

Tunnelling Times in Quantum Mechanics

James Puleston

April 7, 2020

1 Time in Quantum Mechanics

1.1 Time in Classical Mechanics

In the Hamiltonian formulation of classical mechanics, a system with n degrees of freedom possesses $2n$ independent first-order differential equations in terms of $2n$ independent variables. These variables are the coordinates of the *phase space* of the system, and the $2n$ equations of motion describe the evolution of system in the phase space. n of the independent variables are conventionally chosen to be the generalised coordinates q_i and the other n set to be the conjugate momenta p_i , which obey the Poisson bracket relations (Goldstein 2002):

$$\{q_i, p_j\} = \delta_{ij} \quad \{q_i, q_j\} = \{p_i, p_j\} = 0, \quad i, j = \{1, \dots, n\} \quad (1)$$

The time evolution of the canonical variables is governed by the Hamiltonian $H = H(q_i, p_i)$:

$$\frac{dq_i}{dt} = \{q_i, H\} \quad \frac{dp_i}{dt} = \{p_i, H\} \quad (2)$$

For an infinitesimal variation in time, $\delta t = \delta\tau$, the associated variation in the dynamical variables is:

$$\delta q_i = \{q_i, H\}\delta\tau \quad \delta p_i = \{p_i, H\}\delta\tau \quad (3)$$

q_i and p_i are generalised variables; they are not necessarily positions and momenta, but in the case of a dynamical system comprised of a collection of point particles, the canonical variables are usually the particles' positions (\mathbf{q}_i) and momenta (\mathbf{p}_i).

In classical mechanics, physical systems are embedded in a 4-dimensional continuous space-time background, the points of which are assigned coordinates $(t, x, y, z) = (t, \mathbf{x})$. It is essential that the *definitions* of these two spaces and their associated coordinates are not conflated (Hilgevoord 2002). In particular we must distinguish the position variable \mathbf{q} from the space-time coordinate \mathbf{x} . The former defines a point in the phase space of the system (when accompanied by its associated momentum \mathbf{p}) and is a property of a point particle, whereas the latter is the coordinate of a fixed point in the space-time background in which the dynamical system is embedded. Note we can still introduce both sets of quantities in to equations and relate them, as equations (2) and (3) show.

Immediately this raises the question of whether there exists physical systems that possess a dynamical variable that *resembles* the time coordinate of space-time. Such systems are called *clocks*, more precisely defined as physical systems with a dynamical 'clock' or 'time' variable that behaves similarly to the space-time time coordinate t under time translations. For example, under time translation in which the space-time coordinates transform as (cf. Hilgevoord 2002, (9), (10), (11)):

$$\mathbf{x} \rightarrow \mathbf{x} \quad t \rightarrow t + \tau \quad (4)$$

a *linear* clock variable θ and its conjugate momentum η transform as:

$$\eta \rightarrow \eta \quad \theta \rightarrow \theta + \tau \quad (5)$$

Comparing with (3) we see in the infinitesimal case of (5):

$$\delta\eta = \{\eta, H\}\delta\tau \quad \delta\theta = \{\theta, H\}\delta\tau \quad (6)$$

which implies

$$\{\eta, H\} = 0 \quad \{\theta, H\} = 1 \quad (7)$$

The equation of motion given by (2), $\frac{d\theta}{dt} = 1$ has solution $\theta = t + t_0$.

1.2 Time in Quantum Mechanics

3 definitions for time in QM? In quantum mechanics the state of a particle is encoded in a vector $|\psi\rangle$ in Hilbert space \mathcal{H} . Introducing a 1-dimensional continuum position basis to \mathcal{H} , $\{|q\rangle\}$, $q \in \mathbb{R}$, the state vector $|\psi\rangle$ can be expanded as the integral Sakurai (2017):

$$|\psi\rangle = \int_{\mathbb{R}} dq \psi(q) |q\rangle \quad (8)$$

where $\psi(q)$ is the wave function of the particle. More generally, to describe a system in 3 dimensions requires a wave function $\psi(q_x, q_y, q_z)$. It is important to note that the domain of the wave function is the *configuration space* of the system, \mathbb{R}^3 , whose coordinates are the generalised coordinates q_i of the system. It is common in elementary quantum mechanics literature for elements of the domain of the wave function to be expressed as (x, y, z) , i.e. $\psi = \psi(x, y, z)$. This is clearly in notational conflict with the use of (x, y, z) as coordinates of points of the background space-time in which the quantum system resides. In agreement with the literature surveyed in this essay I retain this notation throughout, but the distinction between space-time coordinates and dynamical variables should be maintained.

Measurable quantities or ‘observables’ are represented by operators on \mathcal{H} :

$$\mathcal{O} : \mathcal{H} \rightarrow \mathcal{H} \quad (9)$$

Such operators arise through a procedure called canonical quantisation, which prescribes that *dynamical variables* of the Hamiltonian formalism are promoted to operators on \mathcal{H} and their Poisson bracket relations replaced by commutation relations according to:

$$\{, \} \rightarrow \frac{1}{i\hbar} [,] \quad (10)$$

One notable omission in this process is the promotion of the time coordinate t to an operator. Given the emphasis placed on distinguishing between space-time coordinates and dynamical variables, the reason is clear: time t is a *space-time coordinate*, and canonical quantisation prescribes that *dynamical variables* are promoted to operators. However this raises the question of whether a time operator exists in quantum mechanics. The resolution of this problem has been historically hindered by a ‘proof’ offered by Wolfgang Pauli showing that the introduction of a time operator in quantum mechanics is forbidden. It proceeds roughly along the following lines:

Add Pauli proof c.f. Butterfield On Time in Quantum Physics

Observing that this issue arose from attempts to erroneously quantise the *space-time* coordinate t , the problem becomes void and progress can be made by considering the quantisation of timelike *dynamical variables* of physical systems, namely clocks in analogy with the case in classical mechanics mentioned above.

Despite this clarification, approaches to the question *how long does a quantum particle take to tunnel through a classically forbidden potential barrier?* have not yielded a satisfactory answer universally agreed upon by the physics community. The question can be more formally posed as *when a particle with energy less than the barrier potential traverses the barrier region and is ultimately transmitted, how much time did it, on the average, spend in the barrier region?* Many solutions to this question have been offered within the orthodox interpretation of quantum mechanics. In section 2.1 I describe the physical system (quantum tunnelling experiment) of interest, and in sections 2.2-2.6 I survey of definitions within the orthodox viewpoint. The de Broglie-Bohm interpretation of quantum mechanics offers a clear and unambiguous answer to the question at hand. In section 3.1 I introduce the requisite theory, in section 3.2 I present the natural

definition of tunnelling time within the de Broglie-Bohm interpretation, and in section 3.3 I conclude with a numerical analysis of a quantum tunnelling experiment.

2 Tunnelling Times in the Orthodox Interpretation

In this section I survey a number of contenders for calculating the tunnelling time through a barrier. The definitions in sections 2.2-2.5 are ‘intrinsic’ quantities, in that they make no reference to a measuring apparatus (other than the implied particle detector to determine whether or not an incident electron is eventually transmitted) (Leavens 1996). Section 2.6 offers an ‘experimental’ definition, making reference to a specific physical system.

2.1 Tunnelling Through a Quantum Barrier

Throughout this essay I use the physical system described in (Büttiker 1983). The systems used in other literature surveyed in this essay differ by choice of coordinates and/or barrier location and have been recalculated for the physical system used throughout.

Consider the case of scattering in one dimension with particles of mass m , velocity $v(k) = \frac{\hbar k}{m}$ and kinetic energy $E = \frac{\hbar^2 k^2}{2m}$. The particles move in the positive y direction and interact with a rectangular barrier:

$$V = \begin{cases} V_0 & -\frac{d}{2} < y < \frac{d}{2} \\ 0 & \text{otherwise} \end{cases} \quad (11)$$

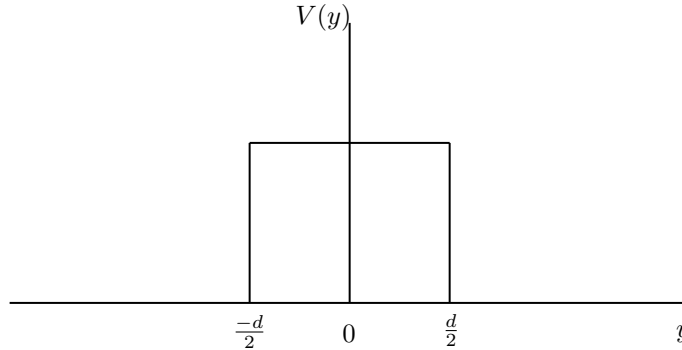


Figure 1: The quantum potential barrier

Note that $E < V_0$ such that this system describes a quantum tunnelling experiment.

The wave function is of the form:

$$\psi(y, k) = \begin{cases} e^{iky} + Ae^{-iky} & y \leq -\frac{d}{2} \\ Be^{\kappa y} + Ce^{-\kappa y} & -\frac{d}{2} \leq y \leq \frac{d}{2} \\ De^{iky} & y \geq \frac{d}{2} \end{cases} \quad (12)$$

where $k = \frac{\sqrt{2mE}}{\hbar}$, $\kappa := \frac{\sqrt{2m(V_0-E)}}{\hbar} = \sqrt{k_0^2 - k^2}$ where $k_0 = \frac{\sqrt{2mV_0}}{\hbar}$ and A, B, C, D are functions of the variables of the system.

The coefficient of the incident wave is set to one, corresponding to one particle per unit length in the incident beam. Note there is no e^{-iky} term on the right of the barrier, as no particles are reflected after being transmitted through the barrier.

Calculation of the wave function coefficients A, B, C, D uses the continuity of the wave function and its first derivative at the barrier boundaries. The results are frequently stated without proof in the literature, but will be used so frequently in this essay that I provide a derivation:

$$\begin{aligned}
D &= T^{\frac{1}{2}} e^{i\Delta\phi} e^{-ikd} & A &= R^{\frac{1}{2}} e^{-i\pi/2} e^{i\Delta\phi} e^{-ikd} \\
B &= \frac{\kappa + ik}{2\kappa} e^{ikd/2} e^{-\kappa d/2} D & C &= \frac{\kappa - ik}{2\kappa} e^{ikd/2} e^{\kappa d/2} D
\end{aligned} \tag{13}$$

where T is the transmission probability and $R = 1 - T$ is the reflection probability (Büttiker 1983).

