dominant behavior of the scattering amplitude.

For a rectangular barrier we have seen, (Eq. (6.72)), that

$$T^{(0)}(k) = \frac{4qk}{(q+k)^2}\exp[i(q-k)a], \tag{19.116}$$

where

$$q(k) = \sqrt{k^2 - 2V_0}. \tag{19.117}$$

We note that in (19.116) only the phase of $T^{(0)}(k)$ has an appreciable k dependence, hence we expand it around $k = k_0 + p$. Thus in this approximation $\Psi_T(x,t)$ becomes

$$\begin{aligned} \Psi_T(x,t) &= \frac{4q_0k_0}{(q_0+k_0)^2}\exp\left\{i\left[k_0(x-x_0-a)+q_0a-E(k_0)t\right]\right\} \\ &\times\ f(x-x_0-a+q'_0a-k_0t), \end{aligned} \tag{19.118}$$

where

$$q_0 = q(k=k_0) \quad \text{and} \quad q'_0 = \left(\frac{dq}{dk}\right)_{k=k_0}. \tag{19.119}$$

From this equation we conclude that a particle which at $t=0$ was at the point x_0, reaches x at the time t, where

$$t = \frac{x-a-x_0+aq'_0}{k_0} = \frac{x-a}{k_0} + \frac{a}{q_0} + \frac{|x_0|}{k_0}, \tag{19.120}$$

and $q_0 = \sqrt{{k_0}^2 - 2V_0}$.
We observe that the time of arrival at x from x_0 is the sum of three classical times:
(a) - the time that takes the particle to move from $x = x_0 = -|x_0|$ to $x = 0$ with speed k_0.
(b) - the travel time from $x = 0$ to $x = a$ with a speed q_0 and
(c) - the time that is needed for the particle to move from $x = a$ to $x = x_0$ with speed k_0.
If we have multiple reflections then this time will be longer.

Now let us consider the tunneling problem where $k^2 < 2V_0$. In this case the term e^{iqa} changes to the tunneling amplitude $T(k) \sim e^{-\gamma(k)a}$, where $\gamma(k) = \sqrt{2V_0 - k^2}$ and also $f(x - x_0 - a - k_0 t + aq'_0)$ is replaced by its analytic continuation $f(x - x_0 - a - k_0 t - ia\gamma'_0)$ provided that the integral over momentum space is sufficiently convergent. By examining this result we note that unlike the term aq'_0, the term $-ia\gamma'_0$ does not indicate a time for the passage through the potential. It only modifies the shape of the wave packet, and this modification is ignorable. Therefore the time of arrival of the wave at the point x is equal to t where $t = \frac{1}{k_0}(x - a - |x_0|)$ and the tunneling time is zero.

Let us study the reason for arriving at this strange conclusion. For this we consider a Gaussian wave packet which at time $t = 0$ is at $x = x_0$ ($x_0 << a$), and is approaching the barrier from the left. The probability of finding the particle to the right will be negligible if

$$\exp\left[-\frac{a^2}{2(\Delta x)^2}\right] << \exp(-\gamma_0 a), \tag{19.121}$$

or

$$\frac{a(\Delta p)^2}{2\gamma_0} >> 1. \tag{19.122}$$

The transmitted wave which was originally of the form (19.104) for $x \ge a$ is proportional to

$$\Psi_T(x,t) \approx \exp\left[-\gamma_0 a + ik_0(x - x_0 - a)\right]$$
$$\times \int_{-\infty}^{\infty} \exp\left\{-\frac{p^2}{2(\Delta p)^2} + ip(x - x_0 - a) - pa\gamma'_0 - \frac{1}{2}p^2 a\gamma''_0\right\} dp. \tag{19.123}$$

The condition for the convergence of the integral is obtained from

$$|a\gamma''_0| < \frac{1}{(\Delta p)^2}, \tag{19.124}$$

or

$$\frac{2aV_0}{(\gamma_0)^3} < \frac{1}{(\Delta p)^2}. \tag{19.125}$$

Now if we combine the two inequalities (19.122) and (19.125) we find that $\gamma_0 >> \sqrt{2V_0}$ and this condition is not compatible with the condition for tunneling, i.e. $\gamma_0 < \sqrt{2V_0}$. Therefore we conclude that for tunneling of a Gaussian wave packet which is close to the barrier, we cannot use the ideas of scattering theory and the motion of the wave packet, and Eq. (19.120) is not useful in this case.

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Chapter 20

Tunneling of a System with Internal Degrees of Freedom

The problem of tunneling of a system of particles with internal degrees of freedom has not received much attention, although in some important physical systems for example α-decay the decaying part is a composite system. In physics and chemistry of molecules there are observable effects attributable to the tunneling of a molecule from one well to the other in symmetric and asymmetric double-wells [1] [2] [3] [4] [5] [6]. We have also seen (Section (19.4)) an attempt to use tunneling of a molecule as a way of measuring tunneling time [7].

20.1 Lifetime of Coupled-Channel Resonances

Here we want to study the time evolution of a particle of mass $m = \frac{1}{2}$ with an internal degree of freedom ρ, when it tunnels through a barrier $U(\mathbf{r}, \rho)$, which, in general, can depend on ρ.

The total Hamiltonian for the system is given by (again setting $\hbar = 1$)

$$H = -\nabla_r^2 + U(\mathbf{r}, \rho) + H_0(\rho), \tag{20.1}$$

where $H_0(\rho)$ is the Hamiltonian describing the internal degrees of freedom [8]. Assuming that the eigenvalues corresponding to these degrees of freedom are discrete, we have the following eigenvalue equation for $H_0(\rho)$;

$$H_0(\rho)\chi_j(\rho) = q_j^2\chi_j(\rho), \quad j = 1, 2, ..., \tag{20.2}$$

where q_j^2 's satisfy the relation

$$q_1^2 < q_2^2 < q_3^2....., \tag{20.3}$$

and that the eigenstates $\{\chi_j(\rho)\}$ form an orthonormal set

$$\int \chi_j^*(\rho)\chi_k(\rho)d\rho = \delta_{kj}. \tag{20.4}$$

The time-dependent Schrödinger equation for this systen is

$$\left[-\nabla_r^2 + H_0(\rho)\right]\Psi(\mathbf{r}, \rho, t) = \left[-i\frac{\partial}{\partial t} + U(\mathbf{r}, \rho)\right]\Psi(\mathbf{r}, \rho, t). \tag{20.5}$$

We expand the wave function $\Psi(\mathbf{r}, \rho, t)$ in terms of the set of eigenfunctions $\{\chi_j(\rho)\}$:

$$\Psi(\mathbf{r}, \rho, t) = \sum_j \sum_E C_j(E)\phi_j(E, \mathbf{r})\chi_j(\rho)\exp(-iEt). \tag{20.6}$$

By substituting (20.6) in (20.5), then multiplying by $\chi_k(\rho)\exp\left(-iE't\right)$ and integrating over ρ and t we find the set of coupled equations:

$$\left[-\nabla_r^2 - q_j^2 + E - U_{jj}(\mathbf{r})\right]C_j(E)\phi_j(E, \mathbf{r}) = \sum_{j \neq k} U_{jk}(\mathbf{r})C_k(E)\phi_k(E, \mathbf{r}),$$
$$j = 1, 2, ..., \tag{20.7}$$

where the matrix potential $U_{jk}(\mathbf{r})$ is given by

$$U_{jk}(\mathbf{r}) = \int \chi_j^*(\rho)U(\mathbf{r}, \rho)\chi_k(\rho)d\rho = U_{kj}(\mathbf{r}). \tag{20.8}$$

The set of wave functions $\{\phi_j(E, \mathbf{r})\}$ also form an orthonormal set provided that the eigenvalues, E_j's, are real;

$$\int \sum_j \left[C_j(E)C_j^*(E')\phi_j(E, \mathbf{r})\phi_j^*(E', \mathbf{r})\right]d^3r = \delta_{E,E'}. \tag{20.9}$$

However this condition of orthogonality breaks down if E_j's have small imaginary parts. For the initial condition, let us assume that (i) the internal motion of the particle is represented by the state $\chi_I(\rho)$ and (ii) $\Phi_I(E, \mathbf{r})$ is the initial wave packet for the particle which is localized behind the barrier. Thus at $t = 0$, we have

$$\psi(\mathbf{r}, \rho, 0) = \chi_I(\rho)\Phi_I(\mathbf{r}) = \sum_E C_I(E)\chi_I(\rho)\phi_I(E, \mathbf{r}), \tag{20.10}$$

where

$$C_I(E) = \int \Phi_I(\mathbf{r})\phi_I^*(E, \mathbf{r})d^3r. \tag{20.11}$$

With the initial condition (20.10) we can determine the time development of the wave packet, viz, $\Psi(\mathbf{r}, \rho, t)$ as the particle escapes from its initial confined position to infinity.

In general, the number of the states $\chi_j(\rho)$'s are infinite. However in practice only a finite number of states contribute significantly to $\Psi(\mathbf{r}, \rho, t)$. As it is evident from Eq. (20.7), for a fixed energy, E, there will be a finite number of channels $j = 1, 2, \ldots.N$ which will be open, i.e. $E - q_j^2 > 0$. For the closed channels, with increasing j, the overlap between $\phi_j(E, \mathbf{r})$ and the barrier becomes smaller, therefore in the right hand side of (20.7) we need to sum over all the open channels and only over the first few of the closed channels.

20.2 Two-Coupled Channel Problem with Spherically Symmetric Barriers

Now let us consider an exactly solvable problem where the internal degree of freedom has two states $\chi_1(\rho)$ and $\chi_2(\rho)$ with the corresponding eigenvalues q_1^2 and q_2^2 [8]. Then the set (20.7) reduces to

$$\left[\frac{d^2}{dr^2} - q_1^2 + E - U_{11}(r)\right] C_1(E)u_1(E, r) = U_{12}(r)C_2(E)u_2(E, r), \tag{20.12}$$

and

$$\left[\frac{d^2}{dr^2} - q_2^2 + E - U_{22}(r)\right] C_2(E)u_2(E, r) = U_{21}(r)C_1(E)u_1(E, r). \tag{20.13}$$

In these relations $u_j(E, r) = \sqrt{4\pi}r\phi_j(E, r)$, $j = 1, 2$ is the reduced wave function for the S-wave ($l = 0$). These differential equations are subject to the boundary conditions:

$$u_1(E,r) \to D_1 \exp(-iK_1 r), \quad r \to \infty, \tag{20.14}$$

and

$$u_2(E,r) \to D_2 \exp(-K_2 r), \quad r \to \infty. \tag{20.15}$$

Here we have assumed that $q_1^2 < E < q_2^2$, i.e. the first channel is open and the second channel is closed. The two constants K_1 and K_2 are given by

$$K_1 = \sqrt{E - q_1^2}, \tag{20.16}$$

and

$$K_2 = \sqrt{q_2^2 - E}. \tag{20.17}$$

For our solvable example we choose the matrix potential $U_{ij}(r)$ as follows [9]:

$$\begin{cases} U_{22} = -v_{22}, \quad U_{11} = -v_{11}, \quad U_{12} = U_{21} = -v_{12}, & \text{for } r \le a \\ U_{22} = U_{11} = v, \quad U_{12} = U_{21} = 0, & \text{for } a \le r \le b \\ U_{22} = U_{12} = U_{11} = U_{21} = 0, & \text{for } r > b \end{cases}. \tag{20.18}$$

For this potential matrix, the solution of the wave equations (20.12) and (20.13) are:

$$u_1^I(r) = \sin(p_- r) + Y\cos(p_+ r), \tag{20.19}$$

$$u_2^I(r) = \alpha\left[\sin(p_- r) + X\cos(p_+ r)\right], \tag{20.20}$$

$$u_1^{II}(r) = A_1 \exp(-Q_1 r) + B_1 \exp(Q_1 r), \tag{20.21}$$

$$u_2^{II}(r) = A_2 \exp(-Q_2 r) + B_2 \exp(Q_2 r), \tag{20.22}$$

$$u_1^{III}(r) = D_1 \exp(-iK_1 r), \tag{20.23}$$

and

$$u_2^{III}(r) = D_2 \exp(-K_2 r). \tag{20.24}$$

In these equations the parameters $p_\pm, \alpha, Q_1$ and Q_2 are defined by

$$p_\pm^2 = \frac{1}{2}\left\{(\gamma^2 + \delta^2) \pm \left[\left(\gamma^2 - \delta^2\right)^2 + 4v_{21}^2\right]^{\frac{1}{2}}\right\}, \tag{20.25}$$

$$\alpha = -\frac{C_1(E)v_{21}}{C_2(E)(\delta^2 - p_-^2)}, \tag{20.26}$$

$$Q_i = \sqrt{v + K_i^2}, \quad i = 1, 2. \tag{20.27}$$

where

$$\gamma^2 = v_{22} - q_2^2 + E, \tag{20.28}$$

and

$$\delta^2 = v_{11} - q_1^2 + E. \tag{20.29}$$

The quantities X, Y, A_i, B_i and D_i are constant amplitudes. By matching these wave functions and their derivatives at a and b, we find the eigenvalue equation which is

$$Y(\delta^2 - p_+^2) - X(\delta^2 - p_-^2) = 0, \tag{20.30}$$

where X and Y are given by

$$X = \frac{G_1 \sin(p_- a) - p_- \cos(p_- a)}{p_+ \cos(p_+ a) - G_1 \sin(p_+ a)}, \tag{20.31}$$

and

$$Y = \frac{G_2 \sin(p_- a) - p_- \cos(p_- a)}{p_+ \cos(p_+ a) - G_2 \sin(p_+ a)}, \tag{20.32}$$

and the constants G_1 and G_2 in (20.32) are given by

$$G_i = \frac{Q_i \{(Q_i - K_i) \exp[-2Q_i(b-a)] - (Q_i + K_i)\}}{(Q_i - K_i) \exp[-2Q_i(b-a)] + (Q_i + K_i)}. \tag{20.33}$$

Here we note that the eigenvalues are independent of the ratio $\frac{C_1(E)}{C_2(E)}$, but the wave functions depend on this ratio. The set of roots of the eigenvalue equation (20.30) with negative imaginary part are the only physically acceptable solutions (Gamow states of Chapter 5).

20.3 A Numerical Example

Consider a two-channel system with the following parameters, $q_1 = 1L^{-1}, q_2 = 5L^{-2}, v_{12} = 1L^{-2}, v_{11} = 3L^{-2}, v = 20L^{-2}, a = 2L$ and $b = 2.3L$, where L is a unit of length. The eigenvalues found from the solution of (20.30) are:

$$E_1 = 7.054 - 0.077i, \quad E_2 = 12.821 - 0.433i, \quad \text{and} \quad E_3 = 22.538 - 1.230i. \tag{20.34}$$

The six functions corresponding to these eigenvalues are shown in Figs. (20.1) and (20.2). Having obtained the eigenfunctions and the eigenvalues,

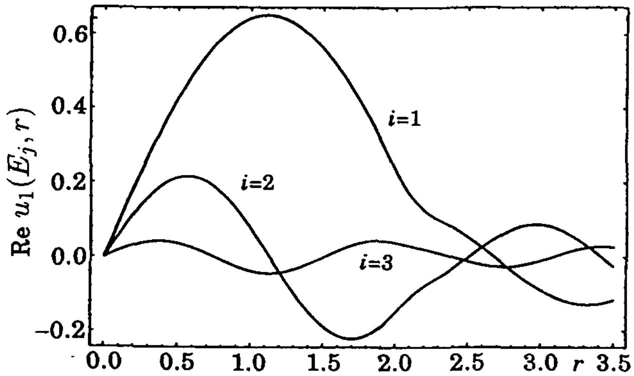

Figure 20.1: The real part of the wave function $u_1(E_j, r)$, $j = 1, 2, 3$ for the open channels for a two-channel problem.

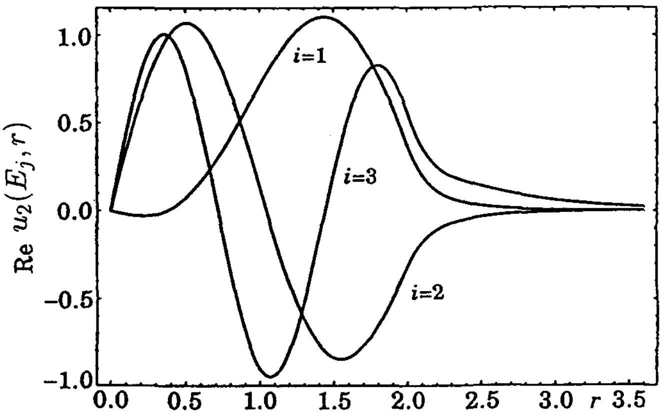

Figure 20.2: The real part of the wave function $u_2(E_j, r)$, $j = 1, 2, 3$ for the closed channels.

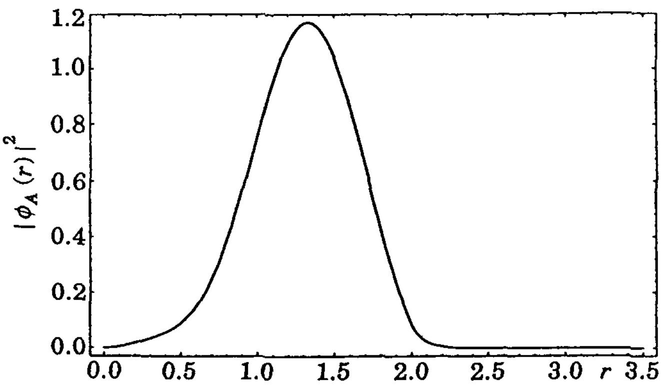

Figure 20.3: The square of the modulus of the wave packet $\phi_A(r)$ plotted as a function of r.

let us consider the motion of the initial wave packet (we choose $I = 2$),

$$\psi(\mathbf{r}, \rho, 0) = \chi_2(\rho)\frac{\phi_2(r)}{\sqrt{4\pi}r}, \tag{20.35}$$

where $\phi_2(r)$ is given by

$$\phi_2(r) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{\pi r}{a}\right) & \text{for } 0 \le r \le a \\ 0 & \text{for } r > a \end{cases}. \tag{20.36}$$

The localized wave function, $\phi_I(r)$, can be expanded in terms of the eigenfunctions $\phi_2(E, r)$ (noting that this expansion, because of the complex nature of the eigenvalues produces a wave packet with a small imaginary part). Let $\phi_A(r)$ be the wave packet obtained from

$$\phi_A(r) = \sum_{i=1}^{3} C_2(E_i)u_2(E_i, r), \tag{20.37}$$

where

$$C_2(E_i) = \int_0^a \phi_2(r)u_2(E_i, r)dr. \tag{20.38}$$

This wave packet is localized behind the barrier (see Fig. (20.3)). The

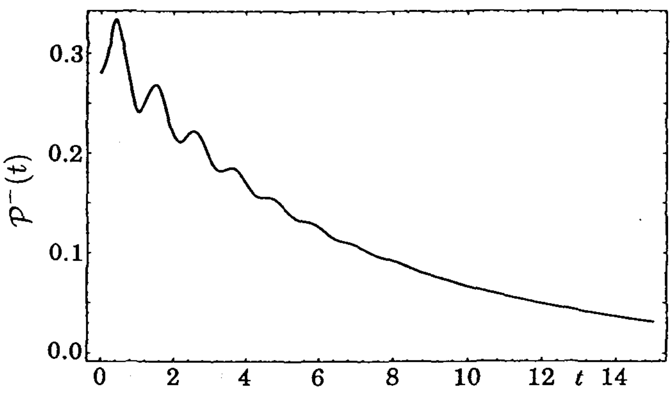

Figure 20.4: The probability $\mathcal{P}^-(t)$ of finding the system in its initial state at time t.

probability of finding the system at time t in its initial state , i.e. $I = 2$ is

$$\mathcal{P}^-(t) = \left| \int \int \Psi^*(\mathbf{r}, \rho, 0)\Psi(\mathbf{r}, \rho, t) d^3r d\rho \right|^2, \tag{20.39}$$

which in this case reduces to

$$\begin{aligned} \mathcal{P}^-(t) &= \left| \sum_i \sum_j C_2^*(E_i) C_2(E_j) \exp(-iE_j t) \int_0^\infty u_2^*(E_i, r) u_2(E_j, r) dr \right|^2, \\ & E_j = \text{Re}\, E_j - \frac{i}{2}\Gamma_j. \end{aligned} \tag{20.40}$$

This probability is shown in Fig. (20.4).

20.4 Tunneling of a Simple Molecule

The simplest system with internal degrees of freedom is a molecule composed of two atoms with a harmonic force binding the two. Here we want to study the one-dimensional tunneling of such a molecule. We begin our study by considering the tunneling of a diatomic molecule in a double-well symmetric or asymmetric potential . We denote the coordinates of the two atoms by x_1 and x_2, and we assume that the two atoms are moving in the potentials $v_1(x_1)$ and $v_2(x_2)$ respectively.

For the simplicity of formulation we take the mass of one of these two atoms as $\frac{1}{2}$ and the other as $\frac{\mu}{2}$, and also we set $\hbar = 1$. Thus the Hamiltonian of this diatomic molecule is

$$H = -\frac{d^2}{dx_1^2} + v_1(x_1) - \frac{1}{\mu}\frac{d^2}{dx_2^2} + v_2(x_2) + \frac{1}{2}K(x_1 - x_2)^2, \tag{20.41}$$

where K is the spring constant for the harmonic binding force. For this Hamiltonian operator we get the Schrödinger equation

$$H\Phi(x_1, x_2, t) = i\frac{\partial}{\partial t}\Phi(x_1, x_2, t), \tag{20.42}$$

which we want to solve subject to the initial condition

$$\Phi(x_1, x_2, 0) = \Phi_0(x_1, x_2). \tag{20.43}$$

Both of the potentials $v_1(x_1)$ and $v_2(x_2)$ are confining double-wells, i.e.

$$\lim_{x_1 \to \pm\infty} v_1(x_1) \to \infty, \qquad \lim_{x_2 \to \pm\infty} v_2(x_2) \to \infty. \tag{20.44}$$

Let us further assume that the central maxima for $v_1(x_1)$ and $v_2(x_2)$ are at $x_1 = x_2 = 0$. If initially the molecule is in the left well, then the probability of finding the molecule in that well at a later time t is given by

$$P^-(t) = \int_{-\infty}^{0}\int_{-\infty}^{0} |\Phi(x_1, x_2, t)|^2\, dx_1 dx_2, \tag{20.45}$$

and at $t = 0$, $P^-(0) \approx 1$.
We denote the Hamiltonians for the atoms 1 and 2 by H_1 and H_2 and their corresponding eigenfunctions by $\psi_m(x_1)$ and $\phi_j(x_2)$ respectively;

$$H_1\psi_m(x_1) = \left[-\frac{d^2}{dx_1^2} + v_1(x_1)\right]\psi_m(x_1) = \varepsilon_m\psi_m(x_1), \tag{20.46}$$

and

$$H_2\phi_j(x_2) = \left[-\frac{1}{\mu}\frac{d^2}{dx_2^2} + v_2(x_2)\right]\phi_j(x_2) = e_j\phi_j(x_2). \tag{20.47}$$

We can expand the eigenfunction of the total Hamiltonian H, Eq. (20.41), in terms of the product of $\psi_m(x_1)$ and $\phi_j(x_2)$;

$$H\Psi = \left[H_1 + H_2 + \frac{1}{2}K\left(x_2 - x_1\right)^2\right]\Psi = E\Psi, \tag{20.48}$$

and

$$\Psi(x_1, x_2) = \sum_{n,j} C_{n,j}\psi_n(x_1)\phi_j(x_2). \tag{20.49}$$

By substituting Ψ from (20.49) in (20.48) and making use of Eqs. (20.46) and (20.47) we find a relation for $E\Psi$. Finally by multiplying the result by $\Psi(x_1, x_2)$ and integrating over the variables x_1 and x_2 we obtain the eigenvalue equation for E;

$$(E - \varepsilon_m - e_k)\, C_{m,k} = \frac{K}{2}\sum_{n,j} \Gamma(m, k; n, j)\; C_{n,j}, \tag{20.50}$$

where in this equation $\Gamma(m, k; n, j)$ is given by

$$\begin{aligned}\Gamma(m, k; n, j) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_m(x_1)\phi_k(x_2)\,(x_1 - x_2)^2\,\psi_n(x_1)\phi_j(x_2)dx_1dx_2 \\ &= \left\langle x_1^2\right\rangle_{mn}\delta_{kj} + \left\langle x_2^2\right\rangle_{kj}\delta_{mn} - 2\left\langle x_1\right\rangle_{mn}\left\langle x_2\right\rangle_{kj}. \end{aligned} \tag{20.51}$$

The numerical coefficients $\langle x_1^s\rangle_{mn}$, $(s = 1, 2)$ are given by the following integrals,

$$\langle x_1^s\rangle_{mn} = \int_{-\infty}^{\infty} \psi_m(x_1)x_1^s\psi_n(x_1)dx_1. \tag{20.52}$$

The same integral can be used to calculate $\langle x_2^s\rangle_{kj}$ except that ψ's are now replaced by ϕ 's. In the set of linear equations (20.50), $\Gamma(m, k; n, j)$ is symmetric;

$$\Gamma(m, k; n, j) = \Gamma(n, j; m, k), \tag{20.53}$$

therefore the eigenvalues are real.

For solving Eq. (20.50) we truncate the sum and assume that the integers n and j each can take values between 1 and N. We write (20.50) in a simpler form by introducing the following symbols:

$$\varepsilon_m + e_j = \Omega_{nj} \to \Omega_{(n-1)N+j}, \tag{20.54}$$

$$\Gamma(m, k; n, j) \to \Gamma\left[(m - 1)N + k; (n - 1)N + j\right], \tag{20.55}$$

and

$$C_{nj} \to C_{(n-1)N+j}. \tag{20.56}$$

With these symbols we write (20.50) as the set of linear equations

$$(E - \Omega_\beta)\, C_\beta = \frac{1}{2}K\sum_{\alpha=1}^{N^2} \Gamma(\beta, \alpha)C_\alpha, \quad \beta = 1, 2, ...N^2, \tag{20.57}$$

where we have replaced n and j by α and m and k by β;

$$\alpha = (n-1)N + j, \quad \beta = (m-1)N + k. \tag{20.58}$$

Thus we find the eigenvalues E of the Eq. (20.57) from the determinant

$$\left|(E - \Omega_\beta)\delta_{\alpha\beta} - \frac{1}{2}K\,\Gamma(\beta,\alpha)\right| = 0. \tag{20.59}$$

From Eqs. (20.59) and (20.57) we obtain the eigenvalues E_γ and the eigenvectors $C_{\gamma\alpha}$. With the help of these we can study the motion of the wave packet $\Phi(x_1, x_2, t)$, Eq. (20.42), as a function of t. Thus we define the eigenfunctions $\Psi_\gamma(x_1, x_2)$ by

$$\Psi_\gamma(x_1, x_2) = \sum_{n,j} C_{\gamma\alpha}\psi_n(x_1)\,\phi_j(x_2), \quad \alpha = (n-1)N + j. \tag{20.60}$$

Then we can expand the initial wave packet $\Phi_0(x_1, x_2)$ in terms of these eigenfunctions

$$\Phi_0(x_1, x_2) = \sum_{\alpha=1}^{N^2} A_\alpha \Psi_\alpha(x_1, x_2), \tag{20.61}$$

and from (20.61) we get the time-dependent wave packet as

$$\Phi(x_1, x_2, t) = \sum_{\alpha=1}^{N^2} A_\alpha \Psi_\alpha(x_1, x_2)\exp(-iE_\alpha t). \tag{20.62}$$

Finally from Eq. (20.45) we calculate the probability of finding the molecule at the time t in the well to the left of the central barrier. If this probability $P^-(t)$ is less than 0.5 we can say that the diatomic molecule has tunneled through the barrier to the second well.

As the first example let us consider the case of a homonuclear molecule, i.e. when the two atoms are identical, and take the mass of each to be $\frac{1}{2}$, and let us denote the harmonic force by $K = \frac{1}{2}\omega^2$. Furthermore let this molecule move in the symmetric potential given by

$$v_1(x) = v_2(x) = \begin{cases} +\infty & \text{for } x < 0, \quad x > c \\ 0 & \text{for } x < 0 \le a, \quad b \le x < c \\ v_0 & \text{for } a < x < b \end{cases}, \quad c = b + a. \tag{20.63}$$

For the wave packet we take $\Phi_0(x_1, x_2)$ to be

$$\Phi_0(x_1, x_2) = \begin{cases} \frac{2\sqrt{2}}{\sqrt{a(a+b)}}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a+b}\right) & \text{for } 0 \le x_1 \le a, \quad 0 \le x_2 \le \frac{a+b}{2} \\ 0 & \text{otherwise} \end{cases}. \tag{20.64}$$

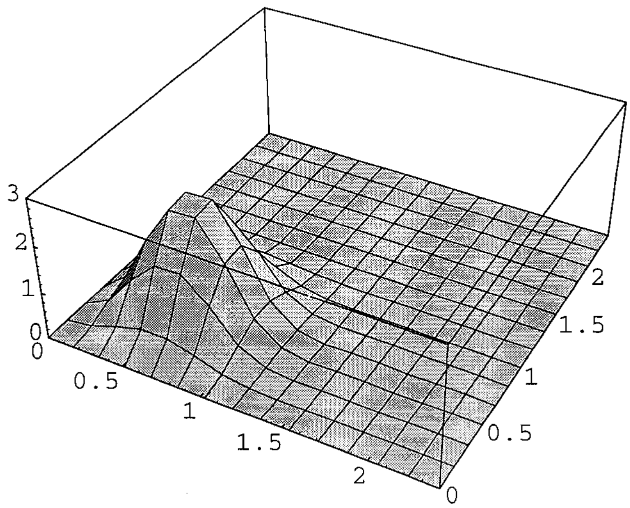

Figure 20.5: The wave packet $\Phi_0(x_1, x_2)$ plotted as a function of the variables x_1 and x_2. This wave packet is confined to the left well of the asymmetric double-well potential when the widths of the two wells are equal (see Eq. (20.64)).

The two-dimensional plot of this wave packet is shown in Fig. (20.5). The constants used are : $a = 1L$, $b = 1.4L$, $c = 2.4L$ and $v_0 = 40L^{-2}$ (L is the unit of length).

In the next two figures the wave packet $\Phi(x_1, x_2, t)$ is shown at the times when $P^-(t)$ takes its minimum value. In Fig. (20.6) the wave function at $t = 5.547L^2$ is plotted for a loosely bound molecule (spring constant $K = \frac{1}{2}L^{-4}$).

When K is small, then when $P^-(t)$ is minimum the molecule has not completely tunneled through to the well in the right. Thus a part of the wave function moves to the right and the rest remains in the left well. When K is large, e.g. $K = 50L^{-4}$, then the two atoms are tightly bound and they act more or less as a single particle. Hence when $P^-(t)$ takes its minimum value, $t = 71.84$, the probability of finding the molecule in the right well is large (see Fig. (20.7)). As we can see in Fig. (20.8) when $K = 50L^{-4}$, $P^-(t)$ which is defined here by

$$P^-(t) = \int_0^a dx_1 \int_0^{\frac{a+b}{2}} |\Phi(x_1, x_2, t)|^2 \, dx_2, \tag{20.65}$$

oscillates with a period T_0. Finally the time $\frac{T_0}{2}$ when $P^-(\frac{T_0}{2})$ takes its

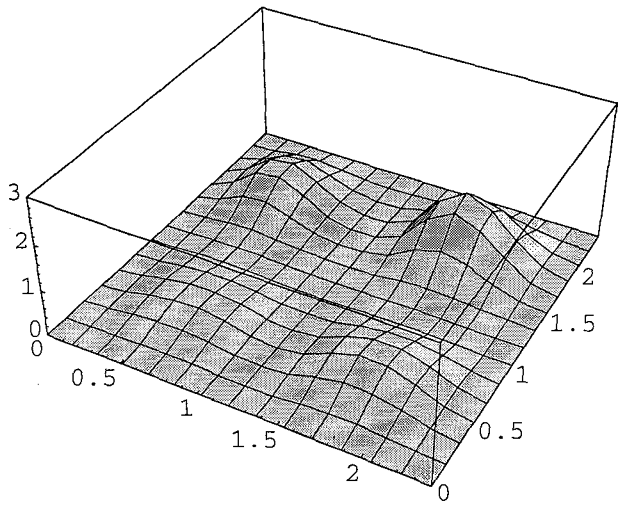

Figure 20.6: The two-dimensional plot of the wave function at the time $t = 5.547L^2$ when $P^-(t)$ assumes its minimum value and the spring constant is small (loosely bound molecule). The wells are of equal width but different depths.

