Quantum Mechanics Notes

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Part I
# Introduction

1 Double Slit Experiment

We can try to understand the quantum behavior of electrons we shall consider the double slit experiment.

1.1 Bullet Interference

In this system bullets are shot with a uniform angle distribution and through a wall, reach a backstop where their position is saved by the detector. $P_1(x)$ and $P_2(x)$ are the probabilities of a bullet to reach any position x on the backstop when either one (but not both) of the slits are open. The probabilities were calculated experimentally by shooting many bullets and keeping track of where they hit the backstop.

We shall notice two key important results which may seem obvious:

- Bullets always arrive in identical lumps

- The probability when both slits are open is just the sum of the probabilities of each seperate slit open. This means there was *no interference.*
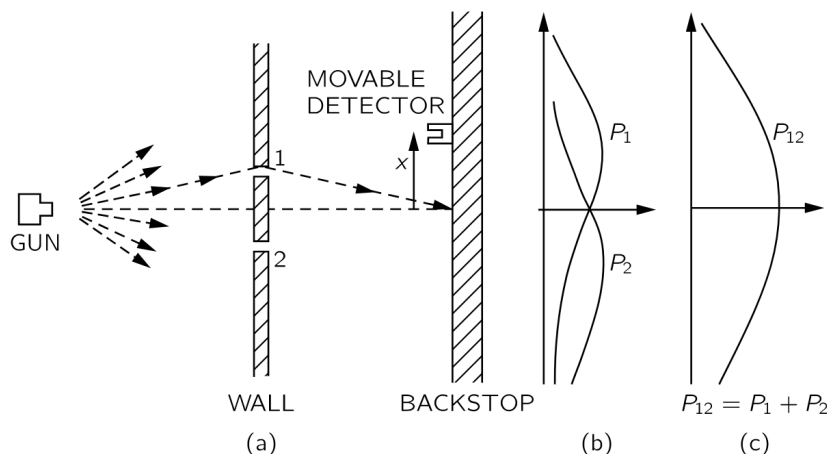
1.2 Wave Interference

Next, we will apply the same experiment but with water waves (or any wave for that matter). Instead of shooting bullets, we have a "wave source" making circular waves. Now the backstop is an "absorber" so there is no reflection of the waves. Instead of counting an amount of some quantity that comes in lump, the wave is continuous, so we measure it's intensity at any x value on the absorber. The intensity is proportional to the height of the wave squared.

Either one of the slits alone result in an intensity function quite similar to the probability of the waves, but together they add up as $|h_1 + h_2|^2$ and not $|h_1|^2 + |h_2|^2$, unlike the bullets.

We can write (using the cosine law):

$$h_j e^{i\omega t}, \quad I_j = |h_j|^2$$
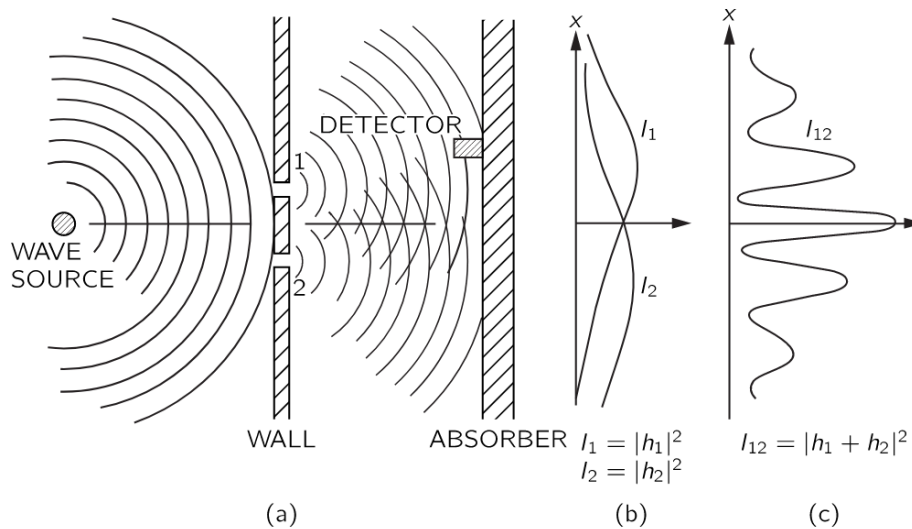
$$|h_1 + h_2|^2 = |h_1|^2 + |h_2|^2 + 2|h_1||h_2|cos\delta$$

$$\boxed{I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2}cos\delta}$$

δ is the phase difference between h_1 and h_2. So far everything is classical.

- Waves arrive continuously.

- The intensity when both slits are open is *not* the sum of the intensities of each seperate slit open. Waves interfere with each other.

WAVE SOURCE

DETECTOR

1

2

WALL   ABSORBER $I_1 = |h_1|^2$ $I_{12} = |h_1 + h_2|^2$
                         $I_2 = |h_2|^2$

I_1

I_2

I_{12}

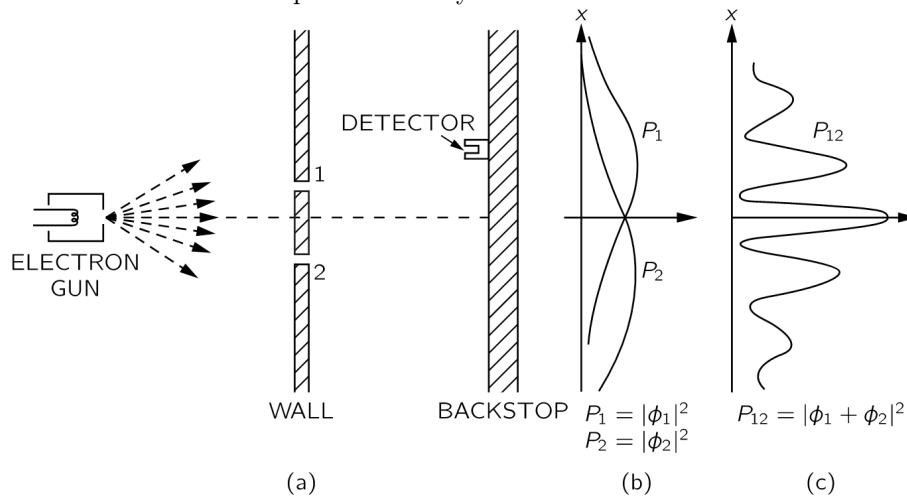(a)   (b)   (c)

1.3   Electron Interference

Recreating the bullet experiment with electrons we get the following results:

- Electrons always arrive in identical lumps (particle behavior).

- $P_{12} \neq P_1 + P_2$. *Electrons have interference* (wave behavior).

This is what we call the wave-particle duality.

