

Quantum Mechanics

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Schrödinger Equation

$$H\psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\mathbf{r}) \right] \psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t)$$

Where H is a hamiltonian operator. If H is time independent separation of variables gives:

$$\begin{aligned} \psi(\mathbf{r}, t) &= \Phi(\mathbf{r}) \cdot e^{-\frac{i}{\hbar}Et} \\ \left[-\frac{\hbar^2}{2m}\Delta + \mathcal{U}(\mathbf{r}) \right] \Phi(\mathbf{r}) &= E\Phi(\mathbf{r}) \end{aligned}$$

The general time dependent solution is:

$$\psi(\mathbf{r}, t) = \sum_n a_n \cdot \Phi(\mathbf{r}) e^{-\frac{i}{\hbar}Et}$$

Where a_n are found through the boundary conditions ($t = 0$):

$$a_n = \int \Phi_n^*(\mathbf{r}) \cdot \psi(\mathbf{r}, t=0) d^3r$$

Operators

Linear Operator

$$F(a\Phi_1 + b\Phi_2) = a \cdot F\Phi_1 + b \cdot F\Phi_2 \quad \forall \Phi_1, \Phi_2$$

Eigenvalue, Eigenfunction

$$Fu_n = f_n u_n$$

u_n is a eigen function to the operator F with corresponding eigenvalue f_n .

Hermitian Operator

$$\int (Hu) \cdot v d^3r = \int u \cdot Hv d^3r, \quad \forall u, v$$

A hermitian operator has real eigenvalues and corresponding eigenfunctions can be chosen to be orthonormal. Practically all operators in quantum mechanics are linear and hermitian.

Eigenfunction Expansion

$$\psi(\mathbf{r}) = \sum_n a_n \Phi_n(\mathbf{r}), \quad a_n = \int \Phi_n^* \cdot \psi \cdot d^3r$$

Expansion Postulate

At a measurement of an observable F on a system described by a wavefunction ψ only eigenvalues of the operator F can be found. The probability of the result $F = f_n$ is given by

$$P(F = f_n) = \left| \int \Phi_n^* \cdot \psi d^3r \right|^2, \quad Fu_n = f_n u_n$$

Momentum Operators

$$L^2 = -\hbar^2 \left[\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right]$$

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \varphi}$$

L^2 and L_z have normalized eigenfunctions $\Upsilon_l^m(\theta, \varphi)$ for which it holds that:

$$L^2 \Upsilon_l^m = \hbar^2 l(l+1) \Upsilon_l^m$$

$$L_z \Upsilon_l^m = m\hbar \Upsilon_l^m$$

l	m	$\Upsilon_l^m(\theta, \varphi)$
0	0	$\Upsilon_0^0 = \frac{1}{\sqrt{4\pi}}$
1	0	$\Upsilon_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$
1	± 1	$\Upsilon_1^{\pm 1} = \pm \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\varphi}$
2	0	$\Upsilon_2^0 = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$
2	± 1	$\Upsilon_2^{\pm 1} = \pm \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\varphi}$
2	± 2	$\Upsilon_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\varphi}$

Commutators and Momentum Operators

$$\epsilon_{ijk} = \begin{cases} 1 & ijk \text{ even} \\ -1 & ijk \text{ odd} \\ 0 & \text{otherwise} \end{cases}$$