Proof. First I introduce a new coordinate system so that the boundaries of the barrier become $0, d$ i.e. $\tilde{y} = y + \frac{d}{2}$. Then, denoting the wave functions to the left of, inside, and to the right of the barrier as ψ_1, ψ_2, ψ_3 respectively, yields:

$$\psi_1 = e^{-ikd/2} e^{ik\tilde{y}} + \tilde{A} e^{-ik\tilde{y}} \quad \psi'_1 = ik e^{ikd/2} e^{ik\tilde{y}} - ik \tilde{A} e^{-ik\tilde{y}} \tag{14a}$$

$$\psi_2 = \tilde{y} B e^{\kappa\tilde{y}} + \tilde{C} e^{-\kappa\tilde{y}} \quad \psi'_2 = \kappa \tilde{B} e^{\kappa\tilde{y}} - \kappa \tilde{C} e^{-\kappa\tilde{y}} \tag{14b}$$

$$\psi_3 = \tilde{D} e^{ik\tilde{y}} \quad \psi'_3 = ik \tilde{D} e^{ik\tilde{y}} \tag{14c}$$

where $\tilde{A} = A e^{ikd/2}, \tilde{B} = B e^{-\kappa d/2}, \tilde{C} = C e^{\kappa d/2}, \tilde{D} = D e^{-ikd/2}$.

Imposing continuity of the wave function and its first derivative at the barrier boundaries:

$$\psi_1(0) = \psi_2(0) \implies e^{-\frac{ikd}{2}} + \tilde{A} = \tilde{B} + \tilde{C} \tag{15a}$$

$$\psi'_1(0) = \psi'_2(0) \implies ik e^{-\frac{ikd}{2}} - ik \tilde{A} = \kappa \tilde{B} - \kappa \tilde{C} \tag{15b}$$

$$\psi_2(d) = \psi_3(d) \implies e^{\kappa d} \tilde{B} + e^{-\kappa d} \tilde{C} = e^{ikd} \tilde{D} \tag{15c}$$

$$\psi'_2(d) = \psi'_3(d) \implies \kappa e^{\kappa d} \tilde{B} - \kappa e^{-\kappa d} \tilde{C} = ik e^{ikd} \tilde{D} \tag{15d}$$

$$\tag{15e}$$

$$ik(15a) + (15b) \implies 2ike^{-ikd/2} = (ik + \kappa) \tilde{B} + (ik - \kappa) \tilde{C} \tag{15f}$$

$$\kappa(15c) + (15d) \implies 2\kappa e^{\kappa d} \tilde{B} = (\kappa + ik) e^{ikd} \tilde{D} \tag{15g}$$

$$\kappa(15c) - (15d) \implies 2\kappa e^{-\kappa d} \tilde{C} = (\kappa - ik) e^{ikd} \tilde{D}. \tag{15h}$$

Inserting equations (15g) and (15h) into equation (15f) one arrives at:

$$2ike^{-ikd/2} = -\frac{(ik - \kappa)^2}{2\kappa} e^{(ik+\kappa)d} \tilde{D} + \frac{(ik + \kappa)^2}{2\kappa} e^{(ik-\kappa)d} \tilde{D} \tag{16a}$$

$$\implies 4ik\kappa e^{-ikd} e^{-ikd/2} = \tilde{D}[(k^2 - \kappa^2)(e^{\kappa d} - e^{-\kappa d}) + 2ik\kappa(e^{\kappa d} + e^{-\kappa d})] \tag{16b}$$

$$= \tilde{D}[2(k^2 - \kappa^2) \sinh \kappa d + 4ik\kappa \cosh \kappa d]. \tag{16c}$$

Hence one arrives at the first result, the transmission probability $T = |\tilde{D}|^2 (= |D|^2)$:

$$T = \left[1 + \frac{(k^2 + \kappa^2)^2 \sinh^2 \kappa d}{4k^2 \kappa^2} \right]^{-1} \tag{17}$$

\tilde{D} can be written in polar form $\tilde{D} = |\tilde{D}| e^{i\theta} = T^{\frac{1}{2}} e^{i\theta}$.

$$\tilde{D} = \frac{2ik\kappa e^{-ikd} e^{-ikd/2} [(k^2 - \kappa^2) \sinh \kappa d - 2ik\kappa \cosh \kappa d]}{(k^2 - \kappa^2)^2 \sinh^2 \kappa d + 4k^2 \kappa^2 \cosh^2 \kappa d} \tag{18a}$$

$$\implies \theta = \arg(\tilde{D}) = \arctan\left(\frac{\text{Im}(\tilde{D})}{\text{Re}(\tilde{D})}\right) = -\frac{3ikd}{2} + \arctan\left(\frac{k^2 - \kappa^2}{2k\kappa} \tanh \kappa d\right) \tag{18b}$$

Evaluating the phase change across the barrier:

$$\Delta\phi := \text{Arg}(|\tilde{D}|e^{i\theta}e^{ikd}) - \text{Arg}(e^{-ikd/2}) = -\frac{3ikd}{2} + \arctan\left(\frac{k^2 - \kappa^2}{2k\kappa} \tanh \kappa d\right) + ikd - \frac{-ikd}{2} \quad (19a)$$

$$= \arctan\left(\frac{k^2 - \kappa^2}{2k\kappa} \tanh \kappa d\right) \quad (19b)$$

Hence

$$\tilde{D} = T^{\frac{1}{2}} e^{i\Delta\phi} e^{-3ikd/2} \quad (20a)$$

$$D = T^{\frac{1}{2}} e^{i\Delta\phi} e^{-ikd} \quad (20b)$$

The result for A follows along similar lines and results for B and C follow immediately from equations (15g) and (15h). \square

2.2 Phase Times

Plane wave solutions to the quantum potential barrier (12)(13) are delocalised over all space. Superposition of plane waves with different momenta k yields waves which are localised in space, called wave packets. For example, one can construct a Gaussian wave packet from plane waves e^{iky} :

$$\psi(t, y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \phi(k) e^{i(ky - w(k)t)} \quad w(k) = \frac{\hbar k^2}{2m} \quad (21a)$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \psi(0, y) e^{-iky} \quad \psi(0, y) = e^{-y^2 + ik_0 y} \quad (21b)$$

$$= \frac{1}{\sqrt{2}} e^{-(k - k_0)^2 / 4} \quad (21c)$$

where $\psi(0, y)$ is the initial profile of the wave function and $\phi(k)$ is the Fourier coefficient which is assumed to be sharply localised around k_0 .

In this instance the integral in (21a) can be accurately calculated by Taylor expansion of the dispersion relation around k_0 to first order. However this will not necessarily work for other plane waves, for example those in (12). To progress one can use the stationary phase approximation; given Fourier coefficient $\phi(k)$ sharply localised around $k = k_0$, the integral (cf. (21a)) has non-zero value by dint of contributions from the integrand only in the region $k \approx k_0$, only if the plane wave term oscillates on scales larger than the region around k_0 (the wave phase is ‘stationary’ in k -space).

Applying this method to the incident and transmitted plane waves in (12)(13) (accounting for time evolution under the time evolution operator $U(t) = e^{-iEt/\hbar}$) yields:

$$\text{Incident:} \quad -\frac{1}{\hbar} \frac{dE}{dk} t + y_p(t) = 0 \quad (22a)$$

from which one derives the group velocity of the wave packet $v_g = \frac{1}{\hbar} \frac{dE}{dk} = \frac{\hbar k}{m}$. This is the propagation velocity of the envelope wave and is identified with the particle velocity. This differs from the phase velocity $v_p = \frac{w}{k}$ which is the propagation velocity of the carrier wave.

$$\text{Transmitted:} \quad \frac{d\Delta\phi}{dk} - \frac{1}{\hbar} \frac{dE}{dk} t + y_p(t) - d = 0 \quad (22b)$$

(cf. Hauge and Støvneng 1989 (2.3)). Solving equations (22a) and (22b) for t at $y_p(t) = -\frac{d}{2}$ and $\frac{d}{2}$ respectively, one finds that the difference of these times, i.e. the traversal time of the peak across the barrier for the transmitted wave, is:

Gaussian Wavepacket with Fourier coefficient

$$\phi(k) = \frac{e^{-\frac{1}{4}(k-k_0)^2}}{\sqrt{2}}, \quad t=0, \quad k_0=20, \quad m=1 \quad (\hbar=1)$$

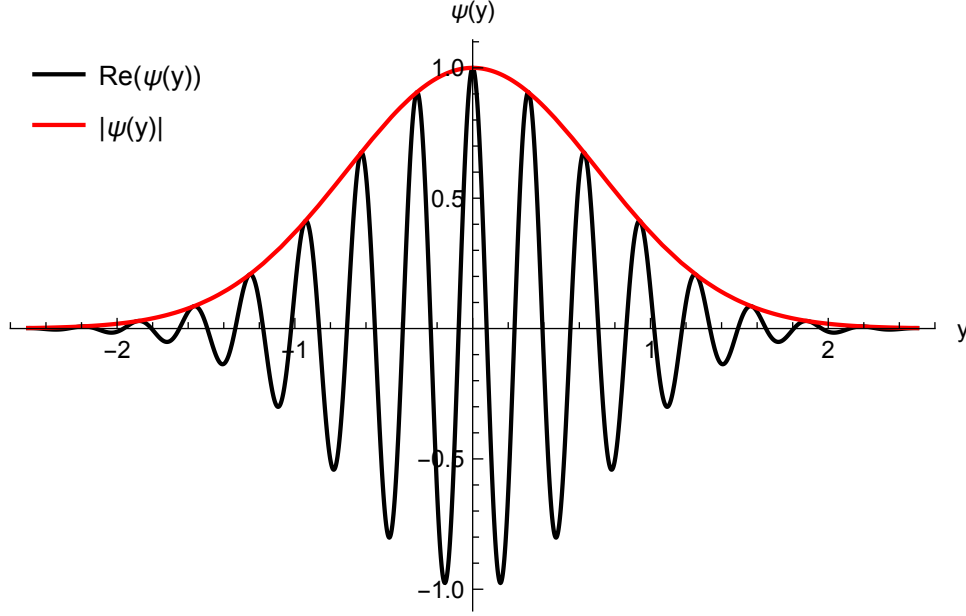


Figure 2: Gaussian wave packet (21a) showing the carrier wave (black) and amplitude modulating envelope wave (red).

$$\tau_\phi = \hbar \frac{d\Delta\phi}{dE} = \frac{m}{\hbar k} \frac{d\Delta\phi}{dk} \quad (23)$$

(An identical result is obtained for a wave packet reflected from the barrier.) (cf. Büttiker 1983 (3.1)). Equation (23) can be calculated explicitly using equation (19b):

$$\frac{m}{\hbar k} \frac{d\Delta\phi}{dk} = \frac{m}{\hbar k} \frac{d}{dk} \left(\arctan \left[\frac{k^2 - \kappa^2}{2k\kappa} \tanh \kappa d \right] \right) \quad (24a)$$

$$= \frac{m}{\hbar k} \frac{1}{\left[\frac{k^2 - \kappa^2}{2k\kappa} \tanh \kappa d \right]^2 + 1} \frac{1}{2} \frac{d}{dk} \left(\frac{k^2 - \kappa^2}{k\kappa} \tanh \kappa d \right) \quad (24b)$$

