1. The Wave Function

1.1 The Schrödinger Equation

$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t)$,
$\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^3}{\partial z^3}$
Solve for the particle's wave function $\Psi(x,t)$
$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34}$ Js

1.2 The Statistical Interpretation

$\int_a^b |\Psi(x,t)|^2 dx = \{\text{P of finding the particle btwn } a \text{ and } b, \text{ at } t\}$

1.3 Probability

Standard deviation: $\sigma = \sqrt{\langle j^2\rangle - \langle j\rangle^2}$
Expectation value of x given Ψ: $\langle x\rangle = \int x|\Psi|^2 dx$
Probability current: $J(x,t) = \frac{i\hbar}{2m}(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x})$

1.4 Normalization

$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$
The Schrödinger equation produces unitary time evolution:
$\vec{J} = -\frac{i\hbar}{2m}(\psi(\vec(r),t)^*\vec{\nabla}\psi(\vec{r},t) - \psi(\vec{r},t)\vec{\nabla}\psi(\vec{r},t)^*)$
The probability density satisfies the continuity equation,
$\frac{\partial}{\partial t}\mathcal{P} + \vec{\nabla}\cdot J = 0$
Because the probability for finding the particle at infinity is 0 (otherwise non-normalizable), $\vec{J} = 0$ at infinity.
Therefore, $\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\mathcal{P}d^3\vec{r} = \frac{\mathrm{d}}{\mathrm{d}t}P = 0$, where P is the total probability $\rightarrow$ the total probability is constant in time.

1.5 Momentum

For a particle in state Ψ, the expectation value of x and p is

$$\langle x\rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 dx \qquad \langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int(\Psi^*\frac{\partial\Psi}{\partial x})dx$$

To calculate the expectation value of any quantity, $Q(x,p)$:

$$\langle Q(x,p)\rangle = \int \Psi^* Q(x, \frac{\hbar}{i}, \frac{\partial}{\partial x})\Psi dx$$

Position and momentum operators: $\widehat{\vec{r}} = \vec{r}$, $\widehat{\vec{p}} = -i\hbar\vec{\nabla}$

1.6: The Uncertainty Principle

The wavelength of Ψ is related to the momentum of the particle by the de Broglie formula: $p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$
Heisenberg's uncertainty principle: $\sigma_x\sigma_p \geq \frac{\hbar}{2}$
Commutation relation btwn position and momentum:

$$\widehat{p}_x(\widehat{x}\psi(x,t)) = -i\hbar\frac{\partial}{\partial x}[x\psi(x,t)] = -i\hbar\psi(x,t) - i\hbar x\frac{\partial}{\partial x}\psi(x,t)$$

$$\widehat{x}(\widehat{p}_x\psi(x,t)) = x(-i\hbar\frac{\partial}{\partial x}\psi(x,t))$$

$\widehat{x}\widehat{p}_x - \widehat{p}_x\widehat{x} = [\widehat{x},\widehat{p}_x] = i\hbar$
$[\widehat{x}_i,\widehat{p}_j] = i\hbar\delta_{ij}, [\widehat{x}_i,\widehat{x}_j] = [\widehat{p}_i,\widehat{p}_j] = 0$,
where $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$
Given three operators $\widehat{A},\widehat{B},\widehat{C}$, we have $[\widehat{A},\widehat{B}\widehat{C}] = [\widehat{A},\widehat{B}]\widehat{C} + \widehat{B}[\widehat{A},\widehat{C}]$.