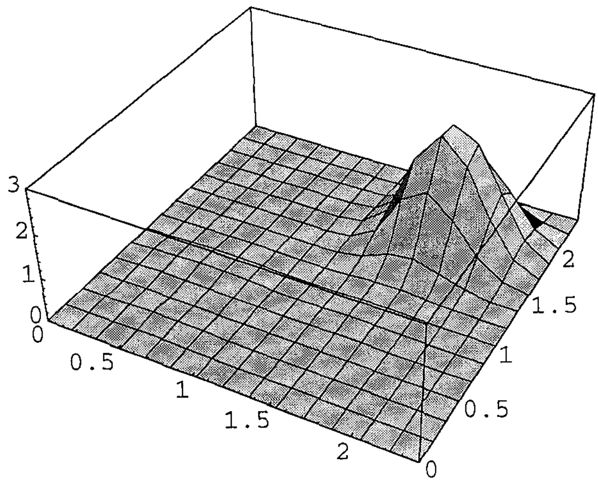

Figure 20.7: Same as in Fig. (20.6) but for a $K = 50L^{-4}$. Here $P^-(t)$ has a minimum at $t = 71.84L^2$ and the wave function is shown for this time.

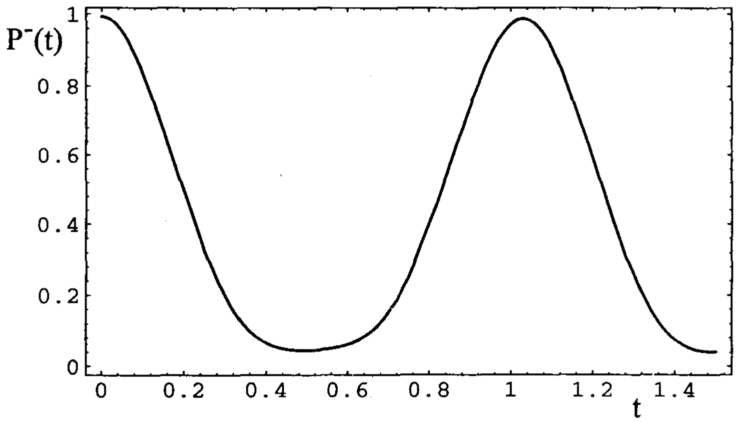

Figure 20.8: The probability of finding the molecule in the left well of a symmetric double-well as a function of time.

minimum value (T_0 corresponds to the period of oscillation) depends on the spring constant or the related quantity ω, where $\omega = \sqrt{2K}$. The dependence of T_0 on ω is shown in Fig. (20.9).

20.5 Tunneling of a Molecule in Asymmetric Double-Wells

As we have seen before in the case of a single particle initially confined in one of the wells, the tunneling to the other well, in general, is not probable unless the resonant conditions are met. Here we first consider molecular tunneling for the resonant case.

(i) - For quantum hopping, we assume a double well potential which is given by (7.1) with the parameters $a = 1L$, $b = 1.4L$, $c = 2.4L$, $v = 21.6L^{-2}$ and $v_1 = 40L^{-2}$.

We consider two cases: the weak binding force $K = \frac{1}{2}$ (i.e. $\omega = 1$ and strong binding force $K = 50$ (or $\omega = 10$), and in each case we study the motion of a wave packet which at $t = 0$ is localized in the left well. For the case of $K = \frac{1}{2}L^{-4}$ at the time $t = \frac{T_0}{2}$, when $P^-(t)$ has its minimum

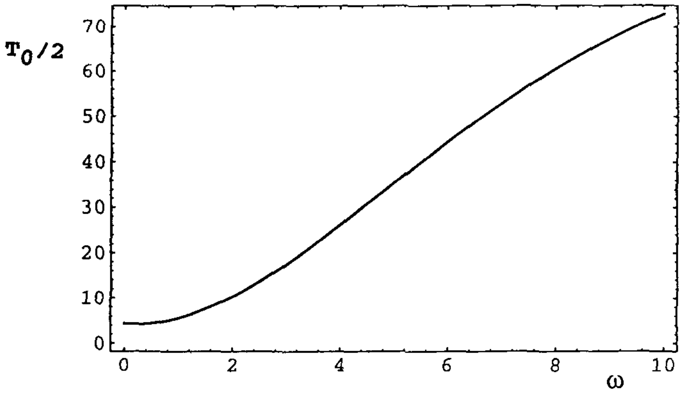

Figure 20.9: The "tunneling time" of a molecule for the symmetric potential (20.63) plotted as a function of ω.

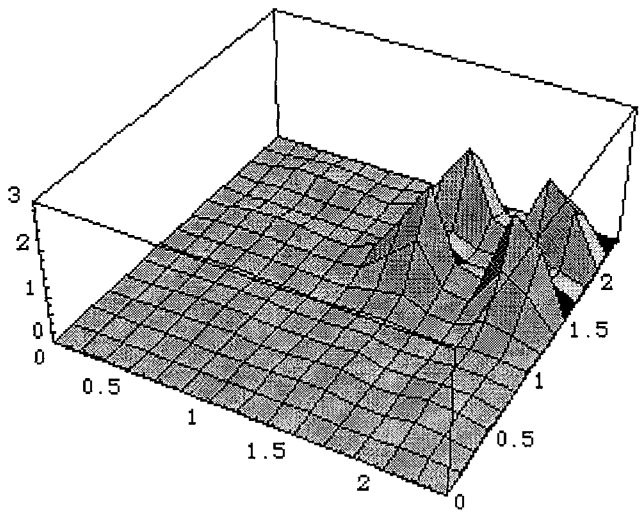

Figure 20.10: The wave packet for loosely bound molecule tunneling through the asymmetric potential (7.1) with equal widths for the wells, at the time $t = \frac{T_0}{2}$ under resonant condition of Chapter 7.

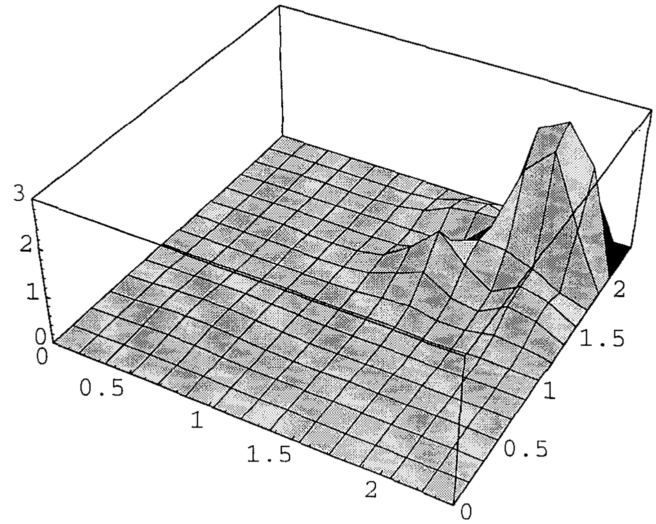

Figure 20.11: Same as in Fig. (20.10) but for tightly bound molecule.

value, the wave packet of each atom appears with two nearly equal peaks in the right well (see Fig. (20.10)). The situation is different when the spring is stiff, e.g. $K = 50$. In this case after tunneling to the second (deeper) well we have two unequal peaks, (Fig. (20.11)). The tunneling time from the left well to the right are $t = 0.972L^2$ and $t = 0.026L^2$ for $K = \frac{1}{2}$ and $K = 50L^{-4}$ respectively.

(ii) - When the wells are of equal depth but with different widths the resonant condition can occur. For instance for the potential (7.1) if we choose $a = 1L$, $b = 1.4L$, $c = 3.46L$, $v_1 = 40L^{-2}$, a $v = 0$, then a single particle can tunnel through the barrier. Now for the molecule we choose an initial wave packet $\Phi_0(x_1, x_2)$ as given by (20.64) (Fig. (20.12)).

After a time $t = \frac{T_0}{2} = 0.011L^2$ we observe that for a stiff spring constant, $K = 50L^{-4}$, in the second well we have unequal peaks, see Fig. (20.13). However in the case of a molecule with small spring constant $K = \frac{1}{2}L^{-4}$, the wave packet spreads everywhere and consists of many maxima Fig. (20.14). Here the probability of finding the molecule in the well to the right of the barrier is small. For the tunneling of a molecule in an asymmetric double-well potential with arbitrary parameters we find that in general $P^-(t)$ is greater than 0.5 for all times, i.e. the probability of tunneling to the second well is small. For instance if we take the parameters used in part (ii) of this section but change c from 3.46 to 2, then the wave packet that we find for $t = \frac{T_0}{2}$ is displayed in Fig. (20.15).

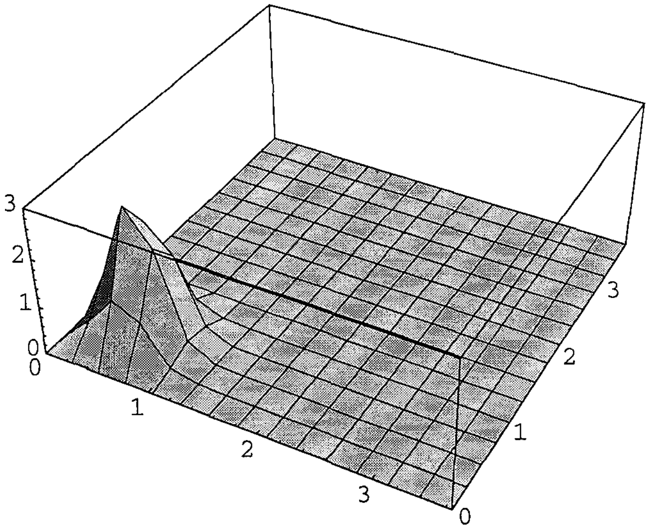

Figure 20.12: The initial wave packet localized in the left well of a double-well ptential (7.1) with the two wells having the same depth but different widths.

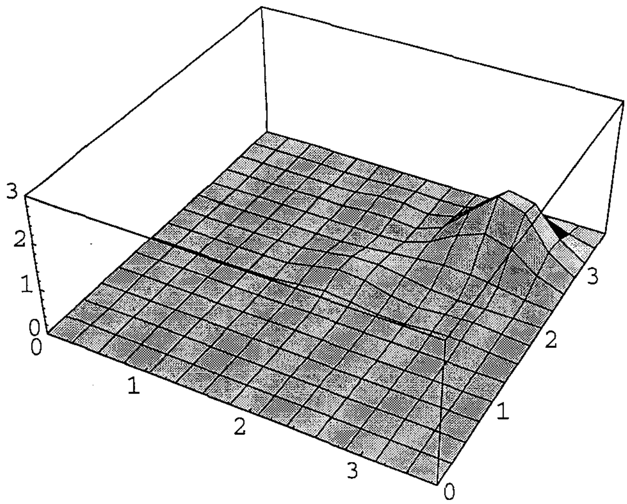

Figure 20.13: The wave packet representing a tightly bound molecule after it has tunneled to the second well. Here the wells have the same depth but different widths.

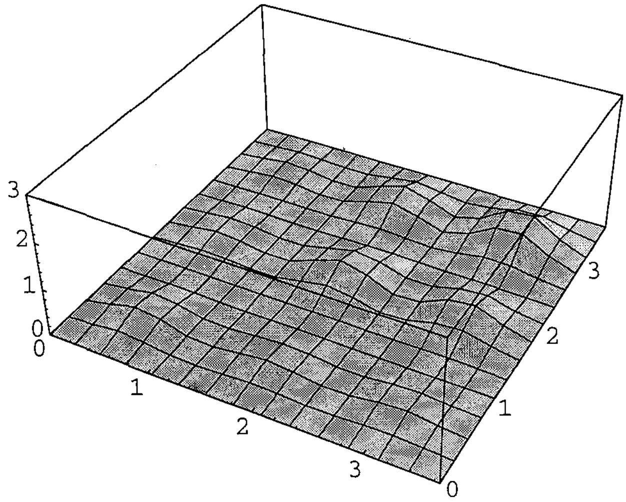

Figure 20.14: Same as in Fig. (20.13) but for loosely bound molecule.

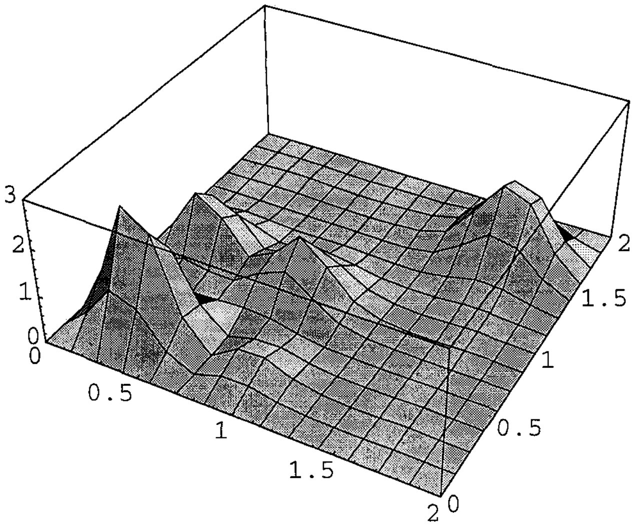

Figure 20.15: The wave packet $\Phi(x_1, x_2, t)$ is shown for $t = \frac{T_0}{2}$. This is the case where resonant condition is not satisfied.

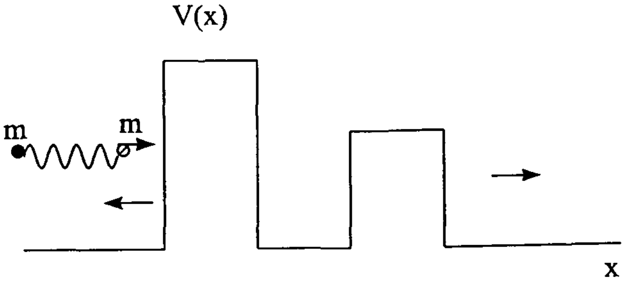

Figure 20.16: A homonuclear molecule tunneling through the potential barrier $V(x)$.

20.6 Tunneling of a Molecule Through a Potential Barrier

Let us consider an arbitrary potential barrier which has a finite extension, i.e. $\lim_{x\to\pm\infty} V(x) \to 0$, and suppose that a homonuclear molecule of mass $2m$ approaches this barrier from the negative side of the x-axis, and by tunneling it moves to $x = \infty$. Here as in the case of a single particle we want to calculate the transmission coefficient for the molecule (see Fig. (20.16)).

If the total energy of the incoming molecule is E, then the Schrödinger equation for this one-dimensional motion is given by

$$\begin{aligned} & -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)\psi \\ & + \left[V(x_1)+V(x_2)+V_0(x_2-x_1)\right]\psi = E\psi, \end{aligned} \tag{20.66}$$

where $V(x)$ represents the barrier and $V_0(x_2 - x_1)$ is the potential acting between the two atoms forming the molecule. It is convenient to use the relative and the center of mass coordinates x and ξ defined by

$$x_1 = x - \frac{1}{2}\xi, \quad x_2 = x + \frac{1}{2}\xi, \tag{20.67}$$

and write (20.66) as [2]

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\left(\frac{1}{2}\frac{\partial^2}{\partial\xi^2}+2\frac{\partial^2}{\partial x^2}\right)\psi(x,\xi)\\
+&\left[V\left(x-\frac{1}{2}\xi\right)+V\left(x+\frac{1}{2}\xi\right)+V_0\left(\xi\right)\right]\psi(x,\xi)=E\psi(x,\xi).
\end{aligned}
\tag{20.68}
$$

We can simplify this equation by taking the following steps:

First we find the solution to the Schrödinger equation

$$
-\frac{\hbar^2}{4m}\frac{d^2\chi_n(\xi)}{d\xi^2}+V_0(\xi)\chi_n(\xi)=e_n\chi_n(\xi), \tag{20.69}
$$

and then we expand $\psi(x,\xi)$ in terms of $\chi_n(\xi)$,

$$
\psi(x,\xi)=\sum_{n=0}^{\infty}\psi_n(x)\chi_n(\xi). \tag{20.70}
$$

Now by substituting this expansion of $\psi(x,t)$ in (20.68) and simplifying the result we find the many-channel Schrödinger equation

$$
\begin{aligned}
&\left(-\frac{\hbar^2}{m}\frac{d^2}{dx^2}-E+e_n\right)\psi_n(x)\\
+&\sum_{j=0}^{\infty}\int_{-\infty}^{\infty}\left[V\left(x+\frac{1}{2}\xi\right)+V\left(x-\frac{1}{2}\xi\right)\right]\chi_j(\xi)\chi_n^*(\xi)d\xi\psi_j(x)=0.
\end{aligned}
\tag{20.71}
$$

We can write (20.71) in a simpler form if we define k_n^2 and $v_{nj}(x)$ by

$$
k_n^2=\frac{m}{\hbar^2}(E-e_n), \tag{20.72}
$$

and

$$
v_{nj}(x)=\frac{m}{\hbar^2}\int_{-\infty}^{\infty}\left[V\left(x+\frac{1}{2}\xi\right)+V\left(x-\frac{1}{2}\xi\right)\right]\chi_j(\xi)\chi_n^*(\xi)d\xi. \tag{20.73}
$$

Then (20.71) can be written as a matrix differential equation

$$
\left(-\frac{\hbar^2}{m}\frac{d^2}{dx^2}-E+e_n\right)\psi_n+\sum_{j=0}^{\infty}v_{nj}(x)\psi_j(x)=0. \tag{20.74}
$$

This equation can be simplified further if $\chi_n(\xi)$ has a definite parity, i.e.

$$\chi_j(-\xi) = (-1)^j \chi_j(\xi). \tag{20.75}$$

Using this, the potential $v_{nj}(x)$ reduces to

$$v_{nj}(x) = \frac{m}{\hbar^2}\int_{-\infty}^{\infty} V\left(x + \frac{1}{2}\xi\right)\left[1 + (-1)^j\right]\chi_j(\xi)\chi_n^*(\xi)d\xi. \tag{20.76}$$

This relation shows that in Eq. (20.74) there is even-even or odd-odd coupling but no even-odd coupling.

The set of equations (20.74) can be solved by the method of variable reflection coefficient which we discussed in detail in Chapter 11.

Let us first study the special case when the spring constant K is large and the molecule is in its ground state. In this case the probability of excitation of the molecule because of the action of the potential $V(x)$ is small. Therefore in Eq. (20.74) we can keep the term $v_{00}(x)$ but ignore all of the other matrix elements of $v_{nj}(x)$ and thus end up with the simple differential equation

$$\frac{d^2}{dx^2}\psi_0(x) + \left[k_0^2 - v_{00}(x)\right]\psi_0(x) = 0. \tag{20.77}$$

If we compare $v_{00}(x)$ with the action of either of the potentials $V(x_1)$ or $V(x_2)$ we observe that $v_{00}(x)$ changes more slowly than $\frac{2m}{\hbar^2}V(x)$. Thus we conclude that tunneling becomes easier for a molecule at higher energies, but more difficult at lower energies. To study this aspect of the problem further, let us consider the special case when the potential between the two atoms is harmonic, $V(\xi) = \frac{1}{2}k\xi^2$. In this case [9]

$$\chi_n(\xi) = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{\frac{1}{2}} H_n(\alpha\xi)\exp\left(\frac{1}{2}\alpha^2\xi^2\right), \tag{20.78}$$

where

$$\alpha^4 = \frac{mK}{\hbar^2}, \tag{20.79}$$

and $H_n(\alpha\xi)$ is the Hermite polynomial .

For the determination of the matrix elements $v_{nj}(x)$ analytically, we assume that $V(x)$ is a Gaussian potential ;

$$V(x) = V_0 \exp\left(-\mu^2 x^2\right), \tag{20.80}$$

then by substituting (20.78) and (20.80) in (20.73) we find $v_{nj}(x)$ [10]

$$\begin{aligned} v_{nj}(x) &= \frac{2mV_0}{\hbar^2}\frac{\alpha}{(2^{n+j}n!j!)^{\frac{1}{2}}}\frac{\exp\left[-\frac{4\mu^2\alpha^2x^2}{(4\alpha^2+\mu^2)}\right]}{(4\alpha^2+\mu^2)} \\ &\times \sum_{k=0}^{min(n,j)} 2^k k! \binom{j}{n}\binom{n}{k}\left(\frac{\mu^2}{4\alpha^2+\mu^2}\right)^{\frac{j+n}{2}-k} \\ &\times H_{j+n-2k}\left[-\frac{2\alpha\mu x}{(4\alpha^2+\mu^2)^{\frac{1}{2}}}\right] \text{ for } \quad (n+j) = \text{even}, \quad (20.81) \end{aligned}$$

otherwise $v_{nj}(x) = 0$. For $j = n = 0$, we have the simple expression

$$v_{00}(x) = \frac{2mV_0\alpha}{\hbar^2\left(\alpha^2+\frac{1}{4}\mu^2\right)^{\frac{1}{2}}}\exp\left(-\frac{4\alpha^2\mu^2x^2}{4\alpha^2+\mu^2}\right). \quad (20.82)$$

This potential should be compared to

$$\frac{2mV(x)}{\hbar^2} = \frac{2mV_0}{\hbar^2}\exp\left(-\mu^2x^2\right). \quad (20.83)$$

Fig. (20.17) shows both $\frac{2mV(x)}{\hbar^2}$ and $v_{00}(x)$ for the parameters $\alpha = 1$ and $\mu = 3$. Here we observe that while $\frac{2mV(x)}{\hbar^2}$ has a higher peak, the width of $v_{00}(x)$ near the base is larger. Thus at higher energies of the incident molecule v_{00} is more transparent, but for lower energies the opacity of $v_{00}(x)$ is greater. In Fig. (20.18) the potentials $v_{00}(x)$, $v_{02}(x)$ and $v_{22}(x)$ are plotted for the same set of parameters ($\alpha = 1$ and $\mu = 3$). We note that the coupling potential $v_{02}(x)$ is quite small compared to $v_{00}(x)$ and $v_{22}(x)$. Furthermore the height and the width of $v_{22}(x)$ together with the fact that $k_2^2 < k_0^2$ shows that the probability of tunneling in $n = j = 0$ channel is greater than to any other channel. For the cases where $k_2^2 < 0$, all higher even channels will be closed and only $n = j = 0$ channel remains open.

In the case of odd-odd coupling with the potentials $v_{11}(x), v_{13}(x)$... we can use a similar argument and solve the problem with $n = j = 1$ only. This will be the first order approximation which can be improved by adding other channels to the set of differential equations.

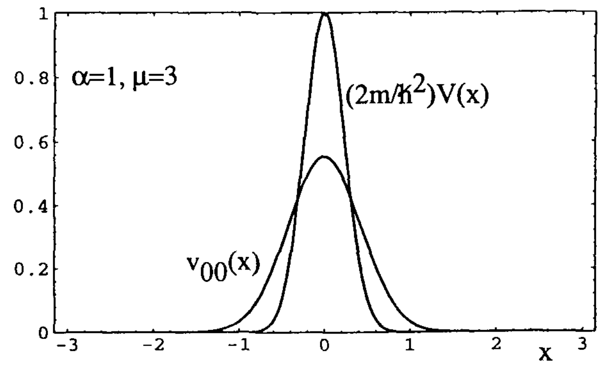

Figure 20.17: The potential barrier for an atom, $\frac{2mV(x)}{\hbar^2}$, and the effective potential $v_{00}(x)$, (see Eq. (20.82)).

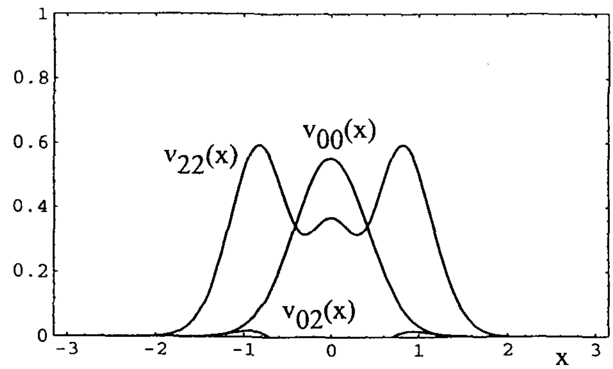

Figure 20.18: The effective potentials for two even channels 0 and 2 calculated from Eq. (20.81).

20.7 Antibound State of a Molecule

At the end of Chapter 10 we discussed the motion of a particle in a potential field which consists of the following three parts: A repulsive part which forms the barrier is followed by an attractive potential and finally there is an impenetrable barrier . There we concluded that for certain energies the particle will be in the "antibound" state. This means that in the neighborhood of this energy the change in the phase shift is discontinuous and the time-delay which is proportional to $\hbar\frac{d\delta(E)}{dE}$ (Chapter 18) is large, i.e. the particle spends a long time in this potential field.

In the example of Chapter 10, we solved this problem for S-wave scattering for a potential consisting of a δ-function barrier and an attractive square well. For the one-dimensional tunneling it is more convenient to consider a smooth potential. In the following calculation we use the potential

$$V(x) = 8\left\{\exp\left[-6(x+3)^2\right] - \exp\left[-(x+1)^2\right]\right\} + e^{4x}, \qquad (20.84)$$

where we have set $\hbar = 2m = 1$. To simplify the problem we assume that the molecule is homonuclear and that the potential between the two atoms is given by (7.62). For this potential the lowest eigenvalues and eigenfunctions are known analytically (Eqs. (7.68), and (7.78)-(7.81)).

Here we need only the lowest energy eigenfunctions, and since the difference between e_2 and e_4 is large, we only include the two levels e_0 and e_2. From Eq. (20.76) it follows that only the even eigenfunctions are needed in the calculation. Since $\chi_0(\xi)$ and $\chi_2(\xi)$ are the same as $u_0(x)$ and $u_2(x)$, Eqs. (7.68) (7.78)-(7.81) of Chapter 7, therefore the potential $v_{nj}(x)$ has the following form ($\hbar = 2m = 1$),

$$v_{nj}(x) = v_{jn}(x) = \int_{-\infty}^{\infty} V\left(x + \frac{1}{2}y\right) u_n(y)u_j(y)dy, \quad n, j = 0, 2, \ldots. \quad (20.85)$$

In Fig. (20.19) these effective potentials are shown. For the solution of the set of equations (20.73) we use the method of variable reflection coefficient of Chapter 11, and solve Eq. (11.24) for each of $U_{00}(y)$, $U_{02}(y)$, and $U_{22}(y)$ with the boundary condition (11.26). Finally from (11.22) we find the reflection coefficient at $y = -\infty$. Since the molecule cannot pass the impenetrable barrier , therefore the transmission coefficient is zero. Now for the open channels where k_n^2 is positive, for large and negative values of y we have

$$\lim_{y\to-\infty} [R_{nj}(y)] = A_{nj} \exp\left[2i\delta_{nj}(E)\right]$$

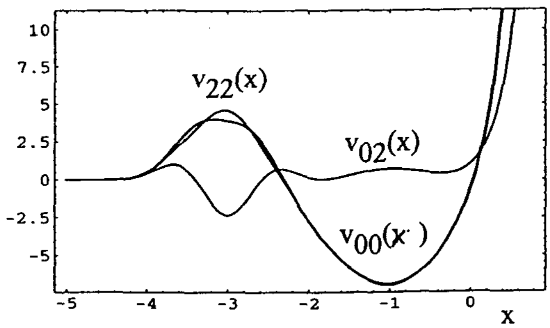

Figure 20.19: The matrix elements of the potential found from $V(x)$, Eq. (20.84) and the wave functions $u_0(x)$ and $u_2(x)$ given by (7.68) (7.78)-(7.81).

$$= \lim_{y \to -\infty} \{\exp\left[i\left(k_n + k_j\right) y\right] \left(2ik_j U_{nj}(y) - \delta_{n,j}\right)\} . \qquad (20.86)$$

In this relation $\delta_{nj}(E)$ is the phase shift and $\delta_{n,j}$ in the right hand side of (20.86) is the Kronecker delta. Here it is assumed that k_n and k_j are real quantities, and therefore the channels corresponding to R_{00}, R_{02}, R_{20} and R_{22} are all open. In Fig. (20.20) the phase shifts $\delta_{00}(E)$, $\delta_{02}(E)$ and $\delta_{22}(E)$ are shown as functions of E. The dependence of $\delta_{20}(E)$ on E which is not shown is similar to that of $\delta_{02}(E)$. In the range of energies shown (in units of L^{-2}) only $\delta_{00}(E)$ is continuous. If the total energy of the molecule is equal to the energies where $\delta_{02}(E)$ .... $\delta_{22}(E)$ are discontinuous, the molecule will be in antibound state in this potential and will spend a long time in this state.

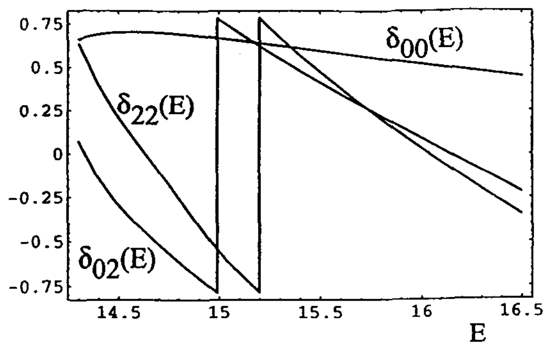

Figure 20.20: The phase shifts $\delta_{00}(E)$, $\delta_{02}(E)$ and $\delta_{22}(E)$ are plotted as a function of energy. Except for $\delta_{00}(E)$ the other phase shifts are discontinuous at certain energies.

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Chapter 21

Motion of a Particle in a Space Bounded by a Surface of Revolution

We have studied the motion of a particle in a confining double-well potential, and have observed that how tunneling causes the splitting between the energy levels. A generalization of this mechanism to three dimensions is the subject that we want to study in this chapter [1].

Let us consider a closed surface similar to a peanut, or to a bowling pin where the cross section in the middle is smaller than the maximum cross section on either sides (see Figs (21.1) and (21.2)). If we assume the boundaries to be impenetrable the energy levels of a particle which is moving within this surface is determined by the geometry of each part and by the possibility of tunneling.

For the mathematical formulation of this problem we consider a closed surface generated by rotating a continuous curve $R(z)$ about the z-axis. The equation for the surface S, thus produced is given by

$$x^2 + y^2 = R^2(z). \tag{21.1}$$

Assuming that there is no force acting on the particle inside the surface we can write the Schrödinger equation in cylindrical coordinates as

$$\frac{\partial^2\psi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\psi}{\partial\rho} + \frac{\partial^2\psi}{\partial z^2} + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + E\psi = 0, \tag{21.2}$$

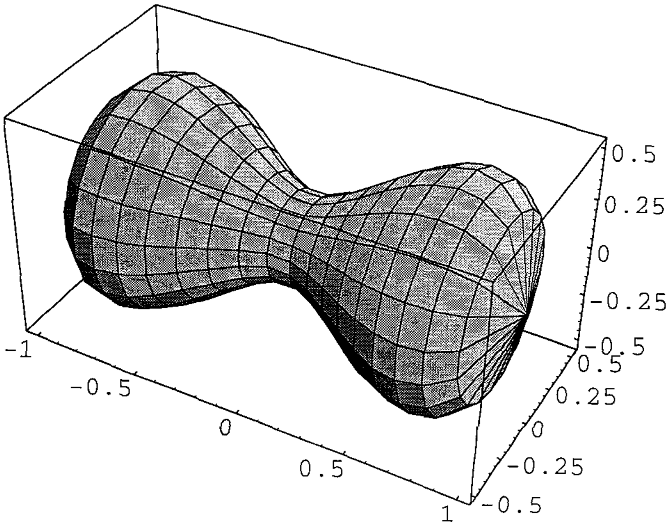

Figure 21.1: A particle trapped inside the symmetric closed surface of rotation shown here has discrete energy levels. The role of tunneling in the determination of the level spacing is the subject of our investigation.