Recalling the relation between k and κ in (12), the derivative term evaluates to:

$$\left[2\kappa^{-1} + \frac{k^2}{\kappa^3} + \frac{\kappa}{k^2} \right] \tanh \kappa d + d \left(-\frac{k^2}{\kappa^2} + 1 \right) \text{sech}^2 \kappa d \quad (24c)$$

Hence

$$\frac{m}{\hbar k} \frac{d\Delta\phi}{dk} = \frac{m}{2\hbar k} \frac{4k^2\kappa^2 \text{sech}^2 \kappa d}{(k^2 - \kappa^2)^2 \tanh^2 \kappa d + 4k^2\kappa^2} \left\{ \left[2\kappa^{-1} + \frac{k^2}{\kappa^3} + \frac{\kappa}{k^2} \right] \sinh \kappa d \cosh \kappa d - \frac{kd}{\kappa} \left(\frac{k}{\kappa} - \frac{\kappa}{k} \right) \right\} \quad (24d)$$

$$= \frac{2m\kappa\kappa^2}{\hbar} \frac{1}{k_0^4 \sinh^2 \kappa d + 4k^2\kappa^2} \left\{ \left[2\kappa^{-1} + \frac{k^2}{\kappa^3} + \frac{\kappa}{k^2} \right] \frac{\sinh 2\kappa d}{2} - \frac{kd}{\kappa} \left(\frac{k}{\kappa} - \frac{\kappa}{k} \right) \right\} \quad (24e)$$

The term in $\{\dots\}$ is easily shown to be:

$$\{\dots\} = \frac{k_0^4}{k^2\kappa^3} \frac{\sinh 2\kappa d}{2} + \frac{d}{\kappa} (\kappa^2 - k^2) \quad \text{where } k_0^2 := k^2 + \kappa^2 \quad (24f)$$

yielding the final result:

$$\tau_\phi = \frac{m}{\hbar k \kappa} \frac{2k^2 \kappa d (\kappa^2 - k^2) + k_0^4 \sinh 2\kappa d}{4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d} \quad (24g)$$

This is defined as the phase-delay time of the scattering process (cf. Büttiker (1983) (3.2)). The same result is achieved via a different approach by Hauge and Støvneng (1989); they introduce an interval (y_1, y_2) containing the barrier (i.e. $y_1 < \frac{-d}{2}, y_2 > \frac{d}{2}$) and using (22a) and (22b) define (cf. Hauge and Støvneng (1989) (2.4)) the spatial delay δy_T as the change in phase induced by the barrier and corresponding temporal delay $\delta \tau_T$ for the transmitted wave packet:

$$\delta y_T = \frac{d\Delta\phi}{dk} - d \quad \delta \tau_T = \frac{1}{v(k)} \left[\frac{d\Delta\phi}{dk} - d \right] \quad \text{where } v(k) = \frac{\hbar k}{m} \text{ is the group velocity} \quad (25)$$

with analogous definitions for the reflected wave packet:

$$\delta y_R = d - \frac{d\Delta\phi}{dk} \quad \delta \tau_R = -\frac{1}{v(k)} \left[d - \frac{d\Delta\phi}{dk} \right] \quad (26)$$

They subsequently define (cf. Hauge and Støvneng (1989) (2.5, 2.6)) the total phase time for transmission:

$$\tau_T(x_1, x_2; k) = \frac{1}{v(k)} [x_2 - x_1 + \delta y_T] \quad (27)$$

and similarly the total phase time for reflection:

$$\tau_R(x_1, x_2; k) = \frac{1}{v(k)} [-2x_1 - \delta y_R] \quad (28)$$

where the minus sign before the spatial delay is picked up due to the wave packet travelling in the opposite direction.

By linearly extrapolating the interval $(y_1, y_2) \rightarrow (-\frac{d}{2}, \frac{d}{2})$, one defines the *extrapolated phase times* (cf. Hauge and Støvneng (1989) (2.7, 2.8)):

$$\Delta\tau_T(-\frac{d}{2}, \frac{d}{2}; k) = \frac{1}{v(k)} [d + \delta y_T] \quad (29)$$

$$\Delta\tau_R(-\frac{d}{2}, \frac{d}{2}; k) = \frac{1}{v(k)} [d - \delta y_R] \quad (30)$$

Substituting in equations (25) and (26) to these results recovers (23).

2.3 Dwell Time

The dwell time τ_D is an expression of the average time spent by a particle in the barrier region, regardless of whether it is ultimately transmitted or reflected (Hauge and Støvneng (1989)). Formally it is defined as the ratio of the average number of particles within the barrier region to the average number entering or leaving the barrier per unit time (quantified by the incident flux j) (Büttiker (1983), Leavens and Aers (1989)):

$$\tau_D = \frac{\int_{-d/2}^{d/2} dy |\psi(t, y)|^2}{j(t, y)} \quad (31)$$

Evaluating this quantity for the wave function inside the barrier region (12) yields:

$$\int_{-d/2}^{d/2} dy |\psi(y)|^2 = \int_{-d/2}^{d/2} dy \frac{T}{4\kappa^2} \left[(\kappa + ik)(\kappa - ik) \left(e^{\kappa(2y-d)} + e^{-\kappa(2y-d)} \right) + (\kappa + ik)^2 + (\kappa - ik)^2 \right] \quad (32a)$$

$$= \int_{-d/2}^{d/2} dy \frac{T}{4\kappa^2} \left[(\kappa^2 + k^2) \left(e^{\kappa(2y-d)} + e^{-\kappa(2y-d)} \right) + 2(\kappa^2 - k^2) \right] \quad (32b)$$

$$= \frac{T}{4\kappa^2} \left[\frac{k_0^2}{\kappa} \sinh 2\kappa d + 2(\kappa^2 - k^2)d \right] \quad (32c)$$

using equation (17) for T :

$$= \frac{k^2}{\kappa} \frac{2\kappa d(\kappa^2 - k^2) + k_0^2 \sinh 2\kappa d}{4k^2\kappa^2 + k_0^4 \sinh^2 \kappa d} \quad (32d)$$

and for the incident flux with $\psi(y) = e^{iky}$:

$$j = -\frac{i\hbar}{2m} \left(\psi^* \frac{\partial \psi}{\partial y} - \psi \frac{\partial \psi^*}{\partial y} \right) \quad (32e)$$

$$= -\frac{i\hbar}{2m} (2ik) = \frac{\hbar k}{m} = v(k) \quad (32f)$$

such that (cf. Büttiker (1983) (3.6)):

$$\tau_D = \frac{1}{v(k)} \frac{k^2}{\kappa} \frac{2\kappa d(\kappa^2 - k^2) + k_0^2 \sinh 2\kappa d}{4k^2\kappa^2 + k_0^4 \sinh^2 \kappa d} \quad (32g)$$

The phase times τ_T and τ_R represent conditional averages over mutually exclusive events (a particle cannot both reflect and transmit). The dwell time τ_D is the average over all scattering channels, and hence the conditional averages must obey the probabilistic rule:

$$\tau_D = T\tau_T + R\tau_R \quad (33)$$

where T and $R = 1 - T$ are transmission and reflection probabilities respectively. Comparison of equations (24g) and (32g) show this consistency check is not satisfied. Resolution of this issue comes from noticing that attaching *physical significance* to the time in (24g) is incorrect, as it requires the assumption that motion outside of the barrier is that of a free particle (Hauge and Støvneng (1989 pp. 924)). This is valid on the transmitted side of the barrier, however during approach to the barrier the incoming wave packet interferes with the reflected wave packet and hence motion can no longer be assumed to be free.

2.4 Continuous Cyclic Quantum Clock

In this section I present a theoretical model of a continuous cyclic quantum clock as provided by Hilgevoord (2002). The angular variable ϕ plays the role of the clock variable and is represented by the operator $\hat{\Phi}$. An angular momentum operator \hat{L} is also introduced and the two operators in the angular representation are given by:

$$\hat{\Phi} = \phi \quad \hat{L} = -i \frac{d}{d\phi} \quad (34)$$

as is familiar from the theory of angular momentum in quantum mechanics. These operators act on a Hilbert space of square integrable functions of ϕ with domain $[0, 2\pi]$ as:

$$\hat{\Phi}f(\phi) = \phi f(\phi) \quad \hat{L}f(\phi) = -i \frac{d}{d\phi} f(\phi) \quad (35)$$

These operators have eigenvalue equations

$$\hat{\Phi}|\phi\rangle = \phi|\phi\rangle, \phi \in [0, 2\pi] \quad \hat{L}|m\rangle = m|m\rangle, m = 0, \pm 1, \pm 2, \dots \quad (36)$$

in which the eigenvectors form complete orthonormal sets such that:

$$\langle \phi | \phi' \rangle = \delta(\phi - \phi') \quad \langle m | m' \rangle = \delta_{mm'} \quad (37)$$

Recalling from the theory of angular momentum in quantum mechanics that the $\hat{L}_z = -i \frac{d}{d\phi}$ operator has eigenfunctions $\propto e^{im\phi}$, $|m\rangle$ has wave function $\langle \phi | m \rangle = A e^{im\phi}$ where A is calculated using the normalisation condition to be $(2\pi)^{-\frac{1}{2}}$:

$$u_m(\phi) := \langle \phi | m \rangle = (2\pi)^{-\frac{1}{2}} e^{im\phi} \quad (38)$$

As $\{|m\rangle\}$ form a complex set, $|\phi\rangle$ can be expressed as:

$$|\phi\rangle = (2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{\infty} e^{-im\phi} |m\rangle \quad (39)$$

Introducing the Hamiltonian $\hat{H} = \omega\hat{L}$, the time evolution operator $U(t) = e^{-iHt}$ acts as:

$$\hat{L}e^{-im\phi} |m\rangle = e^{-im\phi} \hat{L} |m\rangle \text{ by linearity of } \hat{L} \quad (40a)$$

$$= me^{-im\phi} |m\rangle \quad (40b)$$

$$\Rightarrow e^{iHt} |\phi\rangle = \sum_{n=0}^{\infty} \frac{(-i\omega t)^n}{n!} \hat{L}^n (2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{\infty} e^{-im\phi} |m\rangle \quad (40c)$$

$$= (2\pi)^{-\frac{1}{2}} \sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} \frac{(-i\omega m t)^n}{n!} e^{-im\phi} |m\rangle \quad (40d)$$

$$= (2\pi)^{-\frac{1}{2}} \sum_{m=-\infty}^{\infty} e^{-i\omega m t} e^{-im\phi} |m\rangle \quad (40e)$$

$$= |\phi + \omega t\rangle \quad (40f)$$

by setting $\omega = 1$, ϕ plays exactly the same role as a time variable t .

