1. 1D Schrödinger Equation
G chapters 3-4.

1.1 the Free Particle
$V \equiv 0$

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2}$$

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

where $\omega = \frac{k^2\hbar}{2m}$.

Normalization must happen:

$$\int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 = 1$$

Here, however:

$$\int_{-\infty}^{\infty} |A|^2 \, dx \to \infty$$

As this integral represents the probability that the particle can be found, this must always be equal to 1 – anything other than this, and it cannot represent a physical model.

1.2 Wave Packets
Wave packets have to be used to avoid this.
A single plane wave cannot describe a quantum particle, but a wave packet can.

$$\psi(x) = \int g(k) e^{ikx} dk$$

→ $g(k)$ is the Fourier transform of $\psi(x)$.

$\Delta x \Delta k \geq 1$
$\Delta x \Delta p \geq \hbar$
(uncertainty principle)

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\psi}(p) e^{\frac{ipx}{\hbar}} dp$$

$$\tilde{\Psi}(p_x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) e^{-\frac{ip_x x}{\hbar}} dx$$

The latter part is where the wave function depends on the momentum, rather than the position or time. This is denoted by the tilde.

$$P(p) = \left|\tilde{\psi}(p)\right|^2 dp$$

This is the probability that the particle has momentum between p and $p + dp$.

1.3 Time independent potentials

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

Separation of variables – let $\Psi(x,t) = T(t)\psi(x)$.

$$i\hbar \frac{1}{T}\frac{dT}{dt} = -\frac{1}{\psi}\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)$$

Let E be the constant here.

$$i\hbar \frac{dT}{dt} = ET \quad (1.3\text{-}1)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad (1.3\text{-}2)$$

The solution to (1.3-1) is:

$$T(t) = Ae^{-\frac{iEt}{\hbar}}$$

For (1.3-2),

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

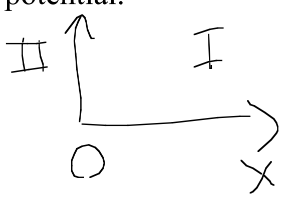
This is the Time Independent Schrödinger Equation. It is an eigenvalue problem involving the Hamilton operator. The complete solution is:

$$\Psi(x,t) = A\psi(x)e^{-\frac{iEt}{\hbar}}\ .$$

Condition $\psi(x)$ must satisfy to correspond to a physically meaningful wave function.

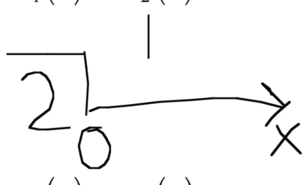
1) $\psi(x)$ must be single-valued.
2) $\int_{-\infty}^{\infty} |\psi(x)|^2$ must be finite.
3) $\psi(x)$ must be continuous everywhere.

   $\frac{d\psi}{dx}$ is continuous everywhere except at an infinite discontinuity of the potential.



infinite wall

$$\psi_1(0) = \psi_2(0)$$

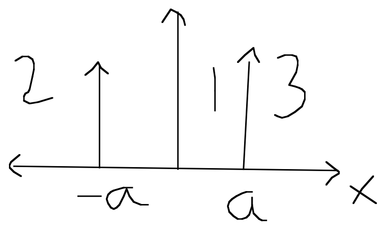


$$\psi_1(0) = \psi_2(0)$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

1.4 Infinite square well

$$V(x) = \begin{cases} 0 & -a \le x \le a \\ \infty & |x|.a \end{cases}$$



$$\psi_2(x) = \psi_3(x) = 0$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + E\psi_1 = 0$$

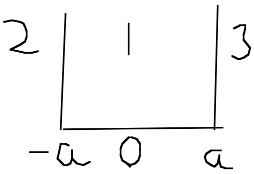
$$\psi_{1(x)} = A_1 e^{k_1 x} + B_1 e^{-k_1 x}$$

$$k_1^{\,2} = -\frac{2m}{\hbar^2}E$$

For $E > 0$, k_1 is purely imaginary.

$$\psi_1(x) = A\cos kx + B\sin kx$$

where $k = \sqrt{\dfrac{2mE}{\hbar^2}}$.



$\psi_1(-a) = 0$, $\psi_1(a) = 0$.

