1. The Wave Function

1.1 The Schrödinger Equation

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

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

where $\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^3}{\partial z^3}$

Solve for the particle's wave function $\Psi(x,t)$

$\hbar = \frac{h}{2\pi} = 1.054572\times10^{-34}$ 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 Φ, 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:

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

The more precisely determined a particle's position is, the less precisely is its momentum. The 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 $[\widehat{A},\widehat{B}\widehat{C}] = [\widehat{A},\widehat{B}]\widehat{C} + \widehat{B}[\widehat{A},\widehat{C}]$.

Other: Blackbody Spectrum

$E = hv = \hbar\omega$

The wave number k is $k = 2\pi/\lambda = \omega/c$

Only two spin states occur (quantum number m is +1 or -1).

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

Wien displacement law: $\lambda_{\text{max}} = \frac{2.90\times10^{-3}\text{mK}}{T}$

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
  $$\psi(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{i}{\hbar}E_nt}$$
  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
  $$\psi(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{i}{\hbar}E_nt}$$
  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 $e^{-i/\hbar E_nt}$ 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: $\cos(\theta) = \frac{1}{2}(e^{i\theta} + e^{-i\theta})$, $\sin(\theta) = \frac{1}{2}(e^{i\theta} - e^{-i\theta})$

Delta function: Given $f(x)$, $\delta(x - x')$ is defined as

$f(x') = \int f(x)\delta(x - x')dx$

$\int\delta(x - x')dx = 1$, note this is not the area

$\delta_\alpha(x) = \frac{1}{\alpha\sqrt{\pi}}e^{-\frac{x^2}{\alpha^2}}$, $\delta_\alpha(x) = \frac{1}{\pi x}\sin(\frac{x}{a})$, $\delta_\alpha(x) = \frac{\alpha}{\pi x^2}\sin^2(\frac{x}{\alpha})$

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, its time dependence follows easily:

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

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 $x = a$.

Futhermore, the wavefunction must vanish at $x = \pm\infty$ for a normalizable wavefunction.

2.2 The Infinite Square Well

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

$$\psi(x) = 0 \text{ for } x < 0 \text{ and } x > a$$

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 $\psi(a) = A\sin(ka) = 0$

Therefore,

$$k_n = \frac{n\pi}{a}, n = 1, 2, ...$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \qquad E_n = \frac{\hbar^2k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

ψ_1 is the ground state, others are excited states.

Properties of $\psi_n(x)$:

1. Alternatively even and odd.
2. As you go up in energy, each successive state has one more node.
3. They are mutually orthogonal, in the sense that $\int\psi_m(x) * \psi_n(x)dx = 0$ whenever $m \neq n$. $\int\psi_m(x) * \psi_n(x)dx = \delta_{mn}$ where δ_{mn} (Kronecker delta) is 0 if $m \neq n$ and 1 if $m = n$. We say that the ϕ's are orthonormal.
4. 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:

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

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

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

$|c_n|^2$ 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

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

Conservation of energy in QM

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

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{j=0}^{\infty} a_j\xi^j$$

The complete solution is $h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi)$

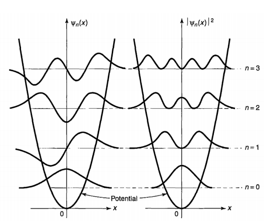
4. Infinite series produces a diverging function

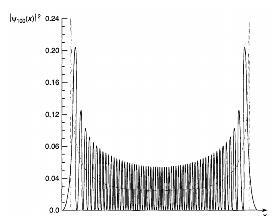
For large n, we have $a_{n+2} \approx \frac{2}{n}a_n$

5. Truncate series

$K = 2n + 1$, so $E_n = (n + \frac{1}{2})\hbar\omega$
The 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: $H_n(\xi) = (-1)^n e^{\xi^2}(\frac{\mathrm{d}}{\mathrm{d}\xi})^n e^{-\xi^2}$
These wavefunctions form a complete orthonormal set for square-integrable wavefunctions of the harmonic oscillator.