2.5 Discrete Cyclic Quantum Clock

A discrete cyclic quantum clock can be modelled by limiting the sum in equation (39) to values of m satisfying $-j \leq m \leq j$, as presented by in Peres (1980). The clock has an odd number $N = 2j + 1$ of states represented by wave functions

$$u_m(\phi) = (2\pi)^{-\frac{1}{2}} e^{im\phi}, m = -j, \dots, j \text{ and } 0 \leq \phi \leq 2\pi \quad (41)$$

One can construct an alternative orthogonal basis for the clock's wave functions

$$v_k(\phi) = N^{-\frac{1}{2}} \sum_{m=-j}^j e^{-2\pi i k m / N} u_m \quad (42a)$$

$$= (2\pi N)^{-\frac{1}{2}} \sum_{m=-j}^j [e^{i(\phi - 2\pi k / N)}]^m \quad \tilde{m} = m + j \quad (42b)$$

$$= (2\pi N)^{-\frac{1}{2}} \sum_{\tilde{m}=0}^{2j} [e^{i(\phi - 2\pi k / N)}]^{\tilde{m} - j} \quad (42c)$$

$$= (2\pi N)^{-\frac{1}{2}} [e^{i(\phi - 2\pi k / N)}]^{\frac{1-N}{2}} \sum_{\tilde{m}=0}^{2j} [e^{i(\phi - 2\pi k / N)}]^{\tilde{m}} \quad (42d)$$

$$= (2\pi N)^{-\frac{1}{2}} [e^{i(\phi - 2\pi k / N)}]^{\frac{1-N}{2}} \left(\frac{1 - (e^{i(\phi - 2\pi k / N)})^N}{1 - e^{i(\phi - 2\pi k / N)}} \right) \quad (42e)$$

$$= (2\pi N)^{-\frac{1}{2}} \frac{\sin \frac{N}{2} (\phi - \frac{2\pi k}{N})}{\sin \frac{1}{2} (\phi - \frac{2\pi k}{N})} \text{ for } k = 0, \dots, N-1. \quad (42f)$$

For large N these functions have a sharp peak at $\phi = \frac{2\pi k}{N}$ which we visualise as pointing to the k^{th} hour with angle uncertainty $\pm \frac{\pi}{N}$:

One can then define projection operators $P_k v_m = \delta_{km} v_m$ and a clock time operator $T_c = \tau \sum k P_k$ where τ is the resolution of the clock. The eigenvectors of T_c are v_k with eigenvalues $t_k = k\tau, k = 0, \dots, N-1$. Hence measuring T_c yields discrete approximations to the true time, just as analog and digital clocks do.

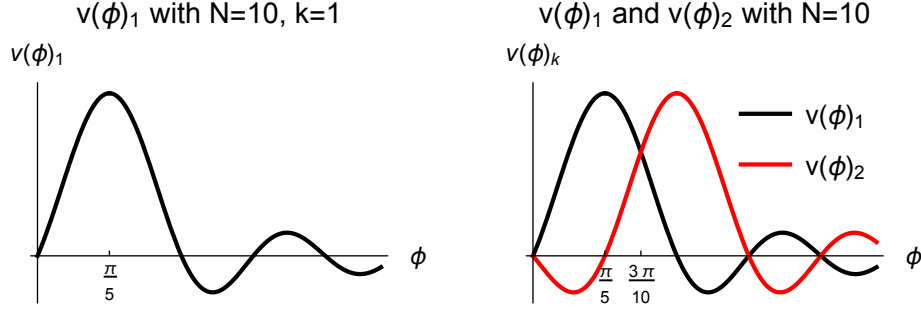


Figure 3: The wave functions of the discrete cyclic quantum clock are sharply peaked around $\phi = \frac{2\pi k}{N}$

The clock's Hamiltonian is:

$$H_c = \omega J \text{ where } \omega = \frac{2\pi}{N\tau} \text{ and } J = -i\hbar \frac{\partial}{\partial \phi} \quad (43)$$

The wave functions u_m are eigenfunctions of the Hamiltonian:

$$H_c u_m = m\hbar\omega u_m \quad (44)$$

whence expanding the time evolution operator as a Taylor series gives:

$$e^{-iH_c t/\hbar} u_m = e^{-im\omega t} u_m = (2\pi)^{-\frac{1}{2}} e^{im(\theta - \omega t)} \quad (45a)$$

$$\implies e^{-iH_c \tau/\hbar} v_k = N^{-\frac{1}{2}} \sum_m e^{-2\pi i k m/N} e^{-2\pi i m/N} u_m \quad (45b)$$

$$= N^{-\frac{1}{2}} \sum_m e^{-2\pi i m(k+1)/N} u_m \quad (45c)$$

$$= v_{k+1} \quad (45d)$$

2.5.1 Application: Atomic Decay

One can apply the construction of the quantum clock to model atomic decay (Peres (1980 Section 4)). The atom-clock system has Hamiltonian $H = H_a + P_0 H_c$ where H_a is the Hamiltonian of the atom, H_c the Hamiltonian of the clock and P_0 the projection operator for the atom's undecayed state, such that the clock stops running when the atom decays. H_a is of the form $H_a = H_0 + V$ where H_0 has a continuous spectrum $H_0 \phi(E) = E \phi(E)$ $E > E_{min}$, plus one discrete eigenstate ϕ_0 with energy $E_0 > E_{min}$. The non vanishing matrix elements of V are denoted $V(E) := \langle \phi(E) | V | \phi_0 \rangle$, which is assumed to be almost constant in E over a large domain on both sides of E_0 .

The wave function for the atom can be expressed as:

$$\psi = a_0 \phi_0 e^{-iE_0 t/\hbar} + \int dE a(E) \phi(E) e^{-iEt/\hbar} \quad (46)$$

Application of the Schrödinger equation for the atom yields:

$$i\hbar \dot{a}(E) = V(E) a_0 e^{i(E-E_0)t/\hbar} \quad (47)$$

Proof.

$$|\psi\rangle = a_0 |\phi_0\rangle e^{-iE_0 t/\hbar} + \int dE a(E) |\phi(E)\rangle e^{-iEt/\hbar} \quad (48a)$$

$$\implies (H_0 + V) |\psi\rangle = a_0 E_0 |\phi_0\rangle e^{-iE_0 t/\hbar} + \int dE a(E) E |\phi(E)\rangle e^{-iEt/\hbar} \quad (48b)$$

$$\begin{aligned} &+ a_0 V |\phi_0\rangle e^{-iE_0 t/\hbar} + \int dE a(E) V |\phi(E)\rangle e^{-iEt/\hbar} \\ &= i\hbar \frac{d|\psi\rangle}{dt} \end{aligned} \quad (48c)$$

Taking the inner product with $\langle\phi(E')|$ on both sides and using the orthogonality conditions yields the final result. \square

a_0 is given by the Weisskopf-Wigner ansatz, $a_0 = e^{-\gamma t/\hbar}$. Substitution into (47) and taking the limit as $t \rightarrow \infty$ yields:

$$\lim_{t \rightarrow \infty} a(E) = \frac{V(E)}{E - E_0 + i\gamma} \quad (49)$$

and

$$\lim_{t \rightarrow \infty} \psi(t) = \int dE \frac{V(E)\phi(E)e^{-iEt/\hbar}}{E - E_0 + i\gamma} \quad (50)$$

Normalisation of the wave function implies:

$$\int dE \frac{|V(E)|^2}{(E - E_0)^2 + \gamma^2} = 1 \quad (51)$$

Utilising the identity:

$$\delta(E - E_0) = \frac{1}{\pi} \lim_{\gamma \rightarrow 0} \frac{\gamma}{(E - E_0)^2 + \gamma^2} \approx \frac{\gamma}{\pi} \frac{1}{(E - E_0)^2 + \gamma^2} \quad (52)$$

in (51) yields $\gamma = \pi|V(E_0)|^2$.

Coupling the atom to a clock using the clock Hamiltonian in (43):

$$H = H_a + P_0 \omega J \quad (53)$$

and setting the initial state of the clock to $v_0 = \frac{1}{\sqrt{N}} \sum u_n$ as in (42a), J can be replaced by the numerical constant $n\hbar$ by virtue of the eigenvalue equation (44). Note this shifts the energy of the initial state $E_0 \rightarrow E_0 + n\hbar\omega$.

In the limit of large t the combined state of the atom and clock is:

$$\psi = N^{-\frac{1}{2}} \sum u_n \int dE \frac{V(E)\phi(E)e^{-iEt/\hbar}}{E - E_0 - n\hbar\omega + i\gamma} \quad (54)$$

The density matrix representing the state of the clock is given by (Peres (1980 pp. 555)):

$$\rho = Tr_a(|\psi\rangle\langle\psi|) = \frac{1}{N} \sum \frac{|u_n\rangle\langle u_m|}{1 + i\alpha(n - m)} \quad (55)$$

where Tr_a indicates the trace is to be taken over the atom degrees of freedom only, and $\alpha = \frac{\hbar\omega}{2\gamma}$ is the angle through which the pointer turns during an average atom lifetime $\frac{\hbar}{2\gamma}$. From this the probability $\langle P_k \rangle$

of finding the clock stopped at time $t_k = k\tau \stackrel{(43)}{=} \frac{2\pi k}{N\omega}$ is given by:

$$\text{Tr}(\rho P_k) = \frac{1}{N} \sum_{m,n} \frac{\langle v_k | u_n \rangle \langle u_m | v_k \rangle}{1 + i\alpha(n-m)} \quad (56a)$$

$$\stackrel{(42a)}{=} \frac{1}{N^2} \sum_{m,n=-j}^j \frac{e^{2\pi i k(n-m)/N}}{1 + i\alpha(n-m)} \quad (56b)$$

The double summation can be evaluated as follows: Let $p = n - m$ and $q = n + m$. The summation becomes:

$$\text{Tr}(\rho P_k) = \frac{1}{N^2} \sum_{p=-2j}^{2j} \sum_{q=q_1(p)}^{q_2(p)} \frac{e^{i\theta p}}{1 + i\alpha p} \quad (57)$$

where $\theta = \frac{2\pi k}{N}$, q_1 and q_2 are bounds that can be determined as follows:

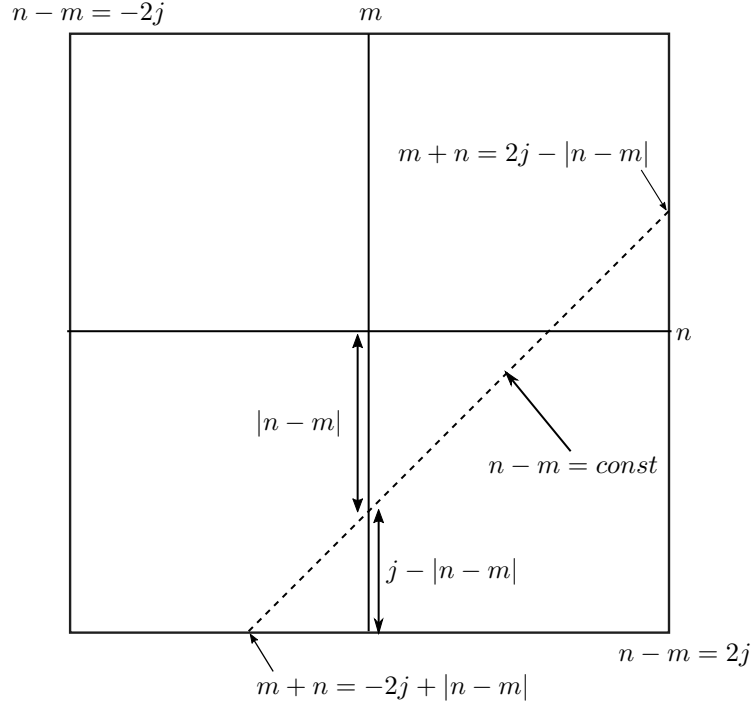


Figure 4: Bounds of the double sum in p, q coordinates

For fixed p , demonstrated by the dashed line in Figure 4, the upper and lower bounds can be read off to be:

$$q_1(p) = -2j + |p| \quad q_2(p) = 2j - |p| \quad (58)$$

Next noting that for fixed p of given parity, all $q \in \{q_1(p), \dots, q_2(p)\}$ have the same parity and hence:

$$Tr(\rho P_k) = \frac{1}{N^2} \sum_{p=-2j}^{2j} \frac{e^{i\theta p}}{1+i\alpha p} \sum_{q=-2j+|p|}^{2j-|p|} 1 \quad (59a)$$

$$= \frac{1}{N^2} \sum_{p=-2j}^{2j} \frac{e^{i\theta p}}{1+i\alpha p} \left[\frac{2j-|p|-(-2j+|p|)}{2} + 1 \right] \quad (59b)$$

$$= \frac{1}{N^2} \sum_{p=-2j}^{2j} \frac{(N-|p|)e^{i\theta p}}{1+i\alpha p} \approx \frac{1}{N} \sum_{p=-2j}^{2j} \frac{e^{i\theta p}}{1+i\alpha p} \quad (59c)$$

This result can be recognised as the Fourier series expansion of $\frac{2\pi e^{-\theta/\alpha}}{N\alpha(1-e^{-2\pi/\alpha})}$, and hence the clocks stop (atoms decay) according to the exponential decay law as expected.

2.6 Larmor Precession

In this section I consider the quantum barrier experiment as in section 2.1, but now with the additional constraints that the particles carry spin $s = \frac{1}{2}$ polarised in the x-direction, and with the presence of a small magnetic field \mathbf{B}_0 parallel with the z-axis and confined to the width of the barrier (Büttiker (1983)):

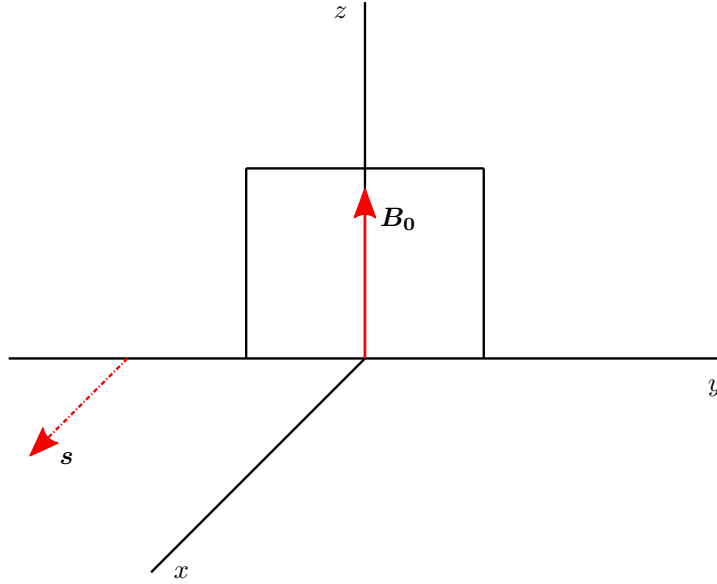


Figure 5: Experimental set up of a quantum barrier with a magnetic field constrained inside.

The magnetic field engenders on the particles in the barrier a Larmor precession of frequency $\omega_L = \frac{g\mu B_0}{\hbar}$, where g is the gyromagnetic ratio and μ is the magnetic moment. This changes the spin of the particles to be polarised in the x-y plane such that:

$$\langle S_x \rangle \approx \frac{\hbar}{2} \quad \langle S_y \rangle \approx -\frac{\hbar}{2} \omega_L \tau_y \quad (60)$$

The presence of the magnetic field and barrier also induces a component of spin in the z-direction, although through an alternative mechanism: Recall from the theory of spin in quantum mechanics that particles with spin in the x-direction can be represented as a linear combination of particles in the $\pm z$ direction:

$$|x; \pm\rangle = \frac{1}{\sqrt{2}} |z; +\rangle \pm \frac{1}{\sqrt{2}} |z; -\rangle \quad (61)$$

with z-components $\pm \frac{\hbar}{2}$ each with probability $\frac{1}{2}$. Inside the barrier the magnetic field induces a Zeeman shift $\pm \frac{\hbar\omega_L}{2}$ to the energies of the particles, giving rise to different exponential decays of the wave functions inside the barrier (12)¹:

$$\kappa_{\pm} = (k_0^2 - k^2 \mp \frac{m\omega_L}{\hbar})^{\frac{1}{2}} \quad (62)$$

where κ_+ (κ_-) corresponds to particles with spin z parallel (antiparallel) to the magnetic field. In the limit $\mathbf{B}_0 \propto \omega_L$ is small, κ_{\pm} can be approximated as:

$$\kappa_{\pm} = \left(k_0^2 - k^2 \mp \frac{m\omega_L}{\hbar}\right)^{\frac{1}{2}} \quad (63a)$$

$$= \kappa \left(1 \mp \frac{m\omega_L}{\hbar\kappa^2}\right)^{\frac{1}{2}} \quad (63b)$$

$$\approx \kappa \left(1 \mp \frac{m\omega_L}{2\hbar\kappa^2}\right) \quad (63c)$$

$$= \kappa \mp \frac{m\omega_L}{2\hbar\kappa} \quad (63d)$$

As $\kappa_+ < \kappa_-$, particles with spin aligned with the magnetic field penetrate more easily than particles with spin anti-aligned with the field, reflected in the transmission probability:

$$T^{(17)} = \left[1 + \frac{(k^2 + \kappa^2)^2 \sinh^2 \kappa d}{4k^2 \kappa^2}\right]^{-1} \quad (64)$$

$$\approx \left[\frac{(k^2 + \kappa^2)^2}{4k^2 \kappa^2} \frac{e^{2\kappa d}}{4}\right]^{-1} \quad (65)$$

$$= \frac{16k^2 \kappa^2}{k^2 + \kappa^2} e^{-2\kappa d} \quad (66)$$

$$\implies T_{\pm} = T e^{\pm \omega_L \tau_z} \quad (67)$$

where $\tau_z = \frac{md}{\hbar\kappa}$ is the time a particle with velocity $v(k) = \frac{\hbar k}{m}$ takes to traverse the barrier. Hence the barrier with the magnetic field induces a net z-component of spin polarisation aligned with the field, quantified the ratio of excess flux to total flux:

$$\langle S_z \rangle = \frac{\hbar}{2} \frac{T_+ - T_-}{T_+ + T_-} = \frac{\hbar}{2} \tanh \omega_L \tau_z \quad (68)$$

The polarisation of the transmitted and reflected particles for all incident energies can be calculated. To do so one must solve the scattering problem with the Hamiltonian:

$$H = \begin{cases} \left(\frac{p^2}{2m} + V_0\right) \mathbb{1} - \left(\frac{\hbar\omega_L}{2}\right) \sigma_z & |y| \leq \frac{d}{2} \\ \left(\frac{p^2}{2m}\right) \mathbb{1} & |y| \geq \frac{d}{2} \end{cases} \quad (69)$$

where $\mathbb{1}$ is the 2×2 identity matrix and $\sigma_x, \sigma_y, \sigma_z$ are the Pauli spin matrices. H acts on spinors

$$\psi = \begin{pmatrix} \psi_+(y) \\ \psi_-(y) \end{pmatrix} \quad (70)$$

As usual $|\psi_{\pm}(y)|^2 dy$ is the probability of finding a particle *upon measurement* with spin $\pm \frac{\hbar}{2}$ in the interval $y, y + dy$. I emphasise 'upon measurement' here as this is an important point of distinction between

¹Note I ignore the exponentially growing term in (12) because it is multiplied by a suppressive pre-factor $e^{-\kappa d/2}$ in equation (13).

the orthodox and pilot-wave interpretations addressed in this essay. The incident beam is polarised in the x -direction:

$$\psi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{iky} \quad (71)$$

i.e. ψ is an eigenvector of S_x

H is diagonal in the spinor basis so one can solve the scattering problem for particles with spin $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ separately. This amounts to solving the quantum barrier in (12) with the following adjustments:

For particles with spin aligned(anti-aligned) with the magnetic field:

- $\kappa \rightarrow \kappa_+(\kappa_-)$
- $V_0 \rightarrow V_0 + (-)\frac{\hbar\omega_L}{2}$
- A, B, C, D in (13) $\rightarrow A_{+(-)}, B_{+(-)}, C_{+(-)}, D_{+(-)}$ by replacing $\kappa \rightarrow \kappa_+(\kappa_-)$

2.6.1 The Strong-Field Limit

The transmitted particles have spinor:

$$\psi_T = (|D_+|^2 + |D_-|^2) \begin{pmatrix} D_+ \\ D_- \end{pmatrix} \quad (72)$$

Recalling the Pauli sigma matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (73)$$

one finds for the expectation values of spin for the transmitted particles:

$$\langle S_z \rangle_T = \frac{\hbar}{2} \langle \psi_T | \sigma_z | \psi_T \rangle = \frac{\hbar}{2} \frac{|D_+|^2 + |D_-|^2}{|D_+|^2 + |D_-|^2} \quad (74a)$$

$$\langle S_y \rangle_T = \frac{\hbar}{2} \langle \psi_T | \sigma_y | \psi_T \rangle = i \frac{\hbar}{2} \frac{D_+ D_-^* - D_+^* D_-}{|D_+|^2 + |D_-|^2} \quad (74b)$$

$$\langle S_x \rangle_T = \frac{\hbar}{2} \langle \psi_T | \sigma_x | \psi_T \rangle = \frac{\hbar}{2} \frac{D_+ D_-^* + D_+^* D_-}{|D_+|^2 + |D_-|^2} \quad (74c)$$

Using (13) and the adjustments for the magnetic field outlined above, one finds:

$$\langle S_z \rangle_T = \frac{\hbar}{2} \frac{T_+ - T_-}{T_+ + T_-} \quad (75)$$

Proof. Follows immediately from the fact that $T = |D|^2$. □

$$\langle S_y \rangle_T = -\hbar \sin(\Delta\phi_+ - \Delta\phi_-) \frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \quad (76)$$

Proof.

$$\langle S_y \rangle_T = i \frac{\hbar}{2} \left(\frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \right) \left(e^{i(\Delta\phi_+ - \Delta\phi_-)} - e^{-i(\Delta\phi_+ - \Delta\phi_-)} \right) \quad (77a)$$

$$= i \frac{\hbar}{2} \left(\frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \right) (2i \sin(\Delta\phi_+ - \Delta\phi_-)) \quad (77b)$$

$$= -\hbar \sin(\Delta\phi_+ - \Delta\phi_-) \frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \quad (77c)$$

□

$$\langle S_x \rangle_T = \hbar \cos(\Delta\phi_+ - \Delta\phi_-) \frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \quad (78)$$

follows along similar lines to the case of $\langle S_y \rangle_T$.