ELECTRON GUN

DETECTOR

1

2

WALL   BACKSTOP $P_1 = |\phi_1|^2$ $P_{12} = |\phi_1 + \phi_2|^2$
                         $P_2 = |\phi_2|^2$

P_1

P_2

P_{12}

(a)   (b)   (c)

If each electron goes through only one of the two slits, we'd expect P_{12} to be the sum $P_1 + P_2$. Yet it isn't. So does it go through both slits at once? but we know electrons arrive in identical lumps, so it can't split up.

So let's try to measure which slit the electron goes through. We add a very strong light source, placed behind the wall and between the two slits. We know that electric charges scatter light. So when an electron passes, however it does pass, on its way to the detector, it will scatter some light to our eye, and we can see where the electron goes.

When we conduct *this* experiment, we see a flash of light either from slit 1 or slit 2, but never both at once. *Now, $P_{12} = P_1 + P_2$ is true.* We succeeded in watching which slit our electrons come through, but now there is no interference.

It is impossible to design an apparatus to determine which hole the electron passes through, that will not at the same time disturb the electrons enough to destroy the interference pattern. This is the uncertainty principle. If an apparatus is capable of determining which hole the electron goes through, it cannot be so delicate that it does not disturb the pattern in an essential way.

2 Matter Waves

2.1 De Broglie Wavelength

Every particle is a wave with $\left(\frac{E}{c}, \overrightarrow{p}\right) = \hbar\left(\frac{\omega}{c}, \overrightarrow{k}\right)$. The particle's velocity is the wave's group velocity.

$$\boxed{\lambda_{DeBroglie} = \frac{h}{p}}$$

$$v_{group} = \frac{d\omega}{dk} = \frac{dE}{dp} = \frac{d}{dp}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = v$$

2.2 Compton Wavelength

The wavelength of a photon whose energy is the same as the rest energy of a particle.

$$\boxed{\lambda_{compton} = \frac{h}{mc}} \begin{cases} E_e = mc^2 \\ E_\gamma = h\nu = hc/\lambda \end{cases}$$

For example, electron compton wavelength $l_e = \frac{h}{m_e c}$

2.3 Compton Scattering

A photon hits an electron, changing its direction of velocity some angle θ. The increase in wavelength due to lost energy is given by

$$\Delta\lambda = \frac{h}{m_e c}(1 - cos\theta) = l_e(1 - cos\theta)$$

Meaning, if the photon has a scattering angle of 90 degrees, its wavelength is increased by the electron's compton wavelength. If it stays on the same path, it has no energy/wavelength change.

3 The Wave Function

3.1 Properties

We have lost determinism to describe the universe as probabilistic. Each particle has energy and momentum $E = \hbar\omega$, $p = \hbar k$ and can be described by a wave function $\Psi(x,t)$.

- The probability density function is given by[1]

$$\frac{dP}{dx} = \rho(x,t) = |\Psi(x,t)|^2 = \Psi^*\Psi$$

- The probability to find the particle in some range $a \leq x \leq b$ is of course given by (all equivalent)

$$P_{ab} = \int_a^b dP = \int_a^b \frac{dP}{dx}dx = \int_a^b \rho dx = \int_{-\infty}^{\infty} |\Psi|^2 dx$$

- The probability that the patricle is *anywhere* is space must be one. Therefore we say the wavefunction is normalized

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

- (Operators) Operator are functions acting on the wavefunction. Here we say:

$$\hat{f}\Psi = f\Psi$$

Ψ	Wave function	Eigenstate
$\hat{f}$	Operator	Eigenfunction
f	Scalar Quantity	Eigenvalue

- The expectation value of any quantity f(x) is given by $\langle \hat{f} \rangle = \int \Psi^* \hat{f}\Psi dx$.

- The varience of any quantity (for example x) can be expressed as[2]

$$\sigma^2 \equiv \langle \Delta x^2 \rangle = \int_{-\infty}^{\infty} (x - \langle x \rangle)^2 \rho(x)dx = \int_{-\infty}^{\infty} x^2\rho(x)dx + \langle x \rangle^2 \int_{-\infty}^{\infty} \rho(x)dx - 2\langle x \rangle \int_{-\infty}^{\infty} x\rho(x)dx = \boxed{\langle x^2 \rangle - \langle x \rangle^2}$$

3.2 Schrodinger's Equation

Assuming a basic wave function $\phi = e^{i(kx - \omega t)}$ we can find the energy and momentum operators[3].

$$\frac{\partial \phi}{\partial t} = -\frac{iE}{\hbar}\phi \quad \frac{\partial \phi}{\partial x} = \frac{ip}{\hbar}\phi$$

$$\hat{E}\phi = E\phi \quad \hat{p}\phi = p\phi$$

$$\boxed{\hat{E} = -\frac{\hbar}{i}\frac{\partial}{\partial t}} \quad \boxed{\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}}$$

The hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V$ is the total energy, therefore

$$\hat{H}\Psi = E\Psi = \hat{E}\Psi$$

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

This is Schrodinger's equation. Like F=ma of a quantum particle.

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[1] Similarly to the intensity of the of the waves in the double slit experiment that was compared to the probability of the bullets/electrons.

[2] Using the fact that $\int_{-\infty}^{\infty} \rho(x)dx = 1$.

[3] The solution could also be written as such: $p^\mu = i\partial^\mu$

3.3 Time Evolution of SE

The SE must conserve probability as $\int_{-\infty}^{\infty} \rho(x)dx$ must always be 1.

$$\frac{d}{dt} \int_{-\infty}^{\infty} \Psi^* \Psi dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} \left(\Psi^* \Psi \right) dx = \int_{-\infty}^{\infty} \left(\Psi^* \frac{d\Psi}{dt} + \frac{d\Psi^*}{dt} \Psi \right) dx = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} \left(\Psi^* \frac{d\Psi}{dx} - \frac{d\Psi^*}{dx} \Psi \right) dx$$

$$\frac{i\hbar}{2m} \left(\Psi^* \frac{d\Psi}{dx} - \frac{d\Psi^*}{dx} \Psi \right) |_{-\infty}^{\infty} = \mathbf{0}$$

[4]Since the wave function must be normalized, it must be zero at infinities. Therefore we have proved SE conserves probability. We have additionaly found the following relation:

$$\boxed{J = \frac{i\hbar}{2m} \left(\Psi^* \frac{d\Psi}{dx} - \frac{d\Psi^*}{dx} \Psi \right)}$$

$$\frac{\partial \rho}{\partial t} - \frac{\partial J}{\partial x} = 0$$

J is the probability current, and this equation is the probability conservation equation. Generalized to 3 spatial dimensions:

$$\boxed{\frac{\partial \rho}{\partial t} - \nabla \cdot J = 0}$$

3.4 Stationary States

We shall attempt to solve SE by separation of variables. Substituting $\Psi(x,t) = \psi(x)f(t)$. We shall call any solution that satisfies this requirement a stationary state.

