Notes on Quantum Mechanics

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Preface

Part I

History

Chapter 1

A Historical Overview

We begin by a lucid overview of the history of Quantum Mechanics . Here we have avoided going into details of some very important Quantum Mechanical phenomena such as the Hydrogen atom, Spin and theiry history. You may refer to [34] to learn more about them. [] is an excellent exposition of "spin" which we'll come to understand in the next few chapters.

1.1 The Pre-Quantum Era

In the 1850s, when Fraunhofer used his experimental setup to analyze the spectra of sunlight he found something remarkable.

Dark lines

Thus, they concluded that Sun must contain Sodium.

1.2 Blackbody Radiation

We can consider a black body to consist of electromagnetic radiation in thermal equilibrium with the walls of the cavity. When they are in thermal equilibrium, the average rate of emission of radiation equals their average rate of absorption of radiation.

The Rayleigh Jeans theory was constructed on the notion that when the walls of an object is in thermal equilibrium, in other words, the temperature of the walls is equal to the "temperature" of radiation. We will see what we mean by the "temperature" of an electromagnetic wave.

If we take the walls of a cavity to consist of oscillating charged particles (about its equilibrium) coupled to a standing-wave mode of an electromagnetic field. This can be seen from Maxwell's theory of electromagnetic waves, which states that a moving charged particle radiates an electromagnetic wave. A point to be noted is that the frequency of the oscillating charge is equal to the frequency of its coupled electromagnetic wave. So then, it is safe to say that in thermal equilibrium, the average energy of the oscillating charge is equal to the average energy of the coupled standing-wave mode of that electromagnetic field.

Now we can see that the oscillating particle has a quadratic potential energy, H_{pot} of $\frac{1}{2}aq^2$ and a kinetic energy H_{kin} of $\frac{p^2}{2m}$, so according to the equipartition theorem, in thermal equilibrium the average energy is,

$$\langle H|H\rangle = \langle H_{pot}|H_{pot}\rangle + \langle H_{kin}|H_{kin}\rangle = \frac{1}{2}k_BT + \frac{1}{2}k_BT = k_BT \tag{1.1}$$

Hence the energy of the wave is also taken to be k_BT, and can be thought to have a "temperature" of T.

This forms the foundation of the Rayleigh Jeans theory, following which we will derive the Rayleigh-Jeans formula.

1.3 Deriving the Rayleigh-Jeans Formula

We start off with the axiom that the energy distribution of a black-body radiation does not depend on the shape of the cavity (which can be proven experimentally). For ease of calculations, we take te shape of the cavity to be a cube. We also assume that the waves vanish at the walls, or in other words, do not pass through them.
The number of standing electromagnetic waves in a cube of length L needs to be calculated.
Let us take the wave equation for the standing electromagnetic wave,

$$\frac{\partial^2 E_x}{\partial x^2} + \frac{\partial^2 E_x}{\partial y^2} + \frac{\partial^2 E_x}{\partial z^2} + k^2 E_x = 0 \tag{1.2}$$

Where $E_x = E_x(x, y, z)$ and $k = \frac{2\pi}{\lambda} = \frac{2\pi f}{c}$. Assuming that $E_x = u(x)v(y)w(z)$ (by variable separable method), we can separate Equation (2) into three ordinary differential equations of the type,

$$\frac{d^2u}{dx^2} + k_x^2 u = 0 \tag{1.3}$$

Where $k^2 = k_x^2 + k_y^2 + k_z^2$. By inspection, we can see that Equation (3) is an equation for a simple harmonic oscillator and has the solution,

$$u(x) = B\cos k_x x + C\sin k_x x \tag{1.4}$$

Applying necessary boundary conditions so that E_x or u is 0 at $x = 0$ and at $x = L$ leads to $B = 0$ and $k_x L = n_x\pi$ where $n_x = 1, 2, 3, ...,$ (since we are considering standing electromagnetic waves and look at only the positive region of the k-space) similar solutions are obtained for $v(y)$ and $w(z)$, giving the solution,

$$E_x(x, y, z) = A\sin(k_x x)sin(k_y y)\sin(k_z z) \tag{1.5}$$

Where,

$$k^2 = \frac{\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2) \tag{1.6}$$

and n_x, n_y and n_z are postive integers.
Now, we take Equation (6) to give us the distance from the origin to a point in k-space, or often called the "Reciprocal" space (due to the units of k being $(length)^-1$).
Let us take a coordinate system corresponding to the k-space (as shown in Figure 1), with the axes being k_x, k_y and k_z. And we know that $k_x = n_x\pi/l$, $k_y = n_y\pi/L$, and $k_z = n_z\pi/L$, so the points in k-space are separated by π/L along each axis, and there is one standing wave in k-space per $(\pi/L)^3$ of volume. The number of standing waves, $N(k)$ having wavenumbers between k and $k+dk$ is then simply the volume between k and $k+dk$ divided by $(\pi/L)^3$. The volume between k and $k + dk$ is simply the volume of a spherical shell of thickness dk multiplied by 1/8 (since we need only the positive quadrant of the k-space, hence 1/4 of the volume of sphere), so that

$$N(k)dk = \frac{\frac{1}{2}\pi k^2 dk}{(\pi/L)^3} = \frac{Vk^2 dk}{2\pi^2} \tag{1.7}$$

Where $V = L^3$ is the volume of the cavity.
For any electromagnetic wave, there are two perpendicular polarisations for each mode, so Equation (6) should be increased by a factor of 2, becoming,

$$\frac{N(k)dk}{V} = \frac{k^2 dk}{\pi^2} \tag{1.8}$$

From using the expression $k = 2\pi f/c$ to obtain k and dk and substituting in Equation (8) gives us $N(f)$,

$$N(f)df = \frac{8\pi f^2}{c^3}df \tag{1.9}$$

And from this, the number of modes per unit volume between λ and $\lambda + d\lambda$ can be derived from Equation (9) by using the expression $f = c/\lambda$ to get λ and $d\lambda$ to get,

$$N(\lambda)d\lambda = \frac{8\pi}{\lambda^4}d\lambda \tag{1.10}$$

Now, each mode of oscilation has energy of $k_B T$, so the energy in the range λ to $\lambda + d\lambda$ is $k_B T N(\lambda)d\lambda$. Hence the energy density in this region is,

$$u(\lambda)d\lambda = k_B T N(\lambda) = \frac{8\pi k_B T}{\lambda^4}d\lambda \tag{1.11}$$

This is the Rayleigh Jeans expression for spectral density in the range λ to $d\lambda$ Considering the energy to be a continuous variable, then the average energy per oscillator is $k_B T$ and the Rayleigh Jeans formula for $u(\lambda)$ holds true. The Rayleigh Jeans formula also behaves perfectly well for long wavelengths in the electromagnetic spectum. It also agrees with the Wien's scaling formula,

$$u(\lambda) = \frac{8\pi k_B T}{\lambda^4} = \frac{f(\lambda T)}{\lambda^5} \tag{1.12}$$

However, we will see in the next section why this is not a correct scaling function.

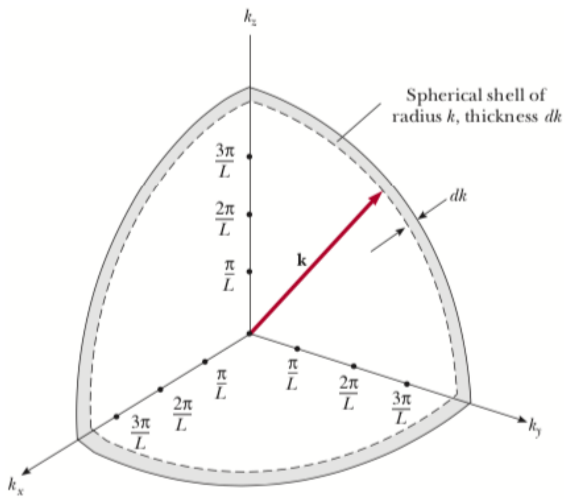


Figure 1.1: Visualising the k-space

1.4 Failure of the Rayleigh Jeans theory in explaining the Stefan-Boltzmann Law

1.4.1 Incorrect Scaling function

From the previous equation for the scaling function, we can see that $f(\lambda T) = 8k_BT$. So from this, we can notice that as λ decreases, the u(λ) also increases. This means that higher the temperature, more lower wavelength waves are emitted, for example, a campfire emits a large amount of short wavelength microwaves (which is very deadly, but thankfully that isnt how things work in nature) according to this law. Hence, the law fails in this regard.

1.4.2 The Ultraviolet Catastrophe

Inspecting the Rayleigh-Jeans formula, and attempting to find the total energy density (by integrating with appropriate limits) of the black body gives us an interesting result,

$$u = \int_{\infty}^{0} = u(\lambda)d\lambda = \int_{\infty}^{0} \frac{8\pi k_BT}{\lambda^4} d\lambda = \infty \tag{1.13}$$

Here we see that the energy density is infinite, which is easy to figure out that this is nonsensical. It implies that if a cavity filled with radiation radiates infinite amount of energy. This was named by Paul Ehrenfest as the "Ultraviolet Catastrophe" However, Stefan found out that the energy radiated is proportional to T^4, hence, trying to explain the Stefan-Boltzmann Law using the Rayleigh-Jeans formula for energy density will end in vain.

1.4.3 Consequences

As the Rayeigh-Jeans formula failed to address shorter wavelengths, Planck decided to use a different approach to explain the black body radiation curve. He decided not to assume that the average energy of an oscillator in the wall to be k_BT. He knew how $u(\lambda)$ varies for short wavelengths, using the Wien's formula and wanted u(λ) to be proportional to T for longer wavelengths. This lead to the formulation of the Planck's formula, which perfectly described the radiation curve.

1.5 Planck's Law

Max Planck, suggested that the energy transfer can radiation i.e. standing waves and walls of container i.e. atoms must be discrete not continuous as fundamental discrete energy units $E = nhv$. Thus he came up with the relation:

$$\langle E\rangle = \frac{\sum_{n=0}^{\infty} nhve^{-nhv/kT}}{\sum_{n=0}^{\infty} e^{-nhv/kT}} \tag{1.14}$$

Now,

$$u(\lambda,T) = N\langle E\rangle = \frac{8\pi}{\lambda^4}.\frac{hc/\lambda}{e^{\frac{hc}{\lambda kT}}-1} \tag{1.15}$$

This turned out to be right distribution! However, nobody at that time understood what it meant. Planck himself considered this to be a mathematical trick. In a sense, it implies that energy transfer is quantized. But almost no one took it seriously. It would take a revolutionary mind to truly understand it and push it to the extreme.

1.6 Photoelectric Effect

It was only Albert Einstein who took Planck's idea to the extreme. He postulated that energy transfer itself must be quantized and transmitted through discrete packets of energy called photons. Einstein drew this conclusion as an interpretation of Phillip Lenard's experimentation of what is called the "Photoelectric effect" i.e. a phenomenon in which electromagnetic radiation incident on a metallic surface causes electron to be emitted from the surface.

1.6.1 Experimental Setup

- Evacuated tube, with a metallic photosurface P, in which light passes through a small opening and causes electrons to be ejected
- These electrons are collected by a collecting surface C
- Since the collecting plate is connected to the negative terminal of the power supply, it will repel normally repel electrons and only absorb the energetic ones
- As the voltage is made more negative, there is a point at which the current ceases, called stopping voltage/potential V_S

1.6.2 Observation

- The intensity of the incident light neither affects the kinetic energy or the stopping voltage, solely the number of electrons emitted

- The frequency of light influences the emitted electrons' energy
- Electrons are emitted without a time delay.
- There is a minimum/threshold frequency, ϕ, below which no electrons are emitted

1.6.3 Interpretation

If light were a wave:

- Intense beams, which have more energy, should cause the emissions of electrons with higher kinetic energy
- Frequency should play a role in the energy of electrons
- Low intensity beams should cause a time delay, since energy would need to accumulate before the emission of an electron.

Einstein created this equation for it,

$$E_{Photon} = h\gamma = T + \phi \tag{1.16}$$

Where,

$$\phi = hv_0$$
$$T = \frac{1}{2}mv^2$$

In summary, Planck said "energy exchange is quantized" whereas Einstein said "energy itself is quantized".

1.7 The de Broglie Hypothesis

In , the French physicist de Brogile proposed that this wave like structure applies to electrons too and follows the equation:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda} \tag{1.17}$$

1.8 The Davidsson-Germer Experiment

1.9 The Compton Effect

Part II

Tools

Chapter 2

Mathematical Preliminaries

This chapter is a discussion of all the mathematical tools and tricks one would require to master Quantum mechanics. Knowledge of basic matrix manipulation and vector calculus is assumed.

2.1 Complex Numbers

A complex number is an order pair $\in \mathbb{C}$ where $a, b \in \mathbb{R}$ where we can denote it as $z = a + ib$ where $i = \sqrt{-1}$

2.1.1 Addition

$z_1 = a_1 + ib_1,\ z_2 = a_2 + ib_2$

$$z_1 + z_2 = (a_1 + a_2) + i(b_1 + b_2)$$

2.1.2 Multiplication

$z_1 = a_1 + ib_1,\ z_2 = a_2 + ib_2$

$$z_1 z_2 = (a_1 + ib_1)(a_2 + ib_2) = (a_1 a_2 - b_1 b_2) + i(a_1 b_2 + a_2 b_1)$$

2.1.3 Properties

Where, $\mathcal{W}, \mathcal{Z}, \lambda \in \mathbb{C}$

Commutativity

$$\mathcal{W} + \mathcal{Z} = \mathcal{Z} + \mathcal{W}$$
$$\mathcal{W}\mathcal{Z} = \mathcal{Z}\mathcal{W}$$

Associativity

$$(\mathcal{Z}_1 + \mathcal{Z}_2) + \mathcal{Z}_3 = \mathcal{Z}_1 + (\mathcal{Z}_2 + \mathcal{Z}_3)$$

$$(\mathcal{Z}_1\mathcal{Z}_2)\mathcal{Z}_3 = \mathcal{Z}_1(\mathcal{Z}_2\mathcal{Z}_3)$$

Identities

$$\mathcal{Z} + 0 = \mathcal{Z}$$

$$\mathcal{Z}1 = \mathcal{Z}$$

Additive Inverse

$$\forall\ \mathcal{Z}\ \exists\ \mathcal{Z}^{-1} \mid \mathcal{Z} + \mathcal{Z}^{-1} = 0$$

Multiplicative Inverse

$$\forall\ \mathcal{Z} \neq 0\ \exists\ \mathcal{W} \mid \mathcal{Z}\mathcal{W} = 1$$

Distributive Property

$$\lambda(\mathcal{W} + \mathcal{Z}) = \lambda\mathcal{W} + \lambda\mathcal{Z}$$

2.1.4 Notation

n-tuple refers to an ordered set of n numbers over a field $\mathcal{F}$.[1]

2.1.5 Wessel Plane

Complex numbers can be represented on a 2-dimentionsal space similar to $\mathbb{R}^2$

2.2 Solving PDEs

What we'll review here is called the variable separable method,

[1]For our case $\mathcal{F}$ simply refers to $\mathbb{C}$

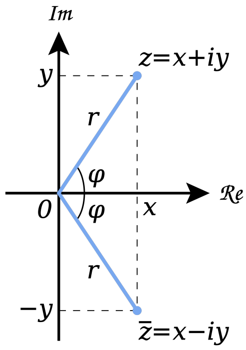


Figure 2.1: Wessel Plane Plot: (Complex conjugate picture.svg from Wikimedia Commons)

2.3 Linear Vector Spaces

A linear vector space or simply a vector space $\mathbb{V}$ is a set along with the regular multiplication and addition operations over a field $\mathcal{F}$, such that the following axioms hold: [2]

2.3.1 Commutativity

$$\mathcal{U} + \mathcal{V} = \mathcal{V} + \mathcal{U}$$

2.3.2 Associativity

$$(\mathcal{U} + \mathcal{V}) + \mathcal{W} = \mathcal{V} + (\mathcal{U} + \mathcal{W})$$

$$(\alpha\beta)\mathcal{V} = \alpha(\beta\mathcal{V})$$

2.3.3 Additive Identity

$$\exists\ 0 \in \mathbb{V} \mid \mathcal{V} + 0 = 0 + \mathcal{V} = \mathcal{V}$$

2.3.4 Additive Inverse

$$\forall\ \mathcal{V}\ \exists\ \mathcal{V}^{-1} \mid \mathcal{V} + \mathcal{V} = 0$$

[2]Here, $\alpha, \beta \in \mathcal{F}$ and $\mathcal{U}, \mathcal{V}$ and $\mathcal{W} \in \mathbb{V}$

2.3.5 Multiplicative identity

$$\exists\, 1 \in \mathbb{V} \mid 1\mathcal{V} = \mathcal{V}$$

2.3.6 Distributive properties

$$\alpha(\mathcal{U} + \mathcal{V}) = \alpha\mathcal{U} + \alpha\mathcal{V}$$
$$(\alpha + \beta)\mathcal{U} = \alpha\mathcal{U} + \beta\mathcal{U}$$

2.4 Inner Product Spaces

An inner product is simply an operation that takes a Dual $|\psi\rangle$ and it's corresponding vector $\langle\psi|$ and maps them to $\mathbb{R}$:

$$\langle expression1|expression2\rangle$$

2.5 Dual Spaces

2.6 Dirac Notation

Operators are represented with respect to a particular basis (in this case $\{e_m, e_n\}$) by their matrix elements

$$\langle e_m|\hat{O}|e_n\rangle = \hat{O}_{mn} \tag{2.1}$$

2.7 Subspaces

Given a vector space $\mathbb{V}$, a subset of its elements that form a vector space among themselves is called a subspace. We will denote a particular subspace i of dimensionality n_i by $\mathbb{V}_i^{n_i}$.
Given two subspaces, and , we define their sum $\mathbb{V}_i^{n_i} \oplus \mathbb{V}_i^{m_i} = \mathbb{V}_i^{l_i}$ [3] as the set containing:

1. All the elements of $\mathbb{V}_i^{n_i}$
2. All the elements of $\mathbb{V}_j^{m_j}$
3. And all possible linear combinations of the above

However for the elements of (3), closure is lost. The dimensionality of such a subspace is $n + m$.

[3] Here $\oplus$ is the direct sum defined as:

2.8 Hilbert Spaces

A Hilbert space H is simply a normed vector space (a Banach space), whose norm is defined as:

$$\|V\| := \sqrt{\langle V|V\rangle} \tag{2.2}$$

This is an axiomatic definition of a Hilbert space, but we are more concerned with the corollaries of it. All the Cauchy sequences [4] of functions in a Hilbert space always converge to a function that is also a memeber of the space i.e. it is said to be **complete** which implies that the integral of the absolute square of a function must converege [5]

$$\int_a^b |f(x)|^2 dx < \infty \tag{2.3}$$

Moreover this means that, any function in Hilbert space can eb expressed as a linear combination of other functions i.e. it is closed/complete

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x) \tag{2.4}$$

Where, $c_n \in \mathbb{C}$

2.9 Linear Operators

2.10 Eigenfunctions of a Hermitian Operator

2.11 Transformations

2.11.1 Active Tranformation

In a loose sense this can be thought of as,

2.11.2 Passive Tranformation

From our discussion before it is also clear that the same transformation can be implemented as,

$$\hat{O} \to U^{\dagger}\hat{O}U \tag{2.5}$$

This is a very different viewpoint, we can understand this by visualizing it to be a

[4] Defintion

[5] we simply state this but a proof can be found in

2.11.3 Equivalence of Transformation types

It's pretty simple to see that both types of transformation constitute the same physical picture. Thus, we can take both viewpoints to mean the same physical transformation in each case, and later on we will see how this leads us two different pictures of Quantum Mechanics and how they are related.