$A\cos ka + B\sin ka = 0 \quad (x = a)$

$A\cos ka - B\sin ka = 0 \quad (x = -a)$

If $\sin ka = 0$, then;

$ka = n\pi$

$n = 0, \pm 1, \pm 2, \ldots$

If $\cos ka = 0$, then:

$ka = \dfrac{n\pi}{2} \quad n = \pm 1, \pm 3, \pm 5, \ldots$

$$\psi(x) = \begin{cases} A\cos\dfrac{n\pi}{2a}x & n = 1,3,5,\ldots \\ B\sin\dfrac{n\pi}{2a}x & n = 2,4,\ldots \end{cases}$$

$$\int_{-\infty}^{\infty} \left|\psi(x)\right|^2 = 1$$

$$\int_{-a}^{a} \left|\psi_1(x)\right|^2 dx = 1$$

$$\int_{-a}^{a} |A|^2 \cos^2\frac{n\pi}{2a}x\,dx = 1$$

$$\int_{-a}^{a} |B|^2 \sin^2\frac{n\pi}{2a}x\,dx = 1$$

$$\int_{-\infty}^{\infty} \cos^2 \frac{n\pi x}{2a} dx = a \to A = \frac{1}{\sqrt{a}}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{8a^2 m}.$$

$$A = B = \frac{1}{\sqrt{a}} \ ?$$

1.5 Probability current

$P(x,t) = |\Psi(x,t)|^2 dx$ probability density.

the probability of finding the particle at time t between x and $x + dx$.
Probability current:

$$j(x,t) = \frac{\hbar}{2mi}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) \quad (1.5\text{-}1)$$

Replacing (1.5-1) into the Schrödinger equation, we obtain:

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0$$

$$\int_a^b \frac{\partial P(x,t)}{\partial t} dx = \frac{\partial}{\partial t}\int_a^b P(x,t)$$

This is the total probability in $[a,b]$.

$$= -\int_a^b \frac{\partial}{\partial x} j(x,t)dx = j(a,t) - j(b,t)$$

Example: at time $t = 0$,

$$\psi(x) = ce^{ikx} = ce^{\frac{ip_x x}{\hbar}}$$

$$j(x) = |c|^2 \frac{p_x}{m}$$

For a particle traveling in the x-axis at velocity v, what is the flux?

$j(x) = v\lambda$ where λ is the density of the particle.

Then a plane wave $ce^{\frac{ip_x t}{\hbar}}$ is equivalent to a beam of particles with density $|c|^2$.

1.6 Finite Well

We want to solve

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

for

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

Let region 1 = $-a < x < a$, region 2 $=< -a$, region 3 $=< a$.

$$\psi_1 = A_1 e^{k_1 x} + B_1 e^{-k_1 x}$$
$$\psi_2 = A_2 e^{k_2 x} + B_2 e^{-k_2 x}$$
$$\psi_3 = A_3 e^{k_3 x} + B_3 e^{-k_3 x}$$

Replacing into the TISE, we obtain:

$$k_2^{\ 2} = k_3^{\ 2} = \frac{2m}{\hbar^2}\left(V_o - E\right)$$
$$k_1^{\ 2} = -\frac{2mE}{\hbar^2}$$

If the energy is positive, then:

$$k_1 = \pm i\sqrt{\frac{2mE}{\hbar^2}} = \pm ik$$

Conditions for $\psi\left(x\right)$:

$$\psi_1\left(a\right) = \psi_3\left(a\right)$$
$$\psi_1\left(-a\right) = \psi_2\left(-a\right)$$

As the jump in the potential is finite, rather than infinite, we must require:

$$\frac{d\psi_1\left(a\right)}{dx} = \frac{d\psi_3\left(a\right)}{dx}$$
$$\frac{d\psi_1\left(-a\right)}{dx} = \frac{d\psi_2\left(-a\right)}{dx}$$

For the bound states $\left(E < V_0\right)$;

$k_3 = k_2 = \sqrt{\frac{2m}{\hbar^2}\left(V_0 - E\right)} = \rho$ (a real, positive number.)

$$\psi_1 = A_1 e^{kx} + B_1 e^{-kx}$$
$$\psi_2 = A_2 e^{\rho x} + B_2 e^{-\rho x}$$
$$\psi_3 = A_3 e^{\rho x} + B_3 e^{-\rho x}$$

B_2 must be zero, otherwise that exponential will diverge. The same for A_3.

$$\psi_1 = A_1 \sin kx + B_1 \cos kx$$
$$\psi_2 = A_2 e^{\rho x}$$
$$\psi_3 = B_3 e^{-\rho x}$$

We obtain non-trivial solutions only for certain values of k and ρ. Through a little algebra:

$$\tan ka = \frac{\sqrt{\frac{2m}{\hbar^2}V_0 - k^2}}{k}$$
$$\tan ka = -\frac{k}{\sqrt{\frac{2mV_0}{\hbar^2} - k^2}}$$

For the unbound state, $E > V_0$.

$$k_2^{\ 2} = k_3^{\ 2} = \frac{2m}{\hbar^2}\begin{pmatrix} V_0 \\ E \end{pmatrix}$$

$$k_2 = k_3 = \pm i\sqrt{\frac{2m}{\hbar^2}\left(V_0 - E\right)} = \pm i\sigma$$

$$k_1 = \pm i\sqrt{\frac{2mE}{\hbar^2}} = \pm ik$$

We are using a stream of particles $e^{i\sigma x}$ of density 1 coming from $-\infty$, going to $+\infty$, and seeing what happens when they arrive at the potential well.