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} f + V\psi f = i\hbar\psi \frac{df}{dt}$$

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} \frac{1}{\psi} + V = i\hbar \frac{df}{dt} \frac{1}{f}$$

The left side is dependent only on x and the right side only on t. Therefore they both must be constant.

Time Independent

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} \frac{1}{\psi} + V = E$$

$$\boxed{\hat{H}\psi = E\psi}$$

Time Dependent

$$i\hbar \frac{df}{dt} \frac{1}{f} = E$$

$$ln|f| = \frac{-iE}{\hbar} t$$

$$\boxed{f(t) = e^{\frac{-iEt}{\hbar}}}$$

These are very important results. We have found the time dependency of stationary states, as well as have found the time independent Schrodinger equation (TISE)[5].

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[4]The time derivatives of the wave function are known from schordingers equation.

[5]Notice key differences from the original SE: Our new equation solves for $\psi(x)$ instead of $\Psi(x,t)$. Therefore we have ordinary derivatives instead of partial. Additionally, the right side of the equation has the total energy as *scalar* and not operator. Applying the energy operator $\hat{E}$ to a time independent wave function gives 0.

Stationary states have no *physical* time dependency. The wave function indeed has a time dependency, but when calculating the probability density we see f(t) has no effect. These states are stationary.

$$\rho = |\Psi(x,t)|^2 = \psi^* e^{\frac{iEt}{\hbar}} \psi e^{\frac{-iEt}{\hbar}} = |\psi(x)|^2$$

Stationary states have $\sigma_E = 0$. Every measurement of the total energy is certain to return the value E.

3.5 Superposition

SE is a homogenous differential equation. Therefore we can create orthonormal basis of solution functions, and the sum of any two solutions of the equations is also a solution. The assumption that the wave function is separable $\Psi(x,t) = \psi(x)f(t)$ gave us the orthonormal basis states, which are stationary; meaning they don't evolve through time. Yet a sum of these stationary states indeed changes with time. The general solution to the SE is

$$\sum_{n=1}^{\infty} c_n \psi_n e^{\frac{-iE_n t}{\hbar}}$$

Just as we had summed the water wave functions in the double slit experiment here we sum the wave functions representing probabilities. Let's normalize the superposition wave function. Since the states are orthonormal we have the identity $\int \psi_i \psi_j dx = \delta_{ij}$.[6] This leaves us with only same-index terms.

$$\int_{-\infty}^{\infty} |\sum_{n=1}^{\infty} c_n \psi_n e^{\frac{-iE_n t}{\hbar}}|^2 dx = \int_{-\infty}^{\infty} \sum_{n=1}^{\infty} |c_n \psi_n e^{\frac{-iE_n t}{\hbar}}|^2 dx = \sum_{n=1}^{\infty} \left(|c_n|^2 \int_{-\infty}^{\infty} |\Psi_n|^2 dx \right) = \boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

From this we see the squares of coefficients must add up to 1. We can interpret this the coefficients be the probabilities associated with measuring each specific stationary state when measuring the system in superposition. So $|c_n|^2$ is the probability of measuring the state with momentum p_n. This is further explored as the principle of uncertainty, and can be shown more rigorously using Fourier transform. Additionally, according to Fourier theory, ANY function can be represented by this sum with a correct choice of coefficients. This means that to find the wave function we substitute our potential function V(x), solve for $\psi_n(x)$, find c_n according to the chosen initial conditions, and finally, we add the time dependency f(t).

A measurement of a wave function in superposition (sum of stationary states) collapses it to a stationary state. The probability of the state ψ_n to be measured is $|c_n|^2$. This is Born's rule.

3.6 Fourier's Trick (Obtaining Coefficients)

As said before, the general wave function solution can be expressed as the linear combination of the stationary solutions. Dirichlet's theorem says any function can be expressed this way.

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

But how do we know what the coefficients are? Fourier's trick is a method of obtaining the set of coefficients c_n to match any function $f(x)$, exploiting the orthnormality of the set $\{\psi_n\}$: multiply both sides by $\psi_m^*(x)$ and integrate. The summing (sum and integral) can be done in any order, and linearity can be applied.

$$\int \psi_m^* f dx = \sum_{n=1}^{\infty} c_n \int \psi_m^* \psi_n dx = \sum_{n=1}^{\infty} c_n \delta_{mn} dx$$

$$\boxed{c_m = \int \psi_m^*(x) f(x) dx}$$

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[6]The kronecker delta is defined as $\delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$. It is very common. It is equal to the components of the identity matrix $I_{ij} = \delta_{ij}$.

This formula can be used as a means of obtaining a solution in any intial value problem. We say $f(x) = \Psi(x,0)$ and substitute the general stationary state $\psi_m(\mathrm{x})$. The time part can be added to find the wave function to be $\Psi(x,t) = \sum_{m=1}^{\infty} c_m \psi_m e^{\frac{-iE_m t}{\hbar}}$.

Part II
Exploring Potentials

4   Infinite Well

4.1   1D

Let us consider the following potential.

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & otherwise \end{cases}$$

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

The wave function must be 0 outside the box for SE to make sense and for the wave function to be normalizable. We can now set the boundary conditions and cosider SE inside the box, with zero potential.

$$\psi(0) = \psi(a) = 0$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

Just like an harmonic oscillator,

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \qquad k^2 \equiv \frac{2mE}{\hbar^2}$$

$$\psi = A\sin(kx) + B\cos(kx)$$

Now using the boundary conditions,

$$\psi(0) = A\sin(0) + B\cos(0) = 0 \ \Rightarrow \ B = 0$$

$$\psi(a) = A\sin(ka) = 0 \ \Rightarrow \ ka = n\pi$$

We learn that k has discrete values since n is an integer. That means the energy must have discrete values as well.

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \boxed{\frac{h^2}{8ma^2}n^2}$$

We get different discrete energy levels. Classical continuous energy has been thrown out - energy comes in discrete amounts/quantities, *"quanta"*. This is *quantized energy*. Our normalized solution to the TISE is then

$$\int_{-\infty}^{\infty} A^2\sin^2(\frac{n\pi x}{a})dx = A^2\int_0^a \sin^2(\frac{n\pi x}{a})dx = \frac{A^2 a}{2} = 1$$

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

Notice our solution is exactly the solution for standing waves between points $x = 0$ and $x = a$. Additionaly, we get *nodes* in the PDE, points where the probability is 0. The higher the energy the more nodes there are.