2. Time-Independent Schrödinger Equation

2.1 Stationary States

Suppose PE is independent of time, $V(\vec{r},t) = V(\vec{r})$.
Separation of variables: $\Psi(\vec{r},t) = \psi(\vec{r})\varphi(t)$
Eq of motion for $\varphi(t)$: $\varphi(t) = e^{-iEt/\hbar}$
Eq of motion for $\psi(\vec{r})$ is the time-independent Schrödinger equation:

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

TD of the wavefunction that corresponds to the constant E is easily written once we solve the TISE: $\Psi_E(\vec{r},t) = \psi_E(\vec{r})e^{-iEt/\hbar}$

Properties of solutions for TI potentials:

- **The constant E must be real.**
- **Stationary wavefunction.**
  $\mathcal{P}(\vec{r},t) = |\psi_E(\vec{r},t)|^2 = |\psi_E(\vec{r})|^2$ (TD cancels out).
- **Stationary wavefunction is a state of definite energy.**
  The total energy (kinetic plus potential) is the Hamiltonian:
  $H(x,p) = \frac{p^2}{2m} + V(x)$.
  Hamiltonian operator: $\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
  Thus the TISE can be written as $\widehat{H}\psi = E\psi$
  $\langle\widehat{H}\rangle = E$, $\langle\widehat{H}^2\rangle = E^2$, $\Delta E = \sqrt{\langle\widehat{H}^2\rangle - \langle\widehat{H}\rangle^2} = 0$
- **Spatial part of stationary wavefunction can be chosen to be real.**
  $\psi^*(\vec{r})$ is a soln w/ same E
  Solns can be chosen to be real: $\psi(\vec{r}) + \psi^*(\vec{r})$ and $\frac{\psi(\vec{r})-\psi^*(\vec{r})}{i}$.
- **Parity symmetry: even and odd wavefunctions.** Suppose $V(-\vec{r}) = V(\vec{r})$. Then, $\psi_E(-\vec{r})$ is a soln w the same energy. $\psi_E(\vec{r}) + \psi_E(-\vec{r})$ is even under reflection, $\psi_E(\vec{r}) - \psi_E(-\vec{r})$ is odd. When the potential is symmetric under reflection, we can choose the stationary states to be either even or odd under reflection.
- **Orthogonality/orthonormality.**
  $\int\psi_m(\vec{r})^*\psi_n(\vec{r})d^3\vec{r} = \delta_{mn}$ where δ_{mn} is 0 if $m \neq n$ and 1 if $m = n$.
- **Linearity.**
  The SE is linear. Given stationary states, a linear combo of these
  $$\psi(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{i}{\hbar}E_n t}$$
  where c_n are complex constants, is a solution to the TDSE
  $$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \widehat{H}\psi(\vec{r},t)$$
- **Time evolution.** Given
  $$\psi(\vec{r},0) = \sum_n c_n\psi_n(\vec{r},0) = \sum_n c_n\psi_n(\vec{r})$$
  at time t, the time evolution is
  $$\psi(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{i}{\hbar}E_n t}$$
  Once we've expanded a given initial wavefunction in terms of a linear combo of the stationary wavefunctions $\psi_n(\vec{r})$, the time evolution follows simply by putting a factor of $e^{-i/\hbar E_n t}$ to each term containing $\psi_n(\vec{r})$.
- **Normalization.**
  The constant coefficients are constrained by $\sum_n |c_n|^2 = 1$
- **Completeness.**
  The stationary states form a complete set if
  $$\sum_n \psi_n(\vec{r'},t)^*\psi_n(\vec{r},t) = \delta^3(\vec{r'} - \vec{r})$$
  where $\delta^3(\vec{r'} - \vec{r})$ is the Dirac-delta function in 3D defined by
  $$\int d^3\vec{r'}\psi(\vec{r'},t)\delta^3(\vec{r'} - \vec{r}) = \psi(\vec{r},t)$$

Euler's formula: $e^{i\theta} = \cos\theta + i\sin\theta$
sin and cos: $\cos(\theta) = \frac{1}{2}(e^{i\theta} + e^{-i\theta})$, $\sin(\theta) = \frac{1}{2}(e^{i\theta} - e^{-i\theta})$

One-dimensional systems

Wavefunction for a system containing a single particle of mass m in 1D with TI potentials.