2.12 Probability

2.12.1 Discrete Variables

Suppose we have a frequency distribution

$$N = \sum_{j=0}^{\infty} N(j) \tag{2.6}$$

The probability of an event N_j is defined as,

$$P(j) = \frac{N(j)}{N} \tag{2.7}$$

In probability theory, the sum of all probabilities is 1,

$$\sum_{j=0}^{\infty} P(j) = \sum_{j=0}^{\infty} \frac{N(j)}{N} = 1 \tag{2.8}$$

The average/mean/expectation value of a value j is given by the formula:

$$\langle j \rangle = \frac{\sum jN(j)}{N} = \sum_{j=0}^{\infty} jP(j) \tag{2.9}$$

and in general, the average of some function of j, is given by,

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j)P(j) \tag{2.10}$$

The spread of a variable's value from it's mean is called it's variance, written as

$$\sigma^2 = \left\langle (\Delta j)^2 \right\rangle \tag{2.11}$$

where,

$$\Delta j = j - \langle j \rangle$$

It's square root is called the standard deviation,

$$\sigma = \sqrt{\left\langle (\Delta j)^2 \right\rangle} = \sqrt{\langle j^2 \rangle - \langle j \rangle^2} \tag{2.12}$$

Which comes from a theorem on variances that we'll find useful later on:

$$\sigma^2 = \left\langle (\Delta j)^2 \right\rangle = \sum (\Delta j)^2 P(j) = \sum (j - \langle j \rangle)^2 P(j)$$

$$= \sum (j^2 - 2j \langle j \rangle + \langle j \rangle^2) P(j)$$

$$= \sum j^2 P(j) - 2 \langle j \rangle \sum j P(j) + \langle j \rangle^2 \sum P(j)$$

$$= \left\langle j^2 \right\rangle - 2 \langle j \rangle \langle j \rangle + \langle j \rangle^2 = \left\langle j^2 \right\rangle - \langle j \rangle^2$$

2.12.2 Continuous Variables

We now move to a continuous probability distribution, we'll create continuous analogs of all the quantities we just introduced. Let's start with probability, the probability of that x lies between a and b

$$P_{ab} = \int_a^b \rho(x) dx \tag{2.13}$$

where $\rho(x)$ is the called the probability density i.e. the probability of getting x, or more concretely,

$\rho(x)dx =$ Probability that an individual is chosend at random lies between x and $x+dx$

Now supposing the rules we held for discrete variables hold, the continuous analogs look like this:

$$1 = \int_{-\infty}^{\infty} \rho(x) dx \tag{2.14}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x \rho(x) dx \tag{2.15}$$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x) \rho(x) dx \tag{2.16}$$

$$\sigma^2 := \left\langle (\Delta x)^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2 \tag{2.17}$$

2.13 Expectation Values

In this section we'll explore how we express the expectation values of a few opeartors. Let's start with the position opeartor in the position representation (i.e. position basis):

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi(\vec{x},t)|^2 dx \tag{2.18}$$

We can differentiate 2.18 with respect to time to find the expectation value for "velocity":

$$\frac{d\langle x \rangle}{dt} =$$

Throwing away

$$\langle v \rangle = \frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} dx \tag{2.19}$$

Therefore we can write the expectation value of momentum as,

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt} = -i\hbar \int \left(\psi^* \frac{\partial \psi}{\partial x}\right) dx \tag{2.20}$$

In general, every observable is a function of position and momentum, thus for an observable $\hat{O}(x,p)$, the expectation value is given by,

$$\left\langle \hat{O}(x,p) \right\rangle = \int \psi^* \hat{O}(x, -i\hbar\nabla)\psi dx \tag{2.21}$$

For example, the expectation value of kinetic energy is,

$$\langle T \rangle = -\frac{\hbar^2}{2m} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} dx \tag{2.22}$$

Or to sum it up in Dirac notation,

$$\left\langle \hat{O} \right\rangle = \langle \psi | \hat{O} | \psi \rangle \tag{2.23}$$

2.14 Fourier Analysis

Fourier analysis is a special case of an integral transform. Fourier analysis is the decomposition of a general wave or oscillation into harmonic components. Because we treat the wave vector as the independent variable of a wave, the Fourier decomposition is typically done in terms of wave vectors. A Fourier series is a sum of sinusoidal functions, each of which is a harmonic of some fundamental wave vector or spatial frequency. A Fourier transform is an integral over a continuous distribution of sinusoidal functions. A Fourier series is appropriate when the system has boundary conditions that limit the allowed wave vectors to a discrete set. For a system where the spatial periodicity is 2L, the Fourier decomposition of a general periodic function is the series

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{ik_n x} \tag{2.24}$$

where,

$$k_n = \frac{n\pi}{L}$$

Here $c_n \in \mathbb{C}$. All $f(x) \in \mathbb{R}$ can be written as:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \right] \tag{2.25}$$

Where,

$$a_n = \frac{1}{L} \int_0^{2L} f(x) \cos\left(\frac{n\pi x}{L}\right) dx \tag{2.26}$$

$$b_n = \frac{1}{L} \int_0^{2L} f(x) \sin\left(\frac{n\pi x}{L}\right) dx \tag{2.27}$$

$$c_n = \frac{1}{2L} \int_0^{2L} f(x) e^{-ik_n x} dx \tag{2.28}$$

obtained by calculating the overlap integrals (i.e., projections or inner products) of the desired function with the harmonic basis functions. That is provided $f(x)$, obeys the following conditions i.e. **Dirichlet conditions**:

- It must be absolutely integrable over a period.
- It must be of bounded variation in any given bounded interval.
- It must have a finite number of discontinuities in any given bounded interval, and the discontinuities cannot be infinite.

A Fourier transform is appropriate when the system has no boundary conditions that limit the allowed wave vectors. In this case, the Fourier decomposition is an integral over a continuum of wave vectors:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(k) e^{ikx} dk \tag{2.29}$$

where the expansion function $a(k)$ is complex. To obtain the expansion function $a(k)$ for a givenspatial function $f(x)$ requires the inverse Fourier transform

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \tag{2.30}$$

which is a projection of the spatial function $f(x)$ onto the harmonic basis functions $e^{ikx}/\sqrt{2\pi}$. The basis functions are orthogonal and normalized in the Dirac sense, which means their projections onto each other are Dirac delta functions

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik'x} e^{-ikx} dx = \delta(k - k') \\ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx'} e^{-ikx} dk = \delta(x - x') \end{aligned} \tag{2.31}$$

2.14.1 Parseval's theorem

Parseval's theorem states that the power is the same whether calculated in position space or wave-vector space:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |a(k)|^2 dk \tag{2.32}$$

2.15 Delta Function

2.15.1 The Divergence of $\frac{\hat{r}}{r^2}$

We can see why the divergence is,

$$\nabla . \frac{\hat{r}}{r^2} = 0 \tag{2.33}$$

But if we calculate this using the Divergence theorem, we find that ,

$$\oint v.da = \int \left(\frac{\hat{r}}{r^2}\right) . \left(r^2 \sin(\theta) d\theta d\phi \hat{r}\right) = \left(\int_0^{\pi} \sin(\theta) d\theta\right) \left(\int_0^{2\pi} d\phi\right) = 4\pi \tag{2.34}$$

This is paradoxical. The issue is that it blows up at $r = 0$ but is is neglible everywhere else. How do we fix this? The Dirac Delta functional!

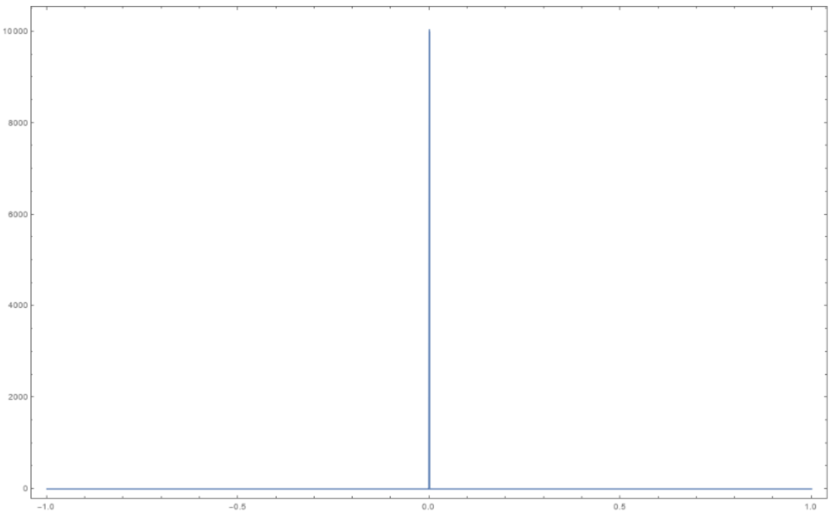


Figure 2.2: A Plot of $\delta(x)$

2.15.2 The One-Dimensional Dirac Delta Functional

The Dirac Delta is a functional [6] which we define as,

$$\delta(x-a) = \begin{cases} 0, & \text{if } x \neq a \\ \infty, & \text{if } x = a \end{cases} \tag{2.35}$$

$$\int_{-\infty}^{+\infty} \delta(x-a)dx = 1 \tag{2.36}$$

$\forall\ a \in \mathbb{R}$ We can visualize it as a sharp peak at a, We can interpret 2.36 as saying "the area of the delta distribution is always 1".

$$f(x)\delta(x-a) = f(a) \tag{2.37}$$

We can combine these to get,

$$\int_{-\infty}^{+\infty} \delta(x-a)f(x)dx = f(a) \tag{2.38}$$

A few interesting properties

$$\delta(kx) = \frac{1}{|k|}\delta(x) \tag{2.39}$$

$$\frac{d}{dx}(\delta(x)) = -\delta(x) \tag{2.40}$$

[6] An object that is a map between functions

where k is a constant

$$\frac{d\theta}{dx} = \delta(x) \tag{2.41}$$

Where θ is the step function defined as,

$$\theta(x) = \begin{cases} 1, & \text{if } x > 0 \\ o, & \text{if } x \leq 0 \end{cases} \tag{2.42}$$

2.15.3 The Three-Dimensional Dirac Delta Function

We generalize (2.35) to three dimensions,

$$\delta^3(\vec{r} - \vec{a}) = \delta(x - a_x)\delta(y - a_y)\delta(z - a_z) \tag{2.43}$$

$$\int_{-\infty}^{+\infty} \delta^3(\vec{r} - \vec{a})dV = 1 \tag{2.44}$$

We can also define the three-dimensional delta function as

$$\delta^3(\boldsymbol{\mathscr{r}}) = \frac{1}{4\pi}\left[\nabla \cdot \left(\frac{\hat{\boldsymbol{\mathscr{r}}}}{\boldsymbol{\mathscr{r}}^2}\right)\right] \tag{2.45}$$

Since,

$$\nabla\left(\frac{1}{\boldsymbol{\mathscr{r}}}\right) = -\frac{\hat{\boldsymbol{\mathscr{r}}}}{\boldsymbol{\mathscr{r}}^2}$$

We can rewrite as,

$$\delta^3(\boldsymbol{\mathscr{r}}) = -\frac{1}{4\pi}\left[\nabla^2\left(\frac{1}{\boldsymbol{\mathscr{r}}}\right)\right] \tag{2.46}$$

2.15.4 Integral representation

We have the relationship for the Fourrier transform,

$$F(x) = \int f(t)e^{-ixt}dt \tag{2.47}$$

and it's inverese

$$f(t) = \frac{1}{2\pi}\int F(x)e^{ixt}dx \tag{2.48}$$

Plugging in Eq. into Eq. we find that

$$F(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(x)dx \int_{-\infty}^{\infty} e^{i(x-y)t}dt \tag{2.49}$$

Now, invoking the definig property of the Delta function,

$$F(y) = \int_{-\infty}^{\infty} F(x)\delta(x-y)dx \tag{2.50}$$

Comparing and we find that,

$$\boxed{\delta(x-y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(x-y)t}dt \tag{2.51}}$$

2.16 Complex Analysis

2.16.1 Complex Differentiation

We call a function to **holomorphic** if it is differentiable in its domain.

2.16.2 Contour Integrals

2.16.3 Cauchy-Goursat Theorem

2.16.4 Cauchy's Integral Formula

2.16.5 A few important relations

Cauchy-Riemann Equations

Laplace Equation

2.17 Gaussian Integrals

In this section we'll try to solve integrals of the form

$$I_0(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx \; \forall \; \alpha > 0 \tag{2.52}$$

We can't directly integrate it, so we consider

$$I_0^2(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha y^2} dy \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\alpha(x^2+y^2)} dxdy \tag{2.53}$$

Switching to polar coordinates in the x-y plane,

$$I_0^2(\alpha) = \int_0^{\infty}\int_0^{2\pi} e^{-\alpha\rho^2} d\rho \; d\phi = \frac{\pi}{\alpha} \tag{2.54}$$

Therefore,

$$I_0(\alpha) = \sqrt{\frac{\pi}{\alpha}} \tag{2.55}$$

2.17.1 Special Cases

By differentiating w.r.t α we can get all integrals of the form:

$$I_{2n}(\alpha) = \int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx \tag{2.56}$$

For example,

$$I_2(\alpha) = \int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = -\frac{\partial}{\partial\alpha} \int_{-\infty}^{\infty} e^{-\alpha x^2} dx$$

$$I_2(\alpha) = \frac{\partial}{\partial\alpha} I_0(\alpha) = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

The integrals $I_{2n+1}(\alpha)$ vanish because they are integrals of odd functions over an even internval ($-\infty$ to ∞).
Note: The integrals discussed so far are valid even if $\alpha \in \mathbb{C}$ Next we'll consider,

$$I_0(\alpha, \beta) = \int_{-\infty}^{\infty} e^{-\alpha x^2 + \beta x} dx \tag{2.57}$$

We can simplify this to be,

$$I_0(\alpha, \beta) = e^{\beta^2/4\alpha} \int_{-\infty}^{\infty} e^{\alpha(x-\beta/2\alpha)^2} dx = e^{\beta^2/4\alpha}\sqrt{\frac{\pi}{\alpha}}$$

This holds even if $\alpha, \beta \in \mathbb{C} : Re(\alpha) > 0$. A corollary of the previous equation,

$$\int_0^{\infty} e^{-\alpha r} dr = \frac{1}{\alpha}$$

if we operate on this with, $(-d/d\alpha)^n$, we get:

$$\int_0^{\infty} r^n e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}}$$

2.17.2 Gamma function

If we consider this integral with $\alpha = 1$ and n replaced with $z - 1$, where z is an abitrary complex number. This lead us to the Gamma function, which is defined as:

$$\Gamma(z) = \int_{\infty}^{0} r^{z-1} e^{-r} dr = (z-1)! \; \forall \; z > 0 \in \mathbb{R} \tag{2.58}$$

2.18 The $i\epsilon$ Prescription

We will now derive and interpret the formula:

$$\frac{1}{x \mp i\epsilon} = \mathscr{P}\frac{1}{x} \pm \pi\delta(x) \tag{2.59}$$

where $\epsilon \to 0$ is a positive infinitesimally small quantity. Now we'll consider the integral

$$I = \lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{f(x)}{x-i\epsilon}dx \tag{2.60}$$

$$I = \lim_{\epsilon'\to 0}\left[\int_{-\infty}^{\epsilon'}\frac{f(x)}{x}dx + \int_{-\infty}^{\epsilon'}\frac{f(x)}{x}dx + i\pi f(0)\right]$$

$$I = \mathscr{P}\int_{-\infty}^{\infty}\frac{f(x)}{x}dx + i\pi f(0) \tag{2.61}$$

$$\frac{1}{(x-a) \mp i\epsilon} = \mathscr{P}\frac{1}{(x-a)} \pm i\pi\delta(x-a) \tag{2.62}$$

2.19 Permutation Functions

2.19.1 Kronecker delta

It simply has the 'function' of 'renaming' an index:

$$\delta^{\mu}_{\nu}x^{\nu} = x^{\mu}$$

it is in a sense simply the identity matrix. Or it is sometimes defined as:

$$\delta_{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases} \tag{2.63}$$

2.19.2 Levi-Civita Pseudotensor

The Levi-Civita Pseudotensor i.e. Tensor density is a completely anti-symmetric i.e. $\epsilon_{ijk} = -\epsilon_{jik} = -\epsilon_{ikj} = -\epsilon_{kji}$, we define it as:

$$\epsilon_{ijk} = \begin{cases} 1 \text{ if } ijk \text{ is an even permuation of } 123 \\ -1 \text{ if } ijk \text{ is an odd permuation of } 123 \\ 0 \text{ if two indices are equal} \end{cases} \tag{2.64}$$

Identities

$$\epsilon_{\alpha\beta\nu}\epsilon_{\alpha\beta\sigma} = \delta_{\mu\rho}\delta_{\nu\sigma} - \delta_{\mu\sigma}\delta_{\nu\rho} \tag{2.65}$$

From this it follows that,

$$\epsilon_{\alpha\beta\nu}\epsilon_{\alpha\beta\sigma} = 2\delta_{\nu\sigma} \tag{2.66}$$

and

$$\epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\beta\gamma} = 6 \tag{2.67}$$

2.20 Tensors

2.20.1 Vector Transformation Rules

The rules:

- For basis vectors forward transformations brings us from old to new coordinate systems and backward brings us from new to old.
- However, with vector components it's the opposite.

Suppose we have a vector $\vec{v}$ in a basis $\vec{e}_j$. We now transform it to a basis $\tilde{\vec{e}}_i$ where it becomes $\tilde{v}$. We call the forward transformation as F_{ij} and the backward as B_{ij} which we define as:

$$\tilde{\vec{e}}_j = \sum_{i=1}^{n} F_{ij}\vec{e}_i$$

$$\vec{e}_j = \sum_{i=1}^{n} B_{ij}\tilde{\vec{e}}_i$$

We can try to derive the statements made previously,

$$\vec{v} = \sum_{j=1}^{n} v_j\vec{e}_j = \sum_{i=1}^{n} \tilde{v}_i\tilde{\vec{e}}_i$$

$$\vec{v} = \sum_{j=1}^{n} v_j\vec{e}_j = \sum_{j=1}^{n} v_j(\sum_{i=1}^{n} B_{ij}\tilde{\vec{e}}_i) = \sum_{i=1}^{n}\sum_{j=1}^{n}(B_{ij}v_j)\tilde{\vec{e}}_i$$

Thus,

$$\tilde{v}_i = \sum_{j=1}^{n} B_{ij}v_j \tag{2.68}$$

Similarly,

$$\vec{v} = \sum_{j=1}^{n} v_j \vec{e}_j = \sum_{i=1}^{n} \tilde{v}_i \tilde{\vec{e}}_i$$

$$\vec{v} = \sum_{j=1}^{n} \tilde{v}_j \tilde{\vec{e}}_j = \sum_{j=1}^{n} \tilde{v}_j (\sum_{i=1}^{n} F_{ij} \vec{e}_i) = \sum_{i=1}^{n} \sum_{j=1}^{n} (F_{ij} \tilde{v}_j) \vec{e}_i$$

Thus,

$$v_i = \sum_{j=1}^{n} F_{ij} \tilde{v}_j \tag{2.69}$$

Now because vector components beehave contrary to the basis vectors, they are said to be ***"Contravariant"***

2.20.2 Index Notation

Einstein Notation i.e. Summing convention

Let us consider the sum[7],

$$x_i = \sum_{j}^{n} \Lambda_{ij} \mathcal{X}^j$$

Is the same as,

$$x_i = \Lambda_{ij} \mathcal{X}^j$$

Here, we define i to be the free index and j to be the summing index or the dummy index that is repeated to signify so.

Index Convention

When we sum from 1 to 3 we use the symbols i, j and k i.e. the English alphabet to signify that we are only considering dimnesions that are spatial/that are not a timme dimension. However, when we use the symbols ν and μ i.e. Greek alphabets we are summing from 0 to 3, we also include the temporal dimension according to the tradition of special relativity in which we name components as $\{x^0, x^1, x^2, x^3\} = \{t, x, y, z\}$ in the Cartesian framework.

2.20.3 Covectors

- Covectors can be thought of as row vector or as functions that act on Vectors such that any covector $\alpha : \mathbb{V} \rightarrow \mathbb{R}$

[7]Mind you there are no exponents there.

- Covectors are linear maps i.e. $\beta(\alpha)\vec{v} = \beta\alpha\vec{v}$ and $(\beta + \alpha)\vec{v} = \alpha\vec{v} + \beta\vec{v}$
- Covectors are elements of a Dual vector space $\mathbb{V}^*$ which has different rules for addition and scaling i.e. scalar multiplication
- You visualize covectors to be some sort of gridline on your vector space such that applying a covector to a vector is equivalent to projecting the vector along the gridline
- Covectors are invariant but their components are not
- The covectors that form the basis for the set of all covectors is called the ***"Dual Basis"***, because they are a basis for the Dual Space $\mathbb{V}^*$ i.e. any covector can be expressed as the linear combination of the dual basis
- However we are free to choose a dual basis
- For covector components, forward transformation brings us from old to new and backwards vice versa
- We can flip between row and column vectors for an orthonormal basis
- Vector components are measured by counting how many are used in the construction of a vector, but covector components are measured by counting the number of covector lines that the basis vector pierces
- The covector basis transforms contravariantly compared to the basis and it's components transform covariantly according to the basis

Contravariant Components

We denote contravariant components using the symbols

$$A^i$$

and their basis like

$$\overrightarrow{e}_i$$

Covariant Components

We denote convariant components using the symbols

$$A_i$$

and their basis like

$$\overrightarrow{e}^i$$

Relationship Between the Two Types of Components

$$|\vec{e}^{\,1}| = \frac{1}{|\vec{e}_1|\cos(\theta_1)}$$

and,

$$|\vec{e}_1| = \frac{1}{|\vec{e}^{\,1}|\cos(\theta_1)}$$

Or with 3 components we have: Since both types of components represent the same vector (as in same magnitude) only inn different bases, we can write

$$\vec{A} = A^i \vec{e}_i = A_i \vec{e}^{\,i}$$

Using Cramer's Method to find Components

2.20.4 Metric Tensor

- Pythagoras' theorem is a lie for non-orthonormal bases
- The metric Tensor is Tensor that helps us compute lengths and angles
- For two dimensions it can be written as:

$$g_{ij} = \begin{bmatrix} e_1 e_1 & e_1 e_2 \\ e_2 e_1 & e_2 e_2 \end{bmatrix}$$

- Or more abstractly

$$g_{ij} = e_i e_j$$

- The dot product between two vectors can be written as

$$||\vec{v}||||\vec{w}|| \cos\theta = v^i w^j g_{ij}$$

- we can see how this allows us to compute angles as well
- To transform the components of the Metric Tensor we have to apply the transformation twice i.e.$\tilde{g}_{\rho\sigma} = \mathbb{F}^{\mu}_{\rho}\mathbb{F}^{\nu}_{\sigma}\tilde{g}_{\mu\nu}$ or $g_{\rho\sigma} = \mathbb{B}^{\mu}_{\rho}\mathbb{B}^{\nu}_{\sigma}\tilde{g}_{\mu\nu}$

2.20.5 Tensor Products

2.20.6 Definition of a Tensor

Part III

Rules

Chapter 3

Formalism

3.1 State Vector

- In Quantum Mechanics, we start with an object called the state vector $|\psi\rangle$. All the information about the system is contained in it.