$\psi_4(x)$ $\rho_4(x)$

$\psi_3(x)$ $\rho_3(x)$

$\psi_2(x)$ $\rho_2(x)$

$\psi_1(x)$ $\rho_1(x)$

0   **x**   **a**   **0**   **x**   **a**
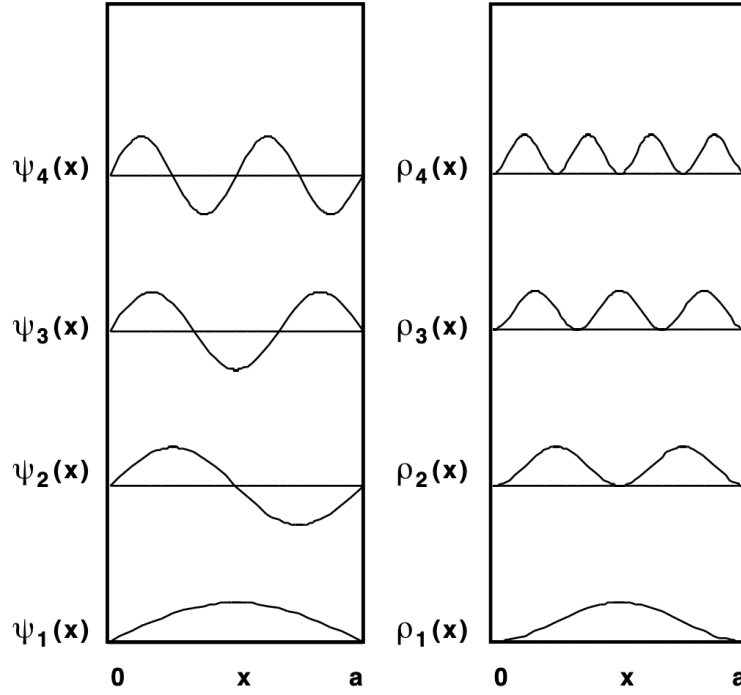
Our stationary solutions found from the TISE are indeed orthonogal:

$$\int_0^a \psi_n \psi_m dx = \int_0^a \frac{2}{a} sin\left(\frac{n\pi x}{a}\right) sin\left(\frac{m\pi x}{a}\right) dx$$

$$sin\alpha \, sin\beta = \frac{1}{2}[cos(\alpha - \beta) - cos(\alpha + \beta)]$$

$$\frac{2}{a} sin\left(\frac{n\pi x}{a}\right) sin\left(\frac{m\pi x}{a}\right) = \frac{1}{a}[cos\left(\frac{\pi x}{a}(n - m)\right) - cos\left(\frac{\pi x}{a}(n + m)\right)]$$

The cosine function completes a whole number of periods from 0 to a, therefore it has an integral of 0 over this interval. This is as long as $n - m \neq 0$. In that case, the function is constant (1) and the integral from 0 to a is a (divided by the coefficient a, the result is 1).

$$\boxed{\int_0^a \psi_n \psi_m dx = \delta_{nm}}$$

Using Fourier's trick to find the set of coefficients, we get:

$$c_n = \sqrt{\frac{2}{a}} \int_0^a sin\left(\frac{n\pi x}{a}\right) \Psi(x,0) \, dx$$

4.2   3D

Our box shall have opposite vertices with coordinates $(0, 0, 0)$ and (a_1, a_2, a_3). To solve this we shall use seperation of variables.

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

$$\frac{-\hbar^2}{2m}\nabla^2\psi = E\psi$$

$$\frac{-\hbar^2}{2m}\left(\frac{d^2X}{dx^2}YZ + X\frac{d^2Y}{dy^2}Z + XY\frac{d^2Z}{dz^2}\right) = E\ X(x)Y(y)Z(z)$$

$$-\frac{X''}{X} - \frac{Y''}{Y} - \frac{Z''}{Z} = \frac{2mE}{\hbar^2}$$

Using the same trick we used to derive the TISE - we notice each term on the left side of the equation depends on a different variable, yet their sum is a constant. Therefore, each term is a constant we'll call α_μ^2. Since all cartesian coordinates are symmetric in this equation we'll use indices to represent the three equations (of each coordinate) in a single equation: X_μ are the seperated functions, a_μ the dimensions of the box. We take a shortcut, having already found the function of a 1D box using the same boundary conditions.

$$X_\mu''(x^\mu) = -\alpha_\mu^2 X_\mu(x^\mu)$$

$$X_\mu(x^\mu) = \sqrt{\frac{2}{a}}sin(\frac{n_\mu\pi}{a_\mu}x^\mu), \qquad \mu = 1, 2, 3.$$

Finally, the energy and the time-independent wave function are

$$E_{n_\mu} = \frac{\hbar^2}{2m}\sum_\mu \alpha_\mu^2 = \boxed{\frac{h^2}{8m}\sum_\mu \left(\frac{n_\mu}{a_\mu}\right)^2}$$

$$\boxed{\psi_{n_1, n_2, n_3}(x, y, z) = \sqrt{\frac{8}{V}}sin\left(\frac{n_1\pi}{a_1}x\right)sin\left(\frac{n_2\pi}{a_2}y\right)sin\left(\frac{n_3\pi}{a_3}z\right)}$$

Note: any two of these functions are orthogonal unless *all three* quantum numbers n_μ match. This can be shown by integrating the product of two time-independent wave functions. The result is a product of kronecker deltas $\prod \delta_{n_\mu m_\mu}$ - *only* if all three are equal to one, the product is one.

5 Harmonic Oscillator

The harmonic oscillator potential is the potential of a body on a spring, $V = \frac{1}{2}m\omega^2 x^2$.

5.1 Ladder Operator Method

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi$$

$$\frac{1}{2m}\left(\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right)\psi = E\psi$$

Let us examine the factorization of the expression operating on the wave function. We shall define the following operators and check whether we can factorize the expression as $u^2 + v^2 = (u + iv)(u - iv)$, with $a_\pm = u \pm iv$. We need to test this, as operators behave differently to scalars - they do not commute $[\hat{u}, \hat{v}] = \hat{u}\hat{v} - \hat{v}\hat{u} \neq 0$.

$$a_\pm \equiv \frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d}{dx} \pm im\omega x\right)$$

$$a_+ a_- f = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega x\right)\left(\frac{\hbar}{i}\hbar\frac{d}{dx} - im\omega x\right)f = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx} + im\omega x\right)\left(\frac{\hbar}{i}\frac{df}{dx} - im\omega x f\right)$$

$$= \frac{1}{2m}\left(-\hbar^2\frac{d^2 f}{dx^2} + m^2\omega^2 x^2 - \hbar m\omega\frac{d}{dx}(xf) + \hbar m\omega x\frac{df}{dx}\right) = \frac{1}{2m}\left(-\hbar^2\frac{d^2 f}{dx^2} + m^2\omega^2 x^2 - \hbar m\omega f\right)$$

$$\frac{1}{2m}\left(\left(i\hbar\frac{d}{dx}\right)^2 + (m\omega x)^2 - \hbar m\omega\right)f$$