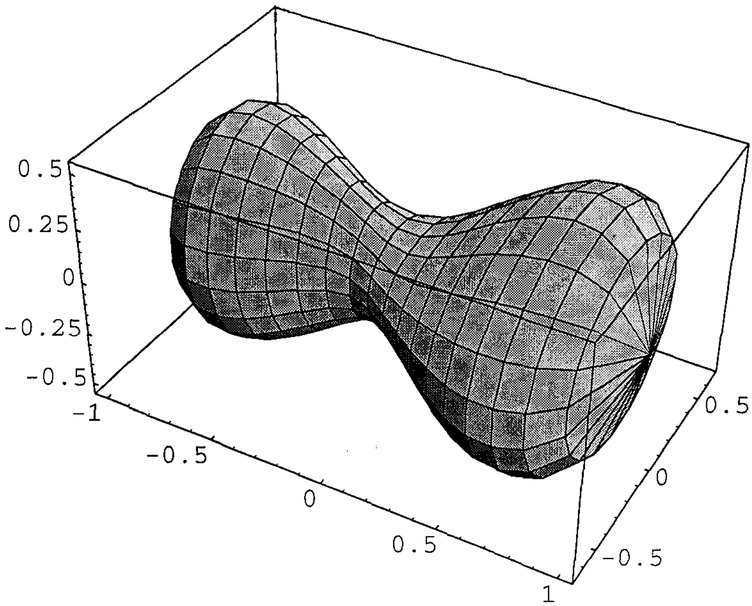

Figure 21.2: An impenetrable surface of rotation in the shape of a bowling pin. The energy eigenvalues for a particle moving inside this surface are affected by tunneling.

where we have set $\hbar = 2m = 1$, and therefore E is measured in units of L^{-2}. The wave function ψ must be finite within S and on the surface it must vanish,

$$\psi(S) = 0. \tag{21.3}$$

While there are open surfaces of rotation for which the Helmholtz (or Schrödinger equation for free particle) is separable [2], but no closed surface of rotation is known with this property [3]. Since the surface S has cylindrical symmetry, $\psi(S)$ is independent of ϕ, and therefore we can separate the ϕ dependence of ψ from the ρ and z dependence, and write $\psi_m(\rho, z, \phi)$ as an expansion in terms of the Bessel function J_m,

$$\psi_m(\rho, z, \phi) = \sum_{j=0}^{\infty} J_m\left[\xi_{mj}\frac{\rho}{R(z)}\right] Z_{mj}(z)e^{im\phi}, \quad 0 \le \rho \le R(z), \tag{21.4}$$

where in this equation ξ_{mj} is the j-th root of J_m, i.e.

$$J_m\left(\xi_{mj}\right) = 0, \quad j = 0, 1, 2, ..., \tag{21.5}$$

and $Z_{mj}(z)$'s are the coefficients of the expansion. On the closed surface S, $\rho = R(z)$, and therefore the boundary condition (21.3) is satisfied. By substituting (21.4) in (21.2) we find

$$\begin{aligned} &\sum_{j=0}^{\infty}\left[\frac{d^2 Z_{mj}}{dz^2} + \left(E - \frac{\xi_{mj}^2}{R^2(z)}\right) Z_{mj}\right] J_m(\mu_j) \\ + &\sum_{j=0}^{\infty}\left\{\left(\frac{dZ_{mj}}{dz}\frac{\partial J_m(\mu_j)}{\partial z} + Z_{mj}\frac{\partial^2 J_m(\mu_j)}{\partial z^2}\right)\right\} = 0, \end{aligned} \tag{21.6}$$

where

$$\mu_j = \frac{\rho\xi_{mj}}{R(z)}. \tag{21.7}$$

To simplify Eq. (21.6), we change the derivatives of $J_m(\mu_j)$ with respect to z to partial derivatives with respect to μ_j;

$$\begin{aligned} &\sum_{j=0}^{\infty}\left[\frac{d^2 Z_{mj}}{dz^2} + \left(E - \frac{\xi_{mj}^2}{R^2(z)}\right) Z_{mj} + \left(\frac{R'}{R}\right)^2\left(m^2 - \left(\frac{\rho\xi_{mj}}{R}\right)^2\right) Z_{mj}\right] \\ \times\ &J_m(\mu_j) - \sum_{j=0}^{\infty}\left[\left(\frac{2R'}{R}\right)\rho\xi_{mj}\frac{dZ_{mj}}{dz} + \rho\xi_{mj}\frac{d}{dz}\left(\frac{R'}{R}\right) Z_{mj}\right. \\ + &\left.\left(\frac{\xi_{mj}\rho}{R}\right)\left(\frac{R'}{R}\right)^2 Z_{mj}\right]\left(\frac{\partial J_m(\mu_j)}{\partial \mu_j}\right) = 0, \end{aligned} \tag{21.8}$$

where $R = R(z)$ and prime denotes derivatives with respect to z. If we multiply (21.8) by $J_m(\mu_j)\rho d\rho$ and integrate over ρ from 0 to ∞ we find the following set of differential equations

$$\frac{d^2 Z_{mj}}{dz^2} + \left[E - \left(\frac{\xi_{mj}}{R}\right)^2 + m^2\left(\frac{R'}{R}\right)^2\right] Z_{mj}$$
$$- \left(\frac{2R'}{R}\right)\sum_{k=0}^{\infty}\xi_{mk}B_m(k,j)\frac{dZ_{mk}}{dz} + \sum_{k=0}^{\infty}\left\{\xi_{mk}^2\left(\frac{R'}{R}\right)^2 C_m(k,j)\right.$$
$$+ \left.\left[\left(\frac{R'}{R}\right)^2 - \frac{R''}{R}\right]\xi_{mk}B_m(k,j)\right\} Z_{mk} = 0. \tag{21.9}$$

In this equation $B_m(k,j)$ and $C_m(k,j)$ are defined by

$$B_m(j,k) = \frac{1}{\left[J_{m+1}(\xi_{mj})\right]^2}\int_0^1 J_m(\xi_{mj}x)x^2$$
$$\times \left[J_{m+1}(\xi_{mk}x) - J_{m-1}(\xi_{mk}x)\right]dx, \tag{21.10}$$

and

$$C_m(j,k) = \frac{-2}{\left[J_{m+1}(\xi_{mj})\right]^2}\int_0^1 J_m(\xi_{mj}x)x^3 J_m(\xi_{mk}x)dx. \tag{21.11}$$

Thus the solution of the problem reduces to the integration of the system of ordinary differential equations

$$\frac{d^2 Z_{mj}}{dz^2} + EZ_{mj} - \sum_k w_{mjk}Z_{mk} = 0, \tag{21.12}$$

where the operator w_{mjk} is the Hermitian potential

$$w_{mjk}(z) = \left[\left(\frac{\xi_{mj}}{R}\right)^2 - m^2\left(\frac{R'}{R}\right)^2\right]\delta_{kj}$$
$$+ \left\{i\left[p\left(\frac{R'}{R}\right) + \left(\frac{R'}{R}\right)p\right] - \frac{d}{dz}\left(\frac{R'}{R}\right)\right\}\xi_{mk}B_m(k,j)$$
$$- \left(\frac{R'\xi_{mk}}{R}\right)^2 C_m(k,j) - \left[\left(\frac{R'}{R}\right)^2 - \left(\frac{R''}{R}\right)\right]\xi_{mk}B_m(k,j), \tag{21.13}$$

and p is the z component of the momentum

$$p = -i\frac{d}{dz}. \tag{21.14}$$

For the j-th channel we can eliminate $\frac{dZ_{mj}}{dz}$ from the differential equation for Z_{mj}. To this end we define the function $\zeta_{mj}(z)$ by

$$Z_{mj}(z) = \zeta_{mj}(z)\exp\left[-\xi_{mj}B_m(j,j)\ln R(z)\right] = \frac{\zeta_{mj}(z)}{R(z)}, \tag{21.15}$$

and replace $Z_{mj}(z)$ by $\zeta_{mj}(z)$ to find

$$\begin{aligned}&\frac{d^2\zeta_{mj}}{dz^2} + \left(E - v_{mj}(z)\right)\zeta_{mj}\\ - &\sum_{k\neq j}\exp\left\{-\left[\xi_{mk}B_m(k,j) - \xi_{mj}B_m(j,j)\ln R(z)\right]\right\}w_{mjk}(z)\zeta_{mk} = 0,\end{aligned} \tag{21.16}$$

in which the matrix potential $v_{mj}(z)$ is given by

$$v_{mj}(z) = \left(\frac{\xi_{mj}}{R}\right)^2 + \left(\xi_{mj}^2\left[(B_m(j,j))^2 - C_m(j,j)\right] - m^2\right)\left(\frac{R'}{R}\right)^2, \tag{21.17}$$

and

$$\xi_{mj}B_m(j,j) = 1. \tag{21.18}$$

The last relation is found from (21.10) by substituting for $(J_{m+1} - J_{m-1})$ in terms of the derivative of J_m and then integrating the result. We observe that since $w_{mjk}(z)$ depends only on m^2, each state for which $m \neq 0$ is degenerate, and the two eigenfunctions $\psi_m(\rho, z, \phi)$ and $\psi_{-m}(\rho, z, \phi)$ correspond to the same energy level. If we want to calculate the low-lying energy levels, we can use the WKB approximation for ζ_{mk}

$$\zeta_{mk} \approx \exp\left[-\int^z \sqrt{v_{mk}(z) - E_{mj\alpha}}\, dz\right], \quad k > j, \tag{21.19}$$

where we have assumed that $v_{mk}(z)$ is larger than the energies $E_{mj\alpha}$. Since the two potentials $w_{mjk}(z)$ and $v_{mk}(z)$ are of the same order of magnitude, therefore for the calculation of these eigenvalues we can ignore the terms in the sum in Eq. (21.16), or include them approximately.

21.1 Testing the Accuracy of the Present Method

We first observe that $v_{mj}(z)$ increases with increasing of m and j. For any given $R(z)$ we find the first few terms of the potential from (21.17);

$$v_{00}(z) = \frac{5.783}{R^2(z)} + 2.261\left(\frac{R'(z)}{R(z)}\right)^2, \tag{21.20}$$

$$v_{10}(z) = \frac{14.682}{R^2(z)} + 4.894\left(\frac{R'(z)}{R(z)}\right)^2, \tag{21.21}$$

$$v_{01}(z) = \frac{30.471}{R^2(z)} + 10.490\left(\frac{R'(z)}{R(z)}\right)^2, \tag{21.22}$$

and

$$v_{11}(z) = \frac{49.218}{R^2(z)} + 16.406\left(\frac{R'(z)}{R(z)}\right)^2. \tag{21.23}$$

In order to test the accuracy of the method we apply it to the problem of a particle confined inside a spherical surface of radius a [1]. In this case the problem is separable in spherical polar coordinates and the wave function is given by

$$\psi_{ljm}(r,\theta,\phi) = j_l\left(\frac{\xi_{lj}r}{a}\right)P_l^m(\cos\theta)\exp(im\phi), \tag{21.24}$$

where ξ_{lj} is the j-th zero of the spherical Bessel function of order l, i.e.

$$j_l(\xi_{lj}) = 0. \tag{21.25}$$

Thus the energy eigenvalues are given by

$$E_{ljm} = \left(\frac{\xi_{lj}}{a}\right)^2. \tag{21.26}$$

Because of the symmetry of the problem the eigenvalues are $(2l+1)$-fold degenerate. The lowest E_{ljm}'s for $a = 1.01L$ are given by

$$(a)\ E_{00} = 9.675,\quad (b)\ E_{10m} = 19.793\ \ (m = 0, \pm 1),$$
$$(c)\ E_{20m} = 32.563\ \ (m = 0, \pm 1, \pm 2),\quad \text{and}\quad (d)\ \ E_{010} = 38.7, \tag{21.27}$$

where all E_{ljm} 's are in units of L^{-2}.

To produce a sphere of radius a by rotation, we choose $R(z)$ to be

$$R(z) = \sqrt{a^2 - z^2}, \tag{21.28}$$

and calculate the potentials $v_{00}(z)......v_{11}(z)$ from Eqs. (21.20)-(21.23). By substituting the resulting potential in the differential equation

$$\frac{d^2\zeta_{mj}}{dz^2} + [E - v_{mj}(z)]\,\zeta_{mj} = 0, \tag{21.29}$$

and solving (21.28) numerically we find the eignvalues $E_{mj\alpha}$. The approximate values of the low-lying eigenvalues are (in units of L^{-2})

$$\begin{aligned} &(a)\ E_{000} \approx 9.707, \quad (b1)\ E_{100} \approx 19.844, \\ &(b2) E_{001} \approx 19.991, \quad (c1)\ E_{200} \approx 31.212, \quad (c2)\ E_{101} \approx 32.837, \\ &(c3)\ \approx 34.784 \quad \text{and} \quad (d)\ E_{010} \approx 37.198. \end{aligned} \tag{21.30}$$

Here (a) and (d) are non-degenerate and $(b1)$ is doubly degenerate. Both $(b1)$ and $(b2)$ correspond to (b) of the exact solution. For (c) we have a non-degenerate state $(c3)$ and two doubly degenerate states $(c1)$ and $(c2)$. As these results indicate the omission of the coupling terms in (21.16) is a reasonable approximation.

21.2 Calculation of the Eigenvalues

Now let us study the energies in the closed surface shown in Fig. (21.1). This surface is produced by rotating the curve

$$R(z) = \left[(z^2 + b^2)(a^2 - z^2)\right]^{\frac{1}{2}}, \quad -a \le z \le a, \tag{21.31}$$

about the z-axis. From (21.31) and (21.20) we find the potential $v_{00}(z)$ to be a symmetric double-well potential shown in Fig. (21.3).

For $a = 1.01$ and $b = 0.2$ this potential has a minimum of $20.58L^{-2}$ at $z = \pm 0.7$ and a maximum of $141.7L^{-2}$ at $z = 0$. The low-lying eigenvalues obtained for this case from Eq. (21.29) are (in units of L^{-2});

$$\begin{aligned} &E_{000} \approx 41.409, \quad E_{001} \approx 41.506, \quad E_{100} \approx 81.716 \\ &E_{101} \approx 81.718 \quad \text{and} \quad E_{002} \approx 84.243. \end{aligned} \tag{21.32}$$

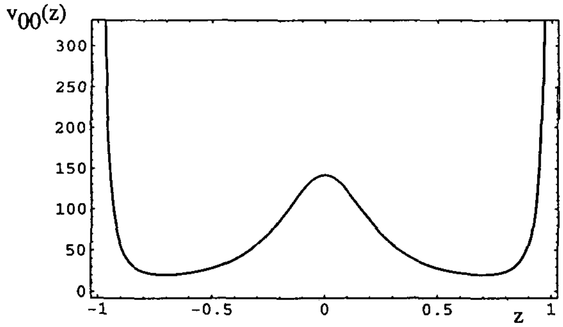

Figure 21.3: The effective potential $v_{00}(z)$ found from Eqs. (21.20) and (21.31).

The level splitting for these levels can be found from the semi-classical expression (Eq.(3.109) of Chapter 3)

$$\Delta E_{mj0} = \frac{E_{mj0}}{\pi} \exp\left[-\int_{z_1}^{z_2} \sqrt{v_{mj}(z) - E_{mj0}}\, dz\right]. \tag{21.33}$$

Using this approximation we find

$$\Delta E_{000} \approx 0.09, \quad \Delta E_{100} \approx 0.001. \tag{21.34}$$

These numbers should be compared to the results of 0.097 and 0.002 obtained from (21.32). These splittings, as we have discussed earlier is caused by quantum tunneling.
If we choose an initial wave packet of the form $\frac{1}{\sqrt{2}}[\zeta_{000}(z) - \zeta_{001}(z)]$ for the $Z(z)$ part, the R and ϕ parts being given as in Eq. (21.4), then this wave packet oscillates between the two parts of the surface shown in Fig. (21.1). *The period of the oscillation is given by* $\frac{2\pi\hbar}{E_{001}-E_{000}}$ *(coherent tunneling).*

As a second example we will determine the lowest eigenvalues for a particle confined to move inside the surface generated by

$$R(z) = \left[(z+c)^2 + b^2\right]^{\frac{1}{2}} \left(a^2 - z^2\right)^{\frac{1}{2}}, \quad -a \le z \le a. \tag{21.35}$$

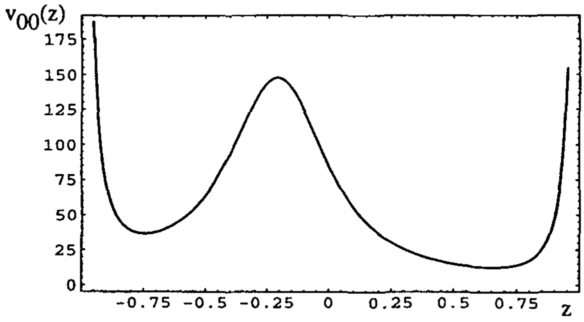

Figure 21.4: Same as in Fig. (21.3) but for the surface of revolution generated by (21.35).

This is the surface shown in Fig. (21.2) when $a = 1.01$ and $b = c = 0.2$. In this problem the potential $v_{ij}(z)$ is asymmetric (see Fig. (21.4) for $v_{00}(z)$) Here the lowest eigenvalues are:

$$E_{000} \approx 28.097, \qquad E_{100} \approx 53.789, \quad E_{001} \approx 61.41 \quad \text{and} \quad E_{002} \approx 67.09. \tag{21.36}$$

In Fig. (21.5) the eigenfunctions corresponding to these levels are shown.

Suppose that a wave packet representing the particle is initially confined to the volume on the right of the constriction in Fig. (21.2). We want to determine whether this wave packet can move to the space to the left or not? For this we choose a wave packet of the form

$$\Phi_0(\rho, z) = \frac{1}{R(z)} J_0\left(\frac{\xi_{00}\rho}{R(z)}\right) \sum_{\alpha=0}^{2} A_\alpha \zeta_{00\alpha}(z), \quad 0 \le \rho \le R(z), \tag{21.37}$$

where A_α 's are the expansion coefficients, for instance

$$A_\alpha = \int_0^1 \sqrt{2} \sin(\pi z) \zeta_{00\alpha}(z) dz. \tag{21.38}$$

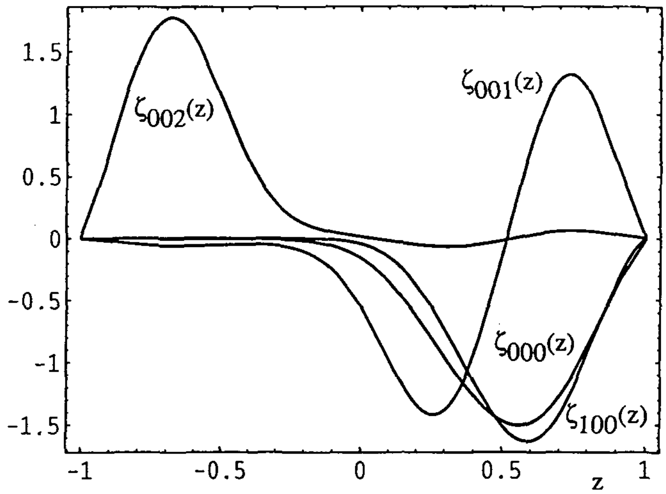

Figure 21.5: The eigenfunctions $\zeta_{00\alpha}(z)$ calculated from the differential equation (21.29) for $m = j = 0$.

By changing the variable from ρ to y, where $y = \frac{\rho}{R(z)}$, we can write $\Phi_0(\rho, z) = \Psi(y, z, t = 0)$, i.e.

$$\Psi(y, z, t = 0) = J_0(\xi_{00}y) \sum_{\alpha=0}^{2} A_\alpha \zeta_{00\alpha}(z). \tag{21.39}$$

Thus the probability of finding the initial wave packet at a point with the coordinates (y, z) is $|\Psi(z, y, t = 0)|^2$ and this probability is shown in Fig. (21.6). Now from equation (21.39) and the eigenvalues (21.36) we can find the motion of the wave packet as a function of time. The motion of the center of the wave packet is given by

$$z_c(t) = \int_{-1}^{1} z dz \int_0^1 y \, |\Psi(z, y, t)|^2 \, dy. \tag{21.40}$$

This motion is dispalyed in Fig. (21.7). We observe that for this closed surface the motion is limited to a narrow range of $0.48 \leq z \leq 0.58$ and this shows that probability of finding the particle to the left of the constriction is very small.

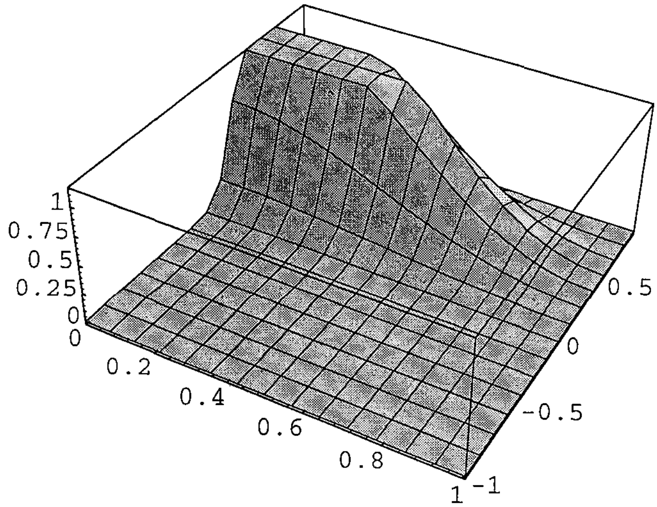

Figure 21.6: The square modulus of the initial wave packet plotted as a function of z and y.

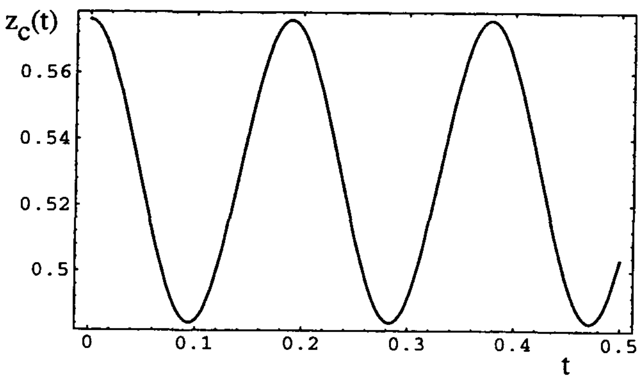

Figure 21.7: The motion of the center of the wave packet is limited to oscillations to the right of constriction shown in Fig. (20.2).

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Chapter 22

Relativistic Formulation of Quantum Tunneling

For most of the problems where quantum tunneling plays a major role, whether the physics of condensed matter or in nuclear physics, the velocity of the tunneling particle is very small compared to the velocity of light. However it is important to know the relative size of the relativistic corrections in any physical situation, and this relativistic correction is the subject that we will address in the first section of this chapter.

22.1 One-Dimensional Tunneling of the Electrons

Here we want to study the relativistic theory of one-dimensional tunneling of an electron of mass m_0 in a potential barrier along the x-axis [1]. The potential barrier will be denoted by $V_j(x)$ where $j = 1, 2$ and 3 denote the three regions where the barrier can have different heights, but for a given j, $V_j(x)$ is a constant.

The motion of electrons are governed by the one-dimensional Dirac equation. We will write the Dirac equation in terms of the Pauli matrices [2], i.e.

$$i\hbar c\sigma_x \frac{d\phi_j(x)}{dx} - m_0 c^2 \sigma_z \phi_j(x) = \left[E - V_j(x)\right]\phi_j(x), \tag{22.1}$$

where m_0 is the rest mass of the electron and σ_x and σ_z are the Pauli matrices;

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{22.2}$$

and the wave function is a 1×2 matrix

$$\phi_j(x) = \begin{bmatrix} \phi_j^{(1)}(x) \\ \phi_j^{(2)}(x) \end{bmatrix}. \tag{22.3}$$

By eliminating $\phi_j^{(1)}$ or $\phi_j^{(2)}$ from Eq. (22.1) we find the second order differential equation

$$\frac{d^2\phi_j^{(i)}(x)}{dx^2} = -\kappa_j^2\phi_j^{(i)}(x), \quad j = 1, 2, \tag{22.4}$$

where

$$\kappa_j^2 = \frac{1}{\hbar^2 c^2}\left[\epsilon - V_j(x)\right]\left[\epsilon - V_j(x) + 2m_0c^2\right], \tag{22.5}$$

and

$$\epsilon = E - m_0c^2. \tag{22.6}$$

Noting that for a given j, $V_j(x)$ is constant, we can solve (22.4) for $\phi_j(x)$ as

$$\phi_j(x) = A_j \exp\left(i\kappa_j x\right) + B_j \exp\left(-i\kappa_j x\right), \tag{22.7}$$

in which the coefficients A_j and B_j are 1×2 matrices;

$$A_j = \begin{bmatrix} \alpha_j^{(1)} \\ \alpha_j^{(2)} \end{bmatrix}, \quad B_j = \begin{bmatrix} \beta_j^{(1)} \\ \beta_j^{(2)} \end{bmatrix}. \tag{22.8}$$

The elements of these matrices are related to the potential parameters by

$$\alpha_j^{(1)} = -\gamma_j\alpha_j^{(2)}, \quad \beta_j^{(1)} = \gamma_j\beta_j^{(2)}, \tag{22.9}$$

where

$$\gamma_j = \frac{1}{\hbar c\kappa_j}\left(\epsilon - V_j\right). \tag{22.10}$$

First let us consider the step potential

$$V_j(x) = \begin{cases} 0 & \text{for } j = 1, \quad x < x_1 \\ V_0 & \text{for } j = 1, \quad x > x_1 \end{cases}. \tag{22.11}$$

Then for $j = 1$, we have the incident wave $A_1 \exp(i\kappa_1 x)$ and the reflected wave $B_1 \exp(-i\kappa_1 x)$ and for $j = 2$ we have also two waves $A_2 \exp(i\kappa_2 x)$ and

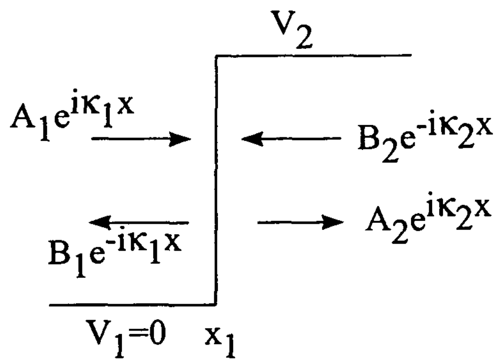

Figure 22.1: A step potential of height V_2 with the incident and reflected waves in the medium $j = 1$.

$B_2 \exp(-i\kappa_2 x)$ (Fig. (22.1)). Note that if V_2 extends to infinity then B_2 will be zero.

Now we define the S-matrix by

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = S_1 \begin{bmatrix} A_2 \\ B_2 \end{bmatrix}, \tag{22.12}$$

which is the generalization of the nonrelativistic S-matrix which we discussed in Chapter 10.

By imposing the continuity of $\phi(x)$ at $x = x_1$ and using the definitions (22.8) and (22.9) we write the S-matrix as

$$S_1 = \frac{1}{2}\begin{bmatrix} \frac{\Gamma_1+1}{\Gamma_1} e^{i(\kappa_2-\kappa_1)x_1} \begin{bmatrix} 1 & 0 \\ 0 & \Gamma_1 \end{bmatrix} & \frac{\Gamma_1-1}{\Gamma_1} e^{-i(\kappa_2+\kappa_1)x_1} \begin{bmatrix} 1 & 0 \\ 0 & -\Gamma_1 \end{bmatrix} \\ \frac{\Gamma_1-1}{\Gamma_1} e^{i(\kappa_2+\kappa_1)x_1} \begin{bmatrix} 1 & 0 \\ 0 & -\Gamma_1 \end{bmatrix} & \frac{\Gamma_1+1}{\Gamma_1} e^{-i(\kappa_2-\kappa_1)x_1} \begin{bmatrix} 1 & 0 \\ 0 & \Gamma_1 \end{bmatrix} \end{bmatrix}, \tag{22.13}$$

where $\Gamma_1 = \frac{\gamma_2}{\gamma_1}$ and γ_1 and γ_2 are given by (22.10) for $j = 1$ and $j = 2$.

According to a theorem in group theory of matrices [3] any non-degenerate $n \times n$ matrix, C, can be written as a product, $C = B\mathcal{D}(\Gamma)$, where B is a unimodular $n \times n$ matrix and $\mathcal{D}(\Gamma)$ is an $n \times n$ diagonal matrix with the diagonal elements $[1, \ 1, \ 1, \ldots\ldots\ldots, \ \Gamma]$. In the present case

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \text{and} \quad \mathcal{D}(\Gamma_1) = \begin{bmatrix} 1 & 0 \\ 0 & \Gamma_1 \end{bmatrix}. \tag{22.14}$$

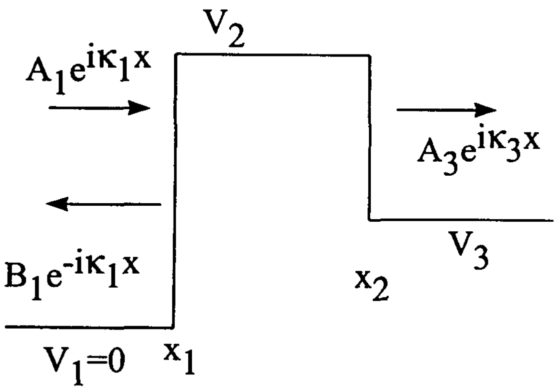

Figure 22.2: A rectangular barrier of height V_2 and width $x_2 - x_1$ joined to a step potential of height V_3.

Using the above theorem we can write S_1, Eq. (22.13), as

$$S_1 = \frac{1}{2}\begin{bmatrix} \frac{\Gamma_1+1}{\Gamma_1}e^{i(\kappa_2-\kappa_1)x_1}\mathcal{D}(\Gamma_1) & \frac{\Gamma_1-1}{\Gamma_1}e^{-i(\kappa_2+\kappa_1)x_1}\sigma_z\mathcal{D}(\Gamma_1) \\ \frac{\Gamma_1-1}{\Gamma_1}e^{i(\kappa_2+\kappa_1)x_1}\sigma_z\mathcal{D}(\Gamma_1) & \frac{\Gamma_1+1}{\Gamma_1}e^{i(\kappa_1-\kappa_2)x_1}\mathcal{D}(\Gamma_1) \end{bmatrix}. \quad (22.15)$$

Now we will use this result to calculate the tunneling of an electron in a rectangular barrier where

$$V_j(x) = \begin{cases} 0 & \text{for } j = 1, \quad x < x_1 \\ V_2 & \text{for } j = 2, \quad x_1 < x < x_2 \\ V_3 & \text{for } j = 3, \quad x > x_2 \quad V_2 > V_3 \end{cases}. \quad (22.16)$$

The width of the barrier is $x_2 - x_1$ (Fig. (22.2)). For this system S is a product of two matrices S_1 and S_2, each for a step potential which we studied earlier (see Section 6.4 for the nonrelaivistic treatment of the problem). Here S is defined by

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = S \begin{bmatrix} A_3 \\ B_3 \end{bmatrix}, \quad (22.17)$$

where

$$S = S_1 S_2. \quad (22.18)$$

In the region $x > x_2$, i.e. $j = 3$, we have only the transmitted wave, and this condition can be expressed as

$$B_3 = \begin{bmatrix} \beta_3^{(1)} \\ \beta_3^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{22.19}$$

From Eqs. (22.17) and (22.18) we conclude that

$$A_1 = \begin{bmatrix} (S_1S_2)_{11} & (S_1S_2)_{12} \\ (S_1S_2)_{21} & (S_1S_2)_{22} \end{bmatrix} A_3. \tag{22.20}$$

The nonrelativistic limit ($c \to \infty$) of (22.20) is the simple expression $A_1 = (S_1S_2)_{11}A_3$.

Now using Eqs. (22.8), (22.9), (22.13) and (22.20) we find the following equation

$$\begin{bmatrix} \alpha_1^{(1)} \\ \alpha_1^{(2)} \end{bmatrix} = (S_1S_2)_{22} \begin{bmatrix} \frac{1}{\Gamma_1\Gamma_2} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_3^{(1)} \\ \alpha_3^{(2)} \end{bmatrix}, \tag{22.21}$$

in which γ_1 and Γ_2 are defined by

$$\Gamma_1 = \frac{\gamma_2}{\gamma_1}, \quad \Gamma_2 = \frac{\gamma_3}{\gamma_2}. \tag{22.22}$$

One conclusion that can be drawn from Eq. (22.21) is that if $\Gamma_1\Gamma_2 = 1$, then the ratio of the reflected to the incident wave will be the same for small and large components of the wave function. But $\Gamma_1\Gamma_2 = 1$ implies the equality of γ_1 and γ_3, i.e. only for the symmetric case $V_1 = V_3 = 0$ this condition is satisfied (see Eq. (22.10)). Let us now consider the potential (22.16) when V_2 satisfies the condition for tunneling, i.e.

$$\epsilon < V_2 < \epsilon + 2m_0c^2. \tag{22.23}$$

For this case κ_2 the wave number inside the barrier is imaginary, and we write it as $\kappa_2 = -iq$. Then from Eq. (22.13) we find $(S_1S_2)_{22}$;

$$\begin{aligned}(S_1S_2)_{22} &= \frac{1}{4i\gamma_1\rho_2} \exp\left[i(\kappa_3x_2 - \kappa_1x_1)\right] \left[\left(\gamma_1^2 + \rho_2^2\right)\left(\gamma_3^2 + \rho_2^2\right)\right]^{\frac{1}{2}} \\ &\times \left(e^{i\alpha+qb} - e^{-i\alpha-qb}\right). \end{aligned} \tag{22.24}$$

where $b = x_2 - x_1$ is the width of the barrier and ρ_2 and α are defined by

$$\rho_2 = \frac{1}{\hbar cq}(V_2 - \epsilon) = i\gamma_2, \tag{22.25}$$

and

$$\alpha = \tan^{-1}\left(\frac{\rho_2}{\gamma_1}\right) + \tan^{-1}\left(\frac{\rho_2}{\gamma_3}\right). \tag{22.26}$$

If the width of the potential is large enough so that e^{-qb} is negligible compared to e^{qb}, then from (22.21) we find the following relation

$$\begin{bmatrix} \alpha_3^{(1)} \\ \alpha_3^{(2)} \end{bmatrix} = \frac{4\gamma_1\rho_2\phi e^{-qb}}{\left[(\gamma_1^2+\rho_2^2)(\gamma_3^2+\rho_2^2)\right]^{\frac{1}{2}}} \begin{bmatrix} \Gamma_1\Gamma_2 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1^{(1)} \\ \alpha_1^{(2)} \end{bmatrix}, \tag{22.27}$$

in which the phase ϕ is given by

$$\phi = ie^{-i\alpha}\exp\left[i\left(\kappa_1 x_1 - \kappa_3 x_2\right)\right], \quad |\phi| = 1. \tag{22.28}$$

The important correction due to relativistic effects comes from the exponential term in (22.27), i.e.

$$\exp(-qb) = \exp\left[-\frac{b}{\hbar c}\sqrt{(V_2-\epsilon)(2m_0c^2+\epsilon-V_2)}\right]. \tag{22.29}$$

By expanding the last term in the exponential we have

$$\exp(-qb) = \exp\left[-\frac{1}{\hbar}\sqrt{2m_0(V_2-\epsilon)}\, b\left\{1+\frac{\epsilon-V_2}{4m_0c^2}+\dots\right\}\right], \tag{22.30}$$

where the first term in the curly bracket is the nonrelativistic penetration factor and the second term is its relativistic correction.