- The position basis representation of the state vector is called the wavefunction $\psi(\vec{x}, t) = \langle x|\psi\rangle$.

- If we wish to know about a particular physical measurable such as an object's position of momentum, we can extract this information from the State vector by means of acting on with an Operator that corresponds to the measurable quantity.

3.1.1 Admissibility Conditions for a Wavefunction

A physically relevant wavefunction must be:

- Continuous i.e. no singularities in it's topology

- Smooth i.e. a Taylor expansion for it exists

- Quadratically integrable with the integral being single valued i.e. finite everywhere and $\psi \to 0$ as $r \to \infty$

- Forming an orthonormal set

- Satisfying the boundary conditions of the quantum mechanical system it represents

3.2 Observables

- Observable quantities such as position and momnetum c

3.3 Time Evolution

3.3.1 Schrodinger Picture

Where
If we consider the Schrodinger picture i.e. the state vector evovles with time whereas the Observables are in a loose sense eternal. The time evolution of the state vector is given by the Schrodinger equation:

$$i\hbar\frac{\partial\left|\psi\right\rangle}{\partial t}=\hat{H}\left|\psi\right\rangle \tag{3.1}$$

Or,

$$i\hbar\frac{\partial\psi}{\partial t}=\hat{H}\psi \tag{3.2}$$

in terms of the Wavefunction. Where, $\hat{H}$ is the Hamiltonian operator, which can be expressed as:

$$\hat{H}=-\frac{\hbar^2\nabla^2}{2m}+V(\vec{x}) \tag{3.3}$$

for a free particle.

3.3.2 Heisenberg Picture

3.4 Measurement

Measurement is defined as a form of time-evolution that is non-unitary and non-deterministic. According to Born's rule

$$\int_a^b \left|\psi(\vec{x},t)\right|^2 dx = \text{Probability of finding the particle at a time t between positions a and b} \tag{3.4}$$

Thus, . Physically speaking this lends a kind of indeterminancy to the wavefunction. We can only speak of probabilities. Therefore, we can only , this brings to the measurement hypothesis, that is the State vector evolves to the state corresponding to the measurement being made. And unlike the Schrodinger equation, this evolution is non-deterministic. This tension is often called the "measurement problem", i.e. why is the measurement of an

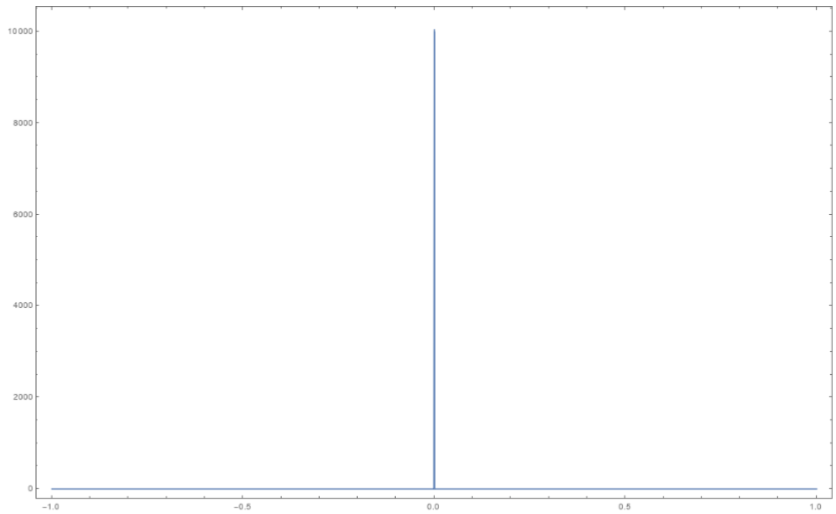


Figure 3.1: A Plot of $\delta(x)$

observable a special process distinct from others? Several theories and models claim to have resolved this, but we shall save that discussion for another time. We will fully focus on understanding the theory of Quantum Mechanics in a pragmatic lens before we question its foundations (although the converse isn't necessarily a bad thing, it isn't the purpose of this manuscript however).

3.5 Summary of Postulates

3.6 Normalization

Normalization is a process through which we ensure that,

$$\int_{-\infty}^{\infty} |\psi(\vec{x},t)|^2 dx = 1 \tag{3.5}$$

This is a natural consequence of Born's rule, we simply want all the probabilities to add up to 1. Thus, to rule out any other absurd scenarios, we make a ruling that non-Normalizable and non-square integrable Wavefunctions are unphysical.
We can also prove that once normalized, the wavefunction always remains normalized, we start by differentiating equation (3.5) with respect to time

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(\vec{x},t)|^2 dx = \frac{\partial}{\partial t}\int_{-\infty}^{\infty} |\psi(\vec{x},t)|^2 dx$$

Dealing with the term inside the integral,

$$\frac{\partial}{\partial t}|\psi(\vec{x},t)|^2 = \frac{\partial}{\partial t}(\psi^*\psi) = \psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}$$

Now the Schrodinger equation for a free particle reads as,

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar}V\psi$$

Conjugating this we can see that,

$$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^*$$

Thus,

$$\frac{\partial}{\partial t}|\psi(\vec{x},t)|^2 = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2 \psi}{\partial x^2} - \psi\frac{\partial^2 \psi^*}{\partial x^2}\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)\right]$$

Now we evaluate the integral,

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(\vec{x},t)|^2 dx = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)_{-\infty}^{\infty}$$

But ψ must go to zero as goes to infinity, otherwise the wave function would not be normalizable. Thus it follows that.

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(\vec{x},t)|^2 dx = 0 \tag{3.6}$$

And hence, the integral is constant i.e. independent of time. Therefore if is normalized at a time $t = 0$, it remains normalized for all future.

3.7 Generalized Uncertainty Principle

Suppose we have a ket $|\psi\rangle$ and two operators $\hat{A}$ and $\hat{B}$, we define two new vectors

,

,

We use the Cauchy-Shwarz inequality,

$$2|X||Y| \geq |\langle X|Y\rangle + \langle Y|X\rangle|$$

Substituting in the left-hand side, $2\sqrt{\langle X|X\rangle\langle Y|Y\rangle} \geq |\langle X|Y\rangle + \langle Y|X\rangle|$ Plugging in Eqs. (4) and (5), $2\sqrt{\langle\psi|A^2|\psi\rangle\langle\psi| - B^2|\psi\rangle} \geq |\langle X|Y\rangle + \langle Y|X\rangle|$ Taking the -1 outside, $2i\sqrt{\langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle} \geq |\langle X|Y\rangle + \langle Y|X\rangle|$ We now substitute in the right hand of the equation $2i\sqrt{\langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle} \geq |\langle\psi|\hat{A}\hat{B}|\psi\rangle - \langle\psi|\hat{B}\hat{A}|\psi\rangle|$ The negative sign is due to the i, this also seems to represent the commutator, so we substitute $2i\sqrt{\langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle} \geq |\langle\psi|[\hat{A},\hat{B}]|\psi\rangle$ Again, the right hand side looks like the expectation value of a quantity, so $2i\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq |\langle[\hat{A},\hat{B}]\rangle|$ $\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq \frac{1}{2i}|\langle[\hat{A},\hat{B}]\rangle|$ We use Eq. (2),

$\sqrt{\sigma_A^2\sigma_B^2} \geq \frac{1}{2i}|\langle[\hat{A},\hat{B}]\rangle|$ Removing the square root we get the expression: $\sigma_A\sigma_B \geq \frac{1}{2i}|\langle[\hat{A},\hat{B}]\rangle|$

This is called the generalized uncertainty principle. This basically states that two variables that do not commute cannot be measured with precision simultaneously.

Talking about position and momentum

We know that observable properties can be represented using operators, here we'll

$\hat{x} = x$ $\hat{P} = -i\hbar\frac{\partial}{\partial x}$ So we now try to find the commutator now $[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$ $[\hat{x},\hat{p}] = -ix\hbar\frac{\partial}{\partial x} + i\hbar\frac{\partial}{\partial x}$ Now let's apply this to state vector to obtain the expectation value $[\hat{x},\hat{p}]|\psi\rangle = -ix\hbar\frac{\partial}{\partial x}|\psi\rangle + i\hbar\frac{\partial x|\psi\rangle}{\partial x}$

$$[\hat{x},\hat{p}]|\psi\rangle = -ix\hbar\frac{\partial}{\partial x}|\psi\rangle + ix\hbar\frac{\partial(|\psi\rangle)}{\partial x} + i\hbar$$

$[\hat{x},\hat{p}]|\psi\rangle = i\hbar$ Substituting this into Eq.(), $\sigma_x\sigma_p \geq \frac{1}{2i}i\hbar$ $\sigma_x\sigma_p \geq \frac{\hbar}{2}$ $\sigma_x\sigma_p \geq \frac{h}{4\pi}$

3.8 Summary of Consequences

3.9 Generalized Statistical Interpretation

. [1] If you measure an observable $\hat{O}$ on a particle in the state $\psi()$, you will certainly get one of the eigenvalues of the observable. If the spetra is discrete, the probability of getting the particular eigenvalue q_n associated with the orthonormalized eigenfunction $f_n(x)$ is

$$P(q_n) = |c_n|^2 = |\langle f_x|\psi\rangle|^2 \tag{3.7}$$

[1]There of course exist other interpretations with subtle variations, we will discuss about these in Chapter 13

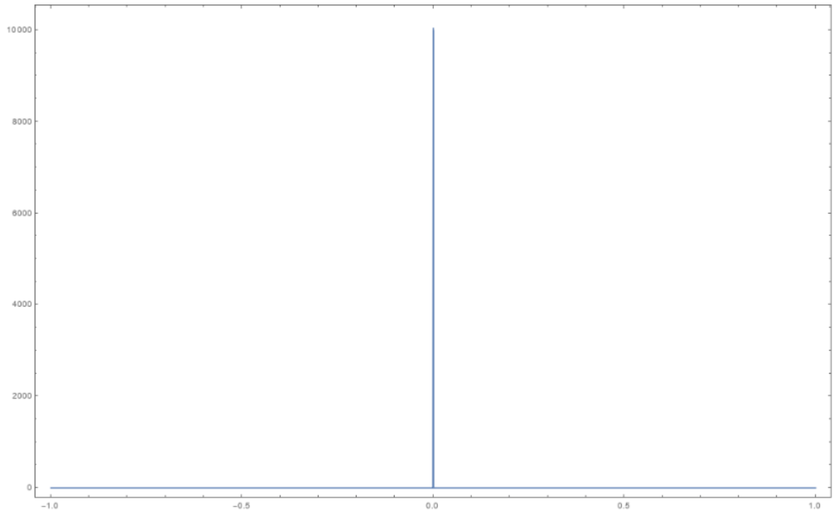


Figure 3.2: A Plot of $\delta(x)$

3.9.1 Position Measurements

3.9.2 Momentum Measurements

3.10 Stationary State

A stationary state ψ_0 is a quantum mechanical state:

- with all observables independent of time
- an eigenvector of the Hamiltonian
- corresponds to a state with a single definite energy

Stationary states themselves are not constant in time but their probability densities $|\psi_0|^2$ are

3.11 The Continuity Equation

$$\boxed{\frac{\partial \rho}{\partial t} = -\nabla.\vec{J} \qquad (3.8)}$$

Where,

$$\rho = \psi\psi^*$$

$$\vec{J} = \frac{\hbar}{2mi}\left[\psi^*\nabla\psi - (\nabla\psi^*)\psi\right]$$

represents an interesting conservation law for quantum mechanics. But first, let's try to quickly prove this.

3.11.1 Proof

W.k.t,

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}|\psi(\vec{x},t)|^2 dv = \frac{\partial}{\partial t}\int_{-\infty}^{\infty}\psi\psi^* dv = \int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial t}dv + \int_{-\infty}^{\infty}\psi\frac{\partial\psi^*}{\partial t}dv = 0$$

3.11.2 Interpretation

- Probability is conserved i.e. $\sum_i^\infty P_i = 1$ [2]
- The probability density evolves deterministically

3.12 The Density Matrix

3.12.1 Properties

- $\rho^\dagger = \rho$
- $\mathrm{Tr}\,\rho = 1$
- For a pure ensemble:
  - $\rho^2 = \rho$
  - $\mathrm{Tr}\,\rho^2 \leq 1$
- For an ensemble uniformly distributed over k states: $\rho = (1/k)\mathbb{I}$

[2]This holds well in the non-relativistic case i.e. when there is no creation or annihilation of particles

Part IV

Toy Models

Chapter 4

Toy Models

4.1 The Infinite Square Well

Suppose,

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{4.1}$$

Thus, inside the well the solutions are:

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)} \tag{4.2}$$

4.1.1 Properties of $\psi_n(x)$

- As you up in energy, each sucessive state has one more node, starting with zero nodes in $\psi_1(x)$

- They are orthonormal i.e. $\int \psi_m^*(x)\psi_n(x)dx = \delta_{mn}$

- They are complete that is any other other eigen function $f(x)$ can be expressed as a linear combination of them i.e. $\int \psi_m^*(x)\psi_n(x)dx = \delta_{mn}$

4.2 Harmonic Oscillator

4.3 Free Particle

4.4 Delta-Function Potential

4.5 Finite Square Well

4.6 Wave-Packets

Part V

Applications

Chapter 5

Symmetries and their Consequences

5.1 What is a Symmetry?

5.2 Translational Invariance in Quantum Mechanics

5.3 Time Translational Invariance

5.4 Parity Invariance

5.5 Time-Reversal Symmetry

5.6 Translationals in Two Dimensions

5.7 Rotations in Two Dimensions

5.8 The Eigenvalue Problem of L_Z

5.9 Angular Momentum in 3-Dimensions

5.10 The Eigenvalue Problem of L^2 and L_Z

5.11 Solution to Rotationally Invariant Problems

5.12 What is Spin?

5.13 Kinematics of Spin

5.14 Spin Dynamics

5.15 Return of Orbital Degrees of Freedom

5.16 Addition of Angular Momentum

5.16.1 The General Problem

5.16.2 Irreducible Tensor Operators

5.16.3 Explaining some "Accidental" Degeneracies

Chapter 6

Addition of Angular Momentum

6.1 The General Problem

How do we add an arbitray J_1 and J_2? If we did what are their $\hat{J}^2$ and $\hat{J}_z$ eigenvalues like? One way to do this would be to construct square matrices of the dimension $2j+1$. However for this we would first need to know the allowed values of j. This we conjecture to be

$$j_1 \otimes j_2 = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus ... \oplus (j_1 - j_2) \tag{6.1}$$

For our example, the total number of kets is:

$$|jm, j_1 j_2\rangle$$

where

$$j_1 + j_2 \geq j \leq j_1 - j_2$$
$$j \geq m \leq -j$$

with the normalization conditions:

$$\alpha + \beta = 0$$

$$\alpha^2 + \beta^2 = 1$$

6.1.1 Clebsch-Gordan Coeeficients

The completeness of the product kets allows us to write,

$$|jm, j_1 j_2\rangle = \sum_{m_1} \sum_{m_2} \langle j_1 m_1, j_2 m_2 | jm, j_1 j_2\rangle \, |j_1 m_1, j_2 m_2\rangle \tag{6.2}$$

Here the coffecients of the expansion are termed "Clebsch-Gordan" coefficients. Here are some of their properties:

- $\langle j_1 m_1, j_2 m_2 | jm \rangle \neq 0$ if and only if $j_1 - j_2 \leq j \leq j_1 + j_2$ or $m_1 + m_2 = m$
- $\in \mathbb{R}$
- $\langle j_1 m_1, j_2 m_2 | jm \rangle > 0$
- $\langle j_1 m_1, j_2 m_2 | jm \rangle = (-1)^{j_1 + j_2 - j} \langle j_1(-m_1), j_2(-m_2) | j(-m) \rangle$

6.1.2 Modified Spectroscopic Notation

In absence of spin using s,p,d.. is sufficient to describe angular momentum. However, in the presence of spin we change out notation to:

- Use capital letters S,P,D or L typically to indicate the value of angular momentum
- Append a subscript J to the right of L i.e. L_J to indicate the j value
- Append a superscript $2S+1$ to the left of L i.e ${}^{2S+1}L$. to indicate the degeneracy due to spin projections

Chapter 7

Systems with N degrees of freedom

7.1 N Particles in One Dimension

7.1.1 The Two-Particle Hilbert Space

Consider two particles described classically by the coordinate system $\{(x_1, p_1), (x_2, p_2)\}$. The rule for quantizing this system now is to promote them to be QM operators () and () that obey the relations:

$$\begin{cases} [\hat{X}_i, \hat{P}_j] & = i\hbar\delta_{ij} \\ [\hat{X}_i, \hat{X}_j] & = 0 \\ [\hat{P}_i, \hat{P}_j] & = 0 \end{cases} \tag{7.1}$$

In a few cases one might be able to extract all the information about the system simply from these equations. Usually they are represented in a basis. In this case we represent them in a basis of simulatneous eigenkets of the position operators

they are normalized,

$$\textit{content...} \tag{7.2}$$

In this basis We may interpret We obviously could have chosen a differeny basis from any two arbitrary commuting operators. We generally denote this Hilbert space as $\mathbb{V}_{1\otimes 2}$.

7.1.2 $\mathbb{V}_{1\otimes 2}$ as a Direct Product Space

Another way to arrive at this space is to construct it out of two one-particle spaces.

7.1.3 N particles in $d = 1$

- All the results in the previous sections generalize to an arbitrary N
- The only exception being the problem for arbitrary N cannot be reduced to N independent one-particle problems by means of any set of coordinates
- There are however exceptions to this including quadratic Hamiltonians which may be reduced to a sum over oscillator hamiltonians by the use of normal coordinates
- In such cases the oscillators become independent and their energies add up in the classical and QM cases

W.k.t that can be decoupled if we use the normal coordinates

$$x_{I,II} = \frac{x_1 \pm x_2}{\sqrt{2}} \tag{7.3}$$

and the corresponding momenta,

$$p_{I,II} = \frac{p_1 \pm p_2}{\sqrt{2}} \tag{7.4}$$

So here's the algorithm

1. Rewrite $\hat{H}$ in terms of normal coordinates
2. Verify that the coordinates are canonical i.e.
$$\{x_i, p_j\} = \delta_{ij} \tag{7.5}$$
3. Now, quantize the system by promoting these variables to operators obeying the equation
$$[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij} \tag{7.6}$$
4. Write the eigenvalue equation for $\hat{H}$ in the simultaneous basis of X_I and X_{II}

Analogously,

1. Qauntize the system directly by promoting the coordinate set $\{x_1, x_2, p_1, p_2\}$ to a set of operators
2. Write the eigenvalue equation for H in the simultaneous eigenbasis of X_1 and X_2
3. Now relabel the coordinates from $\{x_1, x_2\}$ to $\{x_I, x_{II}\}$

7.2 More Particles in More Dimensions

7.2.1 For $d = 2$

- Mathematically, a single particle in $d = 2$ is equivalent to that of 2 particles in $d = 1$
- For the sake of convenience we use different notation in the two cases
- The Cartesian coordinates of the two

7.2.2 For $d = 3$

7.3 Identical Particles

In this section we will apply the formalism that we have developed to identical particles (i.e. particles which are exact replicas of each other in terms of their intrinsic properties such as mass, charge and so on via experiment).

7.3.1 The Classical Case

7.3.2 Two-Particle Systems: Symmetric and Antisymmetric States

7.3.3 Bosons and Fermions

7.3.4 Bosonic and Fermionic Hilbert Spaces

Chapter 8

Approximations

8.1 The Variational Principle

8.1.1 Theorem

Suppose you want to find the ground state energy E_g for a system described by the Hamiltonian H, but you are unable to solve the time-dependent Schrodinger equation. Pick any normalised function ψ whatsoever, then,

$$E_g \leq \langle\psi|H|\psi\rangle \equiv \langle H\rangle \tag{8.1}$$

The expectation value of H in the tate ψ is certain to overestimate the ground-state energy. If ψ is an excited state, then it is obvious that the energy is greater than the ground state energy, but the theorem states that the same holds for any ψ whatsoever.