These derivations have utilised no assumptions about the strength of the field, so hold for arbitrary magnetic field. Using (17) one sees that $T_+ \propto e^{-2\kappa_+ d}$ and $T_- \propto e^{-2\kappa_- d}$. As $\kappa_- > \kappa_+$, for a sufficiently opaque barrier ($k_0 d \gg 1$), $T_+ \gg T_-$, and therefore:

$$\langle S_z \rangle_T \approx \frac{\hbar}{2} \quad \langle S_y \rangle_T = \langle S_x \rangle_T \approx 0 \quad (79)$$

Hence the transmitted beam is almost exclusively polarised parallel to the magnetic field.

By similar arguments, with the spinor:

$$\psi_R = (|A_+|^2 + |A_-|^2)^{-\frac{1}{2}} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \quad (80)$$

one arrives at the analogous results for the reflected wave:

$$\langle S_z \rangle_R = \frac{\hbar}{2} \frac{R_+ - R_-}{R_+ + R_-} \quad (81a)$$

$$\langle S_y \rangle_R = -\hbar \sin(\Delta\phi_+ - \Delta\phi_-) \frac{(R_+ R_-)^{\frac{1}{2}}}{R_+ + R_-} \quad (81b)$$

$$\langle S_x \rangle_R = \hbar \cos(\Delta\phi_+ - \Delta\phi_-) \frac{(R_+ R_-)^{\frac{1}{2}}}{R_+ + R_-} \quad (81c)$$

Using the statement of particle conservation $R_+ - R_- = -(T_+ - T_-)$, one finds that:

$$\langle S_z \rangle_R = -\langle S_z \rangle_T \frac{T_+ + T_-}{R_+ + R_-} \quad (82a)$$

$$\langle S_y \rangle_R = \langle S_y \rangle_T \left(\frac{R_+ R_-}{T_+ T_-} \right)^{\frac{1}{2}} \frac{T_+ + T_-}{R_+ + R_-} \quad (82b)$$

$$\langle S_x \rangle_R = \langle S_x \rangle_T \left(\frac{R_+ R_-}{T_+ T_-} \right)^{\frac{1}{2}} \frac{T_+ + T_-}{R_+ + R_-} \quad (82c)$$

and hence $\langle S_z \rangle_R + \langle S_z \rangle_T = 0$, the statement of conservation of angular momentum.

2.6.2 Infinitesimal Field

In this section I report the study of polarisation of the transmitted and reflected waves in the limit of an infinitesimal field. Using (63d), one finds the result:

$$T_+ - T_- = T(\kappa_+) - T(\kappa_-) \quad (83a)$$

$$= \frac{T(k - \frac{m\omega_L}{2\hbar\kappa}) - T(k + \frac{m\omega_L}{2\hbar\kappa})}{\frac{m\omega_L}{\hbar\kappa}} \times \frac{m\omega_L}{\hbar\kappa} \quad (83b)$$

$$= -\left(\frac{m\omega_L}{\hbar\kappa} \right) \frac{\partial T}{\partial \kappa} \quad (83c)$$

In equation (83c) the Larmor frequency ω_L is multiplied by a time $\frac{m}{\hbar\kappa} \frac{\partial T}{\partial \kappa}$. This motivates the definition of the characteristic times $\tau_{zT}, \tau_{yT}, \tau_{xT}$ such that:

$$\langle S_z \rangle_T = \frac{\hbar}{2} \omega_L \tau_{zT} \quad (84a)$$

$$\langle S_y \rangle_T = -\frac{\hbar}{2} \omega_L \tau_{yT} \quad (84b)$$

$$\langle S_x \rangle_T = \frac{\hbar}{2} \left(1 - \frac{\omega_L^2 \tau_{xT}^2}{2} \right) \quad (84c)$$

Using equations (75), (76) and (78) and the approximation $T_+ + T_- \approx 2T$, one can derive explicit results for the characteristic times:

$$\tau_{zT} = - \left(\frac{m}{\hbar \kappa} \right) \frac{\partial \ln T^{\frac{1}{2}}}{\partial \kappa} \quad (85)$$

Proof.

$$\langle S_z \rangle_T \stackrel{(75)}{=} \frac{\hbar}{2} \frac{T_+ - T_-}{T_+ + T_-} \quad (86a)$$

$$\approx \frac{\hbar}{4} \frac{T_+ - T_-}{T} \quad (86b)$$

$$\stackrel{(83c)}{=} -\frac{m\omega_L}{\hbar \kappa} \frac{\hbar}{4} \frac{1}{T} \frac{\partial T}{\partial \kappa} \quad (86c)$$

$$= -\frac{m\omega_L}{\hbar \kappa} \frac{\hbar}{2} \frac{\partial \ln T^{\frac{1}{2}}}{\partial \kappa} \quad (86d)$$

$$= \frac{\hbar}{2} \omega_L \tau_{zT} \quad (86e)$$

□

$$\tau_{yT} = - \left(\frac{m}{\hbar \kappa} \right) \frac{\partial \Delta \phi}{\partial \kappa} \quad (87)$$

Proof.

$$\langle S_y \rangle_T \stackrel{(76)}{=} -\hbar \sin(\Delta \phi_+ - \Delta \phi_-) \frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \quad (88a)$$

$$\sin(\Delta \phi_+ - \Delta \phi_-) \approx \Delta \phi_+ - \Delta \phi_- \approx \Delta(\Delta \phi) \text{ where } \Delta \phi := \phi_+ - \phi_- \quad (88b)$$

$$\implies \langle S_y \rangle_T \approx -\frac{\hbar}{2} \Delta(\Delta \phi) \text{ as } \frac{(T_+ T_-)^{\frac{1}{2}}}{T_+ + T_-} \approx \frac{1}{2} \quad (88c)$$

$$\Delta \kappa := \kappa_+ - \kappa_- = -\frac{m\omega_L}{\hbar \kappa} \quad (88d)$$

$$\implies \langle S_y \rangle_T = -\frac{\partial \Delta \phi}{\partial \kappa} \left(\frac{m\omega_L}{\hbar \kappa} \right) \quad (88e)$$

$$= -\frac{\hbar}{2} \omega_L \tau_{yT} \quad (88f)$$

□

$$\tau_{xT} = \left(\frac{m}{\hbar \kappa} \right) \left[\left(\frac{\partial \Delta \phi}{\partial \kappa} \right)^2 + \left(\frac{\partial \ln T^{\frac{1}{2}}}{\partial \kappa} \right)^2 \right]^{\frac{1}{2}} \quad (89a)$$

$$= \left(\frac{m}{\hbar \kappa} \right) \left| D^{-1} \frac{\partial D}{\partial \kappa} \right| \quad (89b)$$

Proof. Equation (89a) can be proven using similar methods to above but can be proven more easily by noting that since $\langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2 = \frac{\hbar^2}{4}$ then $\tau_{xT} = (\tau_{yT}^2 + \tau_{zT}^2)^{\frac{1}{2}}$. Equation (89b) follows simply using the form of D in (13). \square

The derivatives in (85), (87) can be evaluated explicitly to give:

$$\tau_{zT} = \frac{mk_0^2 (\kappa^2 - k^2) \sinh^2 \kappa d + \left(\frac{\kappa d k_0^2}{2}\right) \sinh 2\kappa d}{\hbar \kappa^2 (4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d)} \quad (90)$$

Proof.

$$\tau_{zT} \stackrel{(85)}{=} - \left(\frac{m}{\hbar \kappa} \right) \frac{\partial \ln T^{\frac{1}{2}}}{\partial \kappa} \quad (91a)$$

$$\ln T^{\frac{1}{2}} = \frac{m}{2\hbar \kappa} \frac{\partial}{\partial \kappa} \ln \left[1 + \frac{(k^2 + \kappa^2)^2 \sinh^2 \kappa d}{4k^2 \kappa^2} \right] \quad (91b)$$

$$= \frac{m}{2\hbar \kappa} \left[1 + \frac{k_0^4 \sinh^2 \kappa d}{4k^2 \kappa^2} \right]^{-1} \frac{1}{4k^2} \frac{\partial}{\partial \kappa} \left[\frac{k_0^4 \sinh^2 \kappa d}{\kappa^2} \right] \quad (91c)$$

the derivative term evaluates to:

$$\frac{\partial}{\partial \kappa} [\dots] = 2 \left(-\frac{k^4}{\kappa^3} + \kappa \right) \sinh^2 \kappa d + \left(\frac{k^4}{\kappa^2} + 2k^2 + \kappa^2 \right) d \sinh 2\kappa d \quad (91d)$$

$$\Rightarrow \tau_{zT} = \frac{m}{2\hbar} \frac{\kappa}{4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d} \left[2 \frac{\kappa^4 - k^4}{\kappa^3} \sinh^2 \kappa d + \frac{k^4 \kappa + 2k^2 \kappa^3 + \kappa^5}{\kappa^3} d \sinh 2\kappa d \right] \quad (91e)$$

$$= \frac{m}{\hbar \kappa^2} \frac{1}{4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d} \left[(\kappa^2 - k^2) k_0^2 \sinh^2 \kappa d + \frac{1}{2} k_0^4 \kappa d \sinh 2\kappa d \right] \quad (91f)$$

$$= \frac{mk_0^2 (\kappa^2 - k^2) \sinh^2 \kappa d + \frac{1}{2} k_0^2 \kappa d \sinh 2\kappa d}{\hbar \kappa^2 (4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d)} \quad (91g)$$

