1. The Wave Function

1.1 The Schrödinger Equation

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

 $\begin{array}{c} \overline{i\hbar\frac{\partial\Psi}{\partial t}=-\frac{h^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi} \\ \text{Solve for the particle's wave function } \Psi(x,t) \end{array}$

$$\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34} \text{ Js}$$

1.2 The Statistical Interpretation

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

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

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):

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

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:

$$\sigma_x \sigma_p \ge \frac{\hbar}{2}$$

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).

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

Wien displacement law: $\lambda_{max} = \frac{2.90 \times 10^{-3} \text{ mK}}{7}$

2. Time-Independent Schrödinger Equation

2.1 Stationary States

Separation of variables: $\Psi(x,t) = \psi(x)\varphi(t)$

 $\varphi(t) = e^{-iEt/\hbar}$, separable solutions: $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

Time-independent Schrödinger equation:

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

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 $\widehat{\widehat{H}}\psi=E\psi$ Variance of $H\colon \sigma_H^2=\langle H^2\rangle-\langle H\rangle^2=E^2-E^2=0$

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:

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

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

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

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

2.2 The Infinite Square Well Suppose

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

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

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

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

 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: $F = -kx = m \frac{d^2x}{dx^2}$

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

$$\equiv \frac{2E}{\hbar\omega}$$
.

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

The complete solution is $h(\xi)=h_{\rm even}(\xi)+h_{\rm odd}(\xi)$ K=2n+1, so $E_n=(n+\frac{1}{2})\hbar\omega$

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

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:

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

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

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

General solution to the TISE: wave packet,

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

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

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

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

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