22.2 Tunneling of Spinless Particles in One Dimension

For certain problems such as the ionization of atoms in a strong laser field, when the spin of the particle does not play an important role, and when the tunneling is one-dimensional, we can use the method of imaginary time discussed in Chapter 12 and solve the problem [4]. First we observe that the most general form of action for the particle in special theory of relativity is [5]

$$S = \int\left[-a(x,t)\sqrt{1-\left(\frac{dx}{dt}\right)^2} + b(x,t)\right] dt, \tag{22.31}$$

where we have set the speed of light c equal to one.

The equation of motion can be derived from this action and is given by

$$\frac{d}{dt}\left[\frac{a(x,t)}{\sqrt{1-\left(\frac{dx}{dt}\right)^2}}\left(\frac{dx}{dt}\right)\right] = -\sqrt{1-\left(\frac{dx}{dt}\right)^2}\,\frac{\partial a(x,t)}{\partial x} + \frac{\partial b(x,t)}{\partial x}. \tag{22.32}$$

(For relativistic action in electrodynamics which is a special case of this form see [6] and [7]).

By solving Eq. (22.32) the trajectory of the particle can be found as a function of time. From the definition of the turning point we find that the particle reaches this point at the time t_f, where

$$p(t_f) = \left[\frac{a(x,t)}{\sqrt{1-(\frac{dx}{dt})^2}}\left(\frac{dx}{dt}\right)\right]_{t=t_f} = 0. \tag{22.33}$$

This is usually the same time when $\left(\frac{dx}{dt}\right)$ ia also zero.

Since we want to use complex t in the equations of motion, we require the following initial conditions:

Let us assume that the quantities t_f and t_0 are real and complex numbers respectively, then we choose the paths with the following properties [5]

$$p(t_f) = 0, \quad x(t_0) = 0, \quad \left(\frac{dx}{dt}\right)_{t_0} = \infty, \quad x(t) = \text{real}. \tag{22.34}$$

The complex time joins the real time at the turning point $t = t_f$, and since we want $x(t)$ to be real for complex time, we write Eq. (22.32) in the form

$$\frac{d}{dx}\left[\frac{a(x,t)}{\sqrt{t'^2-1}}\right] = -\sqrt{t'^2-1}\,\frac{\partial a(x,t)}{\partial x} + \frac{\partial b(x,t)}{\partial x}t'. \tag{22.35}$$

where $t' = \left(\frac{dt}{dx}\right)$. Thus we have replaced $x(t)$ in the above equation by $t(x)$. With this change, the condition (22.33) becomes

$$p(t_f) = \left[\frac{a(x,t)}{\sqrt{t'^2-1}}\right]_{t_f} = 0, \quad t_0' = 0. \tag{22.36}$$

The advantage of using (22.35) over (22.32) is that we can solve (22.35) numerically and then search for the point $x_f = x(t_f)$ which gives us $t'(0) = 0$.

Having thus found $t(x)$, we can calculate the action S from (22.31) which, by interchanging the function x and the variable t, takes the form

$$S = \int_0^{x_f} \left[-a\,(x, t(x))\,\sqrt{t'^2 - 1} + b\,(x, t(x))\,t'(x)\right] dx. \tag{22.37}$$

The value of the integral taken from 0 to x_f determines the imaginary part of S and this imaginary part gives us the decay width

$$\Gamma(t_f) = D \exp\left[-2\,\mathrm{Im}S(t_f)\right]. \tag{22.38}$$

(Compare with Eqs. (10.2) and (10.3)). In Eq. (22.38) D is a multiplicative constant. We note that $\Gamma(t_f)$ depends on t_f which is the last point of the trajectory for complex time.

As an example of this formulation, let us consider a spinless particle of charge q which is moving in an electric field $\mathcal{E}$. In this case S is given by

$$S = -\int \left[m\sqrt{1 - \left(\frac{dx}{dt}\right)^2} + q\mathcal{E}t\left(\frac{dx}{dt}\right)\right] dt. \tag{22.39}$$

From either (22.32) or (22.35) we derive the equation of motion of the charged particle;

$$m\frac{d}{dt}\left[\frac{\left(\frac{dx}{dt}\right)}{\sqrt{1 - (\frac{dx}{dt})^2}}\right] = q\mathcal{E}. \tag{22.40}$$

This equation can be integrated to yield the position of the particle at the time t;

$$\begin{aligned} x(t) = x(t_0) \quad &+ \quad \frac{m}{q\mathcal{E}}\left\{\sqrt{1 + \left[\frac{q\mathcal{E}}{m}(t - t_0) + \frac{(\frac{dx}{dt})_{t=0}}{\sqrt{1 - (\frac{dx}{dt})^2_{t=0}}}\right]^2}\right. \\ &- \quad \left.\frac{1}{\sqrt{1 - \left(\frac{dx}{dt}\right)^2_{t=0}}}\right\}. \end{aligned} \tag{22.41}$$

Since we are interested in tunneling, therefore we replace t by $-i\tau$ and choose a path with the conditions;

$$\tau_0 = -\frac{m}{q\mathcal{E}}, \quad x(\tau_0) = 0, \quad \left(\frac{dx}{dt}\right)(\tau_0) = i\infty. \tag{22.42}$$

The equation for $x(\tau)$ is a circle given by

$$x^2(\tau) + \tau^2 = \left(\frac{m}{q\mathcal{E}}\right)^2 . \tag{22.43}$$

From this equation we conclude that the motion starts at the point $x = 0$ and the time $\tau = -\left(\frac{m}{q\mathcal{E}}\right)$ and after moving a distance $\Delta x = \frac{m}{q\mathcal{E}}$ at the time $\tau = 0$ its momentum becomes zero. For calculating the action we use Eq. (22.43) for the path and substitute it in the action integral (22.39) to find

$$S = i\int_{\frac{-m}{q\mathcal{E}}}^{0} \left[m\sqrt{1+\left(\frac{dx}{d\tau}\right)^2} + q\mathcal{E}\tau\left(\frac{dx}{d\tau}\right)\right] d\tau = \frac{i\pi m^2}{4q\mathcal{E}}. \tag{22.44}$$

The part of the trajectory between $x = 0$ and $x = \frac{m}{q\mathcal{E}}$ represents the creation of a particle, and the one between $x = -\frac{m}{q\mathcal{E}}$ and $x = 0$ the creation of an antiparticle of charge $-q$. The second path also yields the same action as the particle trajectory. Thus the total action is twice that given by (22.44) and therefore the decay width for this problem is

$$\Gamma = D\exp\left[-\frac{\pi m^2}{q\mathcal{E}}\right], \tag{22.45}$$

where D is a constant.
An alternative approach to the problem of relativistic tunneling of a particle in the presence of external electric and magnetic fields is recently advanced by Karanakov et al [8]. These authors have applied their formulation to the theory of ionization of a relativistic bound state under the influence of the electromagnetic fields when the binding energy is comparable to the electron rest energy m_0c^2.

22.3 Tunneling Time in Special Relativity

In Chapters 17-19 we studied the question of tunneling time in detail, and in particular in the last section of Chapter 19, we discussed the argument of Low and Mende [9] that the tunneling time for a wave packet with certain restriction is zero!

If this is the result in the nonrelativistic formulation, in what way the relativistic tunneling time will manifest itself?

The problem of relativistic tunneling time for a particle of spin $\frac{1}{2}$ has been studied by Krekorta *et al* [10]. Deutch and Low [11] did also investigate the relativistic problem for a spinless particle and found that a Gaussian wave packet subject to plausible conditions can tunnel through the barrier and appear on the other side with a velocity greater than the speed of light (see also [12]). This phenomena apparently violates the principle of causality, but this point will be studied below.

For the relativistic formulation we consider a wave packet which satisfies the Klein-Gordon equation [2];

$$\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} + V(x)\psi = 0, \tag{22.46}$$

where we have set $c = 1$. The simplest potential that we can study is a rectangular barrier of width b and height μ^2;

$$V(x) = \mu^2\theta(x)\theta(b-x). \tag{22.47}$$

We choose the initial conditions such that the causality condition is maintained and thus if the wave profile is zero for $x > a$, i.e.

$$\psi(x,0) = f(x)\theta(a-x), \tag{22.48}$$

and

$$\left[\frac{\partial\psi(x,t)}{\partial t}\right]_{t=0} = g(x)\theta(a-x), \tag{22.49}$$

then we have

$$\psi(x,t) = 0, \quad \text{if} \quad t < x - a, \tag{22.50}$$

and the propagation of the wave is such that the velocity of the wavefront is bounded by the velocity of light. In a similar way if

$$g(x) = f(x) = 0, \quad \text{for} \quad x < a, \tag{22.51}$$

then

$$\psi(x,t) = 0, \quad \text{for} \quad t < a - x. \tag{22.52}$$

The simplest form that we can choose for $f(x)$ is a Gaussian wave packet with its center at x_0, where x_0 is large and negative;

$$\psi(x,0) = f(x) = \exp(i\omega_0 x)\exp\left[-\frac{(x-x_0)^2}{(\Delta x)^2}\right], \tag{22.53}$$

and for $g(x)$ we choose

$$g(x) = -\frac{\partial f}{\partial x}. \tag{22.54}$$

In this case the wave packet moves from left to the right with the velocity of light $c = 1$. Now we want to show that ψ to the right of the barrier is proportional to $f(x - x_0 - t - b)$, i.e. the wave reaches the point x at the time

$$t \approx x - x_0 - b, \tag{22.55}$$

which is less than $x - x_0$ and thus it travels with superluminal velocity.

We impose the condition that the amplitude of the tunneling or the penetration factor must be small;

$$\exp\left[-\gamma(\omega_0)b\right] = \exp\left[-b\sqrt{\mu^2 - \omega_0^2}\right] << 1, \tag{22.56}$$

where in (22.56) $i\gamma(\omega_0)$ is the imaginary wave number under the barrier for the frequency ω_0. In order to solve (22.46) we first find its Laplace transform;

$$\psi_\omega(x) = \int_0^\infty e^{i\omega t}\psi(x,t)dt, \tag{22.57}$$

where Im $\omega > 0$. For the positive values of t, $\psi(x,t)$ is equal to [13]

$$\psi(x,t) = \frac{1}{2\pi}\int_{-\infty+i\epsilon}^{+\infty+i\epsilon} e^{-i\omega t}\psi_\omega(x)d\omega. \tag{22.58}$$

From the Laplace transform (22.57) and its inverse Eq. (22.58) and Eq. (22.46) we find the following relation

$$\left(-\omega^2 - \frac{d^2}{dx^2} + V(x)\right)\psi_\omega(x) = \left[\frac{\partial\psi(x,t)}{\partial t}\right]_{t=0} - i\omega\psi(x,0). \tag{22.59}$$

By substituting from (22.53) and (22.54), we can write (22.59) as

$$\left(-\omega^2 - \frac{d^2}{dx^2} + V(x)\right)\psi_\omega(x) = -i\omega f - \frac{\partial f}{\partial x} = F(x). \tag{22.60}$$

Next we find the Green function for the two solutions of the homogeneous differential equation

$$\left(-\omega^2 - \frac{d^2}{dx^2} + V(x)\right)\phi_\omega(x) = 0, \tag{22.61}$$

for which the two independent solutions are $\phi^+(x)$ and $\phi^-(x)$;

$$\phi^+(x) = \begin{cases} e^{i\omega x} + R(\omega)e^{-i\omega x} & \text{for } x \le 0 \\ Ae^{i\kappa x} + Be^{-i\kappa x} & \text{for } 0 \le x \le b \\ Te^{i\omega x} & \text{for } x \ge b \end{cases}, \tag{22.62}$$

and

$$\phi^-(x) = \begin{cases} e^{-i\omega x} + R'(\omega)e^{i\omega x} & \text{for } x \ge b \\ A'e^{-i\kappa x} + B'e^{i\kappa x} & \text{for } 0 \le x \le b \\ T'e^{-i\omega x} & \text{for } x \le b \end{cases}. \tag{22.63}$$

In these relations $\kappa = \sqrt{\omega^2 - \mu^2}$ is chosen in such a way that in the upper-half ω-plane they are analytic. That is if ω has a small imaginary part, then

$$\kappa = \begin{cases} \sqrt{\omega^2 - \mu^2} & \text{for } \omega \ge \mu \ge 0 \\ i\sqrt{\mu^2 - \omega^2} & \text{for } -\mu \le \omega \le \mu \\ -\sqrt{\omega^2 - \mu^2} & \text{for } \omega \le -\mu \end{cases}. \tag{22.64}$$

In Eq. (22.64) only the positive sign of the square roots are allowed. Imposing the continuity of ϕ and its first derivative at the points where $V(x)$ is discontinuous, we find the coefficients in (22.62) and (22.63) to be

$$R = \frac{1}{D}\left(\omega^2 - \kappa^2\right)\left(1 - e^{2i\kappa b}\right), \quad R' = e^{-2i\omega b}R, \tag{22.65}$$

$$T = T' = \frac{4\omega\kappa}{D}e^{i(\kappa-\omega)b}, \tag{22.66}$$

$$A = \frac{2}{D}\omega(\omega + \kappa), \quad A' = e^{i(\kappa-\omega)b}A, \tag{22.67}$$

$$B = -\frac{2}{D}\omega(\omega - \kappa)e^{2i\kappa b}, \quad B' = e^{-i(\kappa+\omega)b}B, \tag{22.68}$$

and

$$D = (\omega + \kappa)^2 - (\omega - \kappa)^2 e^{2i\kappa b}. \tag{22.69}$$

These equations show that the coefficients $R, T, A, B, D, A', e^{2i\omega b}R'$ and $e^{2i\omega b}B'$ are all analytic in the upper half of the ω-plane. In addition in this half plane D does not vanish. These analytic properties guarantee that in the propagation $f \to \psi$, the causality condition is preserved [14] [15]. For the Wronskian of ϕ^+ and ϕ^- we find the following relation

$$W(\phi^+, \phi^-) = \phi^- \frac{\partial \phi^+}{\partial x} - \phi^+ \frac{\partial \phi^-}{\partial x} = 2i\omega T. \tag{22.70}$$

Now we write the solution of (22.60) as

$$\psi_\omega(x) = -\frac{\phi^+(x)}{2i\omega T}\int_{-\infty}^{x}\phi^-(x')F(x')dx' + \frac{\phi^-(x)}{2i\omega T}\int_{x}^{\infty}\phi^+(x')F(x')dx'. \tag{22.71}$$

From this equation it follows that when $x \to \pm\infty$, and Im $\omega > 0$, $\psi_\omega(x)$ is well-defined. Inversely no solution of (22.61) is finite at both of the boundaries $x \to \pm\infty$. Therefore (22.71) is the only acceptable solution of (22.60).

To calculate $\psi(x,t)$ we find the inverse Laplace transform of (22.71) [13]

$$\psi(x,t) = -\frac{1}{2\pi}\int_{-\infty+i\epsilon}^{\infty+i\epsilon} e^{-i\omega t} \times$$
$$\times \left\{\frac{\phi^+(x)}{2i\omega T}\int_{-\infty}^{x}\phi^-(x')F(x')dx' + \frac{\phi^-(x)}{2i\omega T}\int_{x}^{\infty}\phi^+(x')F(x')dx'\right\} d\omega. \tag{22.72}$$

We observe that the center of $F(x')$ is the point x_0 to the left of the barrier, therefore if we choose $\frac{|x_0|}{\Delta x}$ large enough, in Eq. (22.72) we can replace $\phi^-(x')$ by its value for $x' < 0$ and integrate over all values of x. For the same reason we can ignore the second integral in (22.72). After these simplifications (22.72) becomes

$$\begin{aligned}\psi(x,t) &= \frac{1}{2\pi}\int_{-\infty+i\epsilon}^{\infty+i\epsilon}\frac{e^{-i\omega t}}{2i\omega T(\omega)}e^{i\omega x}T(\omega)d\omega\int_{-\infty}^{\infty}T(\omega)e^{-i\omega x'}\\ &\times \left[i\omega f(x') + \frac{\partial f(x')}{\partial x'}\right]dx'.\end{aligned} \tag{22.73}$$

Finally by integrating the last term in (22.72), we can combine the last two terms and write $\psi(x,t)$ as

$$\psi(x,t) = \frac{1}{2\pi}\int_{-\infty+i\epsilon}^{\infty+i\epsilon} e^{i\omega(x-t)}T(\omega)d\omega\int_{-\infty}^{\infty}e^{-i\omega x'}f(x')dx'. \tag{22.74}$$

With these approximations that we have made, $\psi(x,t)$ has preserved two of its essential features:

(i) - For $T = 1$, $\psi(x,t) = f(x-t)$ as it must be.

(ii) - The wave $\psi(x,t)$ satisfies the requirement of causality, since if $f(x') = 0$ for $x' > 0$, then (22.73) will take the form

$$\psi(x,t) = \frac{1}{2\pi}\int_{-\infty+i\epsilon}^{\infty+i\epsilon} e^{i\omega(x-t-a)}T(\omega)d\omega\int_{-\infty}^{a}e^{-i\omega(x'-a)}f(x')dx'. \tag{22.75}$$

Let us examine this expression for $\psi(x,t)$. First we observe that the integral over x' is analytic in the upper half of the ω-plane and as $\omega \to \infty$, it goes as $\frac{1}{\omega}$. In the upper half of the ω-plane $T(\omega)$ is also analytic and $\lim_{\omega\to\infty} T(\omega) \to 1$. Therefore for $x - t - a > 0$ or $t < x - a$, we can choose the contour integral over ω in the upper half plane. With these results we find $\psi = 0$, and this is consistent with the principle of causality .
For calculating (22.74) we first find $T(\omega)$ from Eqs. (22.66) and (22.69);

$$T(\omega) = \frac{4\omega\kappa e^{i(\kappa-\omega)b}}{(\omega+\kappa)^2 - (\omega-\kappa)^2 e^{2i\kappa b}}. \tag{22.76}$$

Then using (22.53) we have the following integral

$$\int_{-\infty}^{\infty} e^{-i\omega_0 x'} f(x')dx' = \sqrt{\pi}\Delta x \exp\left[-i\omega x_0 - \left(\frac{\omega-\omega_0}{\Delta\omega}\right)^2 + i\omega_0 x_0\right], \tag{22.77}$$

where

$$\Delta\omega = \frac{2}{\Delta x}. \tag{22.78}$$

Thus we can write Eq. (22.74) as

$$\begin{aligned}\psi(x,t) &= \frac{\Delta x}{2\sqrt{\pi}}\int_{-\infty+i\epsilon}^{\infty+i\epsilon} \exp\left[i\omega(x-t)\right] \\ &\times \frac{4\omega\kappa e^{i(\kappa-\omega)b}.}{(\omega+\kappa)^2-(\omega-\kappa)^2e^{2i\kappa b}} \exp\left[-i\omega x_0 - \left(\frac{\omega-\omega_0}{\Delta\omega}\right)^2 + i\omega_0 x_0\right] d\omega.\end{aligned} \tag{22.79}$$

By expanding $\kappa = i\sqrt{\mu^2-\omega^2}$ around $\omega = 0$ and ignoring small terms under the integral, we can use the approximate value of Eq. (22.79) and write $\psi(x,t)$ as

$$\begin{aligned}\psi(x,t) &= \frac{\Delta x}{2\sqrt{\pi}}\left(\frac{-4i}{\mu}\right)\int_{-\mu}^{\mu} \omega e^{i\omega(x-t-x_0-b)} e^{-\mu b} \\ &\times \exp\left[\frac{\omega^2 b}{2\mu} - \left(\frac{\omega-\omega_0}{\Delta\omega}\right)^2\right] d\omega.\end{aligned} \tag{22.80}$$

With this simplification we can evaluate the integral in (22.80) in the limit of $\mu \to \infty$;

$$\begin{aligned}\psi(x,t) &= \frac{4}{\mu}\left\{-i\omega_1 + \frac{x-t-x_0-b}{(\Delta x)^2}\right\} \exp\left[-\mu b\left(1-\frac{\omega_0^2}{2\mu^2}\right)\right] \\ &\times \exp\left[i\omega_0(x-t-x_0-b)\right] \exp\left[-\left(\frac{x-t-x_0-b}{\Delta x}\right)^2\right],\end{aligned} \tag{22.81}$$

where

$$\omega_1 = \frac{\omega_0}{1 - \frac{b(\Delta\omega)^2}{2m}}. \tag{22.82}$$

As we can see from (22.81), the time of arrival of the wave is given by

$$t = x - x_0 - b, \tag{22.83}$$

that is the time that takes the light wave to reach x from x_0, viz, $t_m = x - x_0$ is longer than t, in other words the speed of the propagation exceeds the speed of light!

Low [16] returned to this problem later and asked the following question:

We know that the propagation of the wave $\psi(x,t)$ is subject to the principle of causality. That is if $f(x)$ is zero for $x > x_1$, then the transmitted wave for $x - t - x_1 > 0$ is zero. In other words $\psi(x,t)$ is zero for all values of t satisfying the inequality $t < x - x_1$, where t is the time that takes the light to propagate from x to x_1. Therefore the result obtained in (22.81) comes from a very narrow forerunner part of the wave packet. Then how the transmitted wave knows about the shape of the rest of the wave packet which is given in (22.81)? To answer this question we consider the analytic properties of the Gaussian wave packet that we have used. Thus if we use the analytic properties, from a narrow part of the forerunner, we can determine the shape of the rest of the wave packet through analytic continuation.

To test the validity of this argument Low examined wave packets of other shapes and made the following observations [16]:

Let $\phi(\omega)$ denote the Fourier transform of $f(x)$, then the asymptotic behavior of $\phi(\omega)$ as $\omega \to \infty$, one finds that:

(i) - If $\phi(\omega)$ goes faster than $\exp(-\omega^2)$ to zero as $\omega \to \infty$, one can always choose the parameters so that there is superluminal velocity.

(ii) - If $\phi(\omega) \to 0$ more slowly than $\exp(-|\omega|)$ as $\omega \to \infty$, then there is no superluminal speed .

(iii) - Finally if $\phi(\omega) \to 0$ goes faster than $\exp(-|\omega|)$, but slower than $\exp(-\omega^2)$, as $\omega \to \pm\infty$, then depending on the parameters involved, it is possible to have velocities greater than c.

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Chapter 23

The Inverse Problem of Quantum Tunneling

In this chapter we study three different forms of inverse problems applicable to quantum tunneling [1]:
(i) - In the first one given the reflection amplitude $R(k)$ as a function of the wave number of the particle k, we want to find the shape of the barrier. Here it is assumed that $R(k)$ is known for all k values, corresponding to the energies below as well as above the maximum height of the potential.
(ii) - In the second problem, from the energy dependence of the transmission coefficient $|T(E)|^2$ and the dependence of this coefficient on another parameter λ we want to determine the potential $V(r)$ [2]. In this case $|T(E)|^2$ is known for energies less than or equal to the maximum height of the potential $V(r)$.
(iii) - Finally we discuss the inverse problem of three dimensional decay of unstable states, i.e. the construction of a potential from the empirical data on energies and widths of quasi-stationary states [3].

23.1 A Method for Finding the Potential from the Reflection Amplitude

The differential equation for the variable reflection amplitude for a single channel is (see Eq. (11.16))

$$\frac{dR(y,k)}{dy} = -\frac{v(y)}{2ik}\left(e^{iky} + R(y,k)e^{-iky}\right)^2, \tag{23.1}$$

where $R(y,k)$ is subject to the boundary condition

$$R(y \to \infty, k) \to 0. \tag{23.2}$$

The reflection amplitude is then obtained from the asymptotic solution of (23.1)

$$R(k) = R(y \to -\infty, k). \tag{23.3}$$

For the inverse problem we assume that (23.3) is known for all k values and we want to find $v(r)$. To this end we introduce another function $F(y,k)$ defined by

$$F(y,k) = \frac{1}{2ik}e^{-2iky}R(y,k), \tag{23.4}$$

and substitute for $R(y,k)$ in Eq. (23.1) to get

$$\frac{d}{dy}\left[2ikF(y,k)e^{2iky}\right] = -\frac{v(r)}{2ik}e^{2iky}\left[1 + 2iF(y,k)\right]^2. \tag{23.5}$$

Integrating (23.5) and using (23.2) we find $F(y,k)$;

$$2ikF(y,k)e^{2iky} = \frac{1}{4k^2}\int_y^{\infty} v(y')\exp(2iky')\left[1 + 2iF(y',k)\right]^2 dy'. \tag{23.6}$$

Now replacing $F(y,k)$ by $R(y,k)$ on the left hand side of (23.6), then taking the limit of $y \to -\infty$ and rearranging terms we find

$$\int_{-\infty}^{\infty} v(y)e^{2iky}dy = -2ikR(k) - 4\int_{-\infty}^{+\infty} v(y)e^{2iky}\left[iF(y,k) - F^2(y,k)\right]dy. \tag{23.7}$$

By taking the inverse Fourier transform of (23.7) we obtain an equation for $v(y)$,

$$\begin{aligned} v(y) &= -\frac{2i}{\pi}\int_{-\infty}^{+\infty} kR(k)e^{-2iky}dk - \frac{2}{\pi}\int_{-\infty}^{+\infty} v(y')dy' \\ &\times \int_{-\infty}^{+\infty}\left[iF(y',k) - F^2(y',k)\right]e^{2ik(y'-y)}dk. \end{aligned} \tag{23.8}$$

This equation can be solved by iteration. Thus to the first order we have

$$v_1(y) = -\frac{2i}{\pi}\int_{-\infty}^{+\infty} kR(k)e^{-2iky}dk. \tag{23.9}$$

Substituting this in Eq. (23.6) and ignoring F on the right hand side we get

$$e^{2iky}F_1(y,k) = \frac{1}{4k^2}\int_y^{\infty} v_1(y')e^{2iky'}dy'. \tag{23.10}$$

From this expression and (23.8) we find the potential $v(r)$ to the second order

$$\begin{aligned} v_2(y) &= v_1(y) - \frac{2}{\pi}\int_{-\infty}^{+\infty} v_1(y')dy' \\ &\times \int_{-\infty}^{+\infty}\left[iF_1(y',k) - F_1^2(y',k)\right]e^{2ik(y'-y)}dk. \end{aligned} \tag{23.11}$$

While in principle one can continue this iteration to arbitrary order, in practice the instability of the numerical inversion of the Fourier transform limits the number of iterations [5].

As an example let us consider the reflection amplitude for a δ-function potential $v(x) = s\delta(x)$ which is given by $R(k) = \frac{is}{2k+is}$. If we substitute this amplitude in (23.9) we find the approximate potential,

$$v_1(y) = \frac{s}{\pi}\int_{-\infty}^{+\infty} \frac{2k}{2k+is}e^{-2iky}dy = s\delta(y) - s^2e^{sy}\theta(-y). \tag{23.12}$$

For a similar iterative technique for constructing the potential barrier from the reflection date see [4].

From the reflection and transmission amplitudes one can infer whether the barrier is of finite extent or not. The following important result is found by Portinari [6]. For all values of x for which $V(x) = 0$, the integral

$$\int_{-\infty}^{\infty} k\frac{R(k)}{T(k)}\exp(-2ikx)dk, \tag{23.13}$$

must vanish identically

23.2 Determination of the Shape of the Potential Barrier in One-Dimensional Tunneling

This inverse problem can be solved by using the techniques developed in quantum scattering theory [1] or by using the simpler formulation based on the semi-classical approximation. It is the latter approximate method which we will discuss here.

We have already seen in Chapter 3, Eq. (3.88), that the approximate coefficient of transmission $|T(E)|^2$ is obtained from

$$|T(E)|^2 = \frac{1}{\left\{1 + \exp\left[\sqrt{8m}\frac{f(E)}{\hbar}\right]\right\}}, \tag{23.14}$$

where $f(E)$ is given by

$$f(E) = \int_{x_1}^{x_2} [V(x) - E]^{\frac{1}{2}}\, dx, \tag{23.15}$$

and x_1 and x_2 are the turning points, i.e. the roots of $E = V(x)$. Since we are interested in tunneling then

$$E \le V_{max}, \tag{23.16}$$

with V_{max} being the maximum height of the potential $V(x)$.

Here we assume that $V(x)$ has a minimum or a maximum between the turning points x_1 and x_2. If $|T(E)|^2$ is known then from (23.14) we can determine $f(E)$. Hence to find $V(x)$ we need to invert (23.15). To this end we use the identity [7]

$$\begin{aligned}\int_E^{V(x)} \frac{dE'}{\sqrt{(E' - E)\left[V(x) - E'\right]}} &= \int_0^1 \frac{d\zeta}{\sqrt{\zeta}\sqrt{1-\zeta}} \\ &= B\left(\frac{1}{2}, \frac{1}{2}\right) = \left[\Gamma\left(\frac{1}{2}\right)\right]^2 = \pi,\end{aligned} \tag{23.17}$$

which is true for any $V(x)$. Here $B(x, y)$ and $\Gamma(x)$ are beta and gamma functions respectively. Thus we have the following relation

$$x_2(E) - x_1(E) = \frac{1}{\pi}\int_{x_1}^{x_2} dx \int_E^{V(x)} \frac{dE'}{\sqrt{(E' - E)\left[V(x) - E'\right]}}. \tag{23.18}$$

Now by changing the order of integration in (23.18) and noting that $V(x)$ has a maximum V_{max}, we find

$$x_2(E) - x_1(E) = \frac{1}{\pi}\int_E^{V_{max}} dE' \int_{x_1(E')}^{x_2(E')} \frac{dx}{\sqrt{(E' - E)\left[V(x) - E'\right]}}, \tag{23.19}$$

or

$$x_2(E) - x_1(E) = -\frac{2}{\pi}\int_E^{V_{max}} \frac{df(E')}{dE'}\frac{dE'}{\sqrt{E'-E}}. \tag{23.20}$$

Equation (23.20) shows that from $f(E)$ which is determined directly from the empirical knowledge of $|T(E)|^2$ we can find the width of the potential as a function of E.

As an example consider a potential of the form

$$V(x) = V_{max} - a^2x^2, \tag{23.21}$$

then from Eq. (23.15) we have

$$f(E) = \frac{\pi}{2a}(V_{max} - E). \tag{23.22}$$

If we substitute this $f(E)$ in (23.20) and carry out the integration we find

$$x_2 - x_1 = \frac{2}{a}\sqrt{V_{max} - E}. \tag{23.23}$$

Of course this result can be readily obtained by equating $V(x)$ in (23.21) to E and solving for x.