8.1.2 Proof

Since the eigenfunctions of H form a complete set, we can express ψ as a linear combination of them,

$$\psi = \sum_n c_n\psi_n, \text{ with } H\psi_n = E_n\psi_n$$

Since ψ is normalized,

$$1 = \langle\psi|\psi\rangle = \langle\sum_m c_m\psi_m|\sum_n c_n\psi_n\rangle = \sum_m\sum_n c_m^* c_n\langle\psi_m|\psi_n\rangle = \sum_n |c_n|^2$$

This is under the assumption that the eigenfuctions have been orthornormalized. Meanwhile,

$$\langle H\rangle = \langle\sum_m c_m\psi_m|H\sum_n c_n\psi_n\rangle = \sum_m\sum_n c_m^* E_n c_n\langle\psi_m|\psi_n\rangle = \sum_n E_n|c_n|^2$$

By defintion, ground state energy is the smallest eigenvalue, so $E_g \leq E_n$, and hence,

$$\langle H\rangle \geq E_g\sum_n |c_n|^2 = E_g$$

8.1.3 The Ground State of Helium

The helium atom consists of two electrons in orbit around a nucleus containing two protons, and neutrons, but these are irrelevant as we are only considering charge here. The Hamiltonian for this system, ignoring fine structure and smaller corrections is,

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right) \tag{8.2}$$

The ground state energy has been experimentally found out to be,

$$E_g = -78.975eV$$

We are trying to reproduce this value theoretically. This problem as no exact solution due to the electron-electron repulsion,

$$V_{ee} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \tag{8.3}$$

Ignoring this term, H splits into two independent hydrogen Hamiltonians, and the exact solution is just the product of hydrogenic wave functions,

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) = \frac{8}{\pi a^3}e^{-2(r_1+r_)/a} \tag{8.4}$$

and the energy is $8E_! = -109eV$. We can see that this isnt accurate.
To get a better approximation for E_g, we will apply the variational principle using ψ_0 as the trial wave function.

$$H\psi_0 = (8E_1 + V_{ee})\psi_0 \tag{8.5}$$

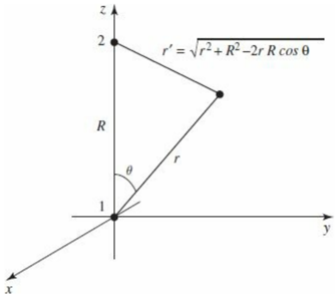
Thus,

$$\langle H\rangle = 8e_1 + \langle V_{ee}\rangle \tag{8.6}$$

Where,

$$\langle V_{ee}\rangle = \left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{8}{\pi a^3}\right)^2\int\frac{e^{-2(r_1+r_)/a}}{|\mathbf{r}_1 - \mathbf{r}_2|}d^3\mathbf{r}_1 d^3\boldsymbol{r}_2 \tag{8.7}$$

The choice of coordinates is as given below,



Integral $\boldsymbol{r}_2$ is done first. From law of cosines,

$$|\mathbf{r}_1 - \mathbf{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos\theta_2} \tag{8.8}$$

And hence,

$$I_2 \equiv \frac{e^{-4r_2/a}}{|\mathbf{r}_1 - \mathbf{r}_2|} = \int \frac{e^{-4r_2/a}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos\theta_2}} r_2^2 sin\theta_2 dr_2 \theta_2 d\phi_2 \tag{8.9}$$

The ϕ_2 integral equates to 2π, the θ_2 integral is,

$$\begin{aligned} \int_0^\pi \frac{sin\theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos\theta_2}} d\theta_2 &= \frac{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 cos\theta_2}}{r_1 r_2}\Big|_0^\pi \\ &= \frac{1}{r_1 r_2}[(r_1 + r_2) - (r_1 - r_2)] = \begin{cases} 2/r_1, & \text{if } r_2 < r_1 \\ 2/r_2, & \text{if } r_2 > r_1 \end{cases} \end{aligned} \tag{8.10}$$

Thus,

$$\begin{aligned} I_2 &= 4\pi \left(\frac{1}{r_1} \int_0^{r_1} e_{-4r_2/a} r_2^2 dr_2 + \int_{r_1}^\infty e^{-4r_2/a} r_2 dr_2 \right) \\ &= \frac{\pi a^3}{8r_1} \left[1 - \left(1 + \frac{2r_1}{a} e^{-4r_1/a} \right) \right] \end{aligned} \tag{8.11}$$

It then follows that $\langle V_{ee} \rangle$ is equal to,

$$\left(\frac{e^2}{4\pi\epsilon_0} \right) \left(\frac{8}{\pi a^3} \right) \int \frac{\pi a^3}{8r_1} \left[1 - \left(1 + \frac{2r_1}{a} e^{-4r_1/a} \right) \right] e^{-4r_1/a} r_1 sin\theta_1 dr_1 d\theta_1 d\phi_1$$

The angular integrals are easy (4π) and the r_1 integral becomes,

$$\int_0^\infty \left[re^{-4r/a} - \left(r + \frac{2r^2}{a} \right) e^{-8r/a} \right] dr = \frac{5a^2}{128}$$

Finally,

$$\langle V_{ee}\rangle = \frac{5}{4a}\left(\frac{e^2}{4\pi\epsilon_0}\right) = -\frac{5}{2}E_1 = 34eV \tag{8.12}$$

And therefore,

$$\langle H\rangle = -109eV + 34eV = -75eV \tag{8.13}$$

This is fairly accurate, but we can improve the result by thinking of a better trial wavefunction. Taking that on average, each electron represents a cloud of negative charge that partially shields the nucleus, so that the other electon sees an effective nucler charge that is somewhat less than 2.
This suggests that we use a trial function of the form,

$$\psi_1(\boldsymbol{r}_1\boldsymbol{r}_2) \equiv \frac{Z^3}{\pi a^3}e^{-Z(r_1+r_2)/a} \tag{8.14}$$

We vary Z as a variational parameter, picking the value that minimizes $\langle H\rangle$. The wavefunction is an eigenstate of the unperturbed hamiltonian, but with Z, instead of 2 in the couloumb terms. We rewrite H,

$$\begin{aligned} H = \frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{Z}{r_1}+\frac{Z}{r_2}\right) \\ + \frac{e^2}{4\pi\epsilon_0}\left(\frac{(Z-2)}{r_1}+\frac{(Z-2)}{r_2}+\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r_2}|}\right) \end{aligned} \tag{8.15}$$

The expectation value of H is evidently,

$$\langle H\rangle = 2Z^2E_1 + 2(Z-2)\left(\frac{e^2}{4\pi\epsilon_0}\right)\langle\frac{1}{r}\rangle + \langle V_{ee}\rangle \tag{8.16}$$

Here the $\langle < 1/r\rangle$ is the expectation value of $1/r$ n the hydrogenic ground state ψ_{100},

$$\left\langle\frac{1}{r}\right\rangle = \frac{Z}{a} \tag{8.17}$$

Now the expectation value of V_{ee} is,

$$\langle V_{ee}\rangle = \frac{5Z}{8a}\left(\frac{e^2}{4\pi\epsilon_0}\right) = -\frac{5Z}{4}E_1 \tag{8.18}$$

Putting everything together,

$$\langle H\rangle = [2Z^2 - 4Z(Z-2) - (5/4)Z]E_1 = [-2Z^2 + (27/4)Z]E_1 \tag{8.19}$$

According to the variational principle, this quantity exceeds E_g for any value of Z. The lowest upper bound occurs when $\langle H \rangle$ is minimised,

$$\frac{d}{dZ}\langle H \rangle = [-4Z + (27/4)]E_1 = 0 \tag{8.20}$$

from which it follows that,

$$Z = \frac{27}{16} = 1.69 \tag{8.21}$$

This says that the other electron partially screens the nucleus, reducing its effective charge from 2 to 1.69. Substituting this in Z, we find,

$$\langle H \rangle = \frac{1}{2}\left(\frac{3}{2}^6\right)E_1 = -77.5eV \tag{8.22}$$

Hence we see that the ground state of helium has been calculated with great precision. We can improve this by selecting better trial wavefunctions, but we do not require that since we have already reached within 2% of the correct answer.

8.1.4 The Hydrogen Molecule Ion

Another classic application of the variational principle is to the hydrogen molecule ion, H , consisting of a single electron in the Coulomb field of two protons . Assuming for the moment that the protons are fixed in position, a specified distance R apart, although one of the most interesting byproducts of the calculation is going to be the actual value of R. The Hamiltonian is,

$$H = \frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r} + \frac{1}{r'}\right) \tag{8.23}$$

Where r and r' are the distances to the electron from the respective protons. Next we try to guess a reasonable trial wavefunction, by taking a hydrogen atom in its ground state,

$$\psi_0(r) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a} \tag{8.24}$$

bringing the second proton in from "infinity," and nailing it down a distance R away. If R is substantially greater than the Bohr radius, the electron's wave function probably isn't changed very much. But we would like to treat the two protons on an equal footing, so that the electron has the same probability of being associated with either one. This suggests that we consider a trial function of the form,

$$\psi = A[\psi_0(r) + \psi_0(r')] \tag{8.25}$$

Normalising this wave function,

$$1 = \int |\psi|^2 d^3r = |A|^2 \left[\psi_0(r)^2 d^3\boldsymbol{r} + \int \psi_0(r')^2 + 2\int \psi_0(r)\psi_0(r')d^3r\right] \tag{8.26}$$

Evaluating the integrals give the normalisation factor to be,

$$|A|^2 = \frac{1}{2(1+I)} \tag{8.27}$$

Where I is,

$$I = e^{-R/a}\left[1 + \frac{R}{a} + \frac{1}{3}\left(\frac{R}{a}\right)^2\right] \tag{8.28}$$

Now computing the expectation value of the Hamiltonian in the trial state ψ,

$$\langle H \rangle = \left[1 + 2\frac{(D+X)}{1+I}\right] E_1 \tag{8.29}$$

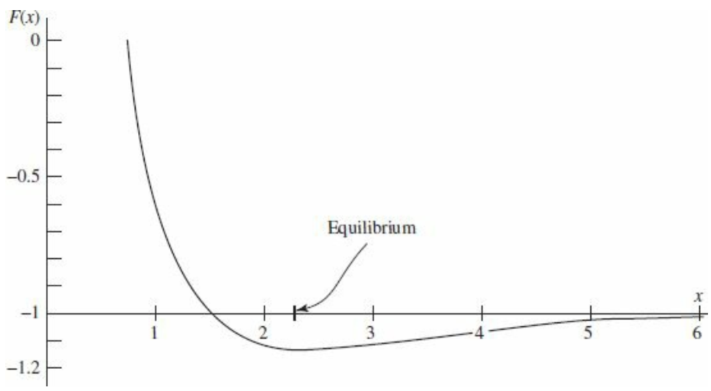
According to the variational principle,

$$V_{pp} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{R} = -\frac{2a}{R}E_1 \tag{8.30}$$

Thus the total energy of the system, in the units of $-E_1$, and expressed as a function of $x \equiv R/\alpha$, is less than,

$$F(x) = -1 + \frac{2}{x}\left\{\frac{(1-(2/3)x^2)e^{-x} + (1+x)e^{-2x}}{1 + (1 + x + (1/3)x^2)e^{-x}}\right\} \tag{8.31}$$

Plotting this function,



Evidently bonding does occur, for there exists a region in which the graph goes below -1 , indicating that the energy is less than that of a neutral atom plus a free proton.

8.2 The WKB Approximation

8.2.1 Introduction

The WKB (Wentzel, Kramers, Brillouin)1 method is a technique for obtaining approximate solutions to the time-independent Schrödinger equation in one dimension (the same basic idea can be applied to many other differential equations, and to the radial part of the Schrödinger equation in three dimensions). It is particularly useful in calculating bound state energies and tunneling rates through potential barriers. Imagine a particle of energy E moving through a region where the potential $V(x)$ is a constant. if $E > V$, the wavefunction is of the form,

$$\psi(x) = Ae^{\pm ikx}, \text{ with } k \equiv \sqrt{2m(E-V)/\hbar}$$

The plus sign indicates that the particle is traveling to the right, and the minus sign means it is going to the left (the general solution, of course, is a linear combination of the two). The wave function is oscillatory, with fixed wavelength and unchanging amplitude . Now suppose that the potential is not constant, but varies rather slowly in comparison to λ , so that over a region containing many full wavelengths the potential is essentially constant. Then it is reasonable to suppose that ψ remains practically sinusoidal, except that the wavelength and the amplitude change slowly with x. This is the inspiration behind the WKB approximation. In effect, it identifies two different levels of x-dependence: rapid oscillations, modulated by gradual variation in amplitude and wavelength.
If $E < V$,

$$\psi(x) = Ae^{\pm kx}, \text{ with } k \equiv \sqrt{2m(V-E)/\hbar}$$

If $V(x)$ is not constant, but varies slowly in comparison with $1/k$, the solution remains practically exponential. The approximation fails at the classical turning point, where $E \approx V$, where λ goes to infinity.

8.2.2 The Classical Region

The Schrodinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

can be rewritten as,

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi \tag{8.32}$$

where,

$$p(x) \equiv \sqrt{2m[E - V(x)]} \tag{8.33}$$

is the classical formula for momentum of a particle with total energy E and potential energy $V(x)$. We assume that $E > V$, and this is the classical region and the particle is confined to this range of x. Writing the complex function ψ in terms of amplitude and phase,

$$\psi(x) = A(x)e^{i\phi(x)} \tag{8.34}$$

Using a prime to denote the derivative with respect to x, we find,

$$\frac{d\psi}{dx} = (A' + iA\phi')e^{i\phi}$$

And,

$$\frac{d^2\psi}{dx^2} = [A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2] \tag{8.35}$$

Putting this in equation (32)

$$\frac{d^2\psi}{dx^2} = [A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2] = -\frac{p^2}{\hbar^2}A \tag{8.36}$$

We can split this into two parts, the real and imaginary,

$$A'' - A(\phi')^2 = \frac{-p^2}{\hbar^2}A, \text{ or } A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right] \tag{8.37}$$

And,

$$2A'\phi' + A\phi'' = 0, \text{ or } (A^2\phi')' = 0 \tag{8.38}$$

From this we get that,

$$\phi(x) = \pm\frac{1}{\hbar}\int p(x)dx \tag{8.39}$$

And then,

$$\psi(x) \approxeq \frac{C}{\sqrt{p(x)}}e^{\pm\frac{1}{\hbar}\int p(x)dx} \tag{8.40}$$

And that the general approximate solution will be a linear combination of two of these terms, one with each sign. See that,

$$|\psi(x)|^2 \approxeq \frac{|C|^2}{p(x)} \tag{8.41}$$

Which says that the probability of finding a particle at point x is inversely proportional to the classical momentum at that point. Sometimes, the WKB approximation is derived from this semiclassical observation.

8.2.3 Tunneling

Now assuming that $E < V$, $p(x)$ becomes imaginary,

$$\psi(x) \approxeq \frac{C}{\sqrt{|p(x)|}} e^{\pm\frac{1}{\hbar}\int |p(x)|dx} \tag{8.42}$$

Take a problem of scattering from a rectangular barrier with a bumpy top, to the left of the barrier,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{8.43}$$

To the right of the barrier,

$$\psi x = Fe^{ikx} \tag{8.44}$$

Where F is the transmitted amplitude and the tunneling probability is,

$$T = \frac{|F|^2}{|A|^2} \tag{8.45}$$

Our WKB approximation gives us,

$$\psi(x) \approxeq \frac{C}{\sqrt{|p(x)|}} e^{\pm\frac{1}{\hbar}\int_0^x |p(x')|dx'} + \frac{D}{\sqrt{|p(x)|}} e^{\pm-\frac{1}{\hbar}\int_0^x |p(x')|dx'} \tag{8.46}$$

If the barrier is sufficiently wide, the exponentially increasing term diminishes, and the relative amplitudes look like,

$$\frac{|F|}{|A|} \approx e^{\pm-\frac{1}{\hbar}\int_0^\alpha |p(x')|dx'}$$

So that,

$$T \approxeq e^{-2\gamma} \tag{8.47}$$

$$\gamma \equiv \frac{1}{\hbar}\int_0^\alpha |p(x')|dx' \tag{8.48}$$

8.2.4 The connection formulas

We have obtained the wavefunctions for before and after the walls of the potential well, now to determine the region within the potential well, or at a turning point ($E = V$), shifting the axes so that the right hand turning point occurs at $x = 0$, in the WKB approximation we have,

$$\psi(x) \approxeq \begin{cases} \frac{1}{\sqrt{|p(x)|}} \left[Be^{\frac{1}{\hbar}\int_x^0 |p(x')|dx'} + Ce^{\pm-\frac{1}{\hbar}\int_x^0 |p(x')|dx'} \right], \text{ if } x < 0 \\ \frac{1}{\sqrt{|p(x)|}} De^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'} \text{ if } x > 0 \end{cases} \tag{8.49}$$

We essentially patch the two WKB solutions, by using the connection formulas,

$$B = -ie^{i\pi/4}D, \text{ and } C = ie^{-i\pi/4}D \tag{8.50}$$

Now providing the final wavefunction,

$$\psi(x) \approxeq \begin{cases} \frac{-2D}{\sqrt{|p(x)|}} sin\left[\frac{1}{\hbar}\int_x^{x^2}|p(x')|dx' + \frac{\pi}{4}\right], \text{ if } x < x_2 \\ \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_{x_2}^{x}|p(x')|dx'} \text{ if } x > x_2 \end{cases} \tag{8.51}$$

Where x_2 is an arbitrary point.

8.3 The Adiabatic Approximation

8.3.1 Adiabatic processes

A gradual change in the external conditions characterises an adiabatic process. There are two characteristic times involved, T_i, the internal time, which governs the motion of the system itself and T_e, the external time regarding the change in external parameters.

Suppose that the Hamiltonian changes gradually from some initial form H^i to some final form H^f, the adiabatic theorem states that if the particle was initially in the nth eigenstate of H^i, it will be carried under the Schrodinger equation into the nth eigenstate of H^f.

Take the example of a particle prepared in the ground state of an infinite square well,

$$\psi^i(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right) \tag{8.52}$$

If we now gradually move the right wall out to 2a. the adiabatic theorem says that the particle will end up in the ground state of the expanded well,

$$\psi^f(x) = \sqrt{\frac{1}{a}}\sin\left(\frac{\pi}{2a}x\right) \tag{8.53}$$

Note that this change in Hamiltonian isnt small, like perturbation theory, the change can be as huge as needed, but the change should happen slowly is what the adiabatic approximation requires.

8.3.2 Berry's Phase

Now we discuss how the Adiabatic approximation is used in nonholonomic processes, where a system does not return to its original state when transported around a closed loop.
If the Hamiton is independent of time, then a particle which starts out in the nth eigenstate $\psi_n(x)$,

$$H\psi_n(x) = E_n\psi_n(x) \tag{8.54}$$

remains in the n^{th} eignstate, simply picking up a phase factor,

$$\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar} \tag{8.55}$$

But the adiabatic theorem states that when H changes gradually, the particle remains in the n^th eignstate, even as the eigenfunction itself evolves,

$$\Psi_n(x,t) = \psi_n(x,t)e^{-\frac{1}{\hbar}\int_0^t E_n(t')dt'}e^{i\gamma_n(t)} \tag{8.56}$$

Where the term,

$$\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')dt' \tag{8.57}$$

Is the dynamic phase and the extra phase, $\gamma_n(t)$ is the geometric phase, which has its significance in the adiabatic theorem.
The net geometric phase change is usually given by,

$$\gamma_n(t) = i\oint\langle\psi_n|\nabla_R\psi_n\rangle \cdot dR \tag{8.58}$$

This is a line integral around a losed loop in parameter space, and its not zero. This is called Berry's phase, and it depends only on the path taken, not on how fast the path is traversed, meanwhile the dynamic phase depends critically on elapsed time

Chapter 9

Perturbation Theory

9.1 Non-Degenerate Perturbation Theory

9.1.1 General Formulation

Suppose we have solved the time-independent Schrodinger wave equation for a given potential (in this case, an infinite potential square well)

$$H^0\psi_n^0 = E_n^0\psi_n^0 \tag{9.1}$$

and obtaining a complete set of orthonormal eigenfunctions ψ_n^0,

$$\left\langle \psi_n^0 \middle| \psi_m^0 \right\rangle = \delta_{nm} \tag{9.2}$$

and the corresponding eigenvalues E_n^0. If we perturb the potential slightly in the potential well and try to solve for the new eigenvalues and eigenfunctions,

$$H\psi_n = E_n\psi_n \tag{9.3}$$

Here, we use perturbation theory to get approximate solutions to the perturbed problem by building on the exact solutions of the unperturbed case. To begin with, we write the perturbed/new Hamiltonian as the sum of two terms,

$$H = H^0 + \lambda H' \tag{9.4}$$

Where H' is the perturbation. We take λ to be a small number, and the H will be the true, exact Hamiltonian. Writing ψ_n and E_n as a power series in λ, we get,

$$\psi_n = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + ... \tag{9.5}$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + ... \tag{9.6}$$

Here E_n^1 is the first-order correction to the n^th eigenvalue, and ψ_n^1 is the first-order correction to the n^th eigenfunction. E_n^2 and ψ_n^2 are the second-order corrections to the eigenvalues and eigenfunctions, and so on. Plugging in Equations (4),(5) and (6) in Equation (3) gives us,

$$\begin{aligned}(H^0 + \lambda H')[\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + ...] = \\ (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + ...)[\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + ...]\end{aligned} \tag{9.7}$$

We can rewrite Equation (7) by collecting like powers of λ in the form,

$$\begin{aligned}H^0\psi^0 + \lambda(H^0\psi_n^1 + H'\psi_n^0) + \lambda^2(H^0\psi_n^2 + H'\psi_n^1) + ... \\ E_n^0\psi^0 + \lambda(E_n^0\psi_n^1 + E_n^1\psi_n^0) + \lambda^2(E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0) + ...\end{aligned}$$

We can get the first order (λ^1) equation from Equation (7),

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^0 + \psi_n^0 \tag{9.8}$$

And the second order (λ^2),

$$H^0\psi_n^2 + H'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0 \tag{9.9}$$

And this can be done for higher powers of λ as well.

