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 $\Psi(x,t)$

$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34}$ 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 Φ, the expectation value of x is

$$\langle x\rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 dx$$

Momentum:

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int(\Psi^*\frac{\partial\Psi}{\partial x})dx$$

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: $\Psi_E(\vec{r},t) = \psi_E(\vec{r})e^{-iEt/\hbar}$

Why separable solutions?

1. Stationary states - time-dependence cancels out

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

Same thing happens in calculating the expectation value of any dynamical variable. Every expectation value is constant in time.

2. There are states of definite total 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 $\widehat{H}\psi = E\psi$

Variance of H: $\sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2 = E^2 - E^2 = 0$

A separable solution has the property that every measurement of the total energy is certain to return the value E.

3. The general solution is a linear combination of separable solutions. There is a different wave function for each allowed energy:

$\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar}, \Psi_2(x,t) = \psi_2(x)e^{-iE_2t\hbar}, \ldots$

Now the time dependent Schrödinger equation has the property that any linear combo of solutions is itself a solution.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar} = \sum_{n=1}^{\infty} c_n\Psi_n(x,t)$$

Euler's formula: $e^{i\theta} = \cos\theta + i\sin\theta$

2.2 The Infinite Square Well

Suppose

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

Classic simple harmonic oscillator, $\psi(x) = A\sin(kx) + B\cos(kx)$

Boundary conditions

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

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

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:

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

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

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

Conservation of energy in QM

2.3 The Harmonic Oscillator

Hooke's law: $F = -kx = m\frac{d^2x}{dt^2}$

Solution is $x(t) = A\sin(\omega t) + B\cos(\omega t)$, where $\omega = \sqrt{\frac{k}{m}}$,

$V(x) = \frac{1}{2}kx^2$.

Taylor series:

$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots$

The Schrödiner Equation for the harmonic oscillator:

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

Introduce $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$, so we have $\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} = (\xi^2 - K)\psi$, where $K \equiv \frac{2E}{\hbar\omega}$.

The recursion formula: $a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j$

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

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

Recursion formula for allowed K: $a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j$

Hermite polynomials: $H_0 = 1$, $H_1 = 2\xi$, $H_2 = 4\xi^2 - 2$,

$H_3 = 8\xi^3 - 12\xi$, $H_4 = 16\xi^4 - 48\xi^2 + 12$, $H_5 = 32\xi^5 - 160\xi^3 + 120\xi$

The normalized stationary states:

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

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

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; grouop 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