The difference $x_2(E) - x_1(E)$ is the maximum information that we can obtain from $f(E)$. But in some problems the potential $V(x)$ may depend linearly on another parameter, say λ, i.e.

$$V(x,\lambda) = V_0(x) - \lambda\phi(x). \tag{23.24}$$

For instance in the case of field emission in a metal (see Chapter 24) where λ is the electric field at the surface of the metal, or in the case of α-decay (Chapter 26) where $\lambda\phi(x) = \frac{l(l+1)}{x^2}$, we have the function f which depends on E as well as λ. Knowing $f(E,\lambda)$, we can establish a second relation between x_1 and x_2, and combining this second result with Eq. (23.20) we can find x_1 and x_2 separately, and thus determine $V(x,\lambda)$. Here we start with the equation

$$\begin{aligned}
\int_{x_1(E,\lambda)}^{x_2(E,\lambda)} \phi(x)dx &= \frac{1}{\pi}\int_{x_1}^{x_2}\phi(x)dx\int_E^{V(x)}\frac{dE'}{\sqrt{(E'-E)\,[V(x)-E']}} \\
&= \frac{1}{\pi}\int_E^{V(x)} dE'\int_{x_1(E',\lambda)}^{x_2(E',\lambda)}\frac{\phi(x)dx}{\sqrt{(E'-E)\,[V(x)-E']}} \\
&= -\frac{2}{\pi}\int_E^{V_{max}}\frac{\partial f(E',\lambda)}{\partial\lambda}\frac{dE'}{\sqrt{E'-E}}.
\end{aligned} \tag{23.25}$$

Since $\phi(x)$ is known, we can calculate $V(x)$ from $f(E,\lambda)$. Let us consider the motion of an electron in the potential field of ions, $V_0(x)$, and assume that there is an additional external field

$$\lambda\phi(x) = e\mathcal{E}x, \tag{23.26}$$

acting on the electron, where $\mathcal{E}$ is the electric field at the surface of the metal and e is the charge of the electron. From (23.25) we find

$$x_2^2(E,\mathcal{E}) - x_1^2(E,\mathcal{E}) = -\frac{4}{\pi e}\int_E^{V_{max}} \left(\frac{\partial f(E',\mathcal{E})}{\partial \mathcal{E}}\right)\frac{dE'}{\sqrt{E'-E}}. \tag{23.27}$$

Combining the two equations (23.20) and (23.27) we obtain x_1 and x_2 separately.

Thus by measuring the coefficient of transmission $|T(E,\mathcal{E})|^2$ we can determine $f(E,\mathcal{E})$ and from it the potential $V(x,\mathcal{E})$.

23.3 Prony's Method of Determination of Complex Energy Eigenvalues

In our discussions of tunneling through two barriers (Chapter 7), the time development of the wave packet in the Heisenberg picture, Chapter 13, and the important problem of lifetime of coupled channel resonances, Chapter 20, we have observed that in general the probability of decay of the initial state is a combination of exponential and sinusoidal functions (see for instance Eq. (20.40)). Suppose that we measure this probability $\mathcal{P}^-(t)$ at $2N$ equal intervals, $\Delta t, 2\Delta t, ...2N\Delta t$, where Δt is an arbitrary time interval.
We want to know whether from these measurements it is possible to find the discrete energy spectrum of the decaying system [8] [9] [10]. For this purpose we write E_j in terms of its real and imaginary parts

$$E_j = \text{Re } E_j - \frac{i}{2}\Gamma_j, \tag{23.28}$$

where Γ_j is positive. We also define ω_{ij} by

$$\omega_{ij} = \text{Re } E_i - \text{Re } E_j. \tag{23.29}$$

Using these we write $\mathcal{P}^-(t)$ as

$$\mathcal{P}^-(t) = M\sum_j |L_j|^2 \exp\left(-\Gamma_j t\right)$$

$$+ \quad M \sum_j \sum_k \exp\left[-\frac{1}{2}(\Gamma_j + \Gamma_k)t\right] \mathrm{Re}\left[L_k^* L_j \exp(-i\omega_{ij}t)\right]. \quad (23.30)$$

where M and $L_k^* L_j$ are defined by

$$M = \sum_j \sum_i \mathrm{Re}\,(L_i^* L_j). \quad (23.31)$$

and

$$L_i^* L_j = C_2^*(E_i) C_2(E_j) \exp\left[-i(E_j - E_i)t\right] \int_0^\infty u_2^*(E_i, r) u_2(E_j, r) dr. \quad (23.32)$$

The measured values of $\mathcal{P}^-(t)$ are

$$\mathcal{P}^-(1), \mathcal{P}^-(2), ...\mathcal{P}^-(j), ...\mathcal{P}^-(2N), \quad (23.33)$$

where $\mathcal{P}^-(j)$ is the probability measured at time $t_j = j\Delta t$. We observe that $\mathcal{P}^-(t)$ is the sum of a number of terms each with an exponential dependence on time. In order to determine Γ_j's and ω_{ij}'s from the measurement of $\mathcal{P}^-(t)$ we use the Prony method [9] [8] [10].
Here we start by solving the set of difference equations

$$\begin{aligned} Z_N \mathcal{P}^-(k) \quad &+ \quad Z_{N-1}\mathcal{P}^-(k+1) + ... + Z_1 \mathcal{P}^-(k+N-1) \\ &+ \quad \mathcal{P}^-(k+N) = 0, \quad k = 1, 2, ...N. \end{aligned} \quad (23.34)$$

where Z_j's are the unknowns. This set of N equations and N unknowns will have real solutions $Z_1.....Z_N$ provided that the determinant of the coefficients in (23.34) does not vanish. From these Z_j's we get the characteristic equation

$$r^N + Z_1 r^{N-1} + ... + Z_N = 0. \quad (23.35)$$

This equation of N-th order will have real and complex roots. Let $r_1, r_2, ...r_J$ denote the real and $r_{J+1}, r_{J+2}, ...r_N$ be the complex roots of (23.35), then

$$r_j = \exp(-\Gamma_j), \quad 1 \le j \le J, \quad (23.36)$$

and

$$\ln\left[\pm r_k \exp(i\theta_k)\right] = -\frac{1}{2}(\Gamma_m + \Gamma_n) - i\omega_{mn}, \quad J+1 \le k \le N. \quad (23.37)$$

The coefficient of $\exp(-\Gamma_j)$ in Eq. (23.30) is positive, therefore r_j is also positive, however the coefficient of $\exp\left[-\frac{1}{2}(\Gamma_m + \Gamma_n)\right]$ in (23.30) can be positive or negative, hence the argument of the logarithm in (23.37) can be positive or negative. From Eqs.(23.36) and (23.37) we find

$$\Gamma_j = -\ln r_j, \quad 1 \le j \le J, \tag{23.38}$$

and

$$\theta_k = \pm 2k\pi - \omega_{nm}, \tag{23.39}$$

or

$$\theta_k = \pm(2k+1)\pi - \omega_{nm}, \tag{23.40}$$

where $J+1 \le k \le N$. From these we find the level widths, Γ_j uniquely, and also we find the multi-valued solution for the level spacing .

23.4 A Numerical Example

In Chapter 20 using a two-channel model, we found the complex eigenvalues with the numerical values given in (20.34) and the function $\mathcal{P}^-(t)$ obtained from (20.40). Let us now assume that $\mathcal{P}^-(t)$ is known at times $t_j = j\Delta t$, $j = 1, 2, \ldots\ldots 2N$. For the present calculation we choose $N = 9$ and we solve Eqs. (23.34), (23.35), (23.36) and (23.37). For Γ_j's we find

$$\Gamma_1 = 0.154, \quad \Gamma_2 = 0.866, \quad \text{and} \quad \Gamma_3 = 2.460, \tag{23.41}$$

and these agree very well with -2 Im E_j's where E_j's are given by (20.34). For ω_{nm}'s of this example we find

$$\omega_{12} = 2\pi - \theta_3, \quad \omega_{23} = 3\pi + \theta_1, \quad \omega_{13} = 5\pi - \theta_2, \tag{23.42}$$

where

$$\theta_1 = 0.224, \quad \theta_2 = 0.292, \quad \text{and} \quad \theta_3 = 0.516. \tag{23.43}$$

These ω_{nm}'s are also in good agreement with the real part of the energy eigenvalues.

For inverting empirical data, which always contain errors, it is better to use a variant of the Prony's method where the best least-square fit to the data is used in the computation [11].

23.5 The Inverse Problem of Tunneling for Gamow States

In Chapters 5 and 10 we studied the problem of determination of the decay width for a central potential, and we found that the decay width Γ is given by Eqs. (5.10) or (5.11) if we use the semi-classical approximation to solve the Schrödinger equation. The essential result was that for the l-th partial wave and for discrete eigenvalues E (or E_0 in Eq. (10.11)), Γ is given by

$$\Gamma(E,l) = \frac{\hbar}{T_0(E,l)} \exp[-2\sigma(E,l)], \tag{23.44}$$

where

$$T_0(E,l) = 2\int_{r_0}^{r_1} \frac{dr}{\sqrt{2m(E - V_{eff}(r))}}, \tag{23.45}$$

$$\sigma(E,l) = \frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m[E - V_{eff}(r)]}\, dr, \tag{23.46}$$

and

$$V_{eff}(r) = V(r) + \frac{\hbar^2\left(l+\frac{1}{2}\right)^2}{2mr^2}. \tag{23.47}$$

The classical turning points r_0, r_1 and r_2 are all functions of E, i.e.

$$V_{eff}(r_i) = E, \quad i = 0, 1 \text{ and } 2. \tag{23.48}$$

Now we can state the inverse problem in the following way [3]:
Suppose that

$$L(E,l) = \frac{1}{\hbar}\int_{r_0}^{r_1} \sqrt{2m(E - V_{eff}(r))}dr = \left(n + \frac{1}{2}\right)\pi \tag{23.49}$$

and $\sigma(E,l)$ are known functions of E and l, then is it possible to determine $V_{eff}(r)$ or $V(r)$ from these data? Note that $L(E,l)$ is just the Bohr-Sommerfeld quantization rule for finding the energy eigenvalues of a particle bound in the well behind the barrier (see Fig. (23.1)), and T_0 is the period of oscillation of this particle in the well. Let us define $I(E,l)$ and $J(E,l)$ by the relations:

$$I(E,l) = \int_{r_0}^{r_1} (E - V_{eff}(r))dr, \tag{23.50}$$

and

$$J(E,l) = \int_{r_1}^{r_2} (V_{eff}(r) - E)dr. \tag{23.51}$$

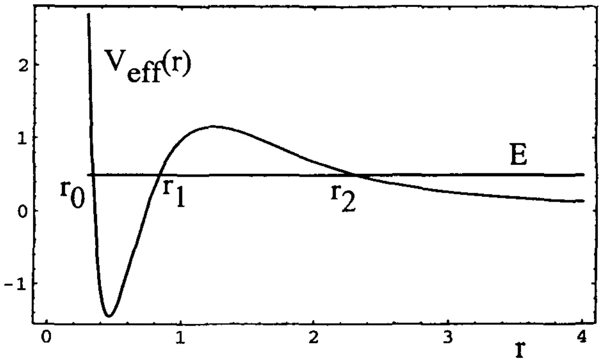

Figure 23.1: A typical potential for three-dimensional tunneling problem. For a given energy E and partial wave l, the turning points are $r_0(E), r_1(E)$ and $r_2(E)$.

Then by differentiating $I(E,l)$ and $J(E,l)$ with respect to E and l we find the following equations:

$$\frac{\partial I(E,l)}{\partial E} = \int_{r_0}^{r_1} dr = r_1(E) - r_0(E), \tag{23.52}$$

$$\begin{aligned} \frac{\partial I(E,l)}{\partial l} &= -\int_{r_0}^{r_1} \frac{\partial V_{eff}(r)}{\partial l} dr = -\int_{r_0}^{r_1} \frac{\hbar^2(2l+1)}{2mr^2} dr \\ &= \hbar^2 \left(\frac{2l+1}{2m}\right) \frac{r_0(E) - r_1(E)}{r_0(E) r_1(E)}, \end{aligned} \tag{23.53}$$

$$\frac{\partial J(E,l)}{\partial E} = -(r_2(E) - r_1(E)), \tag{23.54}$$

and

$$\frac{\partial J(E,l)}{\partial l} = \hbar^2 \left(\frac{2l+1}{2m}\right) \frac{(r_2(E) - r_1(E))}{r_1(E) r_2(E)}. \tag{23.55}$$

Solving these equations for $r_0(E), r_1(E)$ and $r_2(E)$ we find

$$r_{0,1}(E) = \left[\frac{1}{4}\left(\frac{\partial I}{\partial E}\right)^2 - \frac{(2l+1)\hbar^2}{2m}\left(\frac{\frac{\partial I}{\partial E}}{\frac{\partial I}{\partial l}}\right)\right]^{\frac{1}{2}} \pm \left(-\frac{1}{2}\frac{\partial I}{\partial E}\right), \tag{23.56}$$

and

$$r_{1,2}(E) = \left[\frac{1}{4}\left(\frac{\partial J}{\partial E}\right)^2 - \frac{(2l+1)\hbar^2}{2m}\left(\frac{\frac{\partial J}{\partial E}}{\frac{\partial J}{\partial l}}\right)\right]^{\frac{1}{2}} \pm \left(\frac{1}{2}\frac{\partial J}{\partial E}\right). \tag{23.57}$$

In these equations the first subscript on the left corresponds to the plus sign on the right and the second subscript has the minus sign. Thus $r_1(E)$ can be calculated either from (23.56) or from (23.57). Once these turning points are known as functions of E then the shape of the potential will also be known (see also the similar case for the one-dimensional problem in this chapter).

Next we want to show how $I(E, l)$ and $J(E, l)$ can be obtained from the empirical data $L(E, l)$ and $\sigma(E, l)$. For this we use the following identity:

$$E - V_{eff}(r) = \frac{2}{\pi}\int_{V_{eff}(r)}^{E}\left(\frac{E' - V_{eff}(r)}{E - E'}\right)^{\frac{1}{2}} dE'. \tag{23.58}$$

By substituting (23.58) in (23.50) for $I(E, l)$ we find

$$I(E, l) = \frac{2\hbar}{\pi\sqrt{2m}}\int_{V_{eff}^m}^{E}\frac{L(E', l)dE'}{\sqrt{E - E'}}. \tag{23.59}$$

where V_{eff}^m denotes the minimum of $V_{eff}(r)$ in the region of the potential well. By partial integration we can rewrite (23.59) as

$$I(E, l) = \frac{4\hbar}{\pi\sqrt{2m}}\int_{V_{eff}^m}^{E}\frac{\partial L(E', l)}{\partial E'}\sqrt{E - E'}dE'. \tag{23.60}$$

At the bottom of the well from Eq. (23.49) it follows that

$$n(l, V_{eff}^m) = -\frac{1}{2}, \tag{23.61}$$

and this equation can be used to find V_{eff}^m. Similarly using the identity

$$V_{eff}(r) - E = \frac{2}{\pi}\int_{E}^{V_{eff}(r)}\left(\frac{V_{eff}(r) - E'}{E' - E}\right)^{\frac{1}{2}} dE', \tag{23.62}$$

we find

$$J(E, l) = \frac{-4\hbar}{\pi\sqrt{2m}}\int_{E}^{V_{eff}^M}\frac{\partial\sigma(E', l)}{\partial E'}\sqrt{E' - E}\, dE', \tag{23.63}$$

where V_{eff}^M is the maximum height of the barrier which is obtained from

$$\sigma(l, V_{eff}^M) = 0. \tag{23.64}$$

This completes the solution of the inverse tunneling problem for the Gamow states when the WKB approximation is valid.

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Chapter 24

Some Examples of Quantum Tunneling in Atomic and Molecular Physics

There are numerous examples in the physics of atomic and molecular physics where quantum tunneling plays an important role in the explanation of the observed behavior of the system. We have already seen that the splitting of the energy levels in a double-well potential such as in ammonia molecule is due to tunneling [1].

Here we study in greater detail some of the other simple problems in atomic and molecular physics where tunneling dominates the dynamics of the system.

24.1 Torsional Vibration of a Molecule

Let us consider a specific and simple molecule where the torsional vibration is important and has been studied in detail:

The ethylene molecule, C_2H_4, consists of six atoms all in the same plane with angles between various $C-H$ and $C-C$ bonds close to 120^o . By rotating one of the CH_2 group about the $C-C$ axis by an angle α, we change the potential $V(\alpha)$ between the two groups [2] [3]. This potential,

$V(\alpha)$, is a periodic function of α and for C_2H_4 has two and for C_2H_6 has three identical minima. The general form of such a potential is [4]

$$V(\alpha) = \frac{\lambda\hbar^2}{2I}\left[1 - \sum_n A_n \cos(n\alpha)\right], \tag{24.1}$$

where I is the moment of inertia of one CH_2 about the $C - C$ axis, λ is a dimensionless constant which measures the strength of the potential, and A_n's are constant coefficients.

To calculate the energy levels for this potential function we can either solve the Schrödinger equation numerically, or use an approximate technique [3] or in very special cases find wave functionthe exact solution of the problem.

A special form of (24.1) which allows for the determination of the low-lying eigenvalues of the system is a potential which is similar to (7.62) and has the form [5]

$$V(n,\alpha) = \frac{\hbar^2}{2I}\left\{(n+1)\xi[1-\cos(2\alpha)] + \frac{1}{8}\xi^2[1-\cos(4\alpha)]\right\}. \tag{24.2}$$

The potential depends on the integer n and the constant ξ which is a measure of the strength of the potential. Just as $V(n,x)$, Eq. (7.62) this potential is also quasi-solvable, i.e. the low-lying eigenvalues and eigenfunctions can be found exactly [6].

The Schrödinger equation (24.2) is given by

$$\frac{d^2\psi}{d\alpha^2} + \left\{\epsilon + (n+1)\xi\cos(2\alpha) - \frac{1}{8}\xi^2[1-\cos(4\alpha)]\right\}\psi = 0, \tag{24.3}$$

where

$$E = \frac{\hbar^2}{2I}\left[\epsilon + (n+1)\xi\right]. \tag{24.4}$$

The wave function ψ is a sinusoidal function of α which can have periods of π or 2π. The method of solving Eq. (24.3) is similar to the one for the double-well potential discussed in Chapter 7. Thus we change the function $\psi(\alpha)$ to $\phi(\alpha)$ where

$$\phi(\alpha) = \psi(\alpha)\exp\left[-\frac{1}{4}\xi\cos(2\alpha)\right], \tag{24.5}$$

and then substitute for $\psi(\alpha)$ in (24.5) and find the following differential equation for $\phi(\alpha)$

$$\frac{d^2\phi}{d\alpha^2} - \xi\sin(2\alpha)\frac{d\phi}{d\alpha} + \left[\epsilon + n\xi\cos(2\alpha)\right]\phi = 0. \tag{24.6}$$

Now if n is an odd integer, we can write $\phi(\alpha)$ in one of the two forms;

$$\phi(\alpha) = \sum_j C_{2j+1} \cos[(2j+1)\alpha], \tag{24.7}$$

or

$$\phi(\alpha) = \sum_j S_{2j+1} \sin[(2j+1)\alpha]. \tag{24.8}$$

For even n we can also write expansions very similar to (24.7) and (24.8). By substituting (24.7) and (24.8) in (24.6) and requiring that the coefficients of $\cos[(2j+1)\alpha]$ and $\sin[(2j+1)\alpha]$ be zero, we find the following equations for the eigenvectors C_{2j+1} and S_{2j+1} and the eigenvalue ϵ when n is an odd integer

$$\begin{aligned} &\left[\epsilon - (2j+1)^2 + \frac{1}{2}(n+1)\xi\delta_{j0}\right] C_{2j+1} \\ + \; &\frac{1}{2}\xi(n+1-2j)C_{2j-1} + \frac{1}{2}\xi(n+3+2j)C_{2j+3} = 0, \\ &0 \le j \le \frac{1}{2}(n-1), \quad n \text{ odd}, \end{aligned} \tag{24.9}$$

and

$$\begin{aligned} &\left[\epsilon - (2j+1)^2 - \frac{1}{2}(n+1)\xi\delta_{j0}\right] S_{2j+1} \\ + \; &\frac{1}{2}\xi(n+1-2j)S_{2j-1} + \frac{1}{2}\xi(n+3+2j)S_{2j+3} = 0, \\ &0 \le j \le \frac{1}{2}(n-1), \quad n \text{ odd}. \end{aligned} \tag{24.10}$$

In addition we have the conditions

$$C_{-1} = C_{\frac{1}{2}(n+1)} = 0, \tag{24.11}$$

and

$$S_{-1} = S_{\frac{1}{2}(n+1)} = 0. \tag{24.12}$$

The eigenvalues ϵ for C_{2j+1} and S_{2j+1} are found by the diagonalization of a tridiagonal matrix in each case and the corresponding eigenvectors C_{2j+1} and S_{2j+1} are then calculated from (24.9) and (24.10). From these and Eqs. (24.7) and (24.8) $\phi(\alpha)$'s can be determined. In Fig. (24.1) the potential $V(\alpha)$ for $n = 7$ and $\xi = 2$ is shown together with the calculated eigenvalues E_j, Eq. (24.4) in units of $\frac{\hbar^2}{2I}$. Similar results can be found when n is an even integer.

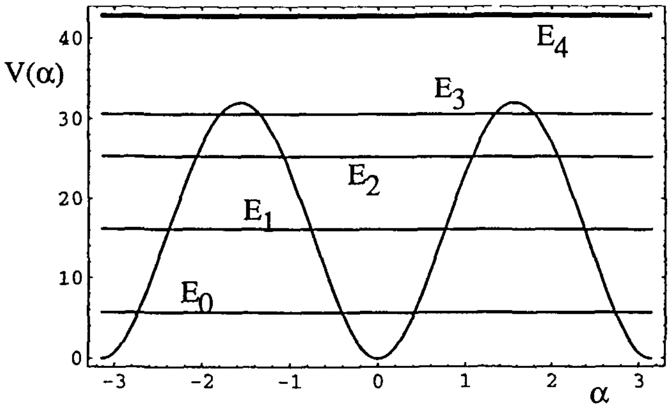

Figure 24.1: The oscillating potential $V(\alpha)$, Eq. (24.2), for $-\pi \leq \alpha \leq \pi$ is shown for the parameters $n = 7$ and $\xi = 2$. Five of the lowest energy levels E_0 to E_4 calculated from (24.4) are also shown.

24.2 Electron Emission from the Surface of Cold Metals

If a metal is placed in a very strong field (about 10^6 volts/cm) so that it forms a cathode, then the electrons are emitted from the surface of the metal and this is called cold emission [7] [8] [9] [10]. This emission of the electrons can be explained on the basis of quantum tunneling.

We know that work must be done in order to remove an electron from the surface of a metal, therefore the potential energy of the electron in the metal is less than its potential energy outside. We take the potential inside to be zero and for the outside to be $V(x) = V_0 > 0$. This model, the so called "free electron gas" model [11], should be considered as an approximate model, since in the metal the potential is a function of the coordinate of the electron, and has a periodicity equal to the separation of the atoms from each other.

The energy distribution among the electrons in this electron gas is such that most of the electrons have energies less than V_0. At the absolute zero temperature these electrons occupy all the energy levels up to the Fermi energy, E_F, and this E_F is less than V_0. Since the energy of these electrons

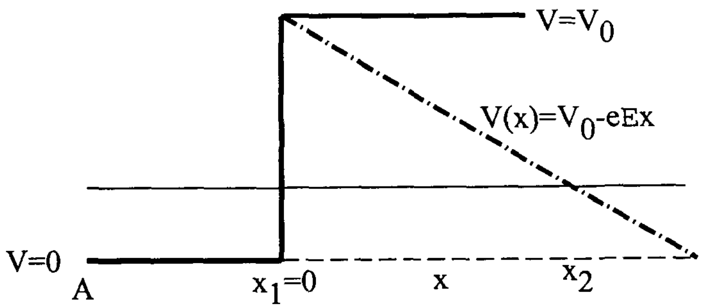

Figure 24.2: The potential energy inside and outside of a metallic surface located at $x = 0$, shown by solid line. When an external electric field $\mathcal{E}$ is added then the total external potential is shown by dashed-dotted line.

is less than the external potential, therefore after reaching the boundary between the metal and outside (vacuum or air), they are reflected back into the metal.

Now if we add the external electric field directed toward the surface of the metal, then the potential energy becomes

$$V(x) = \begin{cases} V_0 - e\mathcal{E}x & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} . \tag{24.13}$$

This potential is shown in Fig. (24.2). Inside the metal there is no electric field, therefore $V(x)$ has a triangular shape. The Schrödinger equation with the potential (24.13) can be solved exactly, (see Section (6.3)), or approximately using the semi-classical (WKB) method.

For simplicity we use the latter to calculate the transmission coefficient. To this end we first find the integral

$$S = \int_{x_1}^{x_2} \sqrt{2m\left[V(x) - E_x\right]}\, dx \tag{24.14}$$

where x_1 and x_2 are the turning points. For those values of E_x where $E_x < V_0$, the first turning point is at $x_1 = 0$ and the second is given by

$$E_x = V_0 - e\mathcal{E}x_2. \tag{24.15}$$

By substituting these in (24.14) and evaluating the integral we find S;

$$S = \frac{2\sqrt{2m}}{3}\frac{(V_0 - E_x)^{\frac{3}{2}}}{e\mathcal{E}}. \tag{24.16}$$

Thus if we denote the transmission coefficient by $|T(E_x)|^2$, then

$$|T(E_x)|^2 = D_0 \exp\left[-\frac{4\sqrt{2m}}{3\hbar}\frac{(V_0 - E_x)^{\frac{3}{2}}}{e\mathcal{E}}\right], \quad D_0 > 0. \tag{24.17}$$

and this transmission coefficient depends on E_x. The average value of $|T(E_x)|^2$ for different energies of the electron, $0 \le E_x \le V_0$, is a function of the electric field $\mathcal{E}$;

$$|T(\bar{E}_x)|^2 = D_0 \exp\left(-\frac{\mathcal{E}_0}{\mathcal{E}}\right), \tag{24.18}$$

where for each metal $\mathcal{E}_0$ and D_0 are constant quantities.

Next we want to calculate the electric current density which in this case is given by

$$J(\mathcal{E}) = e\int \frac{2dp_x dp_y dp_z}{(2\pi\hbar)^3} v_x |T(E_x)|^2, \tag{24.19}$$

where we have used $d^3n = \frac{2}{(2\pi\hbar)^3}dp_x dp_y dp_z$ as the number of conduction electrons per unit volume (see also the discussion in Section 25.3). The range of variations of p_x, p_y and p_z are limited to the points inside the Fermi sphere, i.e.

$$p_x^2 + p_y^2 + p_z^2 \le 2mE_F. \tag{24.20}$$

To calculate $J(\mathcal{E})$ we use cylindrical coordinates

$$p_y = \rho\cos\phi, \quad p_z = \rho\sin\phi, \quad \rho^2 + p_x^2 \le 2mE_F, \tag{24.21}$$

and write (24.19) as

$$J(\mathcal{E}) = \frac{4\pi e}{(2\pi\hbar)^3}\int_0^{\sqrt{2mE_F}} dp_x \int_0^{\sqrt{2mE_F - p_x^2}} |T(E_x)|^2 \frac{p_x}{m}\rho d\rho. \tag{24.22}$$

To simplify the result we change E_x to

$$\epsilon = E_F - E_x, \tag{24.23}$$

and note that $|T|^2$ is now a function of ϵ

$$J(\mathcal{E}) = \frac{2em}{(2\pi)^2}\int_0^{E_F} \epsilon\, |T(\epsilon)|^2\, d\epsilon, \tag{24.24}$$

where

$$|T(\epsilon)|^2 = \exp\left[\frac{4\sqrt{2m}}{\hbar e\mathcal{E}}\left(V_0 - E_F + \epsilon\right)^{\frac{3}{2}}\right], \tag{24.25}$$

and we have set $D_0 = 1$. Since $|T(\epsilon)|^2$ decreases rapidly with increasing ϵ, therefore in (24.25) we can expand $(V_0 - E_F + \epsilon)^{\frac{3}{2}}$;

$$(V_0 - E_F + \epsilon)^{\frac{3}{2}} = (V_0 - E_F)^{\frac{3}{2}} + \frac{3}{2}\epsilon\,(V_0 - E_F)^{\frac{1}{2}} + \ldots.. \tag{24.26}$$

Introducing the parameter Q by

$$Q = \frac{2\sqrt{2m}}{\hbar e\mathcal{E}}\left(V_0 - E_F\right)^{\frac{3}{2}}, \tag{24.27}$$

we find

$$|T|^2 = \exp\left(-\frac{2}{3}Q\right)\exp\left(-\frac{Q\epsilon}{V_0 - E_F}\right). \tag{24.28}$$

Since the integrand in (24.24) decreases rapidly as the function of ϵ, we can extend the range of integration to $(0, \infty)$ and obtain the following expression for $J(\mathcal{E})$;

$$J(\mathcal{E}) = \frac{2me}{4\pi^2\hbar^3}\exp\left(-\frac{2}{3}Q\right)\frac{(V_0 - E_F)^2}{Q^2}. \tag{24.29}$$

This relation shows the dependence of the cold emission current $J(\mathcal{E})$ on the field $\mathcal{E}$.

For more accurate description of this emission with correction due to the image force see Flügge [12].

24.3 Ionization of Atoms in Very Strong Electric Field

A strong electric field can also cause the separation of the electrons from the atoms in a gas [7] [9] [10]. The potential that binds the electron to the atom is of the form of Coulomb potential $V_1(r) = -\frac{C}{r}$ where C is a constant. Now this atom is placed in an electric field $\mathcal{E}$ which is along the z-axis, then the potential that the electron feels changes to

$$V(r) = V_1(r) + e\mathcal{E}z = -\frac{C}{r} + e\mathcal{E}z, \tag{24.30}$$

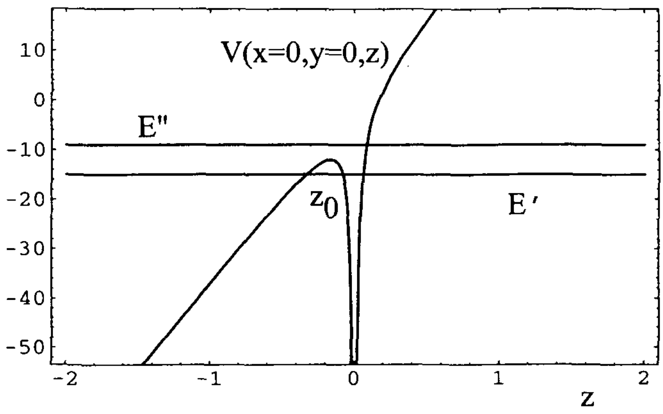

Figure 24.3: The potential energy felt by an electron which is bound to an atom and the atom is placed in a strong electric field along the z-axis.

therefore the potential energy along the z-axis varies as

$$V(x = 0, y = 0, z) = -\frac{C}{|z|} + e\mathcal{E}z, \tag{24.31}$$

and this dependence of V on z is shown in Fig. (24.3). In this case potential forms a barrier around the point

$$z_0 = -\sqrt{\frac{C}{e\mathcal{E}}}, \tag{24.32}$$

and z_0 divides the z-axis into two parts: The interior region $z > z_0$, and the exterior region $z < z_0$ where in both parts the potential energy is less than $V_0 = -\sqrt{Ce\mathcal{E}}$.

In Fig. (24.3) two constant energy lines E' and E'' are shown. For the energy $E = E'' > V(z_0)$ the electron does not remain inside the atom, but moves towards the negative z-axis. On the other hand for the energy $E = E' < V(z_0)$, according to the laws of classical mechanics the electron must stay inside the atom. However in quantum mechanics there is the possibility of tunneling through the barrier. This leads us to the conclusion that if $\mathcal{E}$ is strong enough, then the ionization of the electrons at lower energies is possible, but if the electric field is weak, then the width of the barrier is large and the possibility of tunneling is very small.

24.4 A Time-Dependent Formulation of Ionization in an Electric Field

A one dimensional model of ionization of atoms by an external electric field which has been studied by Geltman [10] [13] [14] is based on time-dependent tunneling. In this model the electron is initially bound by the potential $-\frac{\hbar^2}{2m}s\delta(z)$, but after being exposed to a time-dependent external applied field $(-zF(t))$, the electron is released from the atom and moves away. The wave equation for the electron in this model is given by

$$-i\hbar\frac{\partial\psi(z,t)}{\partial t} - \frac{\hbar^2}{2m}\frac{\partial^2\psi(z,t)}{\partial z^2} - \left[\frac{\hbar^2}{2m}s\delta(z) + zF(t)\right]\psi(z,t) = 0, \qquad (24.33)$$

and is subject to the initial condition

$$\psi(z,t=0) = \sqrt{s}\exp\left(-s|z|\right). \qquad (24.34)$$

This condition shows that the electron at $t = 0$ is in a bound state of a δ-function potential.