Solutions:

$$\psi_1 = A_1 \cos kx + b_1 \sin kx$$

$$\psi_2 = e^{i\sigma x} + \mathrm{Re}^{-i\sigma x}$$

$$\psi_3 = Te^{i\sigma x}$$

Incident beam of density 1 ($e^{i\sigma x}$), with a reflected beam of density R ($\mathrm{Re}^{-i\sigma x}$). Also, a transmitted beam of density T ($Te^{i\sigma x}$).

The extra term in ψ_2 makes the equation inhomogenous.

Now we have four inhomogeneous equations for R, A_1, B_1 and T_1. We then find solutions for any k, and then for any energy.

We obtain:

$$R = \frac{ie^{-zi\sigma a}\left(k^2 - \sigma^2\right)\sin\left(2ka\right)}{2k\sigma\cos\left(2ka\right) - i\left(k^2 + \sigma^2\right)\sin\left(2ka\right)}$$

$$T = \frac{e^{-2i\sigma a}\, 2k\sigma}{2k\sigma\cos\left(2ka\right) - i\left(k^2 - \sigma^2\right)\sin\left(2ka\right)}$$

$|R|^2$ and $|T|^2$ are proportional to the ratios of reflected and transmitted flux of particles to the incident flux.

When $E >> V_0$, then $\sigma \sim k$, and $R \to 0$.

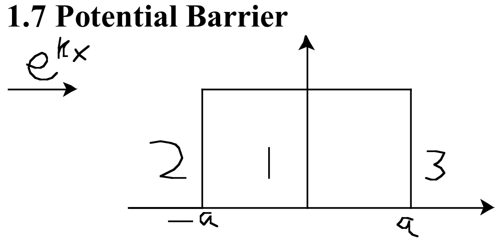
When $E \to V_o$, then $\sigma \to 0$ and $T \to 0$.

If $2ka = n\pi$, then $E = V_0 + \dfrac{n^2\pi^2\hbar^2}{8ma^2}$

$R = 0, T = 1$

This is called transmission resonance.

1.7 Potential Barrier



$E > V_0$

Similar to finite potential well.

$E < V_0$

$\psi_2 = e^{i\sigma z} + \mathrm{R}e^{-i\sigma x}$

$\psi_1 = A_1 e^{k_1 x} + B_1 e^{-k_1 x}$

$\psi_3 = Te^{i\sigma x}$

where $\sigma = \sqrt{\dfrac{2mE}{\hbar^2}}$

$$k_1^{\ 2} = \frac{2m}{\hbar^2}\left(V_0 - E\right)$$

$$k_1 = \sqrt{\frac{2m}{\hbar^2}\left(K - E\right)} = k$$

$$R = \frac{ie^{-2i\sigma a}\left(k^2 + \sigma^2\right)\sinh\left(2ka\right)}{2k\sigma\cosh\left(2ka\right) - i\left(k^2 - \sigma^2\right)\sinh\left(2ka\right)}$$

$$T = \frac{e^{-2ia}2k\sigma}{2k\sigma\cosh\left(2ka\right) - i\left(k^2 - \sigma^2\right)\sinh\left(2ka\right)}$$

$$\left|T\right|^2 = \frac{\left(2\sigma k\right)^2}{\left(\sigma^2 + k^2\right)\sinh^2\left(2ka\right) + \left(2\sigma k\right)^2}$$

(DNLT)

So, as $V_0 \to \infty$,

$k \to \infty$ → $\sinh 2ka \to \infty$. Therefore, $T \to 0$.

$a \to \infty$ → $\sinh 2ka \to \infty$. Therefore $T \to 0$.

For $2ka >> 1$, $\left|T\right|^2 \approx \dfrac{16\sigma^2 k^2}{\left(\sigma^2 + k^2\right)} e^{-4ka}$.

Example, $V_0 = 2eV$, $2a = 1$ Angstrom.

(i) Electron $\dfrac{1}{k} \approx \dfrac{1.96}{\sqrt{V_0 - E}} A$. $\left|T\right|^2 \approx 0.78$

(ii) Proton $\dfrac{1}{k} \approx \dfrac{1.96A}{\sqrt{1890\left(V_0 - E\right)}}$, $\left|T\right|^2 \approx 4 \times 10^{-19}$.

… much more likely to find an electron.