9.1.2 First order perturbation theory

If we take the inner product of Equation (8), with ψ_n^0,

$$\langle\psi_n^0|H^0\psi_n^1\rangle + \langle\psi_n^0|H'\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_0^1\langle\psi_n^0|\psi_n^0\rangle \tag{9.10}$$

Because of the useful property of H^0 to be Hermitian, hence Equation (10) becomes,

$$\langle\psi_n^0|H^0\psi_n^1\rangle = \langle H^0\psi_n^0|\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle = \langle E_n^0\psi_n^0|\psi_n^1\rangle \tag{9.11}$$

And hence the terms in Equation (10) cancel out and the property $\langle\psi_n^0|\psi_n^0\rangle = 1$ give the equation,

$$E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle \tag{9.12}$$

This is a fundamental result in first-order perturbation theory, and it states that first-order correction to energy is the expectation value of the pertubation in the unperturbed state.

Now to get the first-order correction to the wave function, we rewrite Equation (8),

$$(H^0 - E_n^0)\psi_n^1 = -(H'E_n^1)\psi_n^0 \tag{9.13}$$

The right side is a known fucntion, so this amounts to an inhomogenious differential equation for $\psi_n^!$. The unpertubed wave functions constitute a complete set, so ψ_n^1 can be writtten as a linear combination of them,

$$\psi_n^1 = \sum_{m\neq n} c_m^{(n)} \psi_m^0 \tag{9.14}$$

We know that ψ_m^0 satisfies the unpertubed Schrodinger wave equation, so we have,

$$\sum_{m\neq n} (E_m^0 - E_n^0) c_m^{(n)} \psi_m^0 = -(H' - E_n^1)\psi_n^0 \tag{9.15}$$

Taking the inner product with ψ_l^0,

$$\sum_{m\neg n} (E_m^0 - E_n^0) c_m^{(n)} \left\langle \psi_l^0 \middle| \psi_m^0 \right\rangle = -\langle \psi_l^0 | H' | \psi_n^0 \rangle + E_n^1 \left\langle \psi_l^0 \middle| \psi_n^0 \right\rangle \tag{9.16}$$

If $l = n$, is zero, we then get,

$$E_m^0 - E_n^0) c_l^{(n)} = -\langle \psi_l^0 | H' | \psi_n^0 \rangle \tag{9.17}$$

Or that,

$$c_n^{(n)} = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \tag{9.18}$$

So,

$$\psi_n^1 = \sum_{m\neg n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0 \tag{9.19}$$

Note that the perturbed energies are surprisingly accurate, while the wave functions are of poor accuracy.

9.1.3 Second order perturbation theory

We take the inner poduct of the second-order equation with ψ_n^0,

$$\left\langle \psi_n^0 \middle| H^0 \psi_n^2 \right\rangle + \left\langle \psi_n^0 \middle| H' \psi_n^1 \right\rangle = E_n^0 \left\langle \psi_n^0 \middle| \psi_n^2 \right\rangle + E_n^1 \left\langle \psi_n^0 \middle| \psi_n^1 \right\rangle + E_n^2 \left\langle \psi_n^0 \middle| \psi_n^0 \right\rangle \tag{9.20}$$

We exploit the Hermiticity of H^0,

$$\left\langle \psi_n^0 \middle| H^0 \psi_n^2 \right\rangle = \left\langle H^0 \psi_n^2 \middle| \psi_n^2 \right\rangle = E_n^0 \left\langle \psi_n^0 \middle| psi_n^2 \right\rangle \tag{9.21}$$

So the first term on the left cancels the first term on the right. Hence we get the formula for E_n^2 to be,

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n^1 \rangle - E_n^1 \left\langle \psi_n^0 \middle| \psi_n^1 \right\rangle \tag{9.22}$$

But,

$$\left\langle \psi_n^0 \middle| \psi_n^1 \right\rangle = \sum_{m \neq n} c_m^{(n)} \left\langle \psi_n^0 \middle| \psi_m^0 \right\rangle = 0 \tag{9.23}$$

so,

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n^1 \rangle = \sum_{m \neq n} c_m^{(n)} \left\langle \psi_n^0 \middle| \psi_m^0 \right\rangle = \sum_{m \neq n} c_m^{(n)} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle \langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \tag{9.24}$$

Therefore,

$$E_n^2 = \sum_{m \neq n} c_m^{(n)} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} \tag{9.25}$$

This is the fundamental result of second order perturbation theory.

9.2 Degenerate Perturbation Theory

9.2.1 Motivation

If two or more distinct states, take ψ_a^0 and ψ_b^0 share the same energy, ordinary perturbation theory fails since Equation (25) blows up. So hence we need to obtain a different way to handle the problem.

9.2.2 Twofold Degeneracy

Suppose,

$$\begin{aligned} H^0 \psi_a^0 &= E^0 \psi_a^0 \\ H^0 \psi_b^0 &= E^0 \psi_b^0 \\ \left\langle \psi_a^0 \middle| \psi_b^0 \right. &= \left. 0 \right\rangle \end{aligned}$$

And note that any of linear combinations of these states,

$$\psi^0 = \alpha \psi_a^0 + \beta \psi_b^0 \tag{9.26}$$

is still an eigenstate of H^0, with the same eigenvalue E^0,

$$H^0 \psi^0 = E^0 \psi^0 \tag{9.27}$$

When H is perturbed, it breaks the degeneracy. When we increase λ, the common unperturbed energy E^0 splits into two. When we take away the

perturbation, the upper state redyces to one linear combination of ψ_a^0 and ψ_b^0, and the lower state reduces to some other linear combination. We need to figure out the good linear combinations.
Now writing the good unperturbed states in general form, keeping α and β adjustable and solving the Schrodinger equation,

$$H\psi = E\psi \tag{9.28}$$

With $H = H^0 + \lambda H'$ and,

$$E = E^0 + \lambda E^1 + \lambda^2 E^2 + ... \tag{9.29}$$
$$\psi = \psi^0 + \lambda\psi^1 + \lambda^2\psi^2 + ... \tag{9.30}$$

Plugging these into Equation (28) and collecting like powers of λ, as before, we find,

$$H^0\psi^0 + \lambda(H\psi^0 + H^0\psi^1) + ... = E^0\psi^0 + \lambda(E^1\psi^0 + E^0\psi^1) + ... \tag{9.31}$$

But $H^0\psi^0 = E^0\psi^0$, so the first term cancel; at order λ^1 we have,

$$H\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \tag{9.32}$$

Taking inner product with ψ_a^0,

$$\langle\psi_a^0|H^0|\psi^1\rangle + \langle\psi_a^0|H'|\psi^0\rangle = E^0\left\langle\psi_a^0|\psi^1\right\rangle + E^1\left\langle\psi_a^0|\psi^0\right\rangle \tag{9.33}$$

Because H^0 is Hermitian, the first term on the left cancels the term on the right. Putting this in Equation (26), we get,

$$\alpha\langle\psi_a^0|H'|\psi_a^0\rangle = \beta\langle\psi_a^0|H'|\psi_b^0\rangle = \alpha E^1 \tag{9.34}$$

Or in a more compact form,

$$\alpha W_{aa} + \beta W_{ab} = \alpha E^1 \tag{9.35}$$

Where,

$$W_{ab} = langle\psi_a^0|H'|\psi_b^0\rangle$$

Similarly, the inner product with ψ_b^0 gives us,

$$\alpha W_{ba} + \beta W_{bb} = \beta E^1 \tag{9.36}$$

Now using Equation (35) and (36),

$$\alpha[W_{ab}W_{ba} - (E^1 - W_{aa}))(E^1 - W_{bb})] = 0 \tag{9.37}$$

When $\alpha \neq 0$,

$$(E^1)^2 - E^1(W_{aa} + Wbb) + (W_{aa}W_{bb} - W_{ab}W_{ba}) = 0 \tag{9.38}$$

Using the quadratic formula and knowing that $W_{ba} = W_{ab}^*$,

$$E_{\pm}^1 = \frac{1}{2}\left[W_{aa} + W_b b \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\right] \tag{9.39}$$

This is the fundamental result of degenerate pertubration theory, the two roots correspond to the two perturbed energies.
Note that when $\alpha = 0$, we get the nondegenerate perturbation theory (since $\beta = 1$).

9.2.3 Higher-Order Degeneracy

We start by rewriting Equations (35) and(36) in matrix form,

$$\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{9.40}$$

The E^1s are the eigenvalues of the W-matrix, Equation (38) being the characteristic equation for this matrix and the good linear combinations of the unperturbed states are the eigenvectors of W. For n-fold degeneracy, we look for the eigenvalues of the $n \times n$ matrix,

$$W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle \tag{9.41}$$

9.2.4 Lamb Shift

An interesting feature of the fine structure formula is that it depends only on j and not l, moreover in general two different values of l share the same energy. For example, the $2S_{1/2}()$ and $2P_{1/2}()$ states should remain perfectly degenerate. However in 1947 Lamb and Retherford performed an experiment that displayed something to the contrary. The S state is slightly higher in energy than the p state. The explanation of this "Lamb" shift was later explained by Bethe, Feynman, Schwinger and Tomonaga (the founders of QED) as a corollary of the electromagnetic field itself being quantised. Sharply in contrast to the hyperfine structure of Hydrogen, the Lamb shift is a completely novel i.e. non-classical (as the hyperfine structure is explained through Coulomb's law and the Biot-Savart Law) phenomena. It arises from a radiative correction in Quantum Electrodynamics to which classical theories are mute. In Feynman lingo, this arises from loop corrections as potrayed below. Naively,

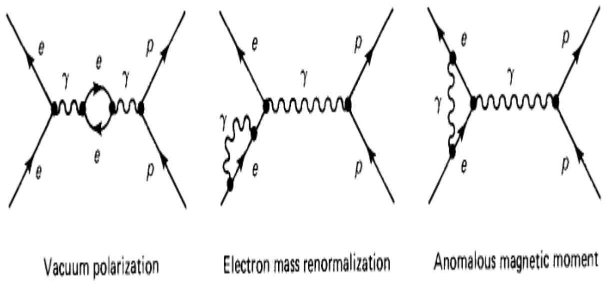


Figure 9.1: Different kinds of radiative corrections

1. the first diagram describes pair-production in the neighbhorhood of a nucleus, leading to a partial screening effect of the proton's charge;

2. the second diagram reflects the fact that the electromagnetic field has a non-zero ground state

3. the third diagram leads to a tiny modification of the electron's magnetic dipole moment (an addition of $a + \alpha/2\pi = 1.00116$)

We shall not discuss the results in depth but rather consider two exemplary cases:
For $l = 0$,

$$\Delta E_{Lamb} = \alpha^5 mc^2 \frac{1}{4n^3} \left[k(n, 0)\right] \tag{9.42}$$

Where $k(n, 0)$ is a numerical factor defined as:

$$k(n,0) = \begin{cases} 12.7, & \text{if } n = 1 \\ 13.2, & \text{if } n \to \infty \end{cases}$$

For $l = 0$ and $j = l \pm \frac{1}{2}$,

$$\Delta E_{Lamb} = \alpha^5 mc^2 \frac{1}{4n^3} \left[k(n, 0) \pm \frac{1}{\pi(l + \frac{1}{2})(l + \frac{1}{2})}\right] \tag{9.43}$$

Here, $k(n, l)$ is a very small number (< 0.05) which varies a little with it's arguments.
The Lamb shift is tiny except for the case $l = 0$, for which it amounts to about 10% of the fine structure. However, since it depends on l, it lifts the degeneracy of the pairs of states with common n and j and in particular it splits $2S_{1/2}$ and $2P_{1/2}$.

9.3 The Zeeman Effect

When an atom is placed in a uniform magnetic field $B_{Ext.}$, the energy levels are shifted, this is known as the Zeeman effect. For the case of a single electron, the shift is:

$$H_Z^{'} = -(\mu_l + \mu_s).B_{Ext.} \tag{9.44}$$

Where,

$$\mu_s = -\frac{e}{m_e}S \tag{9.45}$$

is the magnetic dipole moment associated with electron spin, and

$$\mu_l = -\frac{e}{2m_e}L \tag{9.46}$$

is the dipole moment associated with orbital motion. The gyromagnetic ratio in this case is simply classical i.e. $q/2m$, it is only for spin that we have an extra factor of 2. We now rewrite (9.44) as:

$$H_Z^{'} = \frac{e}{2m_e}(L + 2S).B_{Ext.} \tag{9.47}$$

The nature of the Zeeman splitting depnds on the strength of the external field vs. the internal one that gives rise to spin-orbit/spin-spin coupling. This table provides a short review of the different cases:

Case	**Name**	**Comments**
$B_{Ext.} >> B_{Int.}$	Strong-Field Zeeman Effect	Zeeman effect dominates; fine structure becomes the perturbation
$B_{Ext.} << B_{Int.}$	Weak-Field Zeeman Effect	Fine structure dominates; $H_z^{'}$ can be treated as a small perturbation
$B_{Ext.} = B_{Int.}$	Intermediate Zeeman Effect	Both the fields are equal in strength thus we would need elements of degenerate peturbation theory and will need to diagonlize the necessary portion of the Hamiltonian "by hand"

In the next few sections we'll explore all of them in depth.

9.3.1 Weak-Field Zeeman Effect

Here the fine structure dominates, thus the conserved quantum numbers are n, l, j and m_j, but not m_l and m_s due to the spin-orbit coupling L and S are not separately conserved. Generally speaking, in this problem we have a perturbation pile on top of a perturbation. Thus, the conserved quantum number are those appropriate to the dominant . In first order perturbation theory, the Zeeman correction to energy is,

$$E_Z^1 = \langle nljm_j|H_Z^{'}|nljm_j\rangle = \frac{e}{2m}B_{Ext.}\langle L+2S\rangle \tag{9.48}$$

Now to figure out $\langle L+2S\rangle$, we know that $L+2S = J+S$, this doesn't immediately tell us the expectation value of S but we can figure it out as by understanding that $J = L+S$ is conserved and that the time average of S is simply it's projection along J:

$$S_{Ave} = \frac{(S.J)}{J}J \tag{9.49}$$

But, $L = J - S$, so $L^2 = J^2 + S^2 - 2J.S$, hence:

$$S.J = \frac{1}{2}(J^2 + S^2 - 2J.S) = \frac{\hbar^2}{2}[j(j+1) + s(s+1) - l(l+1)] \tag{9.50}$$

from which it follows that,

$$\langle L+2S\rangle = \left\langle\left(1+\frac{S.J}{J^2}J\right)\right\rangle = \left[1+\frac{j(j+1)-l(l+1)+3/4}{2j(j+1)}\right]\langle J\rangle \tag{9.51}$$

The term in the square brackets is called the Lande g-factor, denoted by g_j. Now, if we choose B_z to lie along $B_{Ext.}$, then:

$$E_Z^1 = \mu_B g_j B_{Ext.} m_j \tag{9.52}$$

where,

$$\mu_B = \frac{e\hbar}{2m} = 5.788\times10^{-5}\ eVT^{-1}$$

is the so called Bohr magneton. The total energy is the sum of the fine-structure part and the Zeeman contribution, in the ground state i.e. $n = 1, l = 0, j = 1/2$ and therefore, $g_J = 2$, it splits into two levels:

$$-13.6\ eV(1+\alpha^2/4) \pm \mu_B B_{Ext.} \tag{9.53}$$

with different signs for different m_j's this is plotted below.

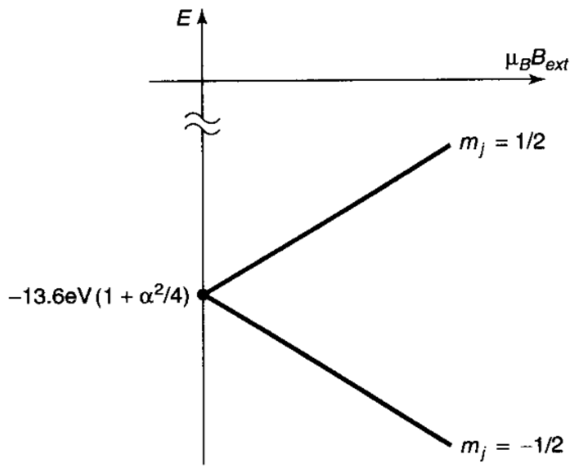


Figure 9.2: Weak-field Zeeman splitting of the ground state of hydrogen; the upper line has a slope of 1 and the lower line a slope of −1

9.3.2 Strong-Field Zeeman Effect

In this case, the Zeeman effect is often referred to as the "Paschen-Back" effect. The conserved quantum numbers are now but and because in the presence of an external torque, the total angular momentum is not conserved but the it's individual components are. The Zeeman Hamiltonian is,

$$H_Z^{'} = \frac{e}{2m} B_{Ext.}(L_z + 2S_z) \tag{9.54}$$

and the unperturbed energies are:

$$E_{nm_lm_s} = -\frac{13.6\ eV}{n^2} + \mu_B B_{Ext.}(m_l + 2m_s) \tag{9.55}$$

This would be our result if we ignore the fine structure completely. However, we need to take that into account as well. In first-order perturbation theory, the fine structure correction to these levels is:

$$E_{fs}^1 = \langle n\ l\ m_l\ m_s | H_r^{'} + H_{so}^{'} | n\ l\ m_l\ m_s \rangle \tag{9.56}$$

The relativistic contribution is the same as before for the spin-orbit term, we need

$$\langle S.L \rangle = \langle S_x \rangle \langle L_x \rangle + \langle S_y \rangle \langle L_y \rangle + \langle S_z \rangle \langle L_z \rangle = \hbar^2 m_l m_s \tag{9.57}$$

Here $\langle S_x \rangle = \langle S_y \rangle = \langle L_x \rangle = \langle L_y \rangle = 0$ for the eigenstates of S_z and L_z. Putting it all together:

$$E_{fs}^1 = \frac{13.6\ eV}{n^3} \alpha^2 \left(\frac{3}{4n} - \left[\frac{l(l+1) - m_l m_s}{l(l+1/2)(l+1)} \right] \right) \tag{9.58}$$

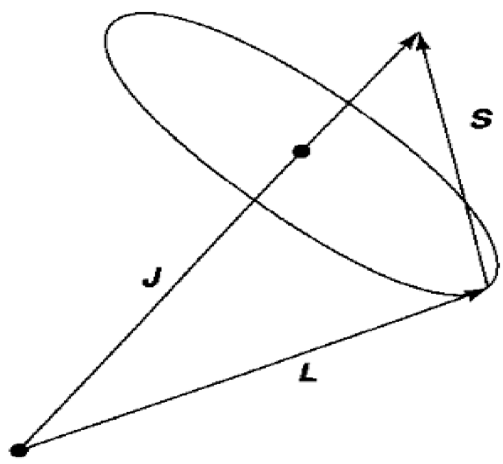


Figure 9.3: In the presence of spin-orbit coupling, L and S are not separately conserved, they precess about the fixed total angular momentum J

Th term in the square brackets is indeterminate for $l = 0$, it's correct value in this case is 1. The total energy here is the sum of the Zeeman part and the fine structure contribution.