Let us introduce the kernel $K_F(z,t;z',t')$ as the solution of the differential equation

$$-i\hbar\frac{\partial K_F}{\partial t} - \frac{\hbar^2}{2m}\frac{\partial^2 K_F}{\partial z^2} - zF(t)K_F = -i\hbar\delta(z-z')\delta(t-t'), \qquad (24.35)$$

subject to the boundary conditions that $K_F(z,t;z',t')$ must remain bounded as $z \to \pm\infty$ [15]. From Eqs. (24.33) and (24.34) it follows that

$$\psi(z,t) = \psi_F(z,t) + \frac{i\hbar s}{2m}\int_0^t K_F(z,t;0,t')\psi(0,t')dt', \qquad (24.36)$$

where $\psi_F(z,t)$ is the solution of the time-dependent Schrödinger equation

$$-i\hbar\frac{\partial\psi_F(z,t)}{\partial t} - \frac{\hbar^2}{2m}\frac{\partial^2\psi_F(z,t)}{\partial z^2} - zF(t)\psi_F(z,t) = 0, \qquad (24.37)$$

or equivalently the solution of the integral equation

$$\psi_F(z,t) = \int_{-\infty}^{\infty} K_F(z,t;z',0)\psi(z',0)dz'. \qquad (24.38)$$

Once $K_F(z,t;z',t')$ is known then from Eqs. (24.34) and (24.38) we can calculate $\psi_F(z,t)$. But as Eq. (24.36) shows we also need to know

$\psi(0,t)$ in order to determine the wave function $\psi(z,t)$. For this we set z in Eq. (24.36) equal to zero to find the integral equation for $\psi(0,t)$;

$$\psi(0,t) = \psi_F(0,t) + \frac{i\hbar s}{2m}\int_0^t K_F(0,t;0,t')\psi(0,t')dt'. \tag{24.39}$$

Noting that $\psi_F(0,t)$ is known, we solve (24.39) for $\psi(0,t)$, and then substitute the result in Eq. (24.36) to obtain $\psi(z,t)$.

Next let us study the propagator $K_F(z,t;z',t')$ which is the kernel for the integral equations (24.38) and (24.39). There are at least two different time-dependent external electric fields for which we have an analytic solution for $K_F(z,t;z',t')$:

(i) - When $F(t) = F_0\theta(t)$ where $\theta(t)$ is the step function. In this case $K_F(z,t;z',t')$ is given by [10]

$$K_F(z,t;z',t') = K_0(z,t;z',t')\exp\left[\frac{iF_0}{2\hbar}(t-t')(z+z') - \frac{i}{24m\hbar}F_0^2(t-t')^3\right] \tag{24.40}$$

where $K_0(z,t;z',t')$ is the free particle propagator (see Eq. (6.22))

$$K_0(z,t;z',t') = \left(\frac{m}{2\pi i\hbar(t-t')}\right)^{\frac{1}{2}}\exp\left[\frac{im\left(z-z'\right)^2}{2\hbar\,(t-t')}\right]. \tag{24.41}$$

(ii) - When $F(t)$ is given by $F(t) = At$, where A is a constant, then from the classical action [16] we can calculate K_F;

$$\begin{aligned} K_F\left(z,t;z',t'\right) &= K_0\left(z,t;z',t'\right) \\ \times\ &\exp\left\{\frac{i}{\hbar}\left[\frac{A}{6}\left(t-t'\right)\left(z\left(2t+t'\right)+z'\left(t+2t'\right)\right)\right]\right\} \\ \times\ &\exp\left\{-\frac{i}{\hbar}\left[\frac{1}{360m}A^2\left(t-t'\right)^3\left(4t^2+7tt'+4t'^2\right)\right]\right\}. \end{aligned} \tag{24.42}$$

It should be pointed out that in the second case since the potential depends on time the kernel $K_F(z,t;z',t')$ is not a function of $t-t'$.
An interesting aspect of the model (i) that we have just discussed is that the decay of the initial state

$$P(t) = \left|\langle\psi(z,t=0)|\psi(z,t)\rangle\right|^2, \tag{24.43}$$

is exponential even after a very long time [15] (compare with the discussion of Section(2.2)). In this formulation we start with the construction of the energy Green function which is the Fourier transform of the propagator K_F. To this end we introduce the dimensionless quantities

$$\zeta = \frac{z}{z_0}, \quad \varepsilon = \frac{E}{E_0}, \quad \tau = \frac{tE_0}{\hbar} \quad \text{and} \quad \sigma = \frac{\hbar^2 s}{2mz_0E_0}, \tag{24.44}$$

where

$$z_0 = \left(\frac{\hbar^2}{2mF_0}\right)^{\frac{1}{3}}, \quad \text{and} \quad E_0 = F_0 z_0, \tag{24.45}$$

are constants with dimensions of length and energy respectively. Using these, we can write the Hamiltonian in the dimensionless form of

$$H_\zeta = -\left[\frac{\partial^2}{\partial \zeta^2} + \zeta + \sigma\delta(\zeta)\right]. \tag{24.46}$$

For this dimensionless form of the Hamiltonian the Green function for a given energy ε is the solution of the differential equation

$$(\varepsilon - H_\zeta)\, G\left(\zeta, \zeta' : \varepsilon\right) = \delta\left(\zeta - \zeta'\right). \tag{24.47}$$

To find this Green function we first calculate $G_F\left(\zeta, \zeta'; \varepsilon\right)$ which is defined as the solution of the differential equation

$$\left(\varepsilon + \frac{\partial^2}{\partial \zeta^2} + \zeta\right) G_F\left(\zeta, \zeta'; \varepsilon\right) = \delta\left(\zeta - \zeta'\right). \tag{24.48}$$

When both $G_F\left(\zeta, \zeta'; \varepsilon\right)$ and $G\left(\zeta, \zeta'; \varepsilon\right)$ satisfy the same boundary conditions, we can express $G\left(\zeta, \zeta'; \varepsilon\right)$ in terms of $G_F\left(\zeta, \zeta'; \varepsilon\right)$;

$$G\left(\zeta, \zeta'; \varepsilon\right) = G_F\left(\zeta, \zeta'; \varepsilon\right) - \sigma \int G_F\left(\zeta, \zeta''; \varepsilon\right) \delta\left(\zeta''\right) G\left(\zeta'', \zeta'; \varepsilon\right) d\zeta''. \tag{24.49}$$

From (24.49) we find $G(\zeta, \zeta'; \varepsilon)$ to be (see also Section (6.2))

$$G\left(\zeta, \zeta'; \varepsilon\right) = G_F\left(\zeta, \zeta'; \varepsilon\right) + \frac{G_F\left(\zeta, 0; \varepsilon\right) G_F\left(0, \zeta'; \varepsilon\right)}{\frac{1}{\sigma} + G_F\left(0, 0; \varepsilon\right)}, \tag{24.50}$$

therefore by knowing G_F we can determine G from (24.50).

To determine G_F we note that the differential equation (24.48) is subject to the conditions:

$$G_F\left(\zeta' + 0, \zeta'; \varepsilon\right) = G_F\left(\zeta' - 0, \zeta'; \varepsilon\right), \tag{24.51}$$

and

$$\left[\frac{\partial}{\partial\zeta}G_F\left(\zeta,\zeta^{'};\varepsilon\right)\right]_{\zeta=\zeta^{'}+0}-\left[\frac{\partial}{\partial\zeta}G_F\left(\zeta,\zeta^{'};\varepsilon\right)\right]_{\zeta=\zeta^{'}-0}=1. \tag{24.52}$$

These conditions together with the outgoing boundary condition give us [15]

$$G_F(\zeta,\zeta^{'};\varepsilon)=-\pi\begin{cases} Ci^{+}\left(-\zeta^{'}-\varepsilon\right)Ai\left(-\zeta-\varepsilon\right) & \text{for } \zeta\leq\zeta^{'} \\ Ci^{+}\left(-\zeta-\varepsilon\right)Ai\left(-\zeta^{'}-\varepsilon\right) & \text{for } \zeta^{'}\leq\zeta \end{cases}, \tag{24.53}$$

where

$$Ci^{+}=Bi+iAi. \tag{24.54}$$

Since Ai and Bi i.e. Airy functions are entire functions of their arguments, and therefore of ε, we can continue $G\left(\zeta,\zeta^{'};\varepsilon\right)$ analytically into the lower half of the complex ε-plane. We have seen that the poles of G in the lower half plane correspond to decaying states (Chapter 10). But first let us consider the time evolution of the initial wave function $\psi(\zeta,0)$ which can be found from the propagator $K\left(\zeta,\tau:\zeta^{'},\tau^{'}\right)$, the latter being the time-Fourier transform of $G\left(\zeta,\zeta^{'};\varepsilon\right)$;

$$K\left(\zeta,\tau;\zeta^{'},\tau^{'}\right)=\frac{i}{2\pi}\int\exp\left[-i\mu\left(\tau-\tau^{'}\right)\right]G\left(\zeta,\zeta^{'};\varepsilon=\mu+i0\right)d\mu, \tag{24.55}$$

or from the identity [10]

$$\begin{aligned} Ai\left(-\zeta-\varepsilon\right)Ci^{+}\left(\zeta^{'}-\varepsilon\right) &= \frac{1}{2\pi}\int_0^{\infty}\sqrt{\frac{i}{\pi\mu}} \\ &\times\ \exp\left\{i\left[\frac{\left(\zeta^{'}-\zeta\right)^2}{4\mu}+\frac{1}{2}\left(\zeta+\zeta^{'}\right)\mu-\frac{1}{12}\mu^3\right]+i\mu\varepsilon\right\}d\mu. \end{aligned} \tag{24.56}$$

From the kernel K we can determine the wave function $\psi(\zeta,\tau)$

$$\psi(\zeta,\tau)=\int K\left(\zeta,\tau;\zeta^{'},\tau^{'}\right)\psi\left(\zeta^{'},0\right)d\zeta^{'}. \tag{24.57}$$

To evaluate (24.57) we observe that the residue of $G\left(\zeta,\zeta^{'};\varepsilon\right)$ at any pole $\varepsilon=\varepsilon_n$ can be written as a product of the eigenfunctions $\psi\left(\zeta,\varepsilon_n\right)\psi\left(\zeta^{'},\varepsilon_n\right)$

[15], where $\psi(\zeta, \varepsilon_n)$ is proportional to $G_F(\zeta, 0; \varepsilon_n)$, and where ε_n is one of the roots of the equation

$$\frac{1}{\sigma} + G_F(0, 0, \varepsilon_n) = 0. \tag{24.58}$$

One way of evaluating the integral in (24.55) is by means of contour integration. Thus for $\tau > 0$, we can close the contour in the lower half of ε-plane and by the theorem of residue find $\psi(\zeta, \tau)$;

$$\psi(\zeta, \tau) = \int \psi\left(\zeta', 0\right) \left[\sum_n \exp(-i\varepsilon_n \tau) \psi(\zeta, \varepsilon_n) \psi\left(\zeta', \varepsilon_n\right)\right] d\zeta'. \tag{24.59}$$

From the analytic properties of the Airy functions, Ci^+ and Ai and Eq. (24.58) we can determine the location of these poles approximately. For instance there is a pole ε_0 which is very close to the negative real axis of the ε-plane, and for $\sigma >> 1$ the position of the pole is given by

$$\varepsilon_0 = -\frac{1}{4}\sigma^2 \left[1 + i \exp\left(-\frac{1}{6}\sigma^2\right)\right]. \tag{24.60}$$

Now if we substitute (24.59) in (24.43) we find $P(t)$ to be

$$\begin{aligned} P(t) &= \Bigg|\sum_n \langle \psi(\zeta, 0) | \psi(\zeta, \varepsilon_n)\rangle \exp\left(-\frac{i\varepsilon_n E_0 t}{\hbar}\right) \\ &\times \int \psi\left(\zeta', \varepsilon_n\right) \psi\left(\zeta', 0\right) d\zeta'\Bigg|^2. \end{aligned} \tag{24.61}$$

Since the root $\varepsilon = \varepsilon_0$ has the smallest imaginary part [15], therefore after a long time we have an exponentially decaying state with the decay width Γ, where

$$\Gamma = \frac{1}{2} E_0 \sigma^2 \exp\left(-\frac{\sigma^2}{6}\right) = \frac{\hbar^2 s^2}{4m} \exp\left(-\frac{\sigma^2}{6}\right). \tag{24.62}$$

24.5 Ammonia Maser

The ammonia maser is of special interest since it was used as the first standard for the molecular frequencies. In this molecule the three hydrogen atoms are at the three corners of an equilateral triangle and the nitrogen atom can move up and down along the axis of the molecule (x-axis), and this

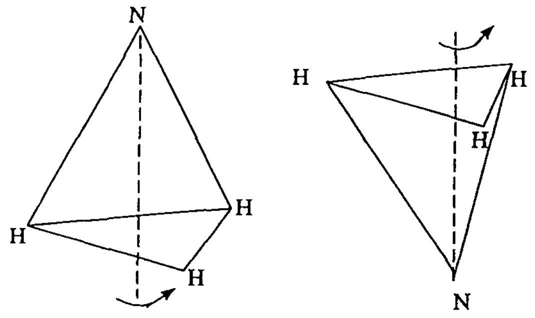

Figure 24.4: In ammonia molecule the motion of the nitrogen atom is along the axis which is shown by the dashed line.

up and down motion is specified in relation to the direction of the rotation of the molecule about its axis (see Fig. (24.4)).

It should be pointed out that in the calculation of the energy levels of NH_3 or similar molecules, none of the normal modes can be approximated by a one-dimensional oscillation of the N atom up and down of the H_3 plane, and in each one of the four normal vibrations the height of the pyramid changes by a small amount. But this change has a very small effect in the splitting of the energy levels [2] [17]. The energy and the parity eigenstates for this system, as we have seen earlier (e.g. Chapter 7, Eq. (7.9)) are a linear combination of the eigenstates shown in Fig. (24.5).

The ammonia maser is driven by a focused stream of ammonia molecules in their antisymmetrical state, $\Psi_-(x)$, through a resonator. The positive polarizability of the symmetric and the negative polarizability of the antisymmetric states enables one to separate these states by means of an electrostatic lens [18]. That is if these molecules are placed in an inhomogeneous electric field, symmetric states can lower their energies by being attracted to the region where the field is stronger while antisymmetric states will have their energies raised and hence they are repelled. For a detailed and clear account of the ammonia maser the reader is referred to Pippard's book [18].

For the ammonia molecule $\Delta E = E_A - E_S \approx 10^{-4}eV = 24000MHz$ and this corresponds to a period of oscillation of $T_0 = \frac{2\pi\hbar}{\Delta E} = 4 \times 10^{-11}s$.

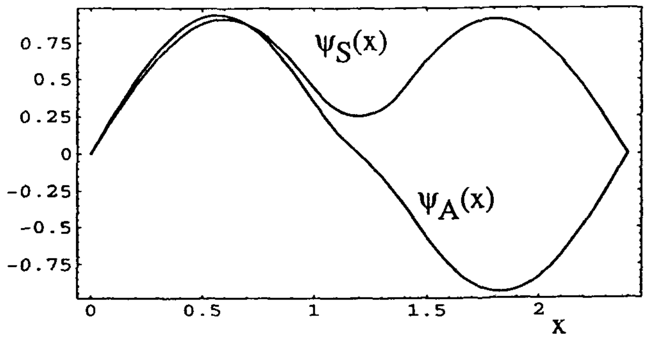

Figure 24.5: The ground and the first excited state for the motion of the nitrogen atom in ammonia molecule.

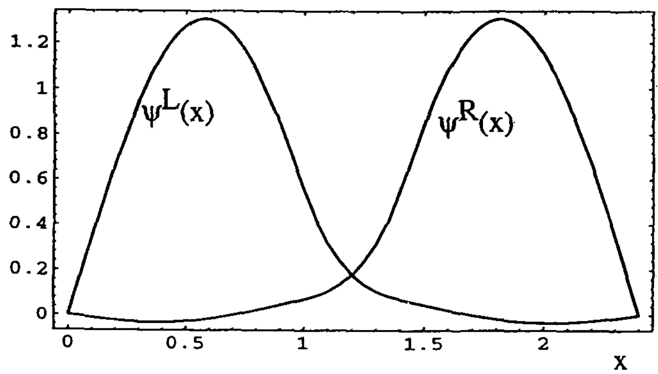

Figure 24.6: Linear combinations of the ground and the first excited states of ammonia molecule forming wave packets.

The wavelength for this problem is about one centimeter which falls in the microwave region.Here the splitting between the energy levels is large and T_0 is very small. But in molecules where ΔE is very small, then T_0 will be very large and if this is the case then the two states $\psi^L(x)$ and $\psi^R(x)$ shown in Fig. (24.6) will change only after a very long time. For instance the molecule PH_3 has an inversion period of $T_0 = 1.1 \times 10^7$ s, and the molecule AsH_3 has level splitting equal to $\Delta E \approx 0.8 \times 10^{-22} eV = 2 \times 10^8 Hz$ and the corresponding period is $T_0 \approx 5 \times 10^7$s $= 2$ years. Thus a small change in the potential can produce a large change in the period of oscillations. Similarly for molecules such as $AsCl_3$ or $BiCl_3$ the time of switching from one configuration to the other can be very large (of the order of hours or even years)[2].

24.6 Optical Isomers

Another example of this type of tunneling is that of optical isomers [2] [17]. Isomers are two forms of a molecule such that one is the mirror image of the other, but the two molecules rotate light rays in equal but opposite directions (enantiomorph). Molecules with asymmetric carbon atom such as $CHClFBr$ have this optical property. The structure of the latter molecule is displayed in Fig. (24.7). None of the two forms shown in Fig. (24.7) is stable. The molecule which rotates the light to the left can change, after a long time, to its optical isomer, and then back to the original molecule.

As before, the period of oscillation is $\frac{2\pi\hbar}{\Delta E}$, where ΔE is the difference between the energies of the antisymmetric and symmetric states. In the case of these isomers the height and the width of the central barrier is large, therefore ΔE calculated from Eq. (3.109) is very small. This means that the period T_0 is extremely long and that the property of the left or right rotation of light for these molecules may be regarded as permanent.

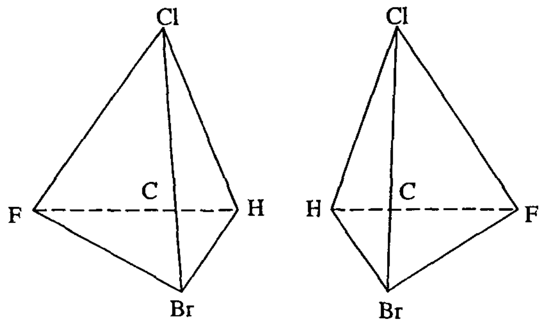

Figure 24.7: An example of optical isomers, the $CHClFBr$ molecule .

24.7 Three-Dimensional Tunneling in the Presence of a Constant Field of Force

One of the few exactly solvable three-dimensional problems is that of tunneling of a particle with ballistic motion. Following Bacher *et al* [19] we discuss the theoretical aspects of this problem and then study the empirical result.

Consider a particle of mass m which is affected by a constant force $\mathbf{F}$. For a classical motion of this particle the Hamilton characteristic function S_{cl} is the solution of the Hamilton-Jacobi equation [20],

$$\frac{\partial S_{cl}}{\partial t} + \frac{1}{2m}\left(\nabla S_{cl}\right)^2 - \mathbf{r}.\mathbf{F} = 0. \tag{24.63}$$

Since $\mathbf{F}$ is constant we can separate the variables in (24.63) and find the complete solution of Eq. (24.63);

$$S_{cl}(\mathbf{r}_f, \mathbf{r}_i; \mathcal{T}) = \frac{m}{2\mathcal{T}}\left|\mathbf{r}_f - \mathbf{r}_i\right|^2 + \frac{1}{2}\mathbf{F}.(\mathbf{r}_f + \mathbf{r}_i)\mathcal{T} - \frac{1}{24m}\mathbf{F}^2\mathcal{T}^3, \tag{24.64}$$

where $\mathcal{T} = t_f - t_i$ is the time that takes the particle to reach $\mathbf{r}_f$ from $\mathbf{r}_i$. We can also find a solution of (24.63) as

$$S_{cl}(\mathbf{r}_f, \mathbf{r}_i; \mathcal{T}) = W_{cl}(\mathbf{r}_f, \mathbf{r}_i; E) - E\mathcal{T}, \tag{24.65}$$

where E, the energy of the particle, is the separation constant and satisfies the equation

$$E(\mathbf{r}_f, \mathbf{r}_i; \mathcal{T}) = -\frac{\partial}{\partial \mathcal{T}} S_{cl}(\mathbf{r}_f, \mathbf{r}_i; \mathcal{T}). \tag{24.66}$$

We can write E as a function of T, by substituting (24.64) in (24.66);

$$E(\mathbf{r}_f, \mathbf{r}_i; \mathcal{T}) = \frac{m}{2\mathcal{T}^2} |\mathbf{r}_f - \mathbf{r}_i|^2 - \frac{1}{2}\mathbf{F}.(\mathbf{r}_f + \mathbf{r}_i) - \frac{1}{8m}\mathbf{F}^2\mathcal{T}^2. \tag{24.67}$$

This is a quadratic equation for $\mathcal{T}$, and if we solve it for $\mathcal{T}$ we find

$$\mathcal{T}_{\pm}(\mathbf{r}_f; \mathbf{r}_f; E) = \frac{\sqrt{m}}{F}(\epsilon_+ \pm \epsilon_-), \tag{24.68}$$

where

$$\epsilon_{\pm}(\mathbf{r}_f, \mathbf{r}_i; E) = \sqrt{2E + \mathbf{F}.(\mathbf{r} + \mathbf{r}_i) \pm F |\mathbf{r}_f - \mathbf{r}_i|}. \tag{24.69}$$

Equation (24.68) shows that for the constant energy E there are, at most, two trajectories connecting $\mathbf{r}_i$ to $\mathbf{r}_f$. But for combinations of $\mathbf{r}_i$, $\mathbf{r}_f$ and E when the quantity under the square root sign in (24.69) becomes negative, there will be no real trajectory. In this case $\mathcal{T}$ becomes complex and this is not an acceptable solution in classical dynamics. However as we have seen a number of times, in quantum mechanics complex or imaginary time appears in problems associated with quantum tunneling.

To simplify the problem let us assume that the starting point of the particle is at $\mathbf{r}_i = 0$, and the force $\mathbf{F}$ is in the direction of the positive z-axis, $(F > 0)$. Then (24.68) can be written in the simpler form of

$$\mathcal{T}_{\pm}(r, 0; E) = \frac{\sqrt{m}}{F}\left[\sqrt{2E + F(r+z)} \pm \sqrt{2E - F(r-z)}\right], \tag{24.70}$$

where in this expression $|\mathbf{r}_f| = r$ and z is the component of $\mathbf{r}_f$ in the direction of z. We observe that depending on the sign of E and the magnitude of $(r-z)$ we can have four different possibilities:
(i-ii)- For positive values of E, $\epsilon_+ = \sqrt{2E + F(r+z)}$ is always real but $\epsilon_- = \sqrt{2E - F(r-z)}$ can be real or imaginary. For large $(r-z)$, ϵ_- is imaginary and $\mathcal{T}_{\pm}(r, 0; E)$ is complex. Since this result depends on F, therefore this, in classical sense, is a "dynamically forbidden" motion . That is, there is no classical path which joins the origin to $\mathbf{r}_f$. But it is interesting that in quantum mechanics this is a special case of quantum tunneling which can occur only in two or three dimensions. Here instead of a turning point we have a "turning plane" with the equation

$$r - z = \frac{2E}{F}. \tag{24.71}$$

(iii-iv) - When E is negative, the quantity $2E+F(r+z)$ can be greater or less than zero, but in either case ϵ_- is imaginary and the motion is forbidden.

On the other hand, depending on the value of $(r+z)$, ϵ_+ can be real or imaginary. For $(r+z) < \frac{2|E|}{F}$, $\mathcal{T}_\pm(r,0;E)$ is imaginary and this is similar to the imaginary time which we introduced in our study of the instantons. The difference between the forbidden motion in (i-ii) and (iii-iv) is that in the latter case the motion is not allowed because of the energy of the particle and is not related to the magnitude of F. Thus this is the case of "forbidden motion due to the energy of the particle". Once we have found $\mathcal{T}_\pm(\mathbf{r}_f,\mathbf{r}_i;E)$ from Eqs. (24.65) and (24.67) we can find $W_{cl}^{\pm}(\mathbf{r}_f,\mathbf{r}_i;E)$;

$$W_{cl}^{\pm}(\mathbf{r}_f,\mathbf{r}_f;E) = \frac{\sqrt{m}}{3F}\left(\epsilon_+^3 \pm \epsilon_-^3\right). \tag{24.72}$$

Now by combining Eqs. (24.65) and (24.72) we calculate $S_{cl}(\mathbf{r}_f,\mathbf{r}_f;E)$ which we need for the quantum mechanical problem. The wave function for this motion can be found by solving the integral equation

$$\psi(\mathbf{r}_f,t_f) = \int K(\mathbf{r}_f,t_f;\mathbf{r}_i,t_i)\psi(\mathbf{r}_i,t_i)d^3r_i, \tag{24.73}$$

where the kernel of this integral equation is a solution of the differential equation

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2 + \mathbf{r}.\mathbf{F}\right] K(\mathbf{r},t;\mathbf{r}_i,t_i) = i\hbar\delta\left(t-t_i\right)\delta\left(\mathbf{r}-\mathbf{r}_i\right). \tag{24.74}$$

Since the Hamiltonian is quadratic in both momenta and coordinates, we can write K in terms of S_{cl} as [21]

$$K(\mathbf{r}_f,t_f;\mathbf{r}_f,t_i) = \left[\det\left\{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{cl}}{\partial\mathbf{r}_f\partial\mathbf{r}_i}\right\}\right]^{\frac{1}{2}} \exp\left[\frac{i}{\hbar}S_{cl}(\mathbf{r}_f,\mathbf{r}_i;\mathcal{T})\right]. \tag{24.75}$$

Using Eq. (24.64) we can simplify K;

$$K(\mathbf{r}_f,t_f;\mathbf{r}_f,t_i) = \left(\frac{m}{2\pi i\hbar\mathcal{T}}\right)^{\frac{3}{2}} \exp\left[\frac{i}{\hbar}S_{cl}(\mathbf{r}_f,\mathbf{r}_i;\mathcal{T})\right]. \tag{24.76}$$

We want to solve this problem with a given energy E, therefore we replace K by its time Fourier transform,

$$G(\mathbf{r}_f,\mathbf{r}_i;E) = \frac{1}{i\hbar}\int_0^\infty e^{\frac{iE\mathcal{T}}{\hbar}}K(\mathbf{r}_f,\mathbf{r}_i;\mathcal{T})d\mathcal{T}. \tag{24.77}$$

By substituting from (24.76) for K, G can be expressed as the following integral;

$$G(\mathbf{r}_f,\mathbf{r}_i;E)=\frac{1}{i\hbar}\int_0^\infty e^{\frac{iE\mathcal{T}}{\hbar}}\left(\frac{m}{2\pi i\hbar\mathcal{T}}\right)^{\frac{3}{2}}\exp\left[\frac{i}{\hbar}S_{cl}(\mathbf{r}_f,\mathbf{r}_i;\mathcal{T})\right]d\mathcal{T}. \quad (24.78)$$

To evaluate the integral in (24.78) we use the method of stationary phase [22] and note that the major contribution to the integral comes from those $\mathcal{T}$ values where the exponent in (24.78) is stationary

$$E=-\frac{\partial}{\partial\mathcal{T}}S_{cl}\left(\mathbf{r}_f,\mathbf{r}_i;\mathcal{T}\right). \quad (24.79)$$

i.e. those $\mathcal{T}$'s around $\mathcal{T}_\pm(\mathbf{r}_f,\mathbf{r}_f;E)$ which contributes significantly to the integral (compare with (24.66)). Next we expand (24.65) around $\mathcal{T}=\mathcal{T}_\pm$;

$$E\mathcal{T}+S_{cl}\left(\mathbf{r}_f,\mathbf{r}_i;\mathcal{T}\right)\approx W_{cl}^{\pm}\left(\mathbf{r}_f,\mathbf{r}_i;E\right)-\frac{1}{2}\left[\frac{\partial E}{\partial\mathcal{T}}\right]_{\mathcal{T}=\mathcal{T}_\pm}\left(\mathcal{T}-\mathcal{T}_\pm\right)^2, \quad (24.80)$$

and then substitute (24.80) in (24.78) and to find $G^\pm$

$$\begin{aligned}G^{\pm}\left(\mathbf{r}_f,\mathbf{r}_i;E\right)&=-\frac{m}{2\pi\hbar^2\mathcal{T}_\pm}\left[-\frac{m}{\mathcal{T}_\pm}\frac{\partial\mathcal{T}_\pm}{\partial E}\right]^{\frac{1}{2}}\exp\left[\frac{i}{\hbar}W_{cl}^{\pm}\left(\mathbf{r}_f,\mathbf{r}_i;E\right)\right]\\ &=\frac{mF}{2\pi i\hbar^2}\left(\frac{1}{\epsilon_+\pm\epsilon_-}\right)\frac{1}{\sqrt{\pm\epsilon_+\epsilon_-}}\exp\left[\frac{i\sqrt{m}}{3\hbar F}\left(\epsilon_+^3\pm\epsilon_-^3\right)\right], \quad (24.81)\end{aligned}$$

where in the last expression ϵ_+ and ϵ_- are given by Eq. (24.69). Since ϵ_+ is real and ϵ_- is imaginary, therefore in Eq. (24.77) we define the contour of integration so that the condition Im $\epsilon_-<0$ is satisfied. This is necessary in order for K to be well-defined. In this case (24.81) takes the simpler form of

$$G\left(\mathbf{r}_f,\mathbf{r}_i;E\right)=\frac{mF}{2\pi i\hbar^2}\left(\frac{1}{\epsilon_++\epsilon_-}\right)\frac{1}{\sqrt{\epsilon_+\epsilon_-}}\exp\left[\frac{i\sqrt{m}}{3\hbar F}\left(\epsilon_+^3+\epsilon_-^3\right)\right]. \quad (24.82)$$

When E is negative we know that only tunneling is possible, and here we discuss this possibility. Again if we choose $\mathbf{r}_i$ to coincide with the origin and $\mathbf{F}$ to be along the z-axis, then the tunneling takes place in the direction of the positive z-axis.

Using the parabolic coordinates [23], $\eta=r-z$ and $\xi=r+z$, we first write $W_{cl}^{\pm}$ as

$$W_{cl}^{\pm}(r,0;E)=\frac{\sqrt{m}}{3F}\left\{(F\xi+2E)^{\frac{3}{2}}\pm i\,(F\eta-2E)^{\frac{3}{2}}\right\}. \quad (24.83)$$

Here the particle moves from the energetically forbidden region, i.e. $r+z=-\frac{2E}{F}$ and enters the dynamically forbidden region. We have already found the Green function for the problem, Eq. (24.82), and we know that the wave function is proportional to this Green's function , thus

$$\psi(\mathbf{r},E)\propto\exp\left\{-\frac{\sqrt{m}}{3\hbar F}\left[F(r-z)-2E\right]^{\frac{3}{2}}\right\}\exp\left\{\frac{i\sqrt{m}}{3\hbar F}\left[F(r+z)+2E\right]^{\frac{3}{2}}\right\}, \tag{24.84}$$

where in (24.84) the prefactor for the exponential terms is not written. This wave function is a good approximation everywhere except in the vicinity of the turning surface $r+z=-\frac{2E}{F}$.

From Eq. (24.84) it is clear that the dependence of the wave function on the variable η and ξ is such that $|\psi(\mathbf{r},E)|^2$ depends only on η, the other variable $\xi=r+z$ appears in the phase of the wave function. Therefore on the surface $\eta=$ constant, $|\psi(\mathbf{r},E)|^2$ will remain constant. In addition from

$$|\psi(\mathbf{r},E)|^2\propto\exp\left\{-\frac{2\sqrt{m}}{3\hbar F}\left[F(r-z)-2E\right]^{\frac{3}{2}}\right\}, \tag{24.85}$$

one can conclude that the current in tunneling is limited only to the positive z-axis and its immediate neighborhood. Using the approximate form of η,

$$\eta=(r-z)=\sqrt{\rho^2+z^2}-z\approx\frac{\rho^2}{2z}, \tag{24.86}$$

and Eq. (24.85) we find the number of particles per unit volume to be proportional to

$$|\psi(\mathbf{r},E)|^2\approx\psi(z,0,E)|^2\exp\left(-\frac{2\kappa\rho^2}{2z}\right), \tag{24.87}$$

where

$$\kappa=\frac{\sqrt{-2mE}}{\hbar}, \tag{24.88}$$

is the inverse length for the problem.

An interesting result that we can get from (24.87) is that the average width of the tunneling current $d(z)$ which can be found from the uncertainty principle is

$$d(z)=\Delta x(z)=\sqrt{\frac{z}{\kappa}}, \tag{24.89}$$

where this $d(z)$ is only a function of the energy of the electron.

Finally from (24.87) it follows that the angular spread of the current filament i.e.

$$\alpha = \frac{d(z)}{z} = \sqrt{\frac{1}{\kappa z}}, \tag{24.90}$$

is inversely proportional to the square root of the distance between the source and the detector, i.e. z.