\square

$$\tau_{yT} = \frac{mk}{\hbar \kappa} \frac{2\kappa d (\kappa^2 - k^2) + k_0^2 \sinh 2\kappa d}{4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d} \quad (92)$$

Proof.

$$\tau_{yT} \stackrel{(87)}{=} - \left(\frac{m}{\hbar \kappa} \right) \frac{\partial \Delta \phi}{\partial \kappa} \quad (93a)$$

$$= - \frac{m}{\hbar \kappa} \frac{1}{1 + \left(\frac{k^2 - \kappa^2}{2k\kappa} \tanh \kappa d \right)^2} \frac{\partial}{\partial \kappa} \left[\left(\frac{k}{2\kappa} - \frac{\kappa}{2k} \right) \tanh \kappa d \right] \quad (93b)$$

$$= - \frac{m}{\hbar \kappa} \frac{4k^2 \kappa^2}{4k^2 \kappa^2 + (k^2 - \kappa^2)^2 \tanh^2 \kappa d} \left[- \left(\frac{k}{2\kappa^2} + \frac{1}{2k} \right) \tanh \kappa d + \left(\frac{k}{2\kappa} - \frac{\kappa}{2k} \right) \text{sech}^2 \kappa d \right] \quad (93c)$$

$$= \frac{mk}{\hbar \kappa} \frac{2\kappa d (\kappa^2 - k^2) + k_0^2 \sinh 2\kappa d}{4k^2 \kappa^2 + k_0^4 \sinh^2 \kappa d} \quad (93d)$$

\square

Note in taking $\frac{\partial \Delta \phi}{\partial \kappa}$, one assumes k and κ are no longer related by the equation in (12) such that taking the derivative with respect to κ whilst keeping k constant makes sense.

One can define characteristic reflection times $\tau_{zR}, \tau_{yR}, \tau_{xR}$ analogous to those in (84) such that:

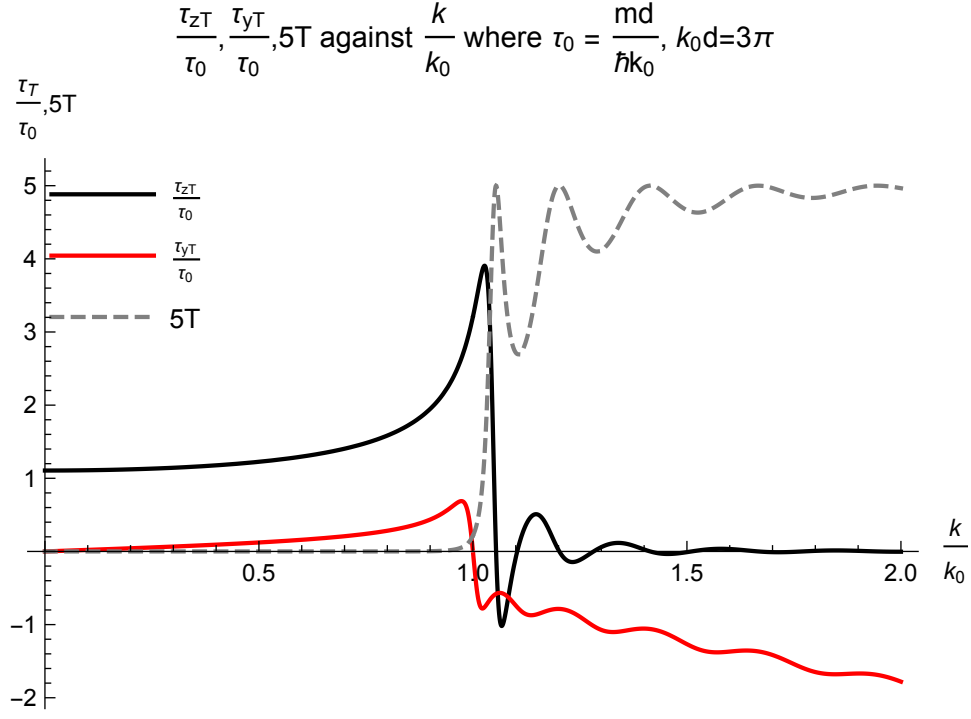


Figure 6: Dependence of the characteristic transmission times and transmission probability on wavenumber.

$$\langle S_z \rangle_R = \frac{\hbar}{2} \omega_L \tau_{zR} \quad (94a)$$

$$\langle S_y \rangle_R = -\frac{\hbar}{2} \omega_L \tau_{yR} \quad (94b)$$

$$\langle S_x \rangle_R = \frac{\hbar}{2} \left(1 - \frac{\omega_L^2 \tau_{xR}^2}{2} \right) \quad (94c)$$

By application of equations (82), one arrives at:

$$\tau_{zR} = -\tau_{zT} \frac{T}{R} \quad (95a)$$

$$\tau_{yR} = \tau_{yT} \quad (95b)$$

$$\tau_{xR} = (\tau_{yR}^2 + \tau_{zR}^2)^{\frac{1}{2}} = \left(\tau_{yT}^2 + \tau_{zT}^2 \frac{T^2}{R^2} \right)^{\frac{1}{2}} \quad (95c)$$

3 Tunnelling Times in the de Broglie-Bohm Interpretation

3.1 de Broglie-Bohm Theory

It is clear from the previous section that no definitive answer to the equation ‘*How long does a particle take to tunnel through a quantum barrier*’ has been agreed upon within the orthodox interpretation of quantum mechanics. In contrast, the de Broglie-Bohm (dBB) interpretation yields a unique and well-defined prescription for defining tunnelling times. The dBB theory is an interpretation of quantum mechanics built upon the following postulates (Holland (1993)):

- P1 Individual physical systems comprise a wave propagating in space and time, and a point particle, the motion of which is guided by the wave.
- P2 The wave is mathematically described by $\psi(t, \mathbf{y}) = Re^{iS/\hbar}$, $R = R(t, \mathbf{y})$ is a real amplitude function, $S = S(t, \mathbf{y})$ is a real phase function and $\psi(t, \mathbf{y})$ satisfies the time dependent Schrödinger equation.
- P3 The velocity of the particle is given by $\mathbf{v} = \frac{1}{m} \nabla S$. The particle motion is obtained by solving this equation along with the specification of the initial condition of the particle, $\mathbf{y}(0)$.
- P4 The probability of a particle *being* between points \mathbf{y} and $\mathbf{y} + d\mathbf{y}$ at time t is given by:

$$|\psi(t, \mathbf{y})|^2 d^3y = R(t, \mathbf{y})^2 d^3y \quad (96)$$

The effect of this postulate is to extract from all possible motions of the particle those compatible with the initial distribution $R(0, \mathbf{y})$. Note how this differs from the orthodox interpretation in which $|\psi(t, \mathbf{y})|^2$ determines the probability density of finding a particle *upon measurement*.

Substituting in $\psi = Re^{iS/\hbar}$ into the time dependent Schrödinger equation yields:

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} + V = 0 \quad (97a)$$

$$\frac{\partial R^2}{\partial t} + \nabla \cdot \left(\frac{R^2 \nabla S}{m} \right) = 0 \quad (97b)$$

Proof.

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi \quad (98a)$$

$$i\hbar \left(\dot{R} + \frac{i}{\hbar} R \dot{S} \right) = -\frac{\hbar^2}{2m} \left(\nabla^2 R + \frac{2i}{\hbar} \nabla R \nabla S - \frac{1}{\hbar^2} R (\nabla S)^2 + \frac{i}{\hbar} R \nabla^2 S \right) + VR \quad (98b)$$

Isolating real and imaginary parts yields:

$$-R\dot{S} = -\frac{\hbar^2}{2m} \left(\nabla^2 R - \frac{R}{\hbar^2} (\nabla S)^2 \right) + VR \quad (98c)$$

$$\implies \frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} + V = 0 \quad (98d)$$

$$\hbar \dot{R} = -\frac{\hbar}{2m} (2\nabla R \nabla S + R \nabla^2 S) \quad (98e)$$

$$\implies \frac{\partial R^2}{\partial t} + \nabla \cdot \left(\frac{R^2 \nabla S}{m} \right) = 0 \quad (98f)$$

□

Note that (97b) can be written as:

$$\frac{\partial P(t, \mathbf{y})}{\partial t} + \nabla \cdot \mathbf{j}(t, \mathbf{y}) = 0 \quad (99)$$

where P is the probability density and \mathbf{j} is the 3-dimensional generalisation of the flux (32e), and hence takes the form of the continuity equation. Note also equation (97a) is a modified Hamilton-Jacobi equation, with additional term $Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$, the ‘quantum potential energy’.

As in P3 one defines the vector field $\mathbf{v} = \frac{1}{m} \nabla S$, which defines at each point in space at each instant in time the tangent to the particle’s trajectory passing through that point. Given the gradient ∇S is orthogonal to level surfaces, the trajectories are orthogonal to surfaces $S = \text{constant}$, and are given by the solution of $\dot{\mathbf{y}} = \frac{1}{m} \nabla S(t, \mathbf{y})$, requiring specification of the initial condition \mathbf{y}_0 . Hence the motion of the particle is completely deterministic once its initial position has been specified. Note one does not have to specify an initial velocity \mathbf{v}_0 as this is encoded in the initial wave $\psi_0(\mathbf{y})$ and is calculated using P2. Note also the important fact that no two different trajectories with the same wave $\psi(t, \mathbf{y})$ intersect. This is because at the point of intersection, both trajectories have the same velocity and position at the same point in time. As the motion of a particle is deterministic given the specification of an initial condition, the two trajectories will subsequently coincide for all times after the time of intersection. By time reversal invariance, the two trajectories must also have coincided for all antecedent times, a contradiction with our initial assumption.

From P3 it is clear that an ensemble of possible motions associated with the same wave is generated by varying the initial condition \mathbf{y}_0 . Once specified, the laws governing the evolution of a physical system are entirely deterministic. The probabilistic nature of quantum mechanics, familiar from experiments such as the double-slit experiment, is recovered from the fact that giving a particle a precisely defined initial condition is empirically unrealisable. Hence given an ensemble of identical physical systems (a wave and point particle), it is the uncertainty of the initial position of the particles that gives rise to the probabilistic nature of quantum mechanics.