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

Once we find the wavefunction $\psi_E(x)$ of energy E, time dependence:

$$\psi_E(x,t) = \psi_E(x)e^{-\frac{i}{\hbar}Et}$$

Boundary conditions
1. When the potential $V(x)$ has a finite jump at $x = a$, both $\psi(x)$ and $\psi'(x)$ are continuous across $x = a$.
2. When the potential $V(x)$ has an infinite jump at $x = a$, $\psi(x)$ is continuous but $\psi'(x)$ is discontinuous across $x = a$.
Wavefunction must vanish at $x = \pm\infty$ to be normalizable.

2.2 The Infinite Square Well

$V(x) = \{0 \text{ if } 0 \leq x \leq a; \quad \infty \text{ otherwise}\}$
$\psi(x) = 0$ for $x < 0$ and $x > a$ For $0 \leq x \leq a$, $V(x) = 0$ and the Schrödinger equation reduces to

$$\psi''(x) + k^2\psi(x) = 0, \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } E > 0$$

Classic **simple harmonic oscillator**: $\psi(x) = A\sin(kx) + B\cos(kx)$
Boundary conditions:
Continuity of $\psi(x)$ at $x = 0$ sets $\psi(0) = B = 0 \rightarrow \psi(x) = A\sin(kx)$ at $x = a$ sets $\psi(a) = A\sin(ka) = 0$

$$k_n = \frac{n\pi}{a}, n = 1,.. \quad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\Big(\frac{n\pi}{a}x\Big) \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

They are complete, in the sense that any other function, $f(x)$, can be expressed as a linear combination of them (Fourier series), Dirichlet's theorem:

$$f(x) = \sum_{n=1}^{\infty} c_n\psi_n(x) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} c_n\sin\Big(\frac{n\pi}{a}x\Big)$$

Fourier's trick: $c_n = \int\psi_n(x)^* f(x)dx$

$$c_m = \frac{2}{a}\int_0^a f(x)\sin\Big(\frac{m\pi x}{a}\Big)dx$$

$|c_n|^2$ tells you the probability that a measurement of the energy would yield the value E_n.
Sum of these probabilities should be 1: $\sum_{n=1}^{\infty}|c_n|^2 = 1$
The expectation value of the energy is $\langle H\rangle = \sum_{n=1}^{\infty}|c_n|^2 E_n$

2.3 The Harmonic Oscillator

Hooke's law (mass m w/ spring constant k): $F = -kx = m\frac{d^2x}{dt^2}$
Solution is $x(t) = A\sin(\omega t) + B\cos(\omega t)$, where $\omega = \sqrt{\frac{k}{m}}$
Potential energy: $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$
Expanding $V(x)$ in a **Taylor series** about the min:
$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots$
Simple harmonic oscillaton, $V(x) \cong \frac{1}{2}V''(x_0)(x - x_0)^2, k = V''(x_0)$
The Schrödiner Equation for the harmonic oscillator:

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

Boundary conditions: $\psi(-\infty) = 0, \qquad \psi(+\infty) = 0$

1. Simplify notation with change of variables
Introduce $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$. SE becomes $\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} = (\xi^2 - K)\psi$, where $K \equiv \frac{2E}{\hbar\omega}$.
2. Asymptotic behavior
Working in the large $\xi^2 >> K$ region,
Hermite eqn: $H''(\xi) - 2\xi H'(\xi) + (K-1)H(\xi) = 0$
Hermite polynomials: $H_0 = 1$, $H_1 = 2\xi$, $H_2 = 4\xi^2 - 2$, $H_3 = 8\xi^3 - 12\xi$, $H_4 = 16\xi^4 - 48\xi^2 + 12$, $H_5 = 32\xi^5 - 160\xi^3 + 120\xi$
3. Method of power series
The recursion formula: $a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j$
Recursion formula for allowed K: $a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j$
$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j\xi^j$
$h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi)$
4. Infinite series produces a diverging function

For large n, we have $a_{n+2} \approx \frac{2}{n} a_n$

5. Truncate series

$K = 2n+1$, so $E_n = (n+\frac{1}{2})\hbar\omega$

Normalized stationary states: $\psi_n(x) = (\frac{m\omega}{\pi\hbar})^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$

Rodrigues formula: $H_n(\xi) = (-1)^n e^{\xi^2} (\frac{\mathrm{d}}{\mathrm{d}\xi})^n e^{-\xi^2}$

2.4 The Free Particle

$E > V(x)$ for all x, $V(x) = 0, -\infty < x < \infty$

We have $x(t) = v_{cl} t$, where v_{cl} is the classical velocity of the particle.