$$[x_i, p_j] = i\hbar \cdot \delta_{ij}$$

$$[x_i, L_j] = i\hbar \cdot \epsilon_{ijk} \cdot x_k$$

$$[L_i, L_j] = i\hbar \cdot \epsilon_{ijk} \cdot L_k$$

$$[x_i, x_j] = [p_i, p_j] = 0$$

$$[p_i, L_j] = i\hbar \cdot \epsilon_{ijk} \cdot p_k$$

$$J_+ = J_x + iJ_y$$

$$J_- = J_x - iJ_y$$

$$J_{\pm} J_{\mp} = J^2 - J_z^2 \pm \hbar \cdot J_z$$

$$[J_+, J_-] = 2\hbar \cdot J_z$$

$$[J_z, J_{\pm}] = \pm \hbar \cdot J_{\pm}$$

$$J_+ \phi_{j,m} = \sqrt{(j-m)(j+m+1)} \cdot \hbar \cdot \phi_{j,m+1}$$

$$J_- \phi_{j,m} = \sqrt{(j+m)(j-m+1)} \cdot \hbar \cdot \phi_{j,m-1}$$

$$\Upsilon_l^l(\theta, \varphi) = (-1)^l \sqrt{\frac{2l+1}{4\pi} \frac{(2l)!}{2^{2l}(l!)^2}} \cdot \sin^l \theta \cdot e^{il\varphi}$$

Applications

0.0.1 Low potential with infinitely rigid walls in one dimension

$$\mathcal{U}(x) = \begin{cases} \infty & x \leq 0, a \leq x \\ 0 & 0 < x < a \end{cases}$$

$$\Phi_n(x) = \begin{cases} 0 & \text{for } x \leq 0 \text{ and } a \leq x \\ \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & \text{for } 0 < x < a \end{cases}$$

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

Harmonic Oscillator 1D

$$\mathcal{U}(x) = \frac{1}{2} m \omega^2 x^2 = \frac{1}{2} k x^2$$

$$N_n = (2^n n!)^{-1/2} \left(\frac{m\omega}{\pi \hbar} \right)^{1/4}$$

Hermite polynom:

$$H_n(\xi) = (-1)^n \cdot e^{\xi^2} \cdot \frac{d^n e^{-\xi^2}}{d\xi^n}$$

$$\Phi_n(x) = N_n \cdot e^{-\frac{m\omega}{2\hbar} x^2} \cdot H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right)$$

$$E_n = \hbar \omega \cdot \left(n + \frac{1}{2} \right)$$

The wave equations can alternatively be written:

$$u_n(x) = N \left(\frac{\partial}{\partial x} - ax \right)^n \cdot u_0(x)$$

$$u_0(x) = e^{-ax^2/2}$$

Spherical Symmetric Potential

$$\mathcal{U}(\mathbf{r}) = \mathcal{U}(r)$$

$$H = -\frac{\hbar}{2mr^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial}{\partial r} \right] + \frac{L^2}{2mr^2} + \mathcal{U}(r)$$

$$H\psi_{nlm}(\mathbf{r}) = E_{nlm}\psi_{nlm}(\mathbf{r})$$

$$\psi_{nlm}(\mathbf{r}) = \frac{G_{nl}(r)}{r} \Upsilon_l^m(\theta, \phi)$$

Radial equation:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} G(r) + \left[\frac{l(l+1)\hbar^2}{2mr^2} + \mathcal{U}(r) \right] G(r) = EG(r)$$

Hydrogen-like Atom

$$\mathcal{U}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

The Schrödinger equation simplifies to:

$$\left[\Delta + \frac{2Z}{a_0 r} + \frac{2mE}{\hbar^2} \right] \Phi(r) = 0$$

Radial wave functions of hydrogenic atoms:

n	l	$R_{nl}(r)$
1	0	$R_{10}(r) = 2 \left(\frac{Z}{a_0} \right)^{3/2} e^{-\rho/2}$
2	0	$R_{20}(r) = \frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \rho) e^{-\rho/2}$
2	1	$R_{21}(r) = \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} \rho e^{-\rho/2}$
3	0	$R_{30}(r) = \frac{1}{9\sqrt{3}} \left(\frac{Z}{a_0} \right)^{3/2} (6 - 6\rho + \rho^2) e^{-\rho/2}$
3	1	$R_{31}(r) = \frac{1}{9\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} \rho(4 - \rho) e^{-\rho/2}$
3	2	$R_{32}(r) = \frac{1}{9\sqrt{30}} \left(\frac{Z}{a_0} \right)^{3/2} \rho^2 e^{-\rho/2}$

$$E - n = -\frac{mZ^2 e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} = -\frac{Z^2 \hbar^2}{2a_0^2 m n^2} = -13.6 \frac{Z^2}{n^2} \text{eV}$$

$$S(x, t) = \frac{\hbar}{2im} \left[\psi^* \cdot \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