9.3.3 Intermediate Zeeman Effect

In this case, we must treat both the effects as perturbations to the Bohr Hamiltonian,

$$H^{'} = H^{'}_{Z} + H^{'}_{fs} \tag{9.59}$$

In section we'll discuss the case $n = 2$, and use it as the basis for degerate perturbation theory. The states here are characterized by l, j and m_j. We could use l,m_l,m_s states but this makes the matrix elements of $H^{'}_{Z}$ easier to deal with but that of $H^{'}_{fs}$ difficult. Using the Clebsch-Gordan coefficients to express $|jm_j\rangle$ as a linear combination of $|lm_l\rangle\,|sm_s\rangle$ we have:

$$l = 0 = \begin{cases} \psi_1 & \left|\frac{1}{2}\frac{1}{2}\right\rangle = |0\ 0\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle \\ \psi_2 & \left|\frac{1}{2}\frac{-1}{2}\right\rangle = |0\ 0\rangle \left|\frac{1}{2}\frac{-1}{2}\right\rangle \end{cases}$$

$$l = 1 = \begin{cases} \psi_3 & \left|\frac{3}{2}\frac{3}{2}\right\rangle = |1\ 1\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle \\ \psi_4 & \left|\frac{3}{2}\frac{-3}{2}\right\rangle = |1\ -1\rangle \left|\frac{1}{2}\frac{-1}{2}\right\rangle \\ \psi_5 & \left|\frac{3}{2}\frac{1}{2}\right\rangle = \sqrt{2/3}\,|1\ 0\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{1/3}\,|1\ 1\rangle \left|\frac{1}{2}\frac{-1}{2}\right\rangle \\ \psi_6 & \left|\frac{1}{2}\frac{1}{2}\right\rangle = -\sqrt{1/3}\,|1\ 0\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{2/3}\,|1\ 1\rangle \left|\frac{1}{2}\frac{-1}{2}\right\rangle \\ \psi_7 & \left|\frac{3}{2}\frac{-1}{2}\right\rangle = \sqrt{1/3}\,|1\ -1\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{2/3}\,|1\ 0\rangle \left|\frac{1}{2}\frac{-1}{2}\right\rangle \\ \psi_8 & \left|\frac{1}{2}\frac{-1}{2}\right\rangle = -\sqrt{2/3}\,|1\ -1\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{1/3}\,|1\ 0\rangle \left|\frac{1}{2}\frac{-1}{2}\right\rangle \end{cases}$$

In this basis the matrix the non-zero elements of H'_{fs} are all on the diagonal and are given by the Bohr model. H'_z has four off diagonal elements. The complete matrix, W as we will see is more complicated but its eigenvalues are the same since they are independent of the chosen basis.

$$\begin{pmatrix} 5\gamma-\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5\gamma+\beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma-2\beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma+2\beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{1}{3}\beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{1}{3}\beta \end{pmatrix} \tag{9.60}$$

Where,

$$\gamma = (\alpha/8)^2 13.6\ eV$$

and,

$$\beta = \mu_B B_{Ext.}$$

The first four eigenvalues are already displayed along the diagonal. We only need to find the eigenvalues of the two 2×2 blocks. The characteristic equation for the first one is given as:

$$\lambda^2 - \lambda(6\gamma - \beta) + \left(5\gamma^2 - \frac{11}{3}\gamma\beta\right) = 0 \tag{9.61}$$

and the quadratic formula gives the eigenvalues:

$$\lambda_{\pm} = 3\gamma - (\beta/2) \pm \sqrt{4\gamma^2 + (2/3)\gamma\beta + (\beta^2/4)} \tag{9.62}$$

The eigenvalues of the second block are the same but with the sign of β reversed. The eight energy levels are listed in the table and are plotted against in the figure (). In the zero field limit they reduce to the fine structure values. For the other cases, the splitting is seen clearly.

$$\begin{aligned}
\epsilon_1 &= E_2 - 5\gamma + \beta \\
\epsilon_2 &= E_2 - 5\gamma - \beta \\
\epsilon_3 &= E_2 - \gamma + 2\beta \\
\epsilon_4 &= E_2 - \gamma - 2\beta \\
\epsilon_5 &= E_2 - 3\gamma + \beta/2 + \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_6 &= E_2 - 3\gamma + \beta/2 - \sqrt{4\gamma^2 + (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_7 &= E_2 - 3\gamma - \beta/2 + \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4} \\
\epsilon_8 &= E_2 - 3\gamma - \beta/2 - \sqrt{4\gamma^2 - (2/3)\gamma\beta + \beta^2/4}
\end{aligned}$$

Figure 9.4: Energy levels for the $n = 2$ states of hydrogen, with fine structure and Zeeman splitting

9.4 Hyperfine Splitting in Hydrogen

The proton also has a magnetic dipole moment, however this is much smaller than that of the electron due to the mass of the proton. It is given by,

$$\mu_p = \frac{g_p e}{2m_p} S_p \tag{9.63}$$

And the magnetic dipole moment of the electron,

$$\mu_e = -\frac{e}{m_e} S_e \tag{9.64}$$

Classically speaking, the dipole μ sets up a magnetic field:

$$B = \frac{\mu_0}{4\pi r^3}[3(\mu.\hat{r})\hat{r} - \mu] + \frac{2\mu_0}{3}\mu\delta^3(r) \tag{9.65}$$

So the Hamiltonian of the electron, in the magnetic field due to the proton's magnetics dipole moment, is

$$H'_{hf} = \frac{\mu_0 g_p e^2}{8\pi m_p m_e} \frac{[3(S_p.\hat{r})(S_e.\hat{r}) - S_p.S_e]}{r^3} + \frac{\mu_0 g_p e^2}{3m_p m_e} S_p.S_e \delta^3(r) \tag{9.66}$$

According to perturbation theory, the first-order correcction to the energy is the expectation value of the perturbing Hamiltonian:

$$E^1_{hf} = \frac{\mu_0 g_p e^2}{8\pi m_p m_e} \left\langle \frac{3(S_p.\hat{r})(S_e.\hat{r}) - S_p.S_e}{r^3} \right\rangle + \frac{\mu_0 g_p e^2}{3m_p m_e} \langle S_p.S_e \rangle |\psi(0)|^2 \tag{9.67}$$

In the groud state or any other state at which $l = 0$, the wavefunction is spherically symmetrical, and the first expectation value vanishes. Meanwhile,

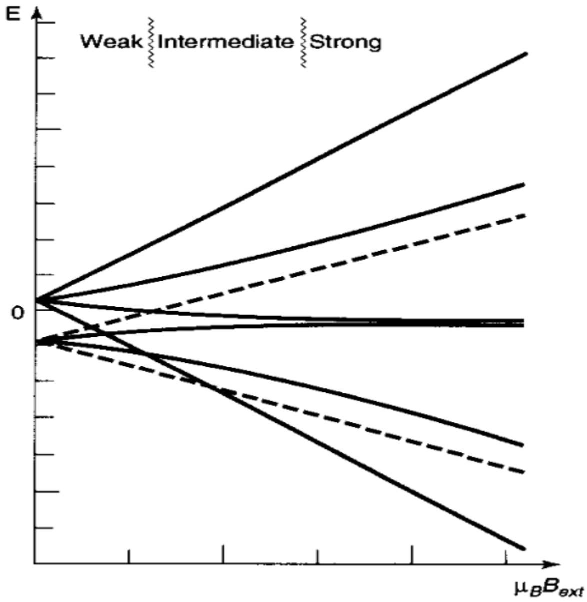


Figure 9.5: Zeeman splitting of the $n = 2$ states of hydrogen, in the weak, intermediate and strong field regimes

from the Schrodinger equation in three dimensions, we find that $|\psi(0)|^2 = 1/(\pi a^3)$, thus,

$$E^1_{hf} = \frac{\mu_0 g_p e^2}{3\pi m_p m_e a^3} \langle S_p . S_e \rangle \tag{9.68}$$

in the groud state. This is called Spin-Spin coupling because it involves the dot product of two spins in contrast with spin-orbit coupling which involves $S.L$. In the presence of spin-spin coupling, the individual spin angular momenta are no longer conserved. However the eigenvectors of the total spin is conserved:

$$S = S_e + S_p \tag{9.69}$$

We square this out to get,

$$S_p . S_e = \frac{1}{2}(S^2 - S_e^2 - S_p^2) \tag{9.70}$$

But the electron and proton both have spin 1/2, so $S_e^2 = S_p^2 = (3/4)\hbar^2$. In the triplet i.e. parallel spin state, the total spin is 1, and hence $S^2 = 2\hbar^2$. In the singlet state the total spin is 0, and $S^2 = 0$. Thus,

$$E^1_{hf} = \frac{4 g_p \hbar^4}{3 m_p m_e^2 c^2 \alpha^4} \begin{cases} +1/4, & \text{(triplet);} \\ -3/4, & \text{(singlet)} \end{cases} \tag{9.71}$$

The Spin-Spin coupling breaks the spin degeneracy of the groud state, lifting the triplet and depressing the singlet, leading to an energy gap. The energy gap is given by:

$$\Delta E = \frac{4g_p\hbar^4}{3m_p m_e^2 c^2 \alpha^4} = 5.88 \times 10^{-6}\ eV \tag{9.72}$$

The frequency of the photon emitted when the triplet transitions to a singlet

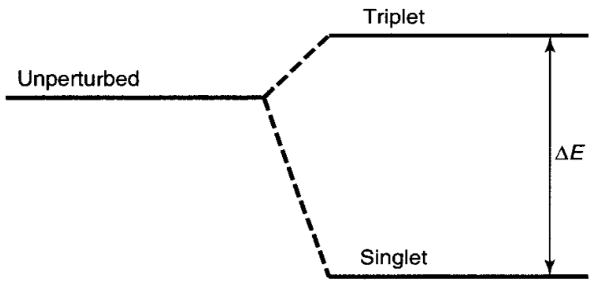


Figure 9.6: Hyperfine splitting in the ground state of Hydrogen

state is:

$$\nu = \frac{\Delta E}{h} = 1420 \text{ MHz} \tag{9.73}$$

The corresponding wavelength is 21 cm which falls in the microwave region. It permeates the universe and is a very important part of Astrophysics.

9.5 Introduction to quantum dynamics

So far, we looked at systems that were time-independent of sorts (quantum statics), and the potentials themselves were time independent, in other words, $V(r,t) = V(r)$. Hence the time-dependent Schrodinger equation took the form,

$$H\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{9.74}$$

And solving by separation of variables,

$$\psi(r,t) = \psi(r)e^{iEt/\hbar} \tag{9.75}$$

where $\psi(r)$ satisfies the time independent Schrodinger equation,

$$H\psi = E\psi \tag{9.76}$$

Due to the nature of the term that carries time dependence, the exponential factor $e^{iEt/\hbar}$, this term cancels out when we construct the physically relevant quantity $|\psi|^2$, which leads to all the expectation values and probabilities to be constant in time, and this is the same case in more complex states where we have linear combinations of these stationary states.
For us, if we want to investigate transitions between one energy level to another, we introduce a time-dependent potential, hence the name of quantum dynamics arises.

9.6 Two level systems

9.6.1 Introduction

Let us suppose that there are two states of the unpertubed sustem, ψ_a and ψ_b. They are eigenstates of the unpertubed Hamiltonian, H_0,

$$H_0\psi_a = E_a\psi_a \text{ and } H_0\psi_b = E_b\psi_b \tag{9.77}$$

and they are orthonormal,

$$\langle\psi_a|\psi_b\rangle = \delta_{ab} \tag{9.78}$$

And any state can be expressed as a linear combination of them, or in particular,

$$\Psi(0) = c_a\psi_a + c_b\psi_b \tag{9.79}$$

In the absence of perturbation, each component evolves with its characteristic exponential factor.

$$\Psi(t) = c_a\psi_a e^{-iE_at/\hbar} + c_b\psi_b e^{-iE_bt/\hbar} \tag{9.80}$$

Calculating $|c_a|^2$ is th probability that the particle is in he state ψ_a, and the measurement of the energy will yield E_a. Normalizing Ψ,

$$|c_a|^2 + |c_b|^2 = 1 \tag{9.81}$$

9.6.2 The perturbed system

Turning on a time-dependent perturbation $H'(t)$, the coefficients c_a and c_b become functions of t and the equation then becomes,

$$\Psi(t) = c_a(t)\psi_a e^{-iE_at/\hbar} + c_b(t)\psi_b e^{-iE_bt/\hbar} \tag{9.82}$$

Now we solve for $c_a(t)$ and $c_b(t)$ by using the time-dependent Schrodinger equation,

$$H\Psi = i\hbar\frac{\partial\Psi}{\partial t}, \text{ where } H = H_0 + H'(t) \tag{9.83}$$

Then we see that,

$$\begin{aligned} c_a[H_0\psi_a]_e^{-iE_at/\hbar} + c_b[H_0\psi_b]e^{-iE_bt/\hbar} + c_a[H'\psi_a]_e^{-iE_at/\hbar} \\ +c_b[H'\psi_b]e^{-iE_bt/\hbar} = i\hbar[\dot{c_a}\psi_a e^{-iE_at/\hbar}\dot{c_b}\psi_b e^{-iE_bt/\hbar} \\ +c_a\psi_a\left(\frac{iE_a}{\hbar}\right)e^{-iE_at/\hbar} + c_b\psi_b\left(\frac{iE_b}{\hbar}\right)e^{-iE_bt/\hbar}] \end{aligned} \tag{9.84}$$

This then simplifies to,

$$c_a[H'\psi_a]_e^{-iE_at/\hbar} + c_b[H'\psi_b]e^{-iE_bt/\hbar} = i\hbar[\dot{c_a}\psi_a e^{-iE_at/\hbar}\dot{c_b}\psi_b e^{-iE_bt/\hbar} \tag{9.85}$$

We isolate $\dot{c_a}$ by taking the inner product with ψ_a and exploiting the orthogonality of ψ_a and ψ_b.

$$c_a\langle\psi_a|H'|\psi_a\rangle_e^{-iE_at/\hbar} + c_b\langle\psi_a|H'|\psi_b]e^{-iE_bt/\hbar} = i\hbar\dot{c_a}e^{-iE_at/\hbar} \tag{9.86}$$

Then we define,

$$H'_{ij} \equiv \langle\psi_i|H'|\psi_j\rangle \tag{9.87}$$

The hermiticity of H' says that $H'_{ji} = (H'_ij)^*$. Now multiplying with $-(i/\hbar)e^{iE_at/\hbar}$, we conclude that,

$$\dot{c_a} = -\frac{i}{\hbar}[c_aH'_{aa} + c_bH'_{ab}e^{-i(En-E_a)t/\hbar}] \tag{9.88}$$

Similarly the inner product with ψ_b isolate $\dot{c_b}$ and gives the result,

$$\dot{c_b} = \frac{i}{\hbar}[c_bH'_{bb} + c_aH'_{ba}e^{-i(En-E_a)t/\hbar}] \tag{9.89}$$

Equations (15) and (16) are equivalent to the time-dependent Schrodinger equation for a two level system. And the diagonal matrix elements of H' vanish giving,

$$H'_{aa} = H'_{bb} = 0 \tag{9.90}$$

And the equations simplify to,

$$\dot{c_a} = -\frac{i}{\hbar}H'_{ab}e^{-i\omega_0t}c_b \tag{9.91}$$

$$\dot{c_b} = -\frac{i}{\hbar}H'_{ab}e^{i\omega_0t}c_a \tag{9.92}$$

Where,

$$\omega_0 = \frac{E_b - E_a}{\hbar}$$

9.6.3 Time-Dependent Perturbation Theory

Defining a size for the perturbation H', considering it to be small, we can obtain solutions for equations (18) and (19) by the process of successive approximations.
Suppoe the particle starts out in the lower state,

$$c_a(0) = 1.\ c_b(0) = 0 \tag{9.93}$$

If there exists no perturbation, these states remain iike this forever.

Zeroth Order:

$$c_a^{(0)}(t) = 1\ c_b^{(0)}(t) = 0 \tag{9.94}$$

To calculate the first-order approximation, we insert these values on the right side of equations (18) and (19)

First Order:

$$\frac{dc_a}{dt} = 0 \rightarrow c_a^{(1)}(t) = 1;$$
$$\frac{dc_b}{dt} = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t} \rightarrow c_b^{(1)} = \frac{i}{\hbar}\int_0^t H'_{ba}(t')e^{i\omega_0 t'}dt' \tag{9.95}$$

Second Order:

$$\frac{dc_a}{dt} = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}\left(\frac{i}{\hbar}\right)\int_0^t H'_{ba}(t')e^{i\omega_0 t'}dt' \rightarrow$$
$$c_a^{(2)}(t) = 1 - \frac{1}{\hbar}\int_0^t H'_{ab}(t')e^{i\omega_0 t'}\left[\int_0^{t'} H'_{ba}(t'')e^{i\omega_0 t''}dt''\right]dt' \tag{9.96}$$

We can continue this process for obtaining n-order approximations.

9.6.4 Sinusoidal Perturbations

If the perturbation has sinusoida time dependence,

$$H'(r,t) = V(r)cos(\omega t) \tag{9.97}$$

so that,

$$H'_{ab} = V_{ab}cos(\omega t) \tag{9.98}$$

Where,

$$V_{ab)} \equiv \langle \psi_a | V | \psi_b \rangle \tag{9.99}$$

For the first order perturbations, using equation (22),

$$c_b(t) \approx -\frac{i}{\hbar}\int_0^t cos(\omega t')dt' = -\frac{iV_ba}{2\hbar}\int_0^t \left[e^{i(\omega_0+\omega)t'} + e^{i(\omega_0-\omega)t'}\right] dt' \tag{9.100}$$

$$= -\frac{V_{ba}}{2\hbar}\left[\frac{e^{i(\omega_0+\omega)t} - 1}{\omega_0+\omega} + \frac{e^{i(\omega_0-\omega)t} - 1}{\omega_0-\omega}\right] \tag{9.101}$$

Simplifying this equation by restricting our attention to driving frequency ω close to transition frequence ω_0, the second term dominates. To be more specific, we assume,

$$\omega_0 + \omega >> |\omega_0 - \omega| \tag{9.102}$$

Perturbation at other frequencies have negligible probabilty for causing a transistion, so this isnt a limitation. Now the equation simplifies to,

$$c_b(t) \approx -\frac{V_{ba}}{2\hbar}\frac{e^{i(\omega_0-\omega)t} - 1}{\omega_0-\omega}[e^{i(\omega_0-\omega)t/2} - e^{-i(\omega_0-\omega)t/2}]$$

$$= -i\frac{V_{ba}}{\hbar}\frac{sin[(\omega_0-\omega)t/2]}{\omega_0-\omega}e^{i(\omega_0-\omega)t/2} \tag{9.103}$$

The transition probability, the probability that a particle which started out in the state ψ_a wil be found at a time t, in the state ψ_b is,

$$P_{a\to b}(t) = |c_b(t)^2 \approx \frac{|V_{ba}|^2}{\hbar^2}\frac{sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2} \tag{9.104}$$

9.7 Emission and Absorption of Radiation

9.7.1 Electromagnetic Waves

An atom, in the presence of a passing light wave, responds to the electric component. It is sinusoidal in nature,

$$E = E_0 cos(\omega t)\hat{k} \tag{9.105}$$

Where q is the charge of the electron. Evidently,

$$H'_{ba} = -\wp E_0 cos(\omega t), \; \wp \equiv q\langle \psi_b | z | \psi_a \rangle \tag{9.106}$$

When ψ is an even or odd function of z, $z|\psi|^2$ is odd and integrates to zero, hence the diagonal matrix elements of H' vanish, hence the perturbation is oscillatory and is of the form,

$$V_{ba} = -\wp E_0 \tag{9.107}$$

9.7.2 Absorption, stimulated emission and spontaneous emission

If an atom starts in the lower state ψ_a and you shine a polarized moochromatic beam of light on it, the probablilty of a transistion to the "upper" state ψ_b is given by,

$$P_{a\to b}(t) = \left(\frac{\wp E_0}{\hbar}\right)^2 \frac{sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2} \tag{9.108}$$

The atom absorbs an energy of $E_B - E_a = \hbar\omega_0$ from the electromagnetic field. We could say that it has absorbed a photon.
Now doing the same derivation for the transition from lower to upper state, we get

$$P_{b\to a}(t) = \left(\frac{\wp E_0}{\hbar}\right)^2 \frac{sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2} \tag{9.109}$$

Here we note that the probability of transition from $a \to b$ is the same as $b \to a$, and this was called stimulated emission. The electromagnetic field gains energy $\hbar\omega_0$ from the atom.
Spontaneous emission is when an atom in the excited state makes a transition downward with a release of a photon without the application of any electromagnetic field.

9.7.3 Incoherent perturbations

The energy density of an electromagnetic wave is,

$$u = \frac{\epsilon_0}{2}E_0^2 \tag{9.110}$$

The transition probablity is proportional to the energy density of the fields,

$$P_{b\to a}(t) = \frac{2u}{\epsilon_0\hbar^2}|\wp|^2\frac{sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2} \tag{9.111}$$

But this is for a monochromatic perturbation for a single frequency ω, now subjecting the system to a range of frequencies, $u \to \rho(\omega)d\omega$ where $\rho(\omega)d\omega$ is the enegy density in the frequency range $d\omega$ and the net transistion probability takes the form of an integral,

$$P_{b\to a}(t) = \frac{2}{\epsilon_0\hbar^2}|\wp|^2\int_0^\infty \rho(\omega)\left\{\frac{sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}\right\}d\omega \tag{9.112}$$

The term in the curly brakets is sharply peaked about ω_0. while $\rho(\omega)$ is relatively broad, so we replace $\rho(\omega)$ with $\rho(\omega_0)$ anf tak it outside the integral,

$$P_{b\to a}(t) \approx \frac{2|\wp|^2}{\epsilon_0\hbar^2}\rho(\omega_0)\int_0^\infty \left\{\frac{sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}\right\} d\omega \tag{9.113}$$

Changing variables from $x \equiv (\omega_0 - \omega)t/2$, extending the limits of integration to $x = +_{-}\infty$, looking up the definite integral,

$$\int_{-\infty}^{\infty} \frac{sin^2 x}{x^2} dx = \pi$$

we find that,

$$P_{b\to a}(t) \approx \frac{\pi|\wp|^2}{\epsilon_0\hbar^2}\rho(\omega_0)t \tag{9.114}$$

The transition probability is proportional to t. The flopping phenomenon characteristic of a monochromatic perturbation gets washed out when we hit the system with an incoherent spread of frequencies. The transition rate is now a constant,

$$R_{b\to a} = \frac{\pi}{\epsilon_0\hbar}|\wp|^2\rho(\omega_0) \tag{9.115}$$

We take all possible polarisations and not only from x and z directions, hence instead of $|\wp|^2$, we have an average $|\hat{n}\cdot\boldsymbol{\wp}|^2$, where

$$\boldsymbol{\wp} = q\langle\psi_b|r|\psi_a\rangle \tag{9.116}$$

And the average is over both polarisations and over all incident directions. This averaging is carried out as follows,

Polarisation: For propogation in the z-direction, the two possible polarisations are $\hat{i}$ and $\hat{j}$, so the polarisation average (p) is,

$$(\hat{n}\cdot\boldsymbol{\wp})_p^2 = \frac{1}{2}[(\hat{i}\cdot\boldsymbol{\wp})^2 + (\hat{j}\cdot\boldsymbol{\wp}^2) = \frac{1}{2}\wp^2 sin^2\theta \tag{9.117}$$

Where θ is the angle between $\boldsymbol{\wp}$ and the direction of propogation.