$\psi''(x) + k^2\psi(x) = 0, k \equiv \sqrt{\frac{2mE}{\hbar^2}}$

$\Psi(x,t) = Ae^{ikx - i\frac{\hbar k^2}{2m}t} + Be^{-ikx - i\frac{\hbar k^2}{2m}t} = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} = Ae^{ik(x-v_p t)} + Be^{-ik(x+v_p t)}$, where $\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}$ is the angular vel, $v_p = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{p}{2m} = \frac{1}{2} v_{cl}$ is the phase velocity.

Not normalizable. General sol to the TISE: wave packet,

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

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

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

$F(k)$ is the Fourier transform of $f(x)$; $f(x)$ is the inverse Fourier transform of $F(k)$

2.5 The Delta-Function Potential

Dirac delta function, area is 1:

$$\delta(x) = \{0, \text{ if } x \neq 0; \quad \infty, \text{ if } x = 0\}$$

$f(x)\delta(x-a) = f(a)\delta(x-a)$ bc the product is 0 anyway except at a.

In particular, $\int_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a)$

Consider $V(x) = -\alpha\delta(x)$, where α is some positive constant.

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

Bound states ($E < 0$):

REGION I, $x < 0, V(x) = 0$

$\frac{\mathrm{d}^2\psi_I}{\mathrm{d}x^2} - \kappa^2\psi_I = 0$, where $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$.

General sol: $\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$ But $A = 0$, so $\psi(x) = Be^{-\kappa x}, (x < 0)$.

REGION II, $x > 0, V(x) = 0$ $\psi(x) = Fe^{-\kappa x} + Ge^{\kappa x}$

But $G = 0$, so $\psi(x) = Fe^{-\kappa x}, (x > 0)$.

The first boundary condition tells us that $F = B$, so $\psi(x) = \{Be^{\kappa x}, (x \le 0), \quad Be^{-\kappa x}, (x \ge 0)\}$

The discontinuity of $\psi'(x)$ across $x = 0$ follows from

$$\psi'_{II}(0) - \psi'_I(0) = \lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\psi''(x)dx = \lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\frac{2m}{\hbar^2}(V(x)-E)\psi(x)dx$$

$$= -\frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon}\alpha\delta(x)\psi(x)dx = \frac{2m}{\hbar^2}\alpha\psi(0) = -\frac{2m}{\hbar^2}\alpha F$$

On the other hand, taking the derivatives directly, $\psi'_{II}(0) - \psi'_I(0) = -\kappa F - \kappa B$. Therefore,

$$\kappa F + \kappa B = \frac{2m}{\hbar^2}\alpha F \to \kappa = \frac{m\alpha}{\hbar^2} \to E = -\frac{m\alpha^2}{2\hbar^2}$$

Only one E, so only one bound state.

Normalizing:

$1 = \int_{-\infty}^{0} B^2 e^{2\kappa x} + \int_0^{\infty} B^2 e^{-2\kappa x} = B^2\frac{1}{2\kappa} + B^2\frac{1}{2\kappa} = \frac{B^2}{\kappa}$, which gives $B = \sqrt{\kappa}$.