And the result is

$$a_+ a_- = \frac{1}{2m}\left(\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right) - \frac{1}{2}\hbar\omega$$

Therefore, we can rewrite

$$(a_+ a_- + \frac{1}{2}\hbar\omega)\psi = E\psi$$

These operators that we have defined are called *ladder operators,* as when acting on the wave function they move it up and down energy levels. They are also called the raising operator and lowering operator. Proof:

$$(a_+ a_- + \frac{1}{2}\hbar\omega)(a_+\psi) = (a_+ a_- a_+ + \frac{1}{2}\hbar\omega a_+)\psi = a_+(a_- a_+ + \frac{1}{2}\hbar\omega)\psi = a_+\left[(a_- a_+ - \frac{1}{2}\hbar\omega)\psi + \hbar\omega\psi\right]$$

$$\boxed{\hat{H}(a_+\psi) = (E + \hbar\omega)(a_+\psi)}$$

We have shown the raising operator gave the state with energy $E + \hbar\omega$. It can be similarly shown that the lowering operator gives a new state with energy $E - \hbar\omega$. But you can't subtract infinitely, There must be some ground zero state, therefore:

$$\boxed{a_-\psi_0 = 0}$$

$$\frac{1}{\sqrt{2m}}\left(\frac{\hbar}{i}\frac{d\psi_0}{dx} - im\omega x\psi_0\right) = 0$$

$$\frac{d\psi_0}{dx} = -\frac{m\omega x}{\hbar}\psi_0$$

$$\boxed{\psi_0 = Ae^{\frac{-m\omega x^2}{2\hbar}}}$$

or more generally,

$$\boxed{\psi_n = A_n(a_+)^n e^{\frac{-m\omega x^2}{2\hbar}}}$$

5.2 Power Series Method

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

First we shall make a change of variables, to clean up the equation of constants: $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$, and $K \equiv \frac{2E}{\hbar\omega}$.

$$\frac{d^2}{dx^2} = \frac{d}{dx}\left(\frac{d}{dx}\right) = \frac{d\xi}{dx}\frac{d}{d\xi}\left(\frac{d\xi}{dx}\frac{d}{d\xi}\right) = \frac{m\omega}{\hbar}\frac{d^2}{d\xi^2}$$

$$\frac{d^2\psi}{d\xi^2} = \left(\xi^2 - K\right)\psi$$

Using a power series is a method of solving differential equations by expressing a the (solution) function as a polynomial power series. Polynomial are great for describing functions near $x = 0$ but as x goes to infinities polynomials tend to infinities as well. Therefore to solve using a power series we must take into account the function's asymptotic behavior first, then express some new function as a power series (this will soon be clear), with our solution being their product.

5.2.1 Asymptotic Solution

So first we shall check for asymptotic behavior, meaning an approximate solution, for $\xi \gg 1$.

$$\frac{d^2\psi}{d\xi^2} = \xi^2\psi$$

$$\psi = Ae^{-\xi^2/2} + Be^{\xi^2/2}$$

$$\psi(\xi) = Ae^{-\xi^2/2}$$

This is our asymptotic solution. We have found that the wave function tends to zero which should be no surprise as it must be normalizable.

5.2.2 Change of Functions

Now to solve for the non-approximate (not $\xi \gg 1$) we will express our function as the following product and use a power series. This will give us the solution for the behavior near x=0 as well as at infinities.

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}$$

$$h(\xi) \equiv \sum_{j=0}^{\infty} a_j \xi^j$$

Calculating the derivatives:

$$\frac{d\psi}{d\xi} = \frac{dh}{d\xi}e^{-\xi^2/2} - h\xi e^{-\xi^2/2}$$

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\frac{dh}{d\xi}\xi + (\xi^2 - 1)h\right)e^{-\xi^2/2}$$

Substituting back to the TISE:

$$\frac{d^2h}{d\xi^2} - 2\frac{dh}{d\xi}\xi + (K - 1)h = 0$$

5.2.3 Power Series - Finding the Coefficients

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$$

$$\frac{dh}{d\xi} = \sum_{j=0}^{\infty} j a_j \xi^{j-1}$$

$$\frac{d^2h}{d\xi^2} = \sum_{j=0}^{\infty} j(j-1)a_j\xi^{j-2} = \sum_{j=-2}^{\infty}(j+2)(j+1)a_{j+2}\xi^j = \sum_{j=0}^{\infty}(j+2)(j+1)a_{j+2}\xi^j$$

The last equality is due to the terms $j = -2$ and $j = -1$ being 0. Substituting back to the TISE, we get a new poer series. We notice there must be only one polynomial whose value is zero everywhere (being the zero polynomial), the polynomial with every coefficient equal to 0.

$$\sum_{j=0}^{\infty}\left[(j+2)(j+1)a_{j+2} + (-2j+K-1)a_j\right]\xi^j = \sum_{j=0}^{\infty} b_j\xi^j = 0$$

$$(j+2)(j+1)a_{j+2} = (2j+K-1)a_j$$

$$\boxed{a_{j+2} = \frac{2j+K-1}{(j+2)(j+1)}a_j}$$

We get a recursive formula of the coefficients of $h(\xi)$. Since this formula relates every *other* coefficient, we get two degrees of freedom. Setting a_0 will get us the series of even coefficients, and setting a_1 will get us the series of odd coefficients.

5.2.4 Termination

For the function to remain normalized, we must have some last non-zero coefficient a_n before the series terminates. This n will be the quantum number corresponding to our energy level. Of course, we get the same energies as in the solution with ladder operators.

$$\frac{2n+K-1}{(n+2)(n+1)}a_n = 0$$

$$K = 2n+1$$

$$\boxed{E = \frac{\hbar\omega}{2} + n\hbar\omega}$$

$$\boxed{a_{j+2} = \frac{2(j+n)}{(j+2)(j+1)}a_j}$$

We can see more clearly now that there can only one coefficient a_n that can terminate series. This means that if *supposedly* the last non-zero term is a_n, but a_{n-1} is non-zero as well, a_{n+1} will be non-zero. This means that for the series to terminate either all odd terms are zero of or all even terms.

$$h(\xi) = a_0 + a_2\xi^2 + a_4\xi^4...$$

$$h(\xi) = a_1\xi + a_3\xi^3 + a_5\xi^5...$$

So we set *either* a_0 or a_1 to be zero, and the solution is given by the following series. What non zero value we pick doesn't matter as it will be set by the normalization. The general solution is then

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\xi^2/2}}, \quad \xi = \sqrt{\frac{m\omega}{\hbar}}x$$

Where H_n are the hermite polynomials.