Propogation direction: Setting the polar axis along $\boldsymbol{\wp}$ and integrate over all propogation directions to get the polarisation-propogation average,

$$(\hat{n}\cdot\boldsymbol{\wp})_p^2 p = \frac{1}{4\pi}\int\left[\frac{1}{2}\wp^2\sin^2\theta\right] sin\theta d\theta d\phi = \frac{\wp^2}{4}\int_0^\pi \sin^3\theta d\theta = \frac{\wp^3}{3} \tag{9.118}$$

So the transition rate for the stimulated emission from state b to state a, under the influence of incoherent, unpolarized light incident from all directions, is,

$$R_{b\to a} = \frac{\pi}{3\epsilon_0\hbar^2}|\wp|^2\rho(\omega_0) \tag{9.119}$$

Where $\wp$ is the matrix element of the electric dipole moment between the two tate and $\rho(\omega_0)$ is the energy density in the fields, per unit frequency, evaluated at $\omega_0 = (E_b - E_a)/\hbar$.

9.8 Spontaneous Emission

9.8.1 Einstein's A and B coefficients

Picture a container of atoms, N_a of them in a lower state ψ_a and N_b of them in the upper state ψ_b. Let A be the spontaneous emission rate, so that the number of particle leaving the upper state by this process per unit time is N_bA. The transition rate for stimulated emission is proportional to the energy density of the electromagnetic field. The number of upper state particles leaving is also similarly found. The absorption rate is proportional to $\rho(\omega_0)$. Now,

$$\frac{dN_b}{dt} = -N_bA - N_bB_{ba}\rho(\omega_0) + N_aB_{ab}\rho(\omega_0) \tag{9.120}$$

Supposing that the atoms are in thermal equlibrium with the ambient field so that the number of particles in each level is constant. $dN_b/dt = 0$, hence,

$$\rho(\omega_0) = \frac{A}{(N_a/N_b)B_{ab} - B_{ba}} \tag{9.121}$$

From statistical mechanics, the number of particles with energy E. in thermal equilibrium at temperature T, is proportional to the Boltzmann factor, e^{-E/k_bT}, so

$$\frac{N_a}{N_b} = \frac{e^{-E_a/k_bT}}{e^{E_b/k_bT}} = e^{\hbar\omega_0/k_bT} \tag{9.122}$$

and hence,

$$\rho(\omega_0) = \frac{A}{e^{\hbar\omega_0/k_bT}}B_{ab} - B_{ba} \tag{9.123}$$

From Planck's blackbody formula,

$$\rho(\omega) = \frac{\hbar}{\pi^2c^3}\frac{\omega^3}{e^{\hbar\omega/k_bT} - 1} \tag{9.124}$$

And from these two equations we can deduce that,

$$B_{ab} = B_{ba} \tag{9.125}$$

And so,

$$A = \frac{\omega^3 \hbar}{\pi^2 c^3} B_{ba} \tag{9.126}$$

We see that from equation (52), that the transition rate for stimulated emission is the same as for absorption. Now, we deduce from equation (46) that,

$$B_{ba} = frac\pi 3\epsilon_0 \hbar^2 |\wp|^2 \tag{9.127}$$

And spontaneous emission rate is,

$$A = \frac{\omega^3 |\wp|^2}{3\pi\epsilon_0 \hbar c^3} \tag{9.128}$$

9.8.2 The lifetime of an excited state

Suppose that you have a bottle full of atoms, with $B_b(t)$ of them in the excited stat. Due to spontaneous emission, this number decreases as time goes on, and to be more specifi, in a time interval dt you will lose a fraction of Adt of them,

$$dN_b = -AN_b dt \tag{9.129}$$

Solving for $N_b(t)$, we get,

$$N_B(t) = N_b(0)e^{-At} \tag{9.130}$$

Here we can see that the number remaining in the excited state decreases exponentially, with a time constant,

$$\tau = \frac{1}{A} \tag{9.131}$$

We call this the lifetime of a state, or to be more technical, it is the time taken for $N_B(t)$ to reach $1/e \approx 0.368$ of its initial value.
Suppose that there are many more states, and many more decays, the transition rates add up, and the net lifetime is,

$$\tau = \frac{1}{A_1 + A_2 + A_3 + ...} \tag{9.132}$$

9.8.3 Selection rules

The calculation of spontaneous emission rates are reduced to a matter of evaluating matrix elements of the form,

$$\langle \psi_b | \mathbf{r} | \psi_a \rangle$$

Specifying the states with quantum numbers n, l and m,

$$\langle b' l' m' | \mathbf{r} | nlm \rangle \tag{9.133}$$

Exploitatio of the angular momentum commutation relations and the hermiticity of the angular momentum operators yield these constraints on this quantity,

Selection rules involving m and m': No transitions occur unless $\Delta m = +_{-}1$ or 0

Selection rules involving l and l': No transitions occur unless $\Delta l = +_{-}1$

Chapter 10

Scattering

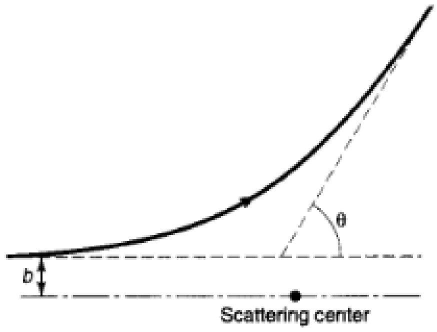
10.1 Classical Scattering

10.1.1 Motivation

We can also define the size/radius of the proton is through its rate of interacting with itself or other particles. This is done by us determining the cross-sectional area. The larger this area is, the more likely it is that you will interact with it. The smaller the area, the less likely to interact. This motivates a connection between proton size and scattering probability. In particle physics, a collision or interaction rate is expressed in effective cross-sectional area, typically just called cross section. As an “area,” we can measure scattering cross sections as the square of some relevant length scale.

10.1.2 The problem

Consider a particle incident on some scattering center. It comes in with an energy $\boldsymbol{E}$ and an impact parameter $\boldsymbol{b}$, and it emerges at some scattering angle θ. The essential problem of classical scattering theory is this: *Given the impact parameter, calculate the scattering angle.* Ordinarily, of course, the smaller the impact parameter, the greater the scattering angle.


θ
b
Scattering center

10.1.3 Solving for differential cross-section

Particles incident within an infinitesimal patch of cross-sectional area dσ will scatter into a corresponding infinitesimal solid angle dQ. The larger dσ is, the bigger dQ will be; the proportionality factor, D(θ) = dσ/dQ, is called the differential (scattering) cross-section, and is given by,

$$d\sigma = D(\theta)d\Omega \tag{10.1}$$

In terms of the impact parameter and the azimuthal angle $\phi, d\sigma = b.db.d\phi$ and $d\Omega = \sin(\theta)d\theta d\phi$, and so,

$$D(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| \tag{10.2}$$

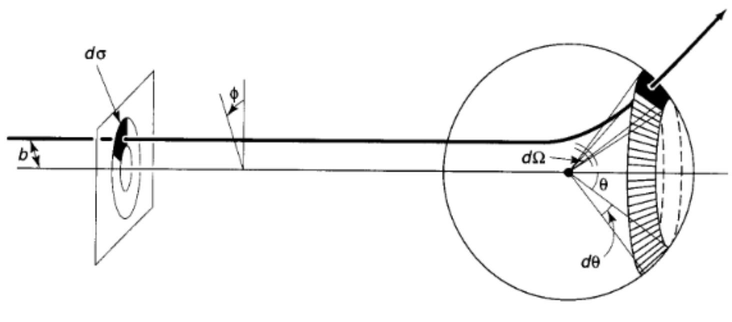
And then the total cross-section is the integral of D(θ) over all solid angles,

$$\sigma = \int D(\theta)d\Omega \tag{10.3}$$

The differential cross-section is the total area of incident beam that is scattered by the target. Beams incident within this area will hit the target, and those farther out will miss it completely.
If we have a beam of incident particles, with uniform intensity/luminosity ($\mathcal{L}$), the number of particles entering area dσ (and hence scattering into solid angle dΩ), per unit time, is dN = $\mathcal{L}$dσ= $\mathcal{L}$D(θ)dΩ, then,

$$D(\theta) = \frac{1}{\mathcal{L}}\frac{dN}{d\Omega} \tag{10.4}$$

This is the definition of the differential cross-section.



10.2 Quantum Scattering

10.2.1 Defining the problem

In the quantum theory of scattering, we imagine an incident plane wave, $\psi(z) = Ae^{ikz}$, traveling in the z direction, which encounters a scattering potential, producing an outgoing spherical wave That is, we look for solutions to the Schrödinger equation of the generic form,

$$\psi(r,\theta) \approx A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}, \text{ for large } r \tag{10.5}$$

The relation between wave number k and energy of incident particles are,

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{10.6}$$

10.2.2 Determining scattering amplitude

Probability of the incident particle travelling with speed v passing through infinitesimal area $d\sigma$ in time dt is,

$$dP = |\psi_{incident}|^2 dV = |A|^2 (vdt) d\sigma \tag{10.7}$$

This is equal to the probability that the particle later emerges into the corresponding solid angle $d\Omega$,

$$dP = |\psi_{scattered}|^2 dV = \frac{|A|^2 |f|^2}{r^2}(vdt) r^2 d\sigma \tag{10.8}$$

And $d\sigma$=$|f|^2 d\Omega$, so,

$$D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \tag{10.9}$$

The differential cross-section (which is the quantity of interest to the experimentalist) is equal to the absolute square of the scattering amplitude. Now we look at different methods to determine this scattering amplitude.

10.3 Partial Wave Analysis

10.3.1 Formalism

We know that the Schrodinger equation for a spherically symmetrical potential $V(r)$ admits the separable solutions,

$$\psi(r,\theta,\phi) = R(r)_l^m(\theta,\phi) \tag{10.10}$$

Where Y_l^m is a spherical harmonic and $u(R) = rR(r)$ satisfies the radial equation,

$$-\frac{\hbar^2}{2m}\frac{dl^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{10.11}$$

At very large r, the potential goes to zero, and the centrifugal term is negligible, so,

$$\frac{d^2u}{dr^2} \approx -k^2u \tag{10.12}$$

Whose general solution is takes the form,

$$u(r) = Ce^{ikr} + De^{-ikr} \tag{10.13}$$

The first term represents an outgoing spherical wave, and the second an incoming one. For the scattered wave, we want $D = 0$. At very large r, then.

$$R(r) \approx \frac{e^{ikr}}{r} \tag{10.14}$$

The radial equation then becomes,

$$\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}u = -k^2u \tag{10.15}$$

The general solution for the radial equation is a linear combinations of spherical Bessel functions,

$$u(r) = Arj_l(kr) + Brn_l(kr) \tag{10.16}$$

We need solutions that are linear combinations analogous to e^ikr and e^-ikr, these are called the spherical Hankel functions,

$$h_l^{(1)} \equiv j_l(x) + in_l(x) \tag{10.17}$$

Below we see some examples of Hankel functions,

$$h_0^{(1)} = -i\frac{e^{ix}}{x} \qquad h_0^{(2)} = i\frac{e^{-ix}}{x}$$

$$h_1^{(1)} = \left(-\frac{i}{x^2} - \frac{1}{x}\right)e^{ix} \qquad h_1^{(2)} = \left(\frac{i}{x^2} - \frac{1}{x}\right)e^{-ix}$$

$$h_2^{(1)} = \left(-\frac{3i}{x^3} - \frac{3}{x^2} + \frac{i}{x}\right)e^{ix} \qquad h_2^{(2)} = \left(\frac{3i}{x^3} - \frac{3}{x^2} - \frac{i}{x}\right)e^{-ix}$$

$$\left.\begin{aligned} h_\ell^{(1)} &\to \frac{1}{x}\,(-i)^{\ell+1}e^{ix} \\ h_\ell^{(2)} &\to \frac{1}{x}\,(i)^{\ell+1}e^{-ix} \end{aligned}\right\} \text{for } x \gg 1$$

The Hankel function of the first kind becomes $e^{-}ikr/r$ for large r, so we use these to get,

$$R(r) = Cj_l^{(1)}(kr) \tag{10.18}$$

10.3.2 Exact wavefunction and the partial wave amplitude

The exact wave function in the exterior region where $V(r) = 0$ is,

$$\psi(r,\theta,\phi) = A\left\{e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\right\} \tag{10.19}$$

Where,

$$f(\theta,\phi) + \frac{1}{k}\sum_{l,m}(-i)^{l+1}C_{l,m}Y_l^m(\theta,\phi) \tag{10.20}$$

The $C_{l,m}$ are called the partial wave amplitudes. Now the cross section is,

$$D(\theta,\phi) = |f(\theta,\phi)|^2 = \frac{1}{k^2}\sum_{l,m}\sum_{l',m'}(i)^{l-l'}C^*_{l,m}C_{l'm'}(Y_l^m)^*Y_{l'}^{m'} \tag{10.21}$$

And the total cross-section is,

$$\sigma = \frac{1}{k^2}\sum_{l,m}\sum_{l',m'}(i)^{l-l'}C^*_{l,m}C_{l'm'}\int(Y_l^m)^*Y_{l'}^{m'}d\Omega = \frac{1}{k^2}\sum_{l,m}|C_{l,m}|^2 \tag{10.22}$$

We know from the Legendre functions that,

$$Y_l^0(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(cos\theta) \tag{10.23}$$

where P_l is the lth Legendre Polynomial. Now the exact wave function in the exterior region is,

$$\psi(r, \theta) = A\left\{e^{ikz} + \sum_{l=0}^{\infty} \sqrt{\frac{2l+1}{4\pi}} C_l h_l^{(1)}(kr) P_l(cos\theta)\right\} \tag{10.24}$$

The scattering amplitude is now given by,

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(-i)^{l+1}\sqrt{\frac{2l+1}{4\pi}} C_l P_l(cos\theta) \tag{10.25}$$

and the total cross-section is,

$$\sigma = \frac{1}{k^2}\sum_{l=0}^{\infty}|C_l|^2 \tag{10.26}$$

To fix the hybrid notation of the cartesian incoming wave and the spherical outgoing wave, we write it in a more consistent form.
We know that the general solution to the Schrodinger equation with $V = 0$ can be written in the form,

$$\sum_{l,m}[A_{l,m} j_l(kr) + B_{l,m} n_l(kr)] Y_l^m(\theta, \phi) \tag{10.27}$$

Expanding the plane wave in terms of spherical waves using Rayleigh's formula,

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l + l) j_l(kr) P_l(cos\theta) \tag{10.28}$$

Substituting this in Equation (24), the consistent exterior region wave function can be written as,

$$\psi(r, \theta) = A\left[l(2l + l) j_l(kr) + \sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}} C_l h_l^{(1)}(kr)\right] P_l(cos\theta) \tag{10.29}$$

10.4 Phase Shift

Let's begin by considering a one-dimensional scattering problem with a localized potential on the half-line $x < 0$ and a brick wall at $x = 0$. So a wave incident from the left,

$$\psi_i(x) = Ae^{ikx} \tag{10.30}$$

is entirely reflected,

$$\psi_r(x) = Be^{-ikx} \tag{10.31}$$

where $x < -a$. No matter what happens in $-a < x < 0$ (the interaction

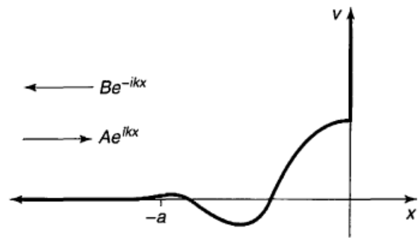


Figure 10.1: 1D scatterubg frin a localized potential bounded on the right by an infinite wall

region), the amplitude (amplitude in the context of waves not probability amplitude) of the reflected wave is the same as the incident wave simply due to conservation of probability. However, the two waves need not have the same phase. If there were no potential at all ($V(x) = 0$), but just at the wall ($x = 0$), then $B = -A$, since the total wave function, incident + reflected must vanish at the origin,

$$\psi_0 = A(e^{ikx} - e^{-ikx}) \tag{10.32}$$

If the potential is not zero ($V(x) \neq 0$), then the wave function ($x < -a$) takes the form:

$$\psi = A\left(e^{ikx} - e^{i(2\delta - kx)}\right) \tag{10.33}$$

Thus, the whole scattering problem reduces to the problem of calculating the phase shift δ as a function of k and hence of the Energy $E = \hbar^2k^2/2m$. Yes there's a factor of 2, before δ, but that's only conventional. We think of the incident wave as being phase shifted once on the way in and again on the way out. Thus, by δ we mean the one-way phase shift and 2δ the total phase shift. We go about this by solving the Schrodinger equation in $-a < x < 0$ along with relevant boundary conditions. Why are we working with δ rather than the complex amplitude B? It makes the physics and math simpler:

- **Physically:** We only need to think of the conservation of probability. The potential merely shifts the phase
- **Mathematically:** We trade a complex number for a real one

Let's return to the 3D case. The incident plane wave carries no angular momentum in the z direction. Thus Rayleigh's formula contains no terms with $m \neq 0$ but insteaed it cfontains all values of the total angular momentum ($l = 0, 1, 2$). Since angular momentum is conserved by a spherically symmetric potential each partial wave labelled by a particular l scatters independently with no change in amplitude (amplitude in this context refer to the amplitude of the wave no the probability amplitude) but differing in phase. If there is no potential then $\psi_0 = Ae^{ikx}$ and the lth partial wave is

$$\psi_0^l = Ai^l(2l+1)j_l(kr)P_l(\cos(\theta)) \tag{10.34}$$

But from our previous considerations,

$$j_l(x) = \frac{1}{2}\left[h^{(1)}(x) + h_l^2(x)\right] \approx \frac{1}{2x}\left[(-i)^{l+1}e^{ix} + i^{l+1}e^{-ix}\right] \tag{10.35}$$

for $x >> 1$. So for large r,

$$\psi_0^{(l)} \approx A\frac{2l+1}{2ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right] P_l(\cos(\theta)) \tag{10.36}$$

The second term in square brackets corresponds to an incoming spherical wave. It is unchanged when we introduce the scattering potential. The first term is the outgoing wave. It picks up a phase shift δ_l:

$$\psi^{(l)} \approx A\frac{2l+1}{2ikr}\left[e^{i(kr+2\delta_l)} - (-1)^l e^{-ikr}\right] P_l(\cos(\theta)) \tag{10.37}$$

Think of it as a converging spherical wave due to the $h_l^{(2)}$ component in e^{ikz}, which is phase shifted by $2\delta_l$ and emerges as an outgoing spherical wave i.e. the h_l^l part of e^{ikz} as well as the scattered wave itself. In the previous section the whole theoryu was expressed in terms of partial wave amplitudes a_l, now we have formulated it in terms of the phase shifts δ_l. There must be a connectioni between the two. Well if we take the assymptotic i.e. large r limit of eq. (10.37):

$$\psi^{(l)} \approx A\left(\frac{(2l+1)}{2ikr}\left[e^{i(kr+2\delta_l)} - (-1)^l e^{-ikr}\right] + \frac{(2l+1)}{r}a_l e^{ikr}\right) P_l(\cos(\theta)) \tag{10.38}$$

With the generic expression in terms of $e^{i\delta_l}$ we find

$$a = \frac{1}{2ik}(e^{2i\delta_l} - 1) = \frac{1}{k}e^{i\delta_l}\sin(\delta_l) \tag{10.39}$$

Although we used the assymptotic form of the wave function to find the connection there's nothing approximate about the result. Both of them are constants independent of r and δ_l means the phase shift in the asymptotic region i.e. where the Hankel functionis have settled down to $e^{\pm ikr}/kr$. It follows in particular that,

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin(\delta_l)P_l(\cos(\theta)) \tag{10.40}$$

and,

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l) \tag{10.41}$$

Voila!