3.2 A Natural Definition of Tunnelling Time

The notion of a particle trajectory in the dBB theory leads one to a natural definition of reflection and transmission times. For a particle with initial condition (restricting to the one-dimensional case) $y = y_0$ at $t = 0$, the time spent in the region $y_1 \leq y \leq y_2$ is given by:

$$t(y_0; y_1, y_2) = \int_0^\infty dt \Theta(y(t, y_0) - y_1) \Theta(y_2 - y(t, y_0)) \quad (100)$$

where $y(t, y_0)$ denotes the trajectory of a particle with initial condition $y = y_0$ at $t = 0$ and Θ is the Heaviside step function. This definition is intuitively clear: $\Theta(y(t, y_0) - y_1)$ has support for particle trajectories $> y_1$, and $\Theta(y_2 - y(t, y_0))$ has support for particle trajectories $< y_2$. When a trajectory satisfies both of these conditions, the particle resides within the interval of interest (y_1, y_2) and increments the measured time.

For empirical purposes, the precise specification of the particle’s initial condition is not possible. For an ensemble of identical systems, one can use P4 at $t = 0$ to state the probability distribution of initial positions, and hence define the mean dwell time:

$$\tau_D(y_1, y_2) = \langle t(y_0; y_1, y_2) \rangle = \int_{-\infty}^\infty dy_0 |\psi(0, y_0)|^2 t(y_0; y_1, y_2) \quad (101a)$$

$$\stackrel{(100)}{=} \int_{-\infty}^\infty dy_0 |\psi(0, y_0)|^2 \int_0^\infty dt \Theta(y(t, y_0) - y_1) \Theta(y_2 - y(t, y_0)) \quad (101b)$$

$$= \int_{-\infty}^\infty dy_0 |\psi(0, y_0)|^2 \int_0^\infty dt \int_{-\infty}^\infty \Theta(y - y_1) \Theta(y_2 - y) \delta(y - y(t, y_0)) \quad (101c)$$

$$= \int_0^\infty \int_{y_1}^{y_2} \int_{-\infty}^\infty dy_0 |\psi(0, y_0)|^2 \delta(y - y(t, y_0)) \quad (101d)$$

$$= \int_0^\infty \int_{y_1}^{y_2} |\psi(t, y)|^2 \quad (101e)$$

where $|\psi(t, y)|^2 = \langle \delta(y - y(t, y_0)) \rangle$. Leavens and Aers (1989 pp. 1204) argue this to be identical to the time derived above (31).

One can use the fact that particle trajectories do not intersect each other to define a starting point y_0^c such that only trajectories $y(t, y_0)$ with $y_0 > y_0^c$ are ultimately transmitted, and trajectories with $y_0 < y_0^c$ are ultimately reflected. y_0^c is defined by:

$$\int_{y_0^c}^{\infty} dy_0 |\psi(0, y_0)|^2 = |T|^2 \quad (102)$$

This definition is intuitively clear - the left hand side is the probability a particle starts in a region that guarantees it will be ultimately transmitted, and this is equal to the transmission probability.

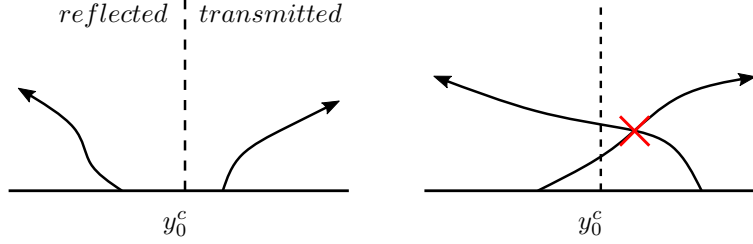


Figure 7: y_0^c separates reflected and transmitted trajectories.

Subsequently one can calculate the mean transmission and reflection times, uniquely given by:

$$\tau_T(y_1, y_2) = \frac{\langle (t(y_0; y_1, y_2) \Theta(y_0 - y_0^c)) \rangle}{\langle \Theta(y_0 - y_0^c) \rangle} \quad (103)$$

$$\tau_R(y_1, y_2) = \frac{\langle (t(y_0; y_1, y_2) \Theta(y_0^c - y_0)) \rangle}{\langle \Theta(y_0^c - y_0) \rangle}. \quad (104)$$

where $|T|^2 = \langle \Theta(y_0 - y_0^c) \rangle$ and $|R|^2 = \langle \Theta(y_0^c - y_0) \rangle$. These are real-valued, non-negative quantities obeying the consistency condition (33):

$$|T|^2 \tau_T(y_1, y_2) + |R|^2 \tau_R(y_1, y_2) = \langle (t(y_0; y_1, y_2) \Theta(y_0 - y_0^c)) \rangle + \langle (t(y_0; y_1, y_2) \Theta(y_0^c - y_0)) \rangle \quad (105a)$$

$$= \langle (t(y_0; y_1, y_2) (\Theta(y_0 - y_0^c) + \Theta(y_0^c - y_0))) \rangle \quad (105b)$$

$$= \langle t(y_0; y_1, y_2) \rangle = \tau_D \quad (105c)$$

The probability distributions of the transmission and reflection times, P_T and P_R are also of interest. These are defined by:

$$\tau_T(y_1, y_2) = \int_0^{\infty} dt P_T(t(y_1, y_2)) t, \quad \tau_R(y_1, y_2) = \int_0^{\infty} dt P_R(t(y_1, y_2)) t. \quad (106)$$

and hence are given by

$$P_T(t(y_1, y_2)) := \frac{\langle (\Theta(y_0 - y_0^c)) \delta[t(y_1, y_2) - t(y_0; y_1, y_2)] \rangle}{\langle \Theta(y_0 - y_0^c) \rangle} \quad (107a)$$

$$P_R(t(y_1, y_2)) := \frac{\langle (\Theta(y_0^c - y_0)) \delta[t(y_1, y_2) - t(y_0; y_1, y_2)] \rangle}{\langle \Theta(y_0^c - y_0) \rangle} \quad (107b)$$

3.3 Numerical Example

Consider tunnelling through barrier with boundaries shifted to $[0, d]$ and an electron with initial Gaussian wave function:

$$\psi(t=0, y) = \frac{1}{(2\pi(\Delta y)^2)^{\frac{1}{4}}} \exp\left(-\left(\frac{(y-y_0)^2}{2\Delta y}\right) + ik_0 y\right) \quad (108)$$

where y_0 is the centroid of $|\psi(0, y)|^2$ and k_0 is the centroid of $|\phi(k)|^2$, the Fourier transform of the wave function into momentum space. This is a minimum-uncertainty product wave function and hence the uncertainties of its position and momentum satisfy $\Delta y \Delta p_y = \frac{1}{2}(\hbar = 1)$. Note that y_0 is chosen such that the wave function is sufficiently far to the left of the barrier region $0 \leq y \leq d$ such that the initial probability density $|\psi(0, y)|^2$ is negligible for $y \geq 0$. Mathematically this is formulated as:

$$\int_0^\infty dy |\psi(0, y)|^2 = 10^{-4} |T|^2 \quad (109)$$

The barrier has height $V_0 = 10eV$ and unfixed width d . The problem is solved numerically. For $E_0 = \frac{1}{2}V_0$, momenta uncertainties $\Delta k = 0.04$ and 0.08\AA and trajectory starting points y_0 near the transmission-reflection bifurcation point y_0^c , a collection of results are presented below:

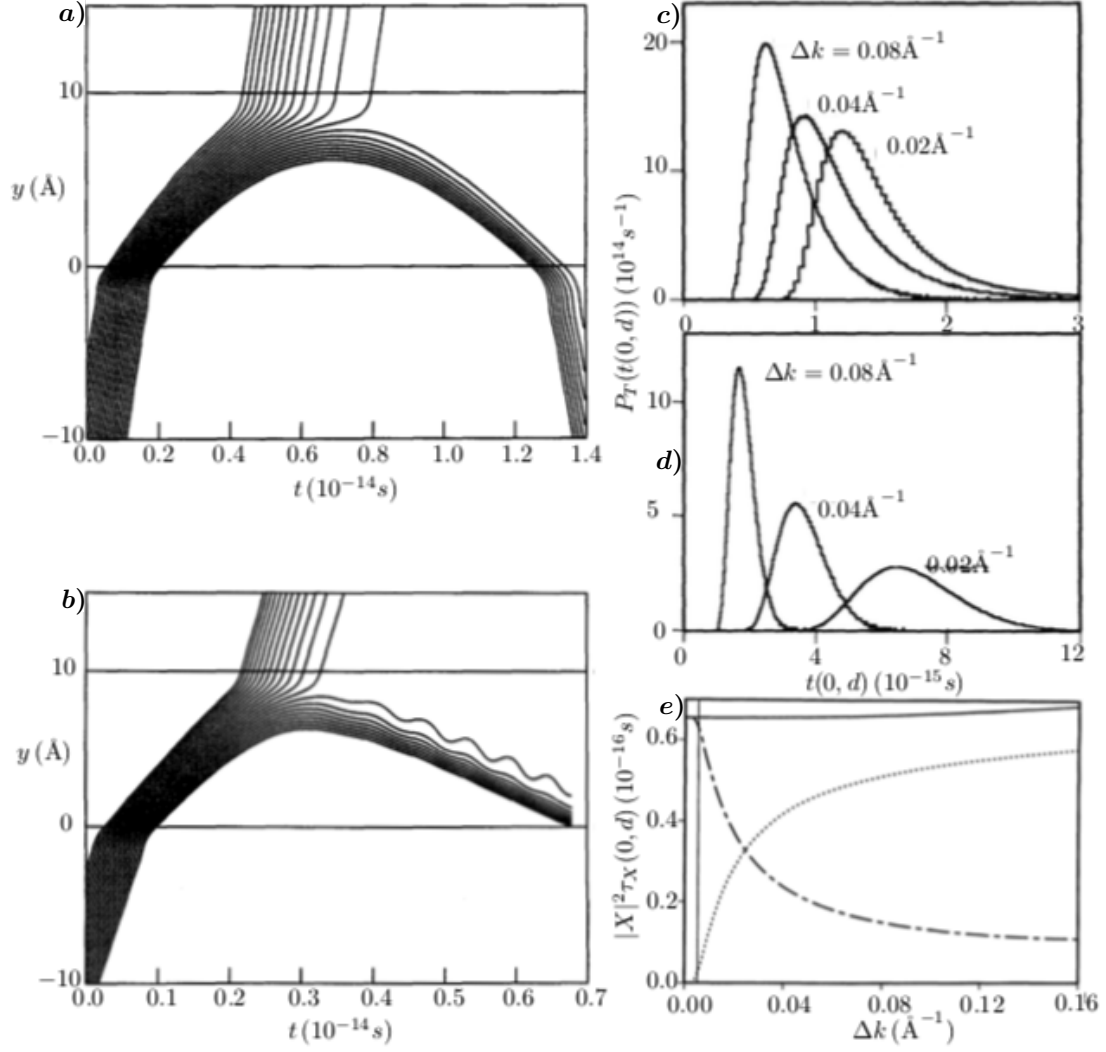


Figure 8: y_0^c separates reflected and transmitted trajectories.

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