6 Free Particle

6.1 Stationary States

A free particle has zero potential everywhere.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

As usual the solution is

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

Adding time dependency

$$\Psi(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x + \frac{\hbar k}{2m}t\right)}$$

Letting k be negative ($k = \frac{\pm\sqrt{2mE}}{\hbar}$),

$$\Psi(x,t) = Ae^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} = Ae^{i(kx - \omega t)}$$

Notice k isn't just any constant, it is the wavenumber given by $p = \hbar k$ and $E = \frac{p^2}{2m}$. We can also use $E = \hbar\omega$ to see that our stationary solution is simply the solution of a plane wave.

6.2 Normalization and Quantization

When attempting to normalize this function we see it cannot be normalized. This means that stationary states of free particles have no physical meaning. Only a superposition, a sum of stationary states, can be normalized and have physical meaning. This means *there is no such thing as a free particle with a definite energy*, and a free particle's probability distribution must change in time.

$$\int_{-\infty}^{\infty} \left(Ae^{-i(kx - \omega t)}\right)\left(Ae^{i(kx - \omega t)}\right)dx = A^2\int_{-\infty}^{\infty} dx = \infty$$

k isn't restricted to discrete values as there aren't any boundaries condition - it isn't quantized, and therefore can have any value. The energy therefore can also have any (non-negative) value. So we can no longer sum the stationary states as usual ($\sum c_n\psi_n$) over the discrete integer quantum number n. Instead we must use an integral to sum over the continuous values of k with a continuous function $\phi(k)$ instead of the set of coefficients.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \phi(k)e^{i(kx - \omega t)}dk$$

We call this a **wave packet**.

6.3 Plancherel's Theorem

6.3.1 Theorem

To find $\phi(k)$ for given initial conditions we use **Plancherel's theorem**.

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} F(k)e^{ikx}dk \iff F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)e^{-ikx}dx}$$

$F(k)$ is the Fourier transform of $f(x)$ and $f(x)$ is the inverse Fourier transform of $F(k)$. Applying the theorem to our wave function:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \phi(k)e^{ikx}dk$$

$$\boxed{\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \Psi(x,0)e^{-ikx}dx}$$

6.3.2 Proof

Any function on the interval $[-a, a]$ can be expressed as a linear combination of sines and cosines.

$$f(x) = \sum_{n=0}^{\infty} \left[a_n sin\left(\frac{n\pi x}{a}\right) + b_n cos\left(\frac{n\pi x}{a}\right) \right]$$

Which can also be written as an exponential (with the following relation to the inital constants

$$\boxed{f(x) = \sum_{n=-\infty}^{\infty} c_n \psi_n} = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/a}$$

$$c_n = \begin{cases} \frac{1}{2}\left(b_{-n} + ia_{-n}\right) & n < 0 \\ b_0 & n = 0 \\ \frac{1}{2}\left(b_n - ia_n\right) & n > 0 \end{cases}$$

Using Fourier's trick, just like before, we get c_n.

$$\int_{-a}^{a} e^{-im\pi x/a} f(x) dx = \sum_{n=-\infty}^{\infty} c_n \int_{-a}^{a} e^{-im\pi x/a} e^{in\pi x/a} dx$$

$$\int_{-a}^{a} e^{-im\pi x/a} e^{in\pi x/a} dx = \int_{-a}^{a} e^{i\pi x(n-m)/a} dx = \frac{ae^{i\pi x(n-m)/a}}{i\pi(n-m)}\Big|_{-a}^{a} \to 2a\delta_{mn}$$

$$\boxed{c_m = \frac{1}{2a}\int_{-a}^{a} \psi_m^*(x) f(x) dx}$$

We shall now make the substitutions $F(k) = \sqrt{\frac{2}{\pi}} a c_n$ and $k = \frac{2\pi}{a}$ to the two boxed equations, and use $\Delta k = \frac{(n+1)\pi}{a} - \frac{n\pi}{a} = \frac{\pi}{a}$.

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} F(k) e^{ikx} \Delta k$$

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

Now taking the limit as $a \to \infty$

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx}$$

All we did was express a function on an interval as a linear combination of periodic functions, found the coefficients using Fourier's trick, and took the limit as the interval becomes $[-\infty, \infty]$ (with a small substitution to make the equations symmetric - we could have just as well integrated over n instead of k).

7 Delta Potential

7.1 Dirac Delta Function

The Dirac delta function can be defined as

$$\delta(x) = \left\{ \begin{array}{ll} 0 & x \neq 0 \\ \infty & x = 0 \end{array} \right\}, \quad \int_{-\infty}^{\infty} \delta(x)dx = 1$$

Some of its properties are:

$$\int_a^b \delta(x-m)f(x)dx = \left\{ \begin{array}{ll} f(m) & a \leq m \leq b \\ 0 & otherwise \end{array} \right.$$

$$\int_a^b \delta'(x-m)f(x)dx = \left\{ \begin{array}{ll} f'(m) & a \leq m \leq b \\ 0 & otherwise \end{array} \right.$$

$\int_a^b \delta(g(x))\,f(x)dx = \sum_i \frac{f(x_i)}{|g'(x_i)|}$, x_i are the zero points of $g(x)$.

Now let us examin the quantum behaivior of a system with a potential proportional to the Dirac delta function $V(x) = -\alpha\delta(x)$.

7.2 Negative Energy (bound)

Anywhere but x=0 the potential is zero. Assuming the energy is negative, k is real and postiive.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta\psi = E\psi$$

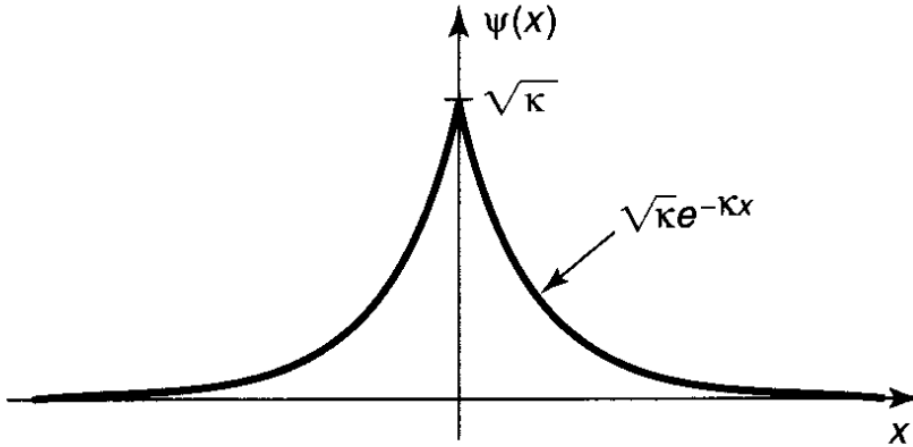$$\frac{d^2\psi}{dx^2} = k^2\psi, \quad k \equiv \frac{\sqrt{-2mE}}{\hbar}$$

$$\psi_{x<0} = Ae^{-kx} + Be^{kx}$$

$$\psi_{x>0} = Fe^{-kx} + Ge^{kx}$$

Taking normalizing into account, for x<0 A=0 and for x>0 G=0. Since the wavefunction must be continuous $\psi_{x>0}(0) = \psi_{x<0}(0)$ and therefore $B = F$.

$$\psi(x) = \begin{cases} Be^{kx} & x \leq 0 \\ Be^{-kx} & x \geq 0 \end{cases}$$

or more compactly $\psi(x) = Be^{-k|x|}$.