2.4 The Free Particle

$$\frac{\partial^2\xi}{\partial x^2} = -k^2\xi, k = \frac{\sqrt{2mE}}{\hbar}$$

General solution to the TISE: wave packet,
$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}\infty\psi(k)e^{i(kx - \frac{\hbar k^2}{2m}t)}dk$

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

Plancherel's theorem:

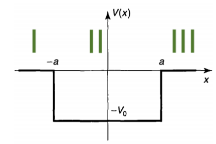
$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}F(k)e^{ikx}dk \leftrightarrow F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-kx}dx$$

$F(k)$ is the Fourier transform of $f(x)$; $f(x)$ is the inverse Fourier transform of $F(k)$
Phase velocity: speed of individual ripples; group velocity: speed of the envelope
Dispersion relation: the formula for ω as a function of k

2.5 The Delta-Function Potential

2.6 The Finite Square Well

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



where V_0 is a positive constant.
Both bound states ($E < 0$) and scattering states ($E > 0$).
Bound states:
Potential is piecewise and discontinuous, can split into regions.

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

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

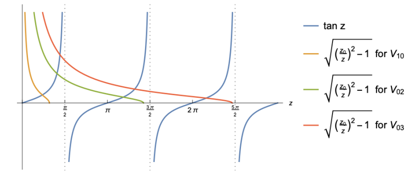
General sol: $\psi(x) = C\sin(lx) + D\cos(lx)$, for $-a < x < a$

REGION III

SE and general sol same as region I, but $x = \infty \to \psi(x) = 0$, 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): $\tan z = \sqrt{(\frac{z_0}{z})^2 - 1}$

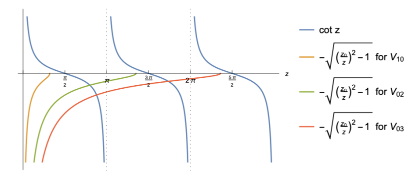


Odd bound states

$\psi_{II}(x) = C\sin(lx)$
$x = -a, \psi_{II}(-a) = \psi_I(-a)$ 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,

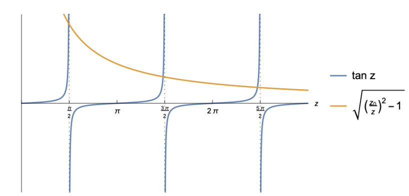
$$\cot(z) = -\sqrt{(\frac{z_0}{z})^2 - 1}$$

Potential V_{01} does not support an odd bound state, since there is no intersection pt, V_{02} produces only one bound state, and V_{03} 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

$z_n \approx \frac{n\pi}{2}, n = 1, 2, 3, \ldots$. Using the def of z and solving for E,
$E_n = -V_0 + \frac{\hbar^2\pi^2n^2}{2m(2a)^2}, n = 1, 2, 3, \ldots$
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

Any shallow or narrow well supports at least one bound state. But we need at least $z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}} \geq \frac{\pi}{2}$ to support any odd state.

Gaussian integrals

$$\int_{-\infty}^{\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}} \text{ and } \int_0^{\infty} e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{\infty} x^{2n+1}e^{-ax^2}dx = 0 \text{ for } n = 0, 1, 2, \ldots$$

$$\int_{-\infty}^{\infty} x^{2n}e^{-ax^2}dx = (-1)^n\frac{\mathrm{d}^n}{\mathrm{d}a^n}\sqrt{\frac{\pi}{a}} \text{ for } n = 0, 1, 2, \ldots$$

$$\int_{-\infty}^{\infty} e^{-ax^2+bx}dx = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}} \qquad \int_{-\infty}^{\infty} x^n e^{-ax^2+bx}dx = \frac{\mathrm{d}^n}{\mathrm{d}b^n}\sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}}$$