10.5 Born Approximation

10.5.1 Integral Form of the Schrodinger Equation

Before we even head to deriving the "Integral Form of the Schrodinger Equation". Why you might ask? It will become evident in the upcoming sections. So let's begin by recalling the time-independent Schrodinger equation

$$\frac{num}{2m} + V\psi = E\psi \tag{10.42}$$

We can rewrite this as,

$$(\nabla^2 + k^2)\psi = Q \tag{10.43}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}$$
$$Q = \frac{2m}{\hbar^2}V\psi$$

This looks pretty similar to the Helmholtz equation from electrodynamics. Here however the "inhomogeneous" term Q itself depends on ψ Suppoase we could find a function that solves the Helmholtz equation with a delta function source:

$$(\nabla^2 + k^2)G(\vec{r}) = \delta^3(\vec{r}) \tag{10.44}$$

We can then express as an integral:

$$\psi(\vec{r}) = \int G(\vec{r} - \vec{r_0}) Q(\vec{r_0}) d^3\vec{r_0} \tag{10.45}$$

$G(\vec{r})$ is called the Green's function for the Helmholtz equation. Moreover, generally speaking the Green's function for a linear differential equation represents the response to a delta function. Our goal now is to solve this differential equation, we start by Fourier transforming it to turn it into an algebraic equation:

$$G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{s}.\vec{r}} g(\vec{s}) d^3\vec{s} \tag{10.46}$$

Then,

$$(\nabla^2 + k^2) G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} (\nabla^2 + k^2) \int e^{i\vec{s}.\vec{r}} g(\vec{s}) d^3\vec{s}$$

But,

$$\nabla^2 e^{i\vec{s}.\vec{r}} = -s^2 e^{i\vec{s}.\vec{r}}$$

and

$$\delta^3(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{s}.\vec{r}} g(\vec{s}) d^3\vec{s}$$

thus,

$$\frac{1}{(2\pi)^{3/2}} \int (-s^2 + k^2) e^{i\vec{s}.\vec{r}} g(\vec{s}) d^3\vec{s} = \frac{1}{(2\pi)^3} \int e^{i\vec{s}.\vec{r}} d^3\vec{s}$$

It follows from Plancherel's theorem that,

$$g(\vec{s}) = \frac{1}{(2\pi)^{3/2}(k^2 - 2^2)}$$

Plugging this back, we see that

$$G(\vec{r}) = \frac{1}{(2\pi)^3} \int e^{i\vec{s}.\vec{r}} \frac{1}{(k^2 - 2^2)} d^3\vec{s}$$

We now switch coordinates for convenience. Now $\vec{r}$ is fixed as far as the s integration matters so we'll choose spherical coordinates with the polar axis along $\vec{r}$. Then

$$\int_0^\pi e^{isr\sin(\theta)} \sin(\theta) d\theta = -\frac{e^{isr\cos(\theta)}}{isr}\Big|_0^\pi = \frac{2\sin(sr)}{sr}$$

We can represent this visually as,

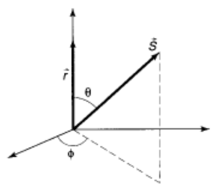


Figure 10.2: New coordinates for the integral

Thus,

$$G(\vec{r}) = \frac{1}{(2\pi)^2}\frac{2}{r}\int_0^\infty \frac{s\sin(sr)}{k^2-s^2}ds = \frac{1}{4\pi^2 r}\int_{-\infty}^\infty \frac{s\sin(sr)}{k^2-s^2}ds$$

We can rewrite this as,

$$G(\vec{r}) = \frac{i}{8\pi^2 r}\left[\int_{-\infty}^\infty \frac{se^{isr}}{(s-k)(s+k)}ds - \int_{-\infty}^\infty \frac{se^{-isr}}{(s-k)(s+k)}ds\right] = \frac{i}{8\pi^2 r}(I_1 - I_2)$$

From Cauchy's integral formula it follows that,

$$I_1 = \oint \left[\frac{se^{isr}}{s+k}\right]\frac{1}{s-k}ds = 2\pi i\left[\frac{se^{isr}}{s+k}\right]\Big|_{s=k} = i\pi e^{ikr}$$

$$I_2 = \oint \left[\frac{se^{-isr}}{s-k}\right]\frac{1}{s+k}ds = -2\pi i\left[\frac{se^{isr}}{s+k}\right]\Big|_{s=-k} = -i\pi e^{ikr}$$

Therfore,

$$G(\vec{r}) = \frac{i}{8\pi^2 r}\left[\left(i\pi e^{ikr}\right) - \left(-i\pi e^{ikr}\right)\right] = -\frac{e^{ikr}}{4\pi r} \tag{10.47}$$

Note that $G + G_0$ still satisfies Equation (10.47). This is simply due to the multivalued nature of the holomorphic function. Thus, the integral form of the Schrodinger equation can be written as,

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|}V(\vec{r}_0)\psi(\vec{r}_0)d^3\vec{r}_0 \tag{10.48}$$

Let's see how this helps us.

10.5.2 The First Born Approximation

Suppose $V(\vec{r}_0)$ is localized about r = 0, that is the potential drops to 0 after a finite region and we want to calculate $\psi(\vec{r})$ at points distant from the scattering center. Then for all points that contribute to the integral form of the Schrodinger equation. So,

$$|\vec{r}-\vec{r}_0| = r^2 + r_0^2 - 2\vec{r}\vec{r}_0 \approxeq r^2\left(1 - 2\frac{\vec{r}.\vec{r}_0}{r^2}\right) \tag{10.49}$$

and hence,

$$|\vec{r}-\vec{r}_0| \approxeq r - \hat{r}.\vec{r}_0 \tag{10.50}$$

Let,

$$\vec{K} = k\hat{z} \tag{10.51}$$

then

$$e^{-i\vec{K}|\vec{r}-\vec{r}_0|} \approx e^{ikr}e^{-i\vec{K}.\vec{r}_0} \tag{10.52}$$

and therefore,

$$\frac{e^{-i\vec{K}|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} \approx \frac{e^{ikr}}{r}e^{-i\vec{K}.\vec{r}_0} \tag{10.53}$$

In the case of scattering, we want:

$$\psi_o(\vec{r}) = Ae^{ikz} \tag{10.54}$$

to represent an incident plane wave. For large r,

$$\psi \approxeq Ae^{ikz} - \frac{m}{2\pi\hbar^2 A}\int e^{-i\vec{K}.\vec{r}_0}V(\vec{r}_0)\psi(\vec{r}_0)d^3\vec{r}_0 \tag{10.55}$$

This is in the standard form. We can read off the scattering amplitude:

$$f(\theta,\phi) = \frac{m}{2\pi\hbar^2 A}\int e^{-i\vec{K}.\vec{r}_0}V(\vec{r}_0)\psi(\vec{r}_0)d^3\vec{r}_0 \tag{10.56}$$

So far this is exact. Now we invoke the Born approximation: "Suppose the incoming plane wave is not substantially altered by the potential; then we can say that

$$\psi(\vec{r}_0) \approxeq \psi_0(\vec{r}_0) = Ae^{ikz_o} = Ae^{i\vec{K}'\vec{r}_o} \tag{10.57}$$

where

$$K' = k\hat{z}$$

inside the integral. This would be just the wave function if V were zero. It is essentially just a weak potential approximation. Generally partial wave analysis is useful when the incident particle has low energy the only the first few terms in the series contribute significantly. The Born approximation applies when the potential is weak when compared to the incident energy, thus the deflection is small. In the Born approximation then,

$$f(\theta, \phi) \approxeq -\frac{m}{2\pi\hbar^2} \int e^{i(k^{'}-k).\vec{r}_0} V(r_0) d^3\vec{r}_0 \tag{10.58}$$

In particular, for low energy scattering, the exponential factor is essentially constant over the scattering region and the Born approximation simplifies to:

$$f(\theta, \phi) \approxeq -\frac{m}{2\pi\hbar^2} \int V(\vec{r}) d^3r \tag{10.59}$$

For a spherically symmetrical potential, $V(\vec{r}) = V(r)$ but not necessarily at low energy. The Born approximation reduces to a simpler form. First we define:

$$\mathcal{K} = k^{'} - k \tag{10.60}$$

and let the polar axis for the r_0, the integral lies along so that;

$$(k^{'} - k).r_0 = \mathcal{K} r_0 \cos(\theta_0) \tag{10.61}$$

Then,

$$f(\theta) \approxeq -\frac{m}{2\pi\hbar^2} \int e^{i\mathcal{K}r_0\cos(\theta_0)} V(\theta_0) r_0^2 \sin(\theta_0) dr_0 d\theta_0 d\phi_0 \tag{10.62}$$

The integral is trivial, 2π, and the integral θ_0 is on we have encountered before in equation (). Dropping the subscript on r, we are left with

$$f(\theta) \approxeq -\frac{2m}{\hbar^2 \mathcal{K}} \int_0^\infty r V(r) \sin(\mathcal{K}r) dr \tag{10.63}$$

The angular dependence of f is carried by $\mathcal{K}$. From our previous considerations we can see that:

$$\mathcal{K} = 2k \sin(\theta/2) \tag{10.64}$$

10.5.3 Examples

Low-energy soft-sphere scattering

Note: We can't apply the Born approximationi to hard-sphere scattering as the integral blows up due to our assumption (i.e. potential does not affect the wave function) here. Suppose,

$$V(\vec{r}) = \begin{cases} V_0, & \text{if } r \leq a \\ 0, & \text{if } r > a \end{cases} \tag{10.65}$$

In this case the low-energy scattering amplitude is,

$$f(\theta, \phi) \approxeq -\frac{m}{2\pi\hbar^2} V_0 \left(\frac{4}{3}\pi a^3\right) \tag{10.66}$$

This is independent of θ and ϕ ! Thus, the differential cross-section is:

$$\frac{d\sigma}{d\Omega} = |f|^2 \approxeq \left[\frac{2mV_0 a^3}{3\hbar^2}\right]^2 \tag{10.67}$$

and the total cross-section:

$$\sigma \approxeq 4\pi \left(\frac{2mV_0 a^3}{3\hbar^2}\right)^2 \tag{10.68}$$

Yukawa Scattering

The Yukawa potential is a toy-model for the binding force in the nucleus of an atom. It has the form,

$$V(r) = \beta \frac{e^{-\mu r}}{r} \tag{10.69}$$

where β and μ are constants. The Born approximation gives,

$$f(\theta) \approxeq -\frac{2m\beta}{\hbar^2 k} \int_0^\infty e^{-\mu r} \sin(kr) dr = -\frac{2m\beta}{\hbar^2(\mu^2 + k^2)} \tag{10.70}$$

Rutherford Scattering

If we substitute $\beta = q_1 q_2 / 4\pi\epsilon_0$ and $\mu = 0$. The scattering amplitude is given by,

$$f(\theta) \approxeq -\frac{2mq_1 q_2}{4\pi\epsilon_0 \hbar^2 k^2} \tag{10.71}$$

or,

$$f(\theta) \approxeq -\frac{q_1 q_2}{16\pi\epsilon_0 E \sin^2(\theta/2)} \tag{10.72}$$

The differential cross-section is the square of this:

$$\frac{d\sigma}{d\Omega} = \left[\frac{q_1 q_2}{16\pi\epsilon_0 E \sin^2(\theta/2)}\right]^2 \tag{10.73}$$

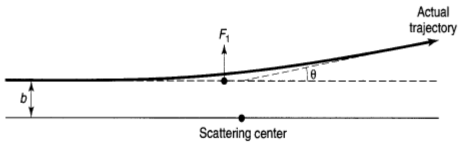


Figure 10.3: An example of the impulse approximation: the particle continues undeflected

10.5.4 The Born series

The Born approximation is very similar to the impulse approximation in the contex of classical scattering. In that sector we start by assuming that the particle keeps going in a straight line and compute the transverse impulse that would be delivered to it in that case:

$$I = \int F_{\perp} dt \tag{10.74}$$

If the deflection is small in comparism to the motion, it would then be a good approximation to the transverse momentum supplied to th particle. Thus we express the scattering angle as:

$$\theta = \arctan(I/p) \tag{10.75}$$

where p is th incident momentum. This is the "first-order" impulse approximation. The zeroth-order is what we started wtih i.e. no deflection at all. Likewise, in the zeroth-order Born approximation the incident plane wave passes by with no modification and what we saw earlier was just the first order correction to this. But the same pattern of thought can lead us to a series which then leads us to higher-order corrections. Let's recall the integral form of the Schrodinger equation:

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int g(\vec{r} - \vec{r}_0) V(\vec{r}_0) \psi(\vec{r}_0) d^3 r_0 \tag{10.76}$$

where is the incident wave and,

$$g(\vec{r}) = -\frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r}$$

is the Green's function with a factor $m/2\pi\hbar^2$ for convenience and V is the scattering potential. Suppose we take the equation for ψ and plug it back into (10.76),

$$\psi = \psi_0 + \int gV\psi_0 + \int\int gVgV\psi$$

Iterating this we obtain the series expasion for ψ,

$$\psi = \psi_0 + \int gV\psi_0 + \int\int gVgV\psi_0 + \int\int\int gVgVgV\psi_0 ... \tag{10.77}$$

We notice the following from (10.77):

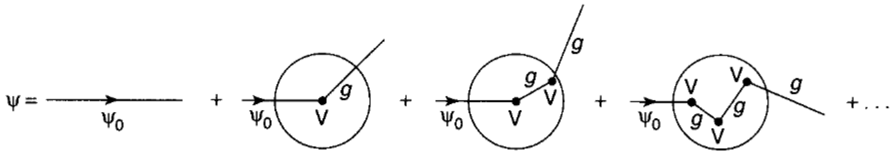


Figure 10.4: A diagram representing the Born series

- The first Born approximation truncates the series after the Next to Leading Order (NLO) term
- In the Leading Order ψ is untouched by V
- In the first order (Next to Leading Order) it is kicked once
- In the second order it is kicked, propagates to a new location and is kicked again and so on
- In this context the Green's function is essentially just the propagator [1]
- This was in fact the inspiration for Feynman diagrams which is expressed in terms of vertex factors (V) and propagators (g)

Figure (10.5.4) might look familiar, because it closely represents Feynman diagrams.

[1]In this context it tells us how the disturbance propagates between one interaction and the next

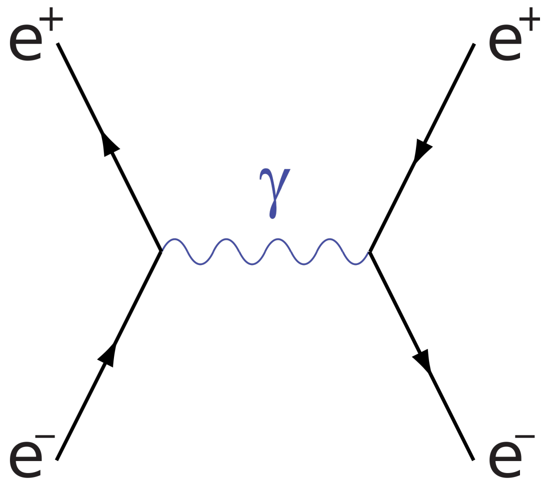


Figure 10.5: Bhabha scattering: Annihilation

Chapter 11

Path Integral Formulation

In this section we'll review the Path integral formulation, it's equivalence to the Schrodinger formalism and a toy model in this context.

11.1 The Path Integral Recepie

So far our stratergy has been to find the eigenstates of H then express the propagator in terms of this. However, the path integral formulation cuts one step and gets to the propagator directly. For a single particle in one dimension we follow the following procedure to find $U(x,t;x^{'},t^{'})$:

1. Draw all paths in the $x-t$ plane connecting $(x^{'},\dot{t})$ and ()
2. Find the action $S[x(t)]$ for each path $x(t)$
3. $U(x,t;x^{'},t^{'}) = A\sum_{Allpaths} e^{i\frac{S[x(t)]}{\hbar}}$; where A is a normalization factor

Here we have in a sense that the classical path taken by the particle corresponds to the stationary path. This is analogous to the Lagrangian formulation of classical mechanics in contrast to the approaches we took earlier involving the Hamiltonian.

11.2 Equivalence to the Schrodinger Equation

In the Schrodinger formalism, the change in the state vector over an infinitesimal time ϵ in the position basis is:

$$\psi(x,\epsilon) - \psi(x,0) = \frac{i\epsilon}{\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right]\psi(x,0) \tag{11.1}$$

to the first order in ϵ, the solution being

$$\psi(x,\epsilon) = \int_{-\infty}^{\infty} U(x,\epsilon;x^{'})\psi(x^{'},0)dx^{'} \tag{11.2}$$

This integral isn't so formidable as ϵ is simply just one slice in time.

$$\psi(x,\epsilon) = \left(\frac{m}{2\pi\hbar i\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right) \exp\left[-\left(\frac{i}{\hbar}\epsilon V\left(x+\frac{\eta}{2},0\right)\right)\right] \psi(x+\eta,0)d\eta \tag{11.3}$$

Where, $\eta = x^{'}$ Now, most of the contribution to the propagator must come from the stationary term, thus if we make the approxiation

$$|\eta| \leq \left(\frac{2\epsilon\hbar\pi}{m}\right)^{1/2}$$

and Taylor expand while avoid the $\epsilon\eta$ terms and treating it to be a Gaussian integral we find that:

$$\psi(x,\epsilon) - \psi(x,0) = \frac{i\epsilon}{\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right]\psi(x,0) \tag{11.4}$$

Which is exactly what we expect to see from the Schrodinger formalism as well.

11.3 Path Integral Evaluation of the Free-Particle Propagator

Let us consider the propagator. The problem is to solve for the integral

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar}\mathfrak{D}[x(t)] \tag{11.5}$$

where

$$\int_{x_0}^{x_N} \mathfrak{D}[x(t)]$$

is essentially the sum over all possible paths in configuration space. To do this we first express x(t) with a discrete approximation which is accurate upto N + 1 points i.e. . The gaps between points are interpolated with straight lines. Now the naive hope is that when $N \to \infty$ the notion of the approximation disappears. Thus we will start by replacing,

$$S = \int_{t_0}^{t_N} \mathcal{L}dt = \int_{t_0}^{t_N} \frac{1}{2}m\dot{x}^2 dt \tag{11.6}$$

with,

$$S = \sum_{i=0}^{N-1} \frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 \epsilon \tag{11.7}$$

where $x_i = x(t_i)$. Then integral then becomes,

$$U(x_N, t_N; x_0, t_0) = \int_{t_0}^{t_N} = \lim_{N\to\infty, \epsilon\to 0} A \int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar} \frac{m}{2} \sum_{i=0}^{N-1} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 \epsilon \right] \prod_{i=1}^{N-1} dx_i \tag{11.8}$$

Two assumptions are present here:

- t_N and t_0 have values that are implicitly defined
- The factor A is chosed so that we have the the correct scale for U when

We can intergrate by means of switching the variables up and then considering it to be a Gaussian integral. We then get

$$U = A \left(\frac{2\pi\hbar\epsilon i}{m} \right)^{N/2} \left(\frac{m}{2\pi\hbar i N\epsilon} \right)^{1/2} \exp\left[\frac{im(x_N - x_0)^2}{2\hbar N\epsilon} \right] \tag{11.9}$$

If we now let , we obtain the right result provided,

$$A = \left[\frac{2\pi\hbar\epsilon i}{m} \right]^{-N/2} = B^{-N}$$

This $1/B$ is in some senses the weighing function for each path. And thus we can understand how even though there are infinite paths, that only the stationary one is realized (because it has the highest weight) since it is most like the first order term. A similar idea is explored in the Born approximation section as well.

Chapter 12

Relativistic Quantum Mechanics

12.1 The Klein-Gordon Equation

In order to develop quantum mechanics relativistically, they started from the relativistic energy–momentum relation,

$$E^2 - \left|\vec{p}\right|^2 c^2 - m^2 c^4 = 0 \tag{12.1}$$

Substituting E and p for their respective operators,

$$E \Rightarrow i\hbar \frac{\partial}{\partial t}, \qquad \vec{p} \Rightarrow -i\hbar\vec{\nabla},$$

and letting the equation act on a wavefunction $\phi(\vec{x}, t)$ the equation becomes,

$$\Big(-\hbar^2 \frac{\partial^2}{\partial t^2} + \hbar^2 c^2 \nabla^2 - m^2 c^4 \Big) \phi(\vec{x}, t) = 0 \tag{12.2}$$

This is the Klein-Gordon Equation. The wave function $\phi(\vec{x}, t)$ is also an object called a field because its arguments extend over all space and time. Another way to say this is that it exists throughout spacetime and its fluctuations are described by the Klein–Gordon equation. In natural units,

$$\Big(\frac{\partial^2}{\partial t^2} + \nabla^2 - m^2 \Big) \phi(\vec{x}, t) = 0$$

This equation was the first attempt at a relativistic quantum mehcanical equation of a wave. it tells us how the field of a particle fluctuates.

The Klein-Gordon equation can also be written in the Lorentz-invariant form,

$$(\partial^\mu \partial_\mu + m^2)\psi = 0 \tag{12.3}$$

Where,

$$\partial^\mu \partial_m u \equiv \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}$$

The Klein-Gordon equation has plane wave solutions,

$$\psi(x,t) = Ne^{i(p\cdot x - Et)} \tag{12.4}$$

Substituting in Equation (3),

$$E^2\psi = p^2\psi + m^2\psi$$

12.2 The Dirac Equation

12.3 Covariant Formalism

12.3.1 The Adjoint Spinor and the Covariant Current

12.4 Solutions to the Dirac Equation

12.4.1 Particles at Rest

12.4.2 General Free-Particle Solutions

12.5 Antiparticles

12.5.1 The Dirac Sea Interpretation

12.5.2 The Feynman-Stuckelberg Interpretation

12.5.3 Antiparticle Spinors

Chapter 13

Epilogue: What lies ahead

With all of what we have discussed, whilst being the most experimentally accurate theory, Quantum Mechanics still remains incomplete due to three key issues that arise from internal consistency and consistency with other theories such relativity:

- **Locality:** Why do non-local effects arise in Quantum Mechanics? Are they artifacts of our ignorance or are they real?
- **Measurement:** Why is measurement distinct from time evolution? Why is it stochastic?
- **Ontology:** Is the wavefunction a calulative device or does it actually exist?

This is a realm that might quickly slip into philosophy[1] so we only mention points here and point to reading material since a subject of this depth deserves several volumes to dissect. Various different interpretations and formulations exist in the community that solve one or more of these problems. Few have suggested that Quantum Mechanics is truly deterministic at heart [2], few more suggest that the measurement problem has a great deal to do with the effect of gravity or some other novel mechanism[3], Rovelli suggests that Quantum Mechanics is about how one system is related to another [4] and a new proposal even goes on to state that classical mechanics is non-deterministic [5]!

[1] For a brief overview refer to [27] and [28]
[2] See [26] and [24]
[3] See [2]
[4] Read [25]
[5] Read [29]

As exemplified by the diversity of proposals, there is absolutely zero consensus in the community as to which approach is the most fruitful [6]. Maybe in the future, people will laugh at our ignorance and foolishness. But as form of anaesthasia [7], I would quote,

> "The aspiration to truth is more precious than its assured possession"
>
> - Gotthold Lessing

[6] See [31]
[7] Or as David Mermim would call it a "pillow"

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