To get some information regarding the center point, x=0, can integrate SE from $-\epsilon$ to ϵ and take the limit as $\epsilon \to 0$.

$$\frac{-\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx - \alpha\int_{-\epsilon}^{\epsilon}\delta(x)\psi dx = E\int_{-\epsilon}^{\epsilon}\psi dx$$

$$\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx = \frac{-2m\alpha}{\hbar^2}\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)dx$$

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

Where $\Delta\left(\frac{d\psi}{dx}\right)$ is the difference of the derivative of ψ from the right and from the left: $\frac{d\psi_{x>0}}{dx}|_{x=0} - \frac{d\psi_{x<0}}{dx}|_{x=0} = -2Bk$. Therefore

$$k = \frac{m\alpha}{\hbar^2} \Rightarrow \boxed{E = -\frac{m\alpha^2}{2\hbar^2}}$$

We have found precisely the energy of the stationary states with negative energy with no dependency on any quantum number: there is *only one such state*. This is *the only bound state* for this potential. Normalizing to find B we get $B = \sqrt{k}$. The bound state is

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha}{\hbar^2}|x|}$$

7.3 Positive Energy (scattering)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_{x<0} = Ae^{-ikx} + Be^{ikx}$$

$$\psi_{x>0} = Fe^{-ikx} + Ge^{ikx}$$

This time we cannot get rid of the A and G terms as no terms go to infinity. We *can* still use the continuity of the wave function to say

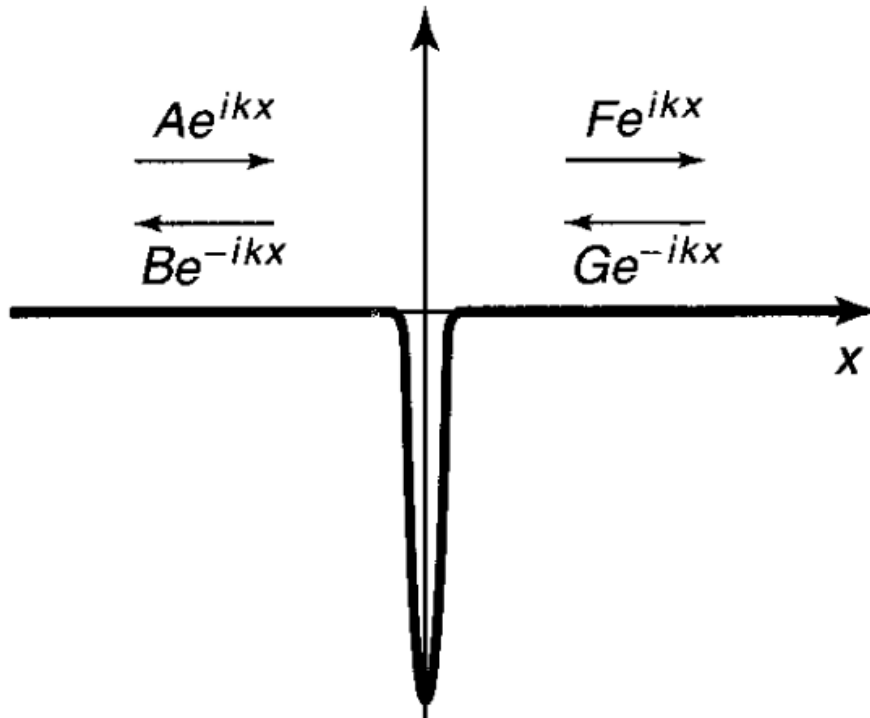$$\psi(0) = \boxed{F + G = A + B}$$

We can also say

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

$$ik(F - G - A + B) = \frac{-2m\alpha}{\hbar^2}(A + B)$$

$$\boxed{F - G = A(1 + 2i\beta) - B(1 - 2i\beta)}, \quad \beta \equiv \frac{m\alpha}{\hbar^2 k}$$

We have found some sort of wave scattering behavior. We can examine scattering from the left to say:

- $G = 0$.

- A is the amplitude of the incident wave.

- B is the amplitude of the reflected wave.

- F is the amplitude of the transmitted wave.

Using the two boxed equations we get

$$B = \frac{i\beta}{1 - i\beta} A, \;\; F = \frac{1}{1 - i\beta} A$$

We can find the reflection and transmission coefficients:

$$R \equiv \frac{|A|^2}{|B|^2} = \frac{\beta^2}{1 + \beta^2}$$

$$T \equiv \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}$$

Substituting β,

$$\boxed{R = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)} \;\; , T = \frac{1}{1 + (m\alpha^2/2\hbar^2 E)}, \;\; R + T = 1}$$

The higher the energy the greater the probability of transmittion (T).

We get a continuous set of scattering states, as none of our variables are quantized and the energy is always higher than the potential V(x).

7.4 Quantum Tunneling

A very strange important thing to notice is that the transmittion and reflection (relative) probabilities depend on α^2 and not α. If we set α to be negative, meaning we get a *barrier potential*, the probabilities would stay the same. In the classical case having an infinite potential barrier means to cross the barrier there needs to be an infinite amount of work done, and zero probability of crossing. In quantum mechanics we have the probability of going trough the barrier and crossing the infinite "pit" equivalent. This is **quantum tunneling**: even though $E < V_{max}$ and $V_{max} = \infty$! The probability to pass through the barrier is non-zero. And in the opposite case with $E > V_{max}$, classicaly we would expect always to be able to cross (assuming no energy loss), yet in the quantum case there is a probability of bouncing back, according to the reflection coefficient.

8 Finite Well

The finite square well potential is

$$V(x) = \begin{cases} -V_0 & -a < x < a \\ 0 & |x| > a \end{cases}$$

It admits both scattering states ($E > 0$) and bound states ($E < 0$). If the potential is even we can assume with no loss of generality that the solution is either even or odd. We shall assume the solution is even.