The normalized wavefunction is:

$$\psi(x) = \begin{cases}\sqrt{\kappa}e^{-\kappa x} = \sqrt{\frac{m\alpha}{\hbar^2}}e^{-\frac{m\alpha}{\hbar^2}}x, & x > 0\\ \sqrt{\kappa}e^{\kappa x} = \sqrt{\frac{m\alpha}{\hbar^2}}e^{\frac{m\alpha}{\hbar^2}}x, & x < 0\end{cases}$$

Scattering states ($E > 0$) – reflection and transmission:

For $x < 0$ the SE reads

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

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

For $x > 0$, $\psi(x) = Fe^{ikx} + Ge^{-ikx}$

Continuity of $\psi(x)$ at $x = 0$: $F + G = A + B$

Reflection coefficient: $R \equiv \frac{|B|^2}{|A|^2}$, Transmission coefficient: $T \equiv \frac{|F|^2}{|A|^2}$

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

Higher $E \to$ greater probability of transmission.

Step potential

Particle of energy $E > V_0$ approaching a step potential from the left in the $x < 0$ region with $V(x) = \{0, x < 0; \quad V_0, x > 0\}$.

Incident and reflected waves in region I, only transmitted wave in region II: $\psi_I(x) = Ae^{ikx} + Be^{-ikx}, \quad \psi_{II}(x) = Ce^{i\kappa x}$

where $k = \sqrt{\frac{2mE}{\hbar^2}}, \kappa = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$\psi(x)$ and $\psi'(x)$ across $x = 0$: $A + B = C$, $ik(A - B) = i\kappa C$

Solving for B and C in terms of A, $B = \frac{k-\kappa}{k+\kappa}A, \quad C = \frac{2k}{k+\kappa}A$

Speed of particle is diff in two regions, use probability current.

$J_{inc} = \frac{\hbar k}{m}|A|^2, \quad J_{ref} = \frac{\hbar k}{m}|B|^2, \quad J_{tra} = \frac{\hbar\kappa}{m}|C|^2$

$R = \frac{J_{ref}}{J_{inc}} = |\frac{B}{A}|^2 = (\frac{k-\kappa}{k-\kappa})^2 = (\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}})^2$

$T = \frac{J_{tra}}{J_{inc}} = \frac{\kappa}{k}|\frac{C}{A}|^2 = \frac{4k\kappa}{(k+\kappa)^2} = \frac{4\sqrt{E}\sqrt{E-V_0}}{(\sqrt{E}+\sqrt{E-V_0})^2}$

$R + T = 1$

Tunneling

Consider a particle mass m and energy $E < V_0$ approaching from the left a potential barrier of height V_0:

$$V(x) = \{V_0, -a < x < a; \quad 0, |x| > a\}$$

$\psi_I(x) = Ae^{ikx} + Be^{-ikx}, \psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}, \psi_{III}(x) = Fe^{ikx}$

where $k = \frac{2mE}{\hbar^2}, \kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

Applying continuity of $\psi(x)$ and $\psi'(x)$ at $x = \pm a$:

$B = \frac{e^{-2iak}(e^{4a\kappa}-1)(k^2+\kappa^2)}{e^{4a\kappa}(k+i\kappa)^2-(k-i\kappa)^2}A, C = ...A, D = ...A, F = ...A$

Bc the speeds of particles in I and II are same,

$T = |\frac{F}{A}|^2 = \frac{(2k\kappa)^2}{(k^2+\kappa^2)^2\sinh^2(2\kappa a)+(2k\kappa)^2}$

$T \approx e^{-2\gamma}$, where $\gamma = \int_a^b \sqrt{\frac{2m(V(x)-E)}{\hbar^2}}dx$

Lifetime of a particle of mass m and energy E:

Particle has velocity $v = \sqrt{\frac{2E}{m}}$ and bounced back and forth in the wall. When it hits the right wall, it has probability $T = e^{-2\gamma}$ for tunneling, where $\gamma = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}(b-a)$ ($b - a$ is width of well). It needs a number N of bounces on the right wall st $NT \sim 1$ for it to tunnel. Therefore, $N \sim \frac{1}{T} = e^{2\gamma}$. The time interval btwn bounces off the right wall is $t = \frac{2a}{v}$ (a is length to the left). Lifetime is

$$\tau \sim Nt = \frac{2a}{\sqrt{\frac{2E}{m}}}e^{2\sqrt{\frac{2m(V_0-E)}{\hbar^2}}(b-a)}.$$

2.6 The Finite Square Well

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

Bound states:

REGION I

$$-\frac{\hbar}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi, \text{ or } \psi_I''(x) - \kappa^2\psi_I(x) = 0, \qquad \kappa \equiv \sqrt{-\frac{2mE}{\hbar}}$$

where $E < 0$ for a bound state.