An experiment related to the solution of this problem is the following: A constant electric field draws electrons from a point source [19] [24], [25], [26] and at a constant rate of about 10^{12} electrons per second, and the current impinges on a screen located at a distance z from the source. The experimental result has verified the relation of the angular spread α to z, i.e. Eq. (24.90).

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Chapter 25

Examples from Condensed Matter Physics

Among the very large number of tunneling problems in solid state physics [1] [2] [3] we will briefly discuss three very important and yet conceptually simple problems. The first one is about the motion of electrons in a periodic potential which is similar to the problem of tunneling through a series of identical barriers discussed in Chapter 6, only now the number of barriers is infinite. Then we discuss the tunneling of electrons in a simple metal-insulator-metal structure . While, in principle, this should be formulated as a many-electron tunneling problem and the current associated with it, we observe that one encounters certain difficulties with such a formulation, and for this reason we replace it with a very simple model for such a tunneling. Finally we discuss an elementary theory of electron tunneling through heterostructures.

25.1 The Band Theory of Solids and the Kronig-Penney Model

Let us consider the solution of the Schrödinger equation with a periodic potential $V(x)$, and let a denote the periodicity of the lattice and the potential, i.e.

$$V(x+a) = V(x). \tag{25.1}$$

Then the solution of the Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} + \left[E - \frac{2m}{\hbar^2}V(x)\right]\psi(x) = 0, \tag{25.2}$$

can also be related to a periodic function with the periodicity a (Floquet's theorem [4], or Bloch's theorem [5]) .

There are a number of periodic potentials for which the Schrödinger equation is exactly solvable. Among these are:
(i) - $V(x) = V_0 \sin x$ for which the solution is given in terms of Mathieu's function [6].
(ii) - $V(x) = -V_0 \csc^2\left(\frac{\pi x}{a}\right)$ for which Eq. (25.2) can be solved in terms of the hypergeometric function [7].
(iii) - An infinite array of identical square wells or an infinite array of δ-functions [8].
Here for simplicity we consider (iii), where the potential is generated by the translation of

$$V(x) = \begin{cases} V_0 & \text{for } -b < x < 0 \\ 0 & \text{for } 0 < x < a-b \end{cases}, \tag{25.3}$$

on both sides of the x-axis (see Fig. (25.1)). As we have seen in Chapter 6, we solve the problem for the regions where $V(x) = V_0$ and also for the part where $V(x) = 0$ separately and then impose the conditions of continuity and periodicity of the wave function.

Let us first discuss the requirement of the periodicity. According to Bloch theorem [5] the solution of the Schrödinger equation (25.2) where $V(x)$ is periodic can be written as

$$\psi(x) = e^{ikx}u_k(x), \tag{25.4}$$

where $u_k(x)$ is periodic;

$$u_k(x) = u_k(x+a). \tag{25.5}$$

This means that the solution is a plane wave multiplied by a function $u_k(x)$ where $u_k(x)$ has the same periodicity as the lattice.

Now let us consider the solution of Eq. (25.2) in the region where $V(x) = 0$;

$$\psi_I(x) = Ae^{i\beta x} + Be^{-i\beta x}, \tag{25.6}$$

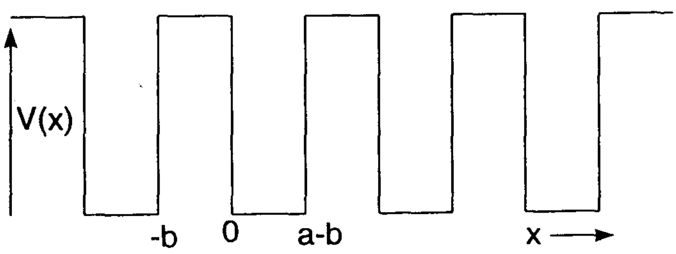

Figure 25.1: A periodic array of identical barriers of height V_0 and width b which is used as a model for a one-dimensional crystal.

where $\hbar\beta = \sqrt{2mE}$. The solution for the part where $V(x) = V_0$ is given by

$$\psi_{II}(x) = Ce^{\alpha x} + De^{-\alpha x}, \tag{25.7}$$

where

$$\alpha = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}. \tag{25.8}$$

For the continuity of ψ at $x = 0$ we have

$$\psi_I(0) = \psi_{II}(0), \tag{25.9}$$

and

$$\left[\frac{d\psi_I(x)}{dx}\right]_{x=0} = \left[\frac{d\psi_{II}(x)}{dx}\right]_{x=0}. \tag{25.10}$$

The periodicity requirement (25.4) and (25.5) can be expressed as

$$\psi_k(x+a) = e^{ika}\psi_k(x). \tag{25.11}$$

If we impose this requirement on the wave function at $x = -b$ and $x = a - b$, a lattice constant apart, we observe that

$$\psi_k(-b) = e^{-ika}\psi_k(a-b). \tag{25.12}$$

We incorporate this last condition in the continuity boundary condition linking the solutions at $x = -b$ and $x = a - b$. Thus we have

$$\psi_{II}(-b) = e^{-ika}\psi_I(a-b), \tag{25.13}$$

and

$$\left[\frac{d\psi_{II}(x)}{dx}\right]_{x=-b} = e^{-ika}\left[\frac{d\psi_I(x)}{dx}\right]_{x=a-b}. \tag{25.14}$$

Using these four boundary conditions, Eqs. (25.9), (25.10), (25.13) and (25.14) we find four equations for four unknowns;

$$A + B = C + D, \tag{25.15}$$

$$\alpha(C - D) = i\beta(A - B), \tag{25.16}$$

$$Ce^{-\alpha b} + De^{\alpha b} = e^{-ika}\left[Ae^{i\beta(a-b)} + Be^{-i\beta(a-b)}\right], \tag{25.17}$$

and

$$\alpha Ce^{-\alpha b} - \alpha De^{\alpha b} = i\beta e^{-ika}\left[Ae^{i\beta(a-b)} - Be^{-i\beta(a-b)}\right]. \tag{25.18}$$

This is a set of homogeneous equations in A, B, C and D. The nontrivial solution of the set of equations is possible only if the determinant of the coefficients is zero. Thus we have

$$\cos(ka) = \left(\frac{\alpha^2 - \beta^2}{2\alpha\beta}\right)\sinh(\alpha b)\sin[\beta(a-b)] + \cosh(\alpha b)\cos[\beta(a-b)], \tag{25.19}$$

where k is a real constant.

A simpler equation can be found when we take the limit of $V_0 \to \infty$ and $b \to 0$ in such a way that $V_0 b$ remains finite. This means that we replace the rectangular barrier with the δ-function barrier. In this limit Eq. (25.19) reduces to

$$P\frac{\sin(\beta a)}{\beta a} + \cos(\beta a) = \cos(ka), \tag{25.20}$$

where

$$P = \frac{mV_0 ba}{\hbar^2}, \tag{25.21}$$

is a dimensionless constant which is a measure of the strength of the potential. In Fig. (25.2), the left hand side of Eq. (25.20), i.e.

$$F(\beta) = P\frac{\sin(\beta a)}{\beta a} + \cos(\beta a) \tag{25.22}$$

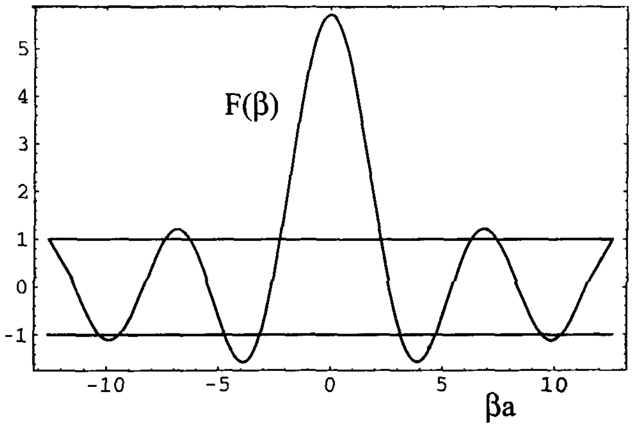

Figure 25.2: The function $F(\beta)$, Eq. (25.22), is plotted as a function of the dimensionless quantity βa. Here β^2 is proportional to the energy of the electron.

is plotted as a function of βa. Since $\cos(ka)$ changes between -1 and $+1$, therefore the acceptable solution of the problem are those parts of the βa-axis which satisfies the relation $-1 \leq F(\beta) \leq 1$.

Thus we reach the following results:

(i) - The energy spectrum of the electrons consists of a number of bands separated from each other by forbidden zones.

(ii) - The width of the allowed energy bands increases with increasing values of $\beta a = \frac{a}{\hbar}\sqrt{2mE}$.

(iii) - The width of a given band decreases with increasing P, i.e. increasing the binding energy of the electron.

25.2 Tunneling in Metal-Insulator-Metal Structures

In the physics of condensed matter tunneling in a system composed of metal-insulator-metal is of great importance [9]. In such an arrangement the insulator forms a barrier and the electron while moving from one metal to the other must tunnel through this barrier. For simplicity we assume that the

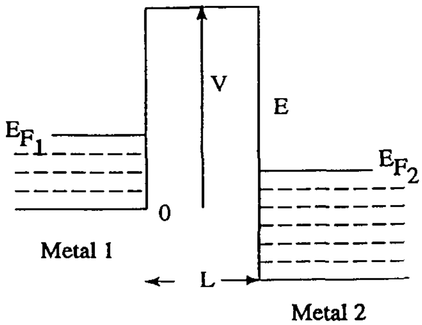

Figure 25.3: A simple metal- insulator -metal structure.

barrier is rectangular with the height V and width L. The two metals on the two sides of the insulator can be different, and for each metal the electrons occupy all of the avialable states up to the Fermi level. This arrangement is shown in Fig. (25.3). The energies E_{F_1} and E_{F_2} are the Fermi energies of the metals 1 and 2. If we place this structure in an external field $\mathcal{E}$, then the potential barrier changes to the shape shown in Fig. (25.4).

25.3 Many Electron Formulation of the Current

If we want to formulate the problem in a way that shows the flow of large number of electrons from the metal on the left to the metal on the right, we write the total Hamiltonian as [10]

$$H = H_L + H_R + H_T \tag{25.23}$$

where in this relation H_L and H_R are the Hamiltonians for the electrons of the left and of the right metals, and H_T is the Hamiltonian operators which shows the conduction of the electrons from left to the right. Since we have defined the Hamiltonian operators for the left and right separately, we have to specify the states for the left and right independent of each other. To simplify our formulation of the problem, instead of the barrier shown in

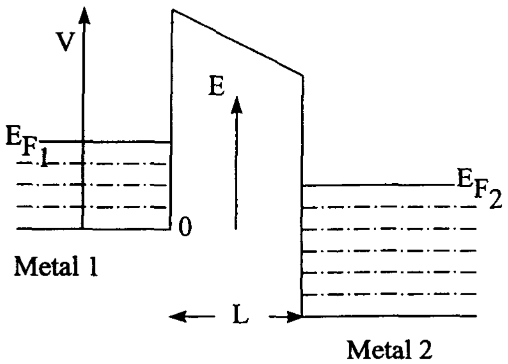

Figure 25.4: The metal-insulator-metal structure placed in an external electric field $\mathcal{E}$.

Fig. (25.3) we choose a confining potential and a barrier in the middle (Fig. (25.4)) and require the wave function to vanish at $|x| = a$. Next we want to see whether it is possible to impose the following conditions on these states [10]:
(i) - The wave functions for the left, in the left, and the wave functions for the right, in the right of the barrier form a complete set of states [10].
(ii) - Every wave function for the left be orthogonal to all the wave functions for the right, and vice versa, so that $[H_R, H_L] = 0$.
(iii) - Finally if we combine all these wave functions, we should have a complete set of states.

If we denote the wave function of an electron for the left by $\Psi_n^l(x)$, and for the right by $\Psi_n^r(x)$, then we can write the annihilation operator as

$$\Psi(x) = \sum_n \left[a_n \Psi_n^r(x) + b_n \Psi_n^l(x)\right]. \tag{25.24}$$

Making use of (25.24) and its complex conjugate, we can express H in second quantized form

$$\begin{aligned} H &= \int \Psi^\dagger(x)\left[\frac{p^2}{2m} + V(x)\right]\Psi(x)dx \\ &+ \frac{1}{2}\int\int \Psi^\dagger(x)\Psi^\dagger(x')W(x-x')\Psi(x')\Psi(x)dxdx'. \end{aligned} \tag{25.25}$$

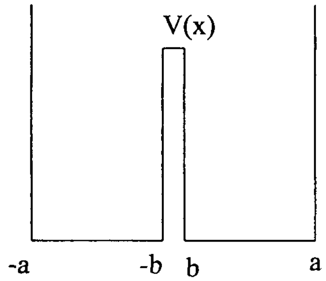

Figure 25.5: A simplified picture of the potential barrier $V(x)$ used for defining the current of electrons.

Now if we substitute for $\Psi(x)$ and $\Psi(x')$ in (25.25) and simplify we get a number of terms depending on a_n, $a_n^\dagger$, b_n and $b_n^\dagger$. We want to know whether it is possible to collect all the terms depending on a_n 's and $a_n^\dagger$'s only, this then will constitute H_R, and collect all terms with b_n's and $b_n^\dagger$'s only, which will be H_L, and the rest of the terms which will be called H_T. But a careful examination shows that such a grouping is not possible.

If the wave functions $\Psi_n^l(x)$ vanish for all positive values of x, either these wave functions do not form a complete set of states for negative x values or they cannot be well defined at $x = 0$. On the other hand if these $\Psi_n^l(x)$ are not zero for $x > 0$ they cannot be orthogonal to all $\Psi_n^r(x)$ (which according to our assumption form a complete set). Therefore we have to make these conditions weaker.

We can choose one of the following alternatives:
(i) - We can keep the condition of orthogonality for all of the states, but abandon the completeness condition for the left states and the right states. At the same time we can require these left- and right- sates be as complete as possible [10].
(ii) - Instead of (i) we can relax the orthogonality condition and replace it with the condition of "maximum orthogonality which is possible". Then we can impose the completeness of the left- and the right- states. If (ii) is adopted, then the commutation relation $[H_R, H_L]$ will not be zero, but it

will be proportional to H_T.

In order to express H, Eq. (25.23), in terms of $a_n^\dagger$, a_n, $b_n^\dagger$ and b_n we first note that the eigenstates for a particle which is moving in the simple symmetric potential (Fig. (25.3)) can be found from the solution of the general relation (7.7) which for this case simplifies to

$$\left[\cos(ka) - \frac{k}{q}\sin(ka)\right]^2 = e^{-2qb}\left[\cos(ka) + \frac{k}{q}\sin(ka)\right]^2, \tag{25.26}$$

where we have set $\hbar = 1$ and k^2 and q denote $2mE$ and $\sqrt{2m(V-E)}$ respectively. If we write Eq. (25.26) in the form of

$$\cot(ka) = \frac{k}{q}\left[\frac{1 \pm e^{-qb}}{1 \mp e^{-qb}}\right], \tag{25.27}$$

we observe that we can expand this equation in terms of the roots of the equation

$$\cot(\sqrt{2mE}a) = \frac{\sqrt{E}}{\sqrt{V-E}}. \tag{25.28}$$

Denoting the n-th root of (25.28) by E_n, from Eqs. (25.27) and (25.28) we can express the approximate solution of (25.27) as

$$E_n \pm T_{nn}, \tag{25.29}$$

where T_{nn} is given by

$$T_{nn} = \frac{2E_n\sqrt{2m(V-E_n)}}{mVa}\exp\left[-2b\sqrt{2m(V-E_n)}\right]. \tag{25.30}$$

In obtaining the approximate solution (25.29) we have assumed that the width of the well $2a$ is large. The quantities T_{nn} are the diagonal elements of the transition operator of Bardeen [10] [11].

Since the potential is symmetric we can write the eigenfunctions of the Hamiltonian as ψ_n^S and ψ_n^A for even and odd parity states. As we have already seen, a linear combination of ψ_n^S and ψ_n^A gives us a wave packet, which can be large on either the left or on the right of the barrier (see Eq.(7.10))

$$\Psi_n^{r,l}(x) = \frac{1}{\sqrt{2}}\left[\psi_n^A(x) \pm \psi_n^S(x)\right]. \tag{25.31}$$

Here $\Psi_n^l(x)$ and $\Psi_n^r(x)$ are wave packets with small tails in the right and the left well respectively. Now we write the Hamiltonian H as

$$\begin{aligned} H &= \sum_n E_n a_n^\dagger a_n + \sum_n E_n b_n^\dagger b_n \\ &- \sum_n T_{nn}\left(a_n^\dagger b_n + b_n^\dagger a_n\right) + W_L + W_R + W_T, \end{aligned} \tag{25.32}$$

where W_L, W_R and W_T are operators which specify the interaction between the three parts of the system. If we ignore these W operators, we can find the rate of change of the particles in the states to the right of the barrier;

$$\frac{dN_R}{dt} = \left(N_L^0 - N_R^0\right)\bar{T}\sin(2\bar{T}t). \tag{25.33}$$

To derive this relation we have assumed that the variation of T_{nn} as a function of time is gradual, and that its average value is $\bar{T}$. In addition the total number of electrons $N_R + N_L$ is constant and that initially $N_R(t = 0) = N_R^{(0)}$ and $N_L(t = 0) = N_L^{(0)}$.

Equation (25.33) shows that the rate of change of N_R is oscillatory while we know that for the case of metal-insulator-metal structure this rate must be constant. The source of this difficulty is the fact that $\Psi_n^r(x)$ is a wave packet which has a small tail to the left and this makes the constant flow of the electrons from left to the right negligible compared to the flow of the electrons because of the presence of this tail. Thus a formulation of the problem of the constant flow of electrons as a many-body problem presents certain difficulties. For other attempts to formulate this problem see [11] and [12].

We next study a simpler model where we consider the characteristic features of a Fermi-Dirac gas and calculate the current. In this approach we utilize three essential concepts:

(i) - For each metal we define a density of states per unit energy, $g(E)$.

(ii) - We know that the electrons obey the Fermi-Dirac statistics.

(iii) - In this model we assume that the insulator forms a barrier, and if this barrier is thin enough, when a potential difference is maintained between the two metals, the tunneling of the electrons is the main source of the electric current.

In order to calculate the current which passes through the insulator we need to know the number of electrons per unit time that reach the barrier and also need to know the transmission coefficient for the barrier. It is also convenient to measure the energies relative to the bottom of the conduction band in the metal to the left, but the final result is independent of the choice of the zeroth of energy. Since the problem is one-dimensional we measure the distance x inside the insulator from the surface of the metal 1 (on the left), and denote the momentum conjugate to x by p_x.

Let $2g(E, p_x)dp_x dE$ be the number of electronic states with energies between E and $E + dE$ and momentum between p_x and $p_x + dp_x$, where the factor of 2 in this relation is introduced for the two spin states of the electron. Then from this definition it follows that

$$g(E) = \int_{-\infty}^{\infty} g(E, p_x) dp_x. \tag{25.34}$$

The occupation probability for the electrons is given by the Fermi-Dirac function $f(E)$ [13]

$$f(E) = \left[1 + \exp\left(\frac{E - E_F}{k_B T}\right)\right]^{-1}. \tag{25.35}$$

Here k_B is the Boltzmann constant and T is the temperature in the Kelvin scale. The number of the occupied states is given by

$$2f(E)g(E, p_x)dE dp_x, \tag{25.36}$$

and the product of this quantity with the x-component of velocity, i.e. $\frac{p_x}{m}$ is the flux of electrons with momenta between p_x and p_x+dp_x as they approach the barrier;

$$\Phi(E, p_x) = 2\left(\frac{p_x}{m}\right) f(E)g(E, p_x)dE dp_x. \tag{25.37}$$

The probability that the electrons hitting the barrier will penetrate in it is directly proportional to the x-component but not to the y and z components of the momentum. If $|T(p_x)|^2$ is the coefficient of transmission through the barrier, which for simplicity is calculated in the WKB approximation, then the maximum number of electrons which can pass through this insulator per second is

$$|T(p_x)|^2 \Phi(E, p_x) = 2|T(p_x)|^2 \left(\frac{p_x}{m}\right) f(E)g(E, p_x)dE dp_x. \tag{25.38}$$

But the electrons can pass the barrier if there are unoccupied states on the other side, hence in order to determine the electron current we multiply (25.38) with the probability of finding these unoccupied states. If we choose the free electron model [14], then the probability of having unoccupied states in the second metal is given by $(1 - f(E))$ and is independent of p_x. Let $J(E, p_x)dE dp_x$ denotes the current in the insulator between the two metals for electrons with energies and momenta between E and $E+dE$ and p_x and $p_x + dp_x$, then we have

$$J(E,p_x)dEdp_x = 2|T(p_x)|^2 \left(\frac{p_x}{m}\right) f(E)g(E,p_x)\left[1 - f(E)\right] dEdp_x. \quad (25.39)$$

In addition to this current we have a current in the opposite direction, i.e. from metal 2 to metal 1. If we use the subscripts 1 and 2 for the metals to the left and to the right of the insulator (see Fig. 25.1), then the net current between the two metals is

$$\begin{aligned} J^{(n)}(E,p_x)dEdp_x &= 2|T(p_x)|^2 \left(\frac{p_x}{m}\right) \\ \times\ &\left\{f_1(E)g_1(E,p_x)\left[1 - f_2(E)\right] - f_2(E)g_2(E,p_x)\left[1 - f_1(E)\right]\right\} dEdp_x. \end{aligned} \quad (25.40)$$

As we mentioned earlier we measure the energies with respect to the bottom of the conduction band of metal 1. Thus $f_1(E)$ and $f_2(E)$ for a given E value are not equal since their Fermi energies E_{F_1} and E_{F_2} are not the same relative to the bottom of the energy band. On the other hand $|T(p_x)|^2$ depends only on $\sqrt{2mV - p_x^2}$ therefore it is the same for the current flowing from 1 to 2 or from 2 to 1, and thus in Eq. (25.40) this term has appeared as a common factor. The total current can be obtained if we integrate (25.40) over E and p_x;

$$J_t^{(n)} = \int\int J^{(n)}(E,p_x)dp_x dE. \quad (25.41)$$

To evaluate this integral we need to know $g(E)$ and $f(E)$. The function $f(E)$ which is the Fermi-Dirac distribution function and is given by (25.35) can also be written as

$$f(E) = \frac{\exp\left[-\frac{E-E_F}{k_BT}\right]}{1+\exp\left[-\frac{E-E_F}{k_BT}\right]}. \quad (25.42)$$

For the determination of the density of states $g(E)$ we observe that electrons are fermions, thus the number of the electrons having momenta between p_x and $p_x + dp_x$ is given by [13]

$$n(E,p_x)dp_x = \frac{\pi}{(2\pi\hbar)^3}\left(2mE - p_x^2\right) dp_x. \quad (25.43)$$

If we integrate this relation between $p_x = -\sqrt{2mE}$ and $p_x = \sqrt{2mE}$ we find

$$n(E) = \frac{\pi}{(2\pi\hbar)^3}\left[\frac{4}{3}(2mE)^{\frac{3}{2}}\right]. \quad (25.44)$$

which is a well known relation in statistical mechanics of the Fermi-Dirac particles [13]. The function $g(E, p_x)$ which is the density of states per unit energy can be found by calculating the partial derivative of $n(E, p_x)$ with respect to E,

$$g(E, p_x) = \frac{\partial n(E, p_x)}{\partial E} = \frac{2m\pi}{(2\pi\hbar)^3}. \tag{25.45}$$

By substituting Eqs. (25.40), (25.42) and (25.43) in (25.41), we find the total current to be

$$J_t^{(n)} = \frac{1}{2\pi^2\hbar^3}\int_0^\infty |T(p_x)|^2 p_x dp_x \int_{\frac{p_x^2}{2m}}^\infty [f_1(E) - f_2(E)]\, dE. \tag{25.46}$$

Now if we change the variables from E to ζ,

$$\zeta = \frac{E - E_F}{k_B T}, \tag{25.47}$$

we can carry out the last integral in (25.46);

$$I = k_B T \int_{\zeta_0}^\infty \frac{e^{-\zeta} d\zeta}{1 + e^{-\zeta}} = k_B T \ln\left[1 + \exp(-\zeta_0)\right], \tag{25.48}$$

where

$$\zeta_0 = \frac{\left(\frac{p_x^2}{2m} - E_F\right)}{k_B T}. \tag{25.49}$$

Combining (25.48) and (25.46) we find the following expression for the total current

$$J_t^{(n)} = \frac{k_B T}{2\pi^2\hbar^3}\int_0^\infty p_x |T(p_x)|^2 \ln\left[\frac{1 + \exp\left(\frac{2mE_{F_1} - p_x^2}{2mk_B T}\right)}{1 + \exp\left(\frac{2mE_{F_2} - p_x^2}{2mk_B T}\right)}\right] dp_x. \tag{25.50}$$

From Eq. (25.50) we can find the total current and its dependence on the temperature T and the potential barrier $V(x)$. For the special case when $V(x)$ is a rectangular barrier of height V_0 and width L, and the temperature is absolute zero, $T = 0$, we can simplify the above integral. Let us assume that $E_{F_1} > E_{F_2}$, then the total current J_t can be written as the integral

$$J_t^{(n)} = \frac{(E_{F_1} - E_{F_2})}{\left(2\pi^2\hbar^3\right)}\int_0^{\sqrt{2mE_{F_2}}} \exp\left[-\frac{2L}{\hbar}\sqrt{2mV_0 - p_x^2}\right] p_x dp_x$$

$$
- \frac{1}{\left(2\pi^2\hbar^3\right)} \int_{\sqrt{2mE_{F_1}}}^{\sqrt{2mE_{F_2}}} \exp\left[-\frac{2L}{\hbar}\sqrt{2mV_0 - p_x^2}\right]
\times \left(E_{F_1} - \frac{p_x^2}{2m}\right) p_x dp_x. \tag{25.51}
$$

Now if we define the parameters α_1, α_2, and α_3 by the following relations

$$
\alpha_1 = \frac{2}{\hbar}\sqrt{2mV_0}, \tag{25.52}
$$

$$
\alpha_2 = \frac{2}{\hbar}\left[2m\left(V_0 - E_{F_1}\right)\right]^{\frac{1}{2}}, \tag{25.53}
$$

and

$$
\alpha_3 = \frac{2}{\hbar}\left[2m\left(V_0 - E_{F_2}\right)\right]^{\frac{1}{2}}, \tag{25.54}
$$

we can calculate the above integrals, and then J_t takes the form

$$
J_t(T=0) = \frac{\hbar}{64\pi^2 mL^4}\left\{\left[e^{-\alpha_1 L}L^2(\alpha_2^2 - \alpha_3^2)\right](1+\alpha_1 L)\right\}
+ \frac{2\hbar}{64\pi^2 mL^4}\left\{(3+\alpha_2^2L^2+3\alpha_2 L)e^{-\alpha_2 L} - (3+\alpha_3^2 L^2 + 3\alpha_3 L)e^{-\alpha_3 L}\right\}. \tag{25.55}
$$

We observe that if $E_{F_1} = E_{F_2}$, i.e. the Fermi surfaces of the two metals are equal then $\alpha_2 = \alpha_3$ and consequently $J_t(T=0) = 0$.

If such a structure is placed in a uniform external electric field $\mathcal{E}$, Fig. (3.4), then we can use Eq. (25.50), but now $T(p_x)$ is given by

$$
T(p_x) = \exp\left[-\frac{2}{\hbar}\int_0^L \sqrt{2m(V_0 - \mathcal{E}) - p_x^2}\, dx\right], \tag{25.56}
$$

provided that

$$
V_0 - \mathcal{E}L > 0, \tag{25.57}
$$

or

$$
T(p_x) = \exp\left[-\frac{2}{\hbar}\int_0^{x_1} \sqrt{2m(V_0 - \mathcal{E}) - p_x^2 dx}\right], \tag{25.58}
$$

where x_1 is the turning point

$$
V_0 - \mathcal{E}x_1 < \mathcal{E}L. \tag{25.59}
$$

25.4 Electron Tunneling Through Heterostructures

As the last problem of this section let us consider the very important case of resonant tunneling of electrons through quantum well structures [15] [16] [17] [18]. An example of such a heterostucture is provided by a double barrier formed from layers $GaAs - GaAlAs - GaAs - GaAlAs - GaAs$. We denote the length of this double barrier, i.e. $GaAlAs - GaAs - GaAlAs$ by L and the separation between the two barriers by d. We also assume that the potential is constant outside the hetrostructure and we take it to be zero at the left and $-V$ at the right when the bias voltage is applied.

The one-dimensional motion of an electron with the effective mass m^* moving from left to the right is given by the Schrödinger equation

$$\frac{-\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \qquad (25.60)$$

For solving this differential equation numerically we choose the finite difference method, i.e. we replace (25.60) by the difference equation

$$\frac{\psi(n+1) + \psi(n-1) - 2\psi(n)}{\Delta^2} = \frac{2m^*}{\hbar^2}[E - V(n)]\psi(n), \qquad (25.61)$$

where Δ is the setp size, $\Delta = \frac{L}{N}$, and N is a large integer. Defining q and Q by

$$q = \frac{\sqrt{2m^*E\Delta^2}}{\hbar} \quad \text{and} \quad Q = \frac{\sqrt{2m^*(E+V(N))\Delta^2}}{\hbar}, \qquad (25.62)$$

we can write the boundary conditions for (25.60) as

$$\psi(n) = \begin{cases} e^{iqn} + Re^{-iqn} & \text{for } n \le 0 \\ Te^{iQn} & \text{for } n \ge N \end{cases}. \qquad (25.63)$$

For calculating R and T we write (25.61) as a matrix equation

$$\begin{bmatrix} \psi(n+1) \\ \psi(n) \end{bmatrix} = \begin{bmatrix} \alpha(n) & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \psi(n) \\ \psi(n-1) \end{bmatrix} = P_n \begin{bmatrix} \psi(n) \\ \psi(n-1) \end{bmatrix}, \qquad (25.64)$$

where

$$\alpha(n) = 2 + \frac{2m^*\Delta^2}{\hbar^2}[V(n) - E]. \qquad (25.65)$$

By iterating (25.64) we find

$$\begin{bmatrix} \psi(N+1) \\ \psi(N) \end{bmatrix} = P_N ....P_0 \begin{bmatrix} \psi(0) \\ \psi(-1) \end{bmatrix} = Z(N) \begin{bmatrix} \psi(0) \\ \psi(-1) \end{bmatrix}. \tag{25.66}$$

In this equation $Z(N)$ is a 2×2 matrix with elements Z_{ij}. From Eqs. (25.63) and (25.66) we obtain

$$|R(E)|^2 = \left| \frac{Z_{12}e^{-iq} + Z_{11} - Z_{21}e^{iQ} - Z_{22}e^{i(Q-q)}}{Z_{11}e^{-iq} + Z_{12} - Z_{22}e^{iQ} - Z_{21}e^{i(Q-q)}} \right|^2, \tag{25.67}$$

then the transmission coefficient can be found from

$$|T(E)|^2 = 1 - |R(E)|^2 . \tag{25.68}$$

As a specific example consider the heterostructure system where

$$V(x) = V_0(x) = \begin{cases} V_0 & \text{for } 0 < x < \frac{L-d}{2} \\ 0 & \text{for } \frac{L-d}{2} < x < \frac{L+d}{2} \\ V_0 & \text{for } \frac{L+d}{2} < x < L \end{cases}, \tag{25.69}$$

and is zero otherwise (Fig.(25.6 (a))). For $L = 150$ *Angstrom*, $d = 50$ *Angstrom* $V_0 = 0.25\ eV$ and for $m^* = 0.067m$, where m is the mass of a free electron, one finds discrete quasi-bound states for the electron trapped between the barriers. The potential given in (25.69) is for the unbiased device. If we apply a constant electric field, $\frac{xV}{L}$, to the sample then $V(x)$ becomes

$$V(x) = \begin{cases} 0 & \text{for } x < L \\ V_0(x) - \frac{x}{L}V & \text{for } 0 < x < L \\ -V & \text{for } x > L \end{cases}. \tag{25.70}$$

Here $V > 0$ is the applied bias (see Fig (25.6(b))). By varying the applied voltage V, we observe that the current as a function of V changes as is depicted in Fig. (25.7).

We have already seen that the current depends on $|T(E)|^2$ (Eqs. (25.39) and (25.40)). For a small applied voltage the tunneling probability of the electrons with energies near the Fermi energy E_F is very small, and thus little current flows through the sample. By increasing V we reach a point where the Fermi energy is about the same as the energy of the quasi-bound state of the system, i.e. when $|T(E)|^2 = 1$. Under this condition the maximum amount of current flows through the system. Further increase in the bias voltage lowers $|T(E)|^2$ and therefore the current decreases accordingly.