8.1 Negative Energy (bound)

As usual, for zero potential (at $|x| > a$):

$$\frac{d^2\psi}{dx^2} = k^2\psi, \quad k \equiv \frac{\sqrt{-2mE}}{\hbar}$$

$$\psi = Be^{-k|x|}$$

and in the region $-a < x < a$:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -l^2\psi, \quad l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\psi(x) = D\cos(lx)$$

We have

$$\psi(x) = \begin{cases} D\cos(lx) & -a < x < a \\ Be^{-k|x|} & |x| > a \end{cases}$$

Using the continuity of the wave function and its derivative we find

$$Be^{-ka} = D\cos(la)$$

$$-kBe^{-kx} = -lD\sin(la)$$

Therefore

$$k = l\tan(la)$$

9 Bound and Scattering States

Imagining a body with energy E in a classical potential V(x), if $E < V(\pm\infty)$ the body is in a **bound state**. The body cannot pass the turning points where $E = V(x)$. It will go back and forth between those points, bounded by its low energy. *Bound states are normalizable and quantized.* Examples of potentials that "generate" bound states are harmonic oscillator and the infinite well. To create a superposition of such states we simply sum them in a linear combination.
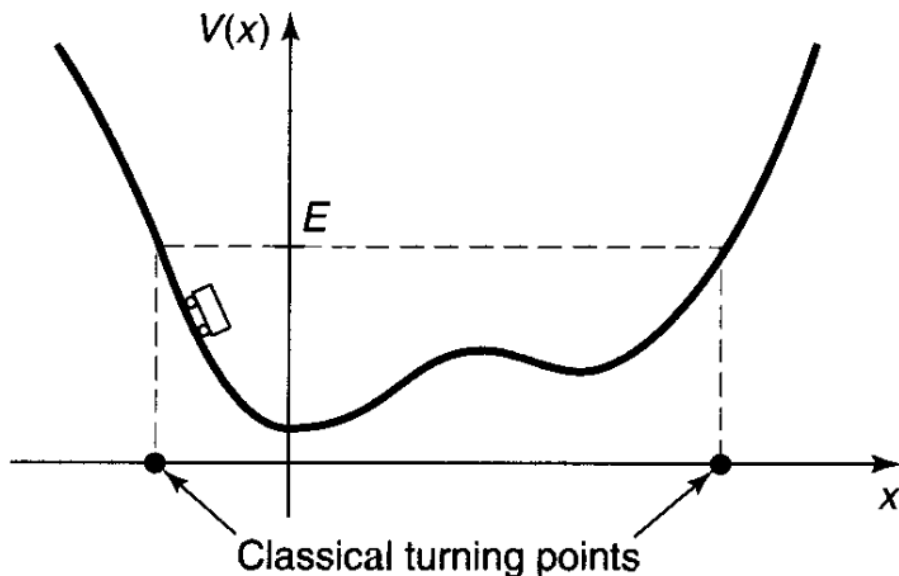
Now imagining a potential for which $E > V(\pm\infty)$, we get a **scattering state**. The classical body can go anywhere from $x = -\infty$ to $x = \infty$. Scattering states aren't normalizable and can't be quantized. An example of a potential with scattering states is the free particle potential, $V(x) = 0$. To create a superposition of such states the sum must be on a continuous variable, therefore the linear combination becomes an integral.
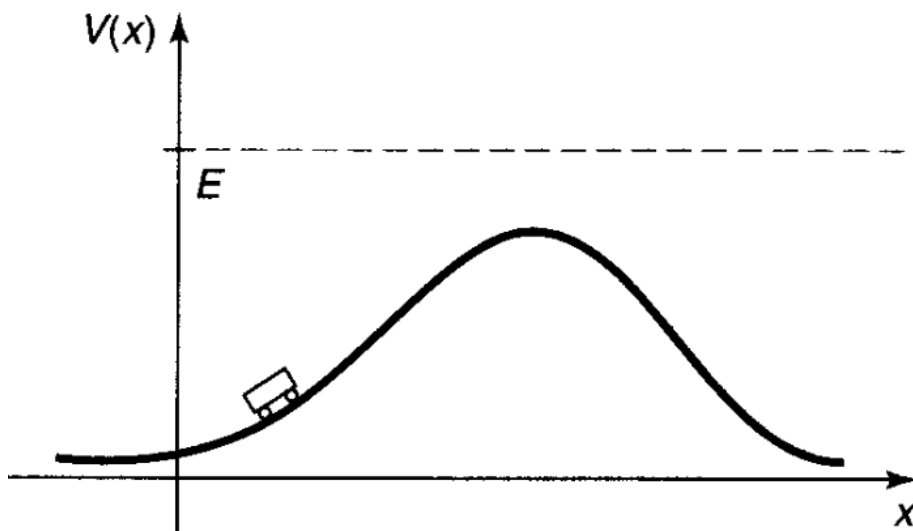
Some potentials generate both scattering states and bound states, depending on the energy. For example the dirac delta potential has one bound state with negative energy (as the potential goes to zero at $\pm\infty$) and infinite continuous (=not quantized) scattering states with postivie energy.

As opposed to the classical case where a body in a potential $V(x)$ with energy $E < V(x)$ has zero probability of reaching $E > V(x)$, in the quantum case there is a non zero probability to cross a potential bigger than the body's energy.

10 Drawing Wave Functions

Schrodinger's equation can be written as

$$\frac{d^2\psi}{dx^2} \propto [V(x) - E]\,\psi$$

1) If $E < V(x)$ the function curves away from the axis ($\psi = 0$). This means $|\psi|^2$ will continue to grow: There cannot exist a state $E < V_{min}$, otherwise the state is not normalizable, and not even a superposition of such states is normalizable.

2) If $E > V(x)$ the function curves towards the axis. This means ψ has wave behavior.

We can use these two facts to draw a qualitative approximation to the states admitted by any potential.

11   Even/Odd Solutions

If the potential is even, then we can say $\hat{H}\psi(-x) = E\psi(-x)$, and we have both $\psi(x)$ and $\psi(-x)$ as solutions to TISE. We can construct even and odd solutions from these two solutions.

$$\psi_{even} = \psi(x) + \psi(-x)$$

$$\psi_{odd} = \psi(x) - \psi(-x)$$

Therefore we can simply solve for these odd/even solutions instead of solving for the "original" solutions.

12 Scattering Matrix

13 Continuous

Assuming some wave function ψ isn't continuous at point x_1, we have $\frac{d\psi}{dx}|_{x_1} = \infty$. The second derivative will then also have point with infinite value, $\frac{d^2\psi}{dx^2}|_{x_1-\epsilon} = \infty$. We cannot have this as the kinetic energy operator will result it infinite kinetic energy, which cannot be. Therefore the wave function must be continuous.

Now assuming some wave function has a first derivative that isn't continuous. This is allowed only if the potential is also infinite at that point.