General sol: $\psi_I(x) = Ae^{-\kappa x} + Be^{\kappa x}$.

$x = -\infty \to \psi(x) = 0$, so $A = 0$, and we have $\psi_I(x) = Be^{\kappa x}$

REGION II

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - V_0\psi = E\psi, \text{ or } \psi'' = -l^2\psi, \qquad l \equiv \sqrt{\frac{2m(E+V_0)}{\hbar}}$$

General sol: $\psi(x) = C\sin(lx) + D\cos(lx)$, for $-a < x < a$

REGION III

$x = \infty \to \psi(x) = 0$, so $G = 0$ and $\psi_{III}(x) = Fe^{-\kappa x}$

Even bound states

$\psi(-x) = \psi(x)$, $\psi_{II}(x) = D\cos(lx)$

Bc the potential has only a finite discontinuity at $x = \pm a$, both ψ and ψ' must be continuous at $x = \pm a$.

$x = a$, $\psi_{II}(a) = \psi_{III}(a)$ imposes $D\cos(la) = Fe^{-\kappa a}$

$x = a$, $\psi'_{II}(a) = \psi'_{III}(a)'$ imposes $-lD\sin(la) = -\kappa Fe^{-\kappa a}$

Continuity of $\psi(x)$ and $\psi'(x)$ at $x = -a$ does not add anything new.

Dividing the above two, we get $\kappa = l\tan(la)$

This is a formula for the allowed energies, since κ and l are both functions of E. Let $z \equiv la$, and $z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}$. $\kappa^2 + l^2 = 2mV_0/\hbar^2$, so $\kappa a = \sqrt{z_0{}^2 - z^2}$.

Transcendental eq for z (and hence E) as a function of z_0 (which is a measure of size of well): $\tan z = \sqrt{(\frac{z_0}{z})^2 - 1}$

Odd bound states

$\psi_{II}(x) = C\sin(lx)$

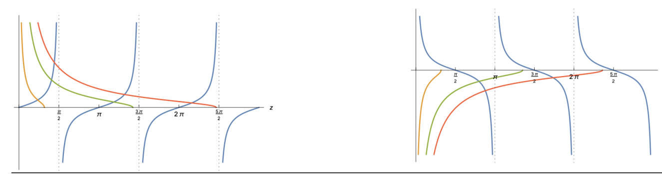
$x = -a, \psi_{II}(-a) = \psi_I(-a)$ imposes $C\sin(la) = Be^{-\kappa a}$

$x = -a, \psi'_{II}(-a) = \psi'_I(-a)$ imposes $lC\cos(la) = -\kappa Be^{-\kappa a}$

Dividing the above two, $l\cot(la) = -\kappa$.

Rewriting this in terms of z and z_0, $\cot(z) = -\sqrt{(\frac{z_0}{z})^2 - 1}$

V_1 does not support an odd bound state, since there is no intersection pt, V_2 produces only one bound state, and V_3 produces two bound states. Finite well potential supports at least one even state, the ground state, and it may not support any of the excited states.



Wide and deep well

$z_n \approx \frac{n\pi}{2}, n = 1, 2, 3, ..., \qquad E_n = -V_0 + \frac{\hbar^2\pi^2 n^2}{2m(2a)^2}, n = 1, 2, ...$

Thus, the energy levels of the infinite square well of width $2a$ are reproduced for $E_n - (-V_0) = E_n + V_0$, which is the energy above the bottom of the well. As $V_0 \to \infty$, finite sq well goes to infinite sq well.

Shallow and narrow well

Need at least $z_0 = \sqrt{\frac{2mV_0 a^2}{\hbar^2}} \ge \frac{\pi}{2}$ to support any odd state.