Disturbance Calculations

Time independent disturbance:

$$\left. \begin{aligned} (H^0 + H') \psi'_m &= E'_m \psi'_m \\ H^0 \psi_n &= E_n^0 \psi_n \end{aligned} \right\} \Rightarrow$$

$$E'_m = E_m^0 + \langle m | H' | m \rangle + \sum_{n \neq m} \frac{|\langle m | H' | n \rangle|^2}{E_m^0 - E_n^0}$$

$$\psi'_m = \psi_m + \sum_{n \neq m} \frac{\int \psi_n^* H' \psi_m d^3r}{E_m^0 - E_n^0} \psi_n$$

Time dependent disturbance:

$$\left. \begin{aligned} H &= H^0 + H' \\ H^0 &\text{ Time independent} \\ H^0 \psi_n &= E_n^0 \psi_n \\ H \psi' &= i\hbar \frac{\partial}{\partial t} \psi' \end{aligned} \right\} \Rightarrow$$

$$\psi'_m = \sum_n a_{mn}(t) \psi_n$$

$$\dot{a}_{mn} = -\frac{i}{\hbar} e^{-i(E_m - E_n)t/\hbar} \cdot H'_{nm}$$

”Golden Rule”

The transition probability per unit of time $w_{f \leftarrow i}$ for a transition from the state ψ_i to a group of states $F = \{\psi_f\}$ with energy $\sin E_i^0$ for a system characterized by the state density $\rho(E)$ is given by:

$$w_{f \leftarrow i} = \frac{2\pi}{\hbar} |\langle f | H' | i \rangle|^2_{E_i^0 \approx E_f^0} \cdot \rho(E_f^0)$$

Dispersion (Born Approximation)

$$\frac{d\sigma}{d\Omega} = |f(\xi, \eta)|^2$$

$$f(\xi, \eta) = \frac{m}{2\pi\hbar^2} \int e^{i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}} \cdot v(\mathbf{r}) d^3r$$

For spherical symmetrical potential:

$$f(\xi, \eta) = \frac{2m}{\hbar^2 K} \int_0^\infty \sin(Kr) \cdot r \cdot v(r) dr, \quad |K| = 2k \cdot \sin\left(\frac{\xi}{2}\right)$$

Spherical box-potential:

$$V(r) = \begin{cases} -V_0 & r \leq a \\ 0 & r > a \end{cases}$$

$$f(\xi, \eta) = -\frac{2mV_0}{\hbar^2} \cdot \frac{\sin(Ka) - Ka \cos(Ka)}{K^3}$$

Screened Coulomb Potential:

$$v(r) = -\frac{A}{r} \cdot e^{-\alpha r}$$

$$\frac{d\sigma}{d\Omega} = \left(\frac{2mA}{\hbar^2 (\alpha^2 + 4k^2 \sin^2(\xi/2))} \right)^2$$

$$\sigma = \left(\frac{Am}{\hbar^2} \right)^2 \frac{16\pi}{\alpha^2 (\alpha^2 + 4k^2)}$$

$$\text{When } \alpha \rightarrow 0, \quad \frac{d\sigma}{d\Omega} \rightarrow \left(\frac{Am}{\hbar^2} \right)^2 \frac{1}{4(k \sin(\xi/2))^4}$$

Periodic Potential

$$V(x) = \begin{cases} 0 & n(a+b) < x < n(a+b) + a \\ V_0 & n(a+b) + a < x < (n+1)(a+b) \end{cases}$$

Continuity Requirements:

$$\cos k_1 a \cdot \cos k_2 b - \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin k_1 a \cdot \sin k_2 b = \cos(k(a+b)), \quad V_0 < E$$

$$\cos k_1 a \cdot \cosh \kappa b - \frac{k_1^2 + \kappa^2}{2k_1 \kappa} \sin k_1 a \cdot \sinh \kappa b = \cos(k(a+b)), \quad V_0 < E$$

Phase and group speed:

$$v_f = \frac{\omega}{k}, \quad v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$$

Effective mass:

$$m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$$