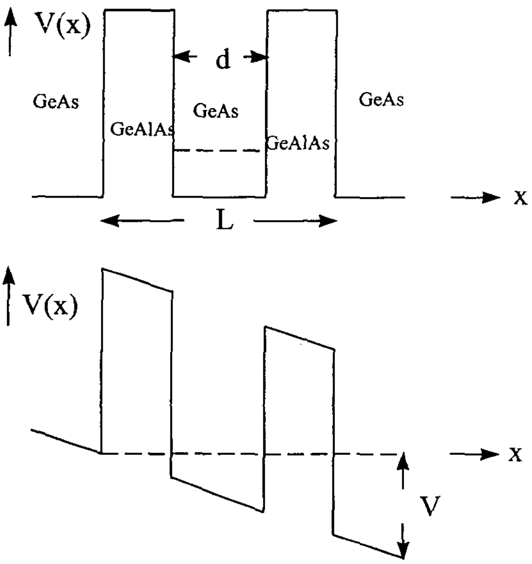

Figure 25.6: The potential energy in the double-well heterostructure (a) unbiased case and (b) when an external constant field is applied to the sample.

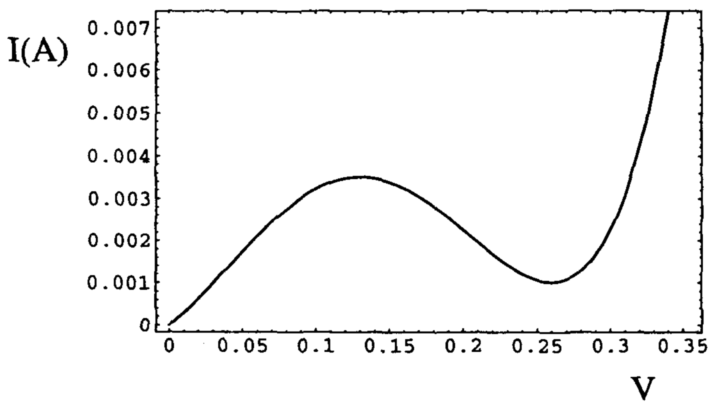

Figure 25.7: Typical current-voltage for the resonant tunneling diode

By applying a stronger external field we reach a situation where thermionic emission current becomes dominant and the current increases rapidly (Fig. (25.7)).

The interesting part of the voltage-current curve is the negative resistance region which is of great interest for low power high speed digital devices and for generating microwaves.

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Chapter 26

Alpha Decay

As we mentioned in our historical review of the subject of quantum tunneling, R.E. Rutherford in 1908 showed that α particles are indeed the nucleus of He^4. There are three chains of radioactive elements which can be found in nature. These are uranium, actinium and thorium. In these three chains there are thirty α-emitting nuclei. They start with U^{238}, U^{235} and Th^{232} and after a number of transmutation these nuclei end up with Pb^{206} , Pb^{207} and Pb^{208} (for the condition of stability of nuclei see [1]). Since there are 82 protons in the lead, the Pb nucleus is stable.

One of the important characteristics of α-decay is that the half-life of these radioactive substances can vary by many orders of magnitude. If Γ is the probability of the decay in a second then $\tau = \frac{\ln 2}{\Gamma}$ is the half-life . When there are a number of ways that a given nucleus can decay and the i-th way of the decay has the corresponding Γ_i, then the total decay constant of the nucleus is $\Gamma_t = \sum_i \Gamma_i$.

As an example of the large variation in the half-life of nuclei let us consider the Po^{213} nucleus which by emitting α particles of energy $8.336 MeV$ decays and its half-life is $4.2 \times 10^{-6} s$ or 1.33×10^{-13} years. On the other hand the Th^{232} nucleus emits α particles of energy $3.98 MeV$ and has a half-life of about 1.39×10^{10} years [2] [3] [4].

In spite of its large variation the half-life of α-decay is very long compared to the typical times of nuclear motion, whereas the former varies between $10^{-6} s$ to $10^{17} s$ the latter is about $10^{-21} s$. Thus the α-decay can be considered as a quasi-stationary process.

Now let us study the dynamics of this decay. Inside the nucleus the α

particles are affected by a potential for which the exact shape or strength is not known. But we do know that this potential is of short range, i.e. it is appreciable only in a finite radius R which we call it the nuclear radius [5] [6].

Outside this range the α particle is subject to electromagnetic forces. If we assume that the electric charge of the nucleus is distributed uniformly inside a sphere and is static, then the α particle feels the Coulomb potential,

$$V_c = \frac{2Ze^2}{r}. \tag{26.1}$$

In this relation Z is the electric charge of the daughter nucleus [5] [7] and r is the distance between the center of the α nucleus and the center of charge of the nucleus. However this is an approximation, since the protons inside the nucleus are in motion and therefore the potential is neither static nor symmetric. Thus in general we have to include higher multipoles in our calculation of Γ. The most important of these higher multipoles is the contribution of quadrupole moment with its corresponding potential

$$V_Q = \frac{2Qe^2}{r^2}P_2(\cos\Phi), \tag{26.2}$$

where Q is the quadrupole moment and Φ is the angle between $\mathbf{r}$ and the axis of the nucleus. The quadrupole moment Q is proportional to the square of the radius of the nucleus R, and the potentials V_c and V_Q are both defined for $r > R$ [8]. Hence to the first order of approximation we can ignore V_Q compared to V_c, and only use V_Q as a small perturbation in the calculation of the tunneling rate.

Inside the nucleus there are no stable α particles, but there are clusters of particles and that these clusters are changing with time. The probability of formation of certain clusters are more likely than others. If we denote the wave function for a certain cluster i by Ψ_i and if $p_i = |\alpha_i|^2$ is the probability of formation of this cluster, then the wave function of the nucleus is $\Psi = \sum_i \alpha_i\Psi_i$. Occasionally two protons and two neutrons combine to form an α particle. There is a small probability that this α particle will be emitted and a large probability that it will break up into other particles or system of particles. If we assume that Ψ_i is the wave function for a certain cluster which contains an α particle and if $\Gamma_i^{(0)}$ is the probability of emission of this α particle with the energy E_i, from the observed decay rate we find Γ_i, where

$$\Gamma_i = p_i\lambda_i^{(0)} = |\alpha_i|^2\lambda_i^{(0)}. \tag{26.3}$$

So there are two parts to the theoretical determination of the α decay rate:
(i) - The problem of calculation of the formation factor p_i from the knowledge of nuclear forces . With our present knowledge of the nuclear forces and nuclear structure this is a difficult problem to formulate and solve.
(ii) - Calculation of $\lambda_i^{(0)}$ which can be done in quasi-stationary approximation.

Let us suppose that an α particle has been formed in the nucleus and we want to calculate its decay rate. In order to solve this problem we need to know not only the Coulomb force V_c outside the nucleus but also the interaction between the α particle and the nucleus. Since the latter is not sufficiently well known, for the sake of simplicity we choose a constant potential to represent this interaction,

$$V(r) = V_0, \quad r < R. \tag{26.4}$$

The dynamics of this system, i.e. α particle plus nucleus can be described by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r), \tag{26.5}$$

where

$$m = \frac{m_\alpha m_z}{m_\alpha + m_z}, \tag{26.6}$$

is the reduced mass of the system and m_α and m_z are the masses of the α particle and the nucleus respectively, and E is the energy of the α particle. Since the force is central we can write the wave function $\psi(r)$ in terms of the partial waves $u_l = r\psi_l$. The resulting equation can be solved for the wave function inside the nucleus ;

$$u_l = rj_l(Kr), \quad K = \frac{\sqrt{2m(E+V_0)}}{\hbar}, \quad r < R, \tag{26.7}$$

and for the outside $u_l(r)$ is the solution of

$$\frac{d^2u_l}{d\rho^2} + \left(1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right)u_l = 0, \tag{26.8}$$

where $\rho = kr, \quad k = \frac{\sqrt{2mE}}{\hbar}$ and

$$\eta = \left(\frac{2Ze^2}{\hbar}\right)\left(\frac{m}{2E}\right)^{\frac{1}{2}}. \tag{26.9}$$

In general Eq. (26.8) has two independent solutions, one which is finite at $\rho = 0$ and we denote it by F_l and the other which is infinite at $\rho = 0$ and this we denote by G_l. These so called Coulomb wave functions have the following asymptotic properties [9],

$$F_l \to \sin\left[\rho - \frac{l\pi}{2} - \eta\ln(2\rho) + \delta_l\right], \text{ as } \rho \to \infty, \tag{26.10}$$

and

$$G_l \to \cos\left[\rho - \frac{l\pi}{2} - \eta\ln(2\rho) + \delta_l\right], \text{ as } \rho \to \infty. \tag{26.11}$$

In these relations δ_l is given by

$$\delta_l = \arg\Gamma\left(l + 1 + i\eta\right). \tag{26.12}$$

The solution of (26.8) which satisfies the outgoing boundary condition (i.e. Gamow wave function) is a linear combination of F_l and G_l,

$$u_l = N_l(G_l + iF_l), \quad r > R, \tag{26.13}$$

where N_l is the normalization constant. At the nuclear radius, R, the two solutions (26.7) and (26.13) should join smoothly, i.e. their logarithmic derivatives at $r = R$ must be equal

$$\frac{1}{j_l(KR)}\left[\frac{d}{dr}\left\{rj_l(Kr)\right\}\right]_{r=R} = \frac{kR}{\left(G_l + iF_l\right)_{r=R}}\left[\frac{d}{d\rho}\left(G_l + iF_l\right)\right]_{r=R}. \tag{26.14}$$

From (26.14) we can find the complex eigenvalues $E_l - \frac{i}{2}\Gamma_l$ for different l values. A simpler way of solving the tunneling through the Coulomb barrier is by using the WKB approximation (Chapter 3), which is a good approximation for the calculation of these eigenvalues provided that in the definition of the effective potential in (26.8) we replace $l(l+1)$ by $(l+\frac{1}{2})^2$. Consider the nucleus N_Z^A which consists of Z protons and $A - Z$ neutrons. We know that the radius of such a nucleus is [7]

$$R = A^{\frac{1}{3}}R_0. \tag{26.15}$$

in which R_0 is about 1.2 *Fermis* ($1.2 \times 10^{-15}m$). The charge of the α particle is $2e$ and the charge of the daughter nucleus is $(Z-2)e$, and when Z is large we can approximate it by Ze. Thus the Coulomb potential at the nuclear radius is equal to

$$V_m = \frac{2Ze^2}{R} = \frac{2Z}{A^{\frac{1}{3}}}\frac{e^2}{R_0} \approx 3\frac{Z}{A^{\frac{1}{3}}} \quad (MeV). \tag{26.16}$$

For instance for U^{238}, where $A = 238$ and $Z = 92$, V_m is approximately equal to $30MeV$. This nucleus is radioactive and emits α particles with energy of 4.3 MeV. Using Gamow's formula (Eq. (5.11) we can calculate the decay width and the half-life of U^{238} which turns out to be 10^{10} years. But as it can be seen from Gamow's formula, this half-life is very sensitive to the energy of the α particle. Compare this half-life with that of Po^{212} which emits α particles with the energy of 8.9 MeV and has a half-life of only $3 \times 10^{-7}s$. This sensitivity is the result of the rapid decrease of the width of the barrier with increasing of energy (see Fig. (5.1)), and the exponential dependence of the tunneling probability on the integral over the width of the barrier, Eq. (5.11).

Using (5.11) we can write Γ as [10]

$$\Gamma = \frac{8(E+V_0)\hbar}{\sqrt{2mR\left(2Ze^2 - ER\right)}} \exp\left(-2\sigma\right), \tag{26.17}$$

where m is the reduced mass of the α particle, Eq. (26.6), and σ is given by

$$\sigma = 2\int_R^b \sqrt{\frac{2m}{\hbar^2}\left(\frac{2Ze^2}{r} - E\right)}dr, \tag{26.18}$$

and b is the classical turning point

$$b = \frac{2Ze^2}{E}. \tag{26.19}$$

We can evaluate the integral in (26.18) and write σ as

$$\sigma = \left[\frac{32mZ^2e^4}{E\hbar^2}\right]^{\frac{1}{2}} \left\{\cos^{-1}\sqrt{\frac{R}{b}} - \sqrt{\frac{R}{b} - \left(\frac{R}{b}\right)^2}\right\}. \tag{26.20}$$

For low energies i.e. as $E \to 0$, the width of the barrier $b - R$ will be large, and in this limit σ has a simple form. Thus if v_α is the velocity of the emitted α particle then

$$\sigma \approx \frac{4\pi Ze^2}{\hbar v_\alpha}. \tag{26.21}$$

We can relate $\tau = \frac{\ln 2}{\Gamma}$ to the energy E using Eqs. (26.17) and (26.21);

$$\ln \tau = B - \frac{C}{\sqrt{E}}, \tag{26.22}$$

and this is the relation found by Geiger and Nuttall in the early days of experimental work on α decay . In Eq. (26.22) B and C are dependent on

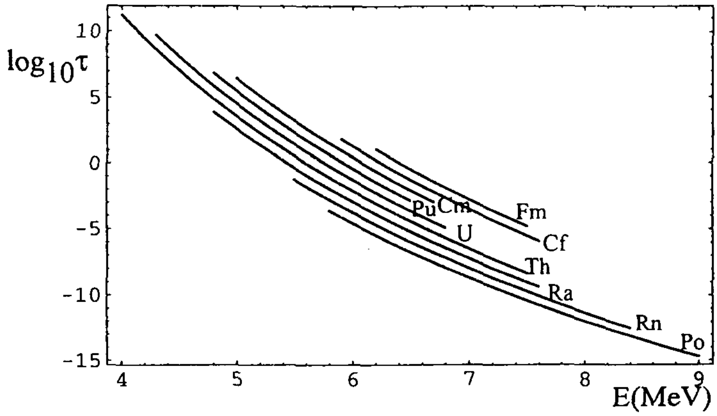

Figure 26.1: The half-lives of different chains of α emitters are shown as a function of the energy of the emitted α particle.

Z but are independent of energy E. In particular if E is measured in MeV and τ in years, then the best fit to τ for the α-emitter nuclei is given by

$$\log_{10}\tau = A(ZE^{-\frac{1}{2}} - Z^{\frac{2}{3}}) - B, \tag{26.23}$$

when the constants A and B are 1.61 and 28.9 respectively. In Fig. (26.1) the half-lives of the nuclei that decay with α emission are shown starting with Po_{84}^{212} and ending with Fm_{100}^{254}.

A more accurate form of the Geiger-Nuttall [11] relation which is obtained from Eqs. (26.17) and (26.18) and is valid for the whole range of lifetime of the isotopes is found by Biswas [12]. For instance for polonium Po_{84}^{216} the relation between the decay rate and the energy of the emitted α particle can be written as

$$\begin{aligned} \log_{10}\Gamma &= 38.0664 - \frac{89.71}{\sqrt{E}}\cos^{-1}(0.1923\sqrt{E}) + \frac{1}{2}\log_{10}E - 0.3225E, \\ & 5.2 \le E \le 8.944. \end{aligned} \tag{26.24}$$

This expression fits well with the experimental points in the middle, $E \sim 6\ MeV$ but on both sides diverges, thus showing that this simple picture of α decay fails to account for very short-lived elements as well as very long-lived ones.

The time-dependent theory of α-decay can be formulated along the lines presented in Chapter 5 (see also [13] [14] and [15] [16]).

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Index

α particle, 536
α particle, 531–533, 535
α-decay, 411, 531, 535, 537
α-emitter, 536

action
relativistic, 458
Airy function, 32, 87, 374, 496, 497
alpha decay, xxi, 53, 475, 531
ammonia maser, xx, 497
ammonia molecule, 485, 498, 499
analytic continuation, 302
anharmonic oscillator , 270
annihilation operator, 517
anti-instanton, 232, 234
antibound, 434
antibound state, 167, 435
applied bias, 526
$AsCl_3$, 500
AsH_3, 500
asymmetric double-well, 260, 267, 290
asymmetric double-wells, 251, 255, 261
asymmetric potential, xvi, 46
asymptotic expansion
of the Bessel function, 27
asymptotic form, 27, 122, 175
atomic clock, 402

ballistic motion, 501
band theory, 511
band theory of solids, xx
barrier
asymmetric, 391
delta function, 434
impenetrable, 434
opaque, 367
rectangular, 87, 375, 404
spherically symmetric, 413
square, 401
time-dependent, 387
barriers
identical, 513
basis set , 257, 262
Bender-Dunn algebra, 256
Bessel function, 26, 153, 194, 265, 286, 441
spherical, 444
beta function, 474
$BiCl_3$, 500
Bloch theorem, 512
Bohr-Sommerfeld quantization rule, xvii, 41, 42, 46, 49, 479
Boltzmann function, 278
boson, xx
bounce, 233
bound state with positive energy, 68
boundary condition
outgoing, 2
Breit-Wigner, 226
Breit-Wigner form, 58

Brueckner method, 116

canonical coordinates, 242
canonical momentum, 241
canonical variables, 242
causality, 462, 466, 467
causality condition, 462, 464
causality, the violation of, 365
CH_2, 486
C_2H_4, 485
$CHClFBr$, 500, 501
Chebyshev polynomial, 94
classical action, 220
classical path, 219, 324
classical trajectory, 278, 280, 316
closed channels, 155, 416
coefficient of transmission, 222, 474, 476, 521
coherent phase, 393
coherent tunneling, 105, 109, 446
cold emission, xx, 488
cold emission current, 491
commutation relation, 253, 256, 257, 261, 268
complex barrier, 132
complex eigenvalues, 167, 478
complex path, 332
complex scaling, xix, 297
complex time, 237, 459, 502
conduction band, 522
conjugate variables, 253
conservation of energy, 179
conservation of probability, 117, 154
conservation of the probability
    law of, 84
Cooper pairs, 4
Coulomb wave function, 534
coupled channel resonances, 476
current density, 490
cylindrical symmetry, 124

Darboux transformation, 128, 129
Darboux's method, 127
daughter nucleus, 532, 534
DeBroglie wavelength, 393
decay
    nonexponential, xvii
    probability of, 171
decay amplitude, 185
decay rate, 1, 532, 536
decay width, xix, 1, 43, 56, 167, 168, 173, 297, 302, 460, 479, 497
decaying states, xviii
decaying system, 56
decy width, 461
degenerate states, 445
degrees of freedom, xvii, xviii, 139, 284
delta-function, 242
delta-function barrier, 83
delta-function potential, 82, 160
density of states, 520, 522
diatomic molecule, xx, 392, 418
digamma function, 374
dilatation transformation, xix, 297, 298, 300
Dirac equation, xx, 453
dispersive medium, 339
distribution function, 278, 291
    Margenau-Hill, 292
    Wigner, 292
double-well potential, 48
    asymmetric, 108
    symmetric, 108
double-well potential , 45
dwell time, 382, 385
dynamically forbidden motion, 502

effective Hamiltonian, 284
effective mass, 525

effective potential, 43, 142
Ehrenfest theorem, 289
eigenvalue equation, 55, 106
eigenvalues
  complex, 53, 131, 330, 476
  discrete, 53
  distinct, 93, 112
electron emission, 488
electron tunneling
  through hetrostructures, xx
enantiomorph, 500
energetically forbidden region, 505
energy band, 515
energy levels
  non-degenerate, 268
  noncommesurable, 260
energy splitting, 231, 235
error function, 19, 81
ethylene molecule, 485
Euclidean action, 227
Euclidean formulation, 240
Euclidean path integral, xviii, 226
exclusion principle, 343
expectation value, 258–260
exponential law, 1
extended paths, 220, 222, 223

Fermi energy, 488, 516, 522, 526
Fermi level, 516
Fermi sphere, 490
Fermi surface, 524
Fermi-Dirac distribution function, 522
Fermi-Dirac function, 521
Fermi-Dirac gas, 520
Fermi-Dirac particles, 523
Fermi-Dirac statistics, 520
fermion, xx, 522
Feynman
  path integration, xviii
field emission, 475
finite difference method, 525
Floquet's theorem, 150
forbidden paths, 245
forbidden region, 221, 224
forbidden zone, 515
force
  state-dependent, 288
forerunner wave, 342
Fourier integral, 244
Fourier series, 150
Fourier transform, 172, 220, 226, 238, 245, 277, 279, 400, 402, 467, 472, 473, 495, 496
free electron gas, 488
free electron model, 521
front velocity, 339

GaAs, 525
GaAlAs, 525
Galiliean invariant, 281
gamma function, 43, 374, 474
Gamow, 2, 53
Gamow formula, 43, 56, 66, 168, 535
Gamow states, 57, 415, 479, 481
Gamow wave function, 60, 534
Gaussian approximation, 290
Gaussian function, 143
Gaussian integral, 228
Gaussian potential, 431
Gaussian wave packet, 126, 127, 144, 252, 254, 258, 260, 264, 280, 282–284, 289, 345, 366, 405, 462, 467
Geiger -Nuttall relation, 535
Geiger-Nuttall formula, xxi
Geiger-Nuttall formula, 2
Geiger-Nuttall relation, 536

Gel'fand-Levitan kernel, 124
Gel'fand-Levitan method, 124, 126
generating function, 395
generator
of the transformation, 241
Green function, 79, 113, 172, 181, 495, 505
Green's function, 171, 463, 505
free particle, 80
Green's theorem, 60
group velocity, 339, 347
Gurney and Condon, 3

half-life, 1, 531, 535, 536
Hamilton canonical equation, 281
Hamilton characteristic function, 318
Hamilton's canonical equations, 141, 280, 289
Hamilton's characteristic function, 501
Hamilton-Jacobi coordinates, 241
Hamilton-Jacobi equation, 308, 316, 318, 324, 501
Hamiltonian, 142, 184, 241, 251, 258, 262, 263, 268, 298, 300, 302, 317, 381, 386, 393, 396, 398, 403, 411, 419, 495, 503, 516, 519
classical, 141
Hermitian, 129
Hamiltonian operator, 157, 226, 253, 373, 393, 395, 419
Hamitonian, 516
Hankel function, 320
harmonic oscillator
multidimensional, 312
Hartman effect, 383
Hartree-Fock method, 116
He, 531
Heisenberg picture, 476
Heisenberg's equation, xviii, 251
Helmhotz equation, 441
Hermite polynomial, 395, 431
Hermitian, 281
Hermitian adjoint, 298
Hermitian Hamiltonian, 56
Hermitian operator, xx, 3, 373, 381
heterostructure, 149, 525–527
heterostructures
tunneling through, 525
hypergeometric function, 97, 512

identical barriers, 284
imaginary phase, 240
imaginary time, 226, 237, 238, 332, 458, 502
impenetrable boundaries, 439
impenetrable surface of rotation, 440
incident channel, 152
infinitesimal generator, 298
instanton, 232–235, 503
integral equation, 206
interaction time, 394, 396
internal degrees of freedom, 392, 411, 418
internal energy of a simple molecule, 392
intrinsic time, 394, 395
inverse problem of tunneling, 471, 479, 481
ionization, 492, 493
ionization of atoms, xx, 458, 491

Jost function, 61, 62, 167

Kapur and Peierls method, 307, 311, 312, 327
Klein's method, 267
Klein-Gordon equation, 462

Kronig-Penney model, 511
Kummer equation, 100

Lagrangian, 251, 278, 332
Laplace transform, 80, 179, 463, 465
Laplacian, 325
Larmor frequency, 389
Larmor precession, 388–390
law of conservation of probability, 60
layered semiconductors, xviii
level spacing, 440, 478
level splitting, 35
loosely bound molecule, 422, 425, 428
Low and Mende's tunneling time, 402, 461
low-lying eigenvalues, 269, 486

magnetic field, 389, 392
many electron tunneling, 511
Margenau-Hill distribution function, 277, 292, 293
Mathieu's function, 512
matrix equation, 525
metal-insulator-metal structure, xx, 511, 515–517, 520
method of characteristics, 280, 324
Miller-Good method, xvii, 23, 31, 66, 222
minimum tunneling time, xx, 351, 375, 377
Mittag-Leffeler's theorem, 62
molecule
  homonuclear, 421, 429, 434
momentum space, 278
Moshinsky function, 61, 63, 81, 161
most probable escape path, xix, 327–329
multichannel tunneling, 205, 368
multidimensional tunneling, 307, 318
multiple reflections, 225, 404

negative resistance, 528
Newton's laws of motion, 237
NH_3, 498
non-degenerate eigenvalues, 445
nuclear forces, 533
nuclear radius, 534
number density, 175

opaque barrier, 383
open channels, 155, 416
operator equation, xix
optical isomer, 500, 501
optical potential, 129
outgoing boundary condition, 42, 53, 56

Paley and Wiener theorem, 12
parabolic cylinder function, 119
parabolic cylinder function, 33, 42, 159
path
  classical, 316
path integral, 219, 240–242
path integral method, 231
Pauli matrices, 453
Pb^{206}, 531
Pb^{207}, 531
periodicity of the wave function, 513
periodicity of the wavefunction, 512
perturbation, 185, 318, 396, 402
perturbation theory, 167, 184
PH_3, 500
phase shift, 352, 354, 372
phase space, 241, 260, 266, 278, 280, 281, 284, 292
phase space trajectory, 261, 286

phase time, 382, 383
phase velocity, 339
Po^{216}, 536
positive energy bound states, 66
potential
    δ-function, 300, 326
    asymmetric, xvii, xx, 105, 121, 125, 127, 131, 143, 419, 424–426, 447
    asymmetric double-well, 114, 119, 126
    central, 222
    centrifugal, 263
    confining, xvi, xix, 73, 75, 105, 121, 142, 251, 261
    Coulomb, 491, 532
    cubic, 251, 252, 289
    cut-off, 207, 213
    delta-function, 79, 84, 85, 473
    double-well, 121, 125, 128, 232, 237, 287–289, 347, 424, 439, 485, 486
    double-well Morse, 99
    Eckart, 96, 99, 245
    effective, xviii, 168, 170, 320, 446
    effective radial, 264
    harmonic, 254
    linear, xx, 87, 373
    matrix, 412, 414
    non-confining, 99, 121
    noncentral, 328
    nonlocal, 112, 116
    nonsymmetric, 205
    optical, 128, 131
    oscillating, 488
    periodic, 150, 486, 511, 512
    quadratic, 374
    quartic, 251, 252, 259
    quasi-solvable, 121, 285
    rectangular, 88, 154
    reflectionless, 355
    separable, 116, 119, 300, 383
    step, 348, 454–456
    sum of inverse powers, 252, 261
    symmetric, xvii, xx, 105, 121, 127, 128, 143, 255, 285, 290, 419, 421, 425
    symmetric double-well, 114, 317, 445
    time-dependent, 205, 385
    triangular, 489
    velocity-dependent, 112
    von Neumann and Wigner, 67
    Yukawa, 300
    multi-well, xvi
potential barrier
    oscillating, 152
potentials
    time-dependent, xviii
potntial
    nonconfining, 73
probability, 405
    time-dependence of, 108
probability amplitude, 12
probability current, 154
probability density, 112
probability of tunneling, 264, 432
Prony method, 477, 478
Prony's method, 259, 260, 476
propagator, 225, 240, 495
    approximate form, 221
    Feynman, 219
    semi-classical, 243

quadrupole moment, 532
quantal trajectory, 284
quantum clock, xx, 398
quantum coherence, 255, 261
quantum hopping, 255, 261, 424

quasi-bound state, 526
quasi-solvable, 121, 486
quasi-stationary, xvii, 77, 173, 174, 531
quasi-stationary states, 471
quasilinear approximation, 327
quasilinearization, 323
 method of, 318, 322, 323

radiating boundary condition, 53
radioactive state, 57
radioactivity
 source of, 56
rectangular barrier, xix, 11, 282, 377, 382, 399, 404, 456, 462, 514, 516
rectangular barriers, 283
 identical, 90
recurrence relations, 123
reflection coefficient, 354
reflection amplitude, 151, 156, 206, 213, 382, 389, 391, 392, 394, 397, 401, 403, 473
reflection coefficient, 83, 98, 392, 400
 for Eckart potential, 99
reflection phase time, 383
reflection time, xx, 351, 371, 391
reflection time operator, 371
relativistic correction, 453, 458
relativistic effects, 458
relativistic quantum tunneling, xx, 453
resolving power, 399
resonance, 58, 89, 370
resonance states, 19
resonant condition, 131, 426, 428
resonant energy, 384
resonant pole, 299
resonant tunneling, 4, 84, 95, 110, 149, 211, 525
resonant tunneling diode., 527
Riccati equation, 24, 25
rotation of spin, 389
rotation of the spin, 392
Rutherford, 1

S-matrix, 167, 297
saddle point, 244
scattering matrix, 151
scattering theory, xviii, 167
Schrödinger equation, 14
Schrödinger operator, 157
Schrödinger equation, 42, 49, 53, 56, 57, 60, 61, 67, 68, 73, 74, 79, 82, 84, 86, 96, 97, 112, 116, 124, 125, 128, 152, 158, 167, 193, 194, 213, 219, 242, 258, 267, 271, 298, 301, 307, 308, 315, 319, 322, 323, 327, 330, 332, 340, 342, 343, 345, 354, 358, 360, 371, 372, 374, 375, 392, 394, 402, 419, 430, 439, 479, 486, 489, 511, 512, 533
 time-dependent, 107, 140, 149, 157, 168, 184, 279, 386, 412, 493
Schrödingrer equation, 525
Schwinger's method, xix, 362
second quantized form, 517
self-adjoint operator, 252
semi-classical approximation, xvii, 221, 225, 244, 357, 376, 446, 474, 479
semi-classical limit, 228, 231
semiconductor, 149
semiconductor structures, 339

separable potential, 118
signal velocity, 339, 342, 343, 347
single-valued, 326
sojourn time, 382
spinless particle, 458
splitting of the energy levels, xix, 38, 49, 439, 446, 485, 498, 500
state-dependent force, 289
stationary phase, 66, 220, 239, 504
steepest decent
  line, 309, 310
  method of, 344
step function, 206, 375, 494
supercurrent, 5
superluminal speed, 467
superluminal velocity, 463
superposition principle, 58
surface of rotation, 440
symmetric double-well, 231, 258, 259, 267, 290, 411
symmetric double-wells, 251
symmetric potential, xvi, 48, 49, 268

Th^{232}, 531
thermionic emission, 528
tightly bound molecule, 423, 426, 427
time of arrival, 238, 345, 346, 467
time of reflection
  classical, 374
time reversal, 281
time reversal transformation, 268, 285
time-delay, xix, 201, 351, 352, 354–357, 361–363, 365, 367, 368, 370, 434
time-dependent barrier, 149
time-dependent barrier, 151, 157
time-dependent problems, 79
time-energy uncertainty, 11
torsional oscillations of a molecule, xx
torsional vibration of a molecule, 485
trajectories
  ensemble, 289
trajectory, 223, 313, 315, 502
  phase space, 284
  complex, 460
  phase space, 126, 127, 143, 146
trajectory of the particle, 221, 459
transfer matrix, 90, 91
transition operator, 519
transmission amplitude, 87, 88, 151, 156, 206, 213, 366, 382, 389, 394, 397, 403, 473
transmission coefficient, 83–85, 117, 354, 400, 429, 471, 490, 520
  for two rectangular barriers, 89
  resonance, 90
transmission phase time, 383, 384
transmission probability, 388, 390
transmission time, 391
transmitted wave, 457
trapped particle, 225
travel time, xx, 404
traversal time, 390
tridiagonal matrix, 487
tunnel diode, 4
tunneling
  classical description, 139
  coherent, xix, 107
  dissipative, 251
  many-channel, 212
  multi-channel, 206
  of a molecule, 205
tunneling of a simple molecule, 418

Tunneling time, 396
tunneling time, 282, 394, 398
turning plane, 502
two-channel problem, 416
two-channel system, 413, 415, 478

U^{235}, 531
U^{238}, 531, 535
uncertainty principle, xvi, 505
uncertainty relation, 402
unitary operator, 158
unitary transformation, 157

variable reflection amplitude, 207, 211, 472
variable reflection coefficient, xx, 431, 434
variable transmission amplitude, 208
variational principle, 309
virial theorem, 298

wave function
  time-dependent, 56
wave packet, 56
  localized, 107
Whittaker function, 374
Wigner distribution function, xix, 277, 278, 280, 281, 284, 285, 287, 290, 291
Wigner inequality, xix
Wigner phase space trajectory, 285, 291
Wigner trajectory, 284, 288, 289
WKB, 66, 376
WKB approximation, xvii, 3, 23, 31, 46, 55, 124, 176, 212, 220, 221, 233, 236, 307, 311, 312, 320, 346, 352, 355, 386, 391, 394, 443, 481, 489, 521, 534
  many-channel problems, 215
WKB connection formula, 321
WKB method, 26, 46
Wronskian, 87, 464

zero eigenvalue, 236