Quantum Mechanics

Basics

$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \hat{H}\Psi(\vec{r},t)$ $\qquad f(x) = \sum_{n=1}^{\infty} c_n|\phi_n\rangle$

$\langle\phi|\hat{A}|\psi\rangle = \langle\phi|\hat{A}\psi\rangle = \langle\hat{A}^\dagger\phi|\psi\rangle = \langle\hat{A}\psi|\phi\rangle^\dagger$

$\hat{H}\psi = E\psi \quad \Psi(\vec{x},t) = e^{\frac{-it\hat{H}}{\hbar}}\Psi(\vec{x},0) \quad c_m = \langle\phi_m|f\rangle \quad P_m = |c_m|^2$

$\hat{p} = -i\hbar\nabla \qquad \hat{E} = i\hbar\frac{\partial}{\partial t} \qquad p = \hbar k \qquad E = \hbar\omega$

$\hat{I} = \sum_i |\phi_i\rangle\langle\phi_i| \qquad \langle\phi_m|\phi_n\rangle = \delta_{nm} \qquad \langle\hat{A}\rangle = \langle\Psi|\hat{A}|\Psi\rangle$

Hermitian: $A^\dagger = A$ $\qquad$ Unitary: $U^\dagger = U^{-1}$

$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ $\qquad$ use test function to calculate this

$(\Delta x)^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 \qquad \langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2$

$[\hat{x},\hat{p}] = i\hbar \qquad [\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$

$\frac{d\langle\hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle$

$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0 \qquad \vec{J} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$

Harmonic Oscillator

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \qquad E_n = \hbar\omega(n+\frac{1}{2})$

$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i\hat{p}}{m\omega}) \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i\hat{p}}{m\omega})$

$\hat{N} = \hat{a}^\dagger\hat{a} \qquad \hat{H} = \hbar\omega(\hat{N}+\frac{1}{2}) \qquad \hat{N}\phi = n\phi$

$[\hat{a},\hat{a}^\dagger] = 1 \qquad [\hat{N},\hat{a}] = -\hat{a} \qquad [\hat{N},\hat{a}^\dagger] = \hat{a}$

$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \qquad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}) \qquad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^\dagger - \hat{a})$

$u_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$

Landau levels:

$\vec{B} = B\hat{z} \qquad A_x = -By/2 \qquad A_y = Bx/2$

$H = (\vec{p} - \frac{e}{c}\vec{A})^2/2m = \frac{\Pi_x^2+\Pi_y^2}{2m} + \frac{p_z^2}{2m}$

use $\Pi_x \equiv p_x - \frac{eA_x}{c} \qquad \Pi_y \equiv p_y - \frac{eA_y}{c} \qquad [\Pi_x,\Pi_y] = i\hbar\left(\frac{eB}{c}\right)$

$a = \sqrt{\frac{c}{2\hbar eB}}(\Pi_x + i\Pi_y) \qquad a^\dagger = \sqrt{\frac{c}{2\hbar eB}}(\Pi_x - i\Pi_y)$

$a^\dagger a = \frac{c}{2\hbar eB}\left(\Pi_x^2 + \Pi_y^2 + i\,[\Pi_x,\Pi_y]\right)$

$E = \frac{eB\hbar}{mc}(n+1/2) + \frac{p_z^2}{2m}$

1D Problems

scattering/bound states:

ψ, ψ' continuous at barrier

$E > V : \psi \sim e^{\pm ikx} \qquad k = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$E < V : \psi \sim e^{\pm\kappa x} \qquad \kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

if $V = \lambda\delta(x-a)$:

$\psi_{a+\epsilon}(a) = \psi_{a-\epsilon}(a)$

$\lim_{\epsilon\to 0}[\psi'(a+\epsilon) - \psi'(a-\epsilon)] = \frac{2m\lambda}{\hbar^2}\psi(a)$

infinite potential well (0 to a):

$\phi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \qquad E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}$

Hydrogen Atom

$H = \frac{p^2}{2\mu} - \frac{Ze^2}{r} \qquad \mu = \frac{m_1 m_2}{m_1+m_2} \qquad E_n = -\frac{Z^2\hbar^2}{2\mu r_B^2 n^2} = \frac{-13.6Z^2}{n^2}$

$\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta,\phi)$

fine: $H_{rel} = \frac{-p^4}{8m^3c^2} \qquad H_{LS} = \left(\frac{1}{2}\frac{1}{m_e^2c^2}\frac{1}{r}\frac{dV_c}{dr}\right)\vec{L}\cdot\vec{S}$

hyperfine: $H_{hf} = \underbrace{\frac{3(\vec{\mu}_e\cdot\hat{r})\hat{r} - \vec{\mu}_e\cdot\vec{\mu}_p}{r^3}}_{only\ for\ l>0} - \frac{8\pi}{3}\vec{\mu}_e\cdot\vec{\mu}_p\delta^{(3)}(\vec{r})$

Zeeman ($\vec{B} = B\hat{z}$): $H_Z = -(\vec{\mu}_{orbital} + \vec{\mu}_{spin})\cdot\vec{B}$

$= -\left(-\frac{e}{2m_ec}\vec{L} - \frac{eg_e}{2m_ec}\vec{S}_e + \frac{eg_p}{2m_pc}\vec{S}_p\right)\cdot\vec{B} = \frac{e}{2m_ec}\vec{B}\cdot\left[\vec{L} + 2\vec{S}_e\right] - \frac{eg_p}{2m_pc}\vec{B}\cdot\vec{S}_p$

$\alpha = \frac{e^2}{\hbar c} \qquad r_B = \frac{\hbar^2}{m_ee^2} = \frac{\hbar}{\alpha m_ec} \qquad \mu_B = \frac{e\hbar}{2m_ec}$

Parity

$\underbrace{\langle a|P^{-1}}_{\eta_a^*\langle a|}\underbrace{PVP^{-1}}_{\eta_V V}\underbrace{P|b\rangle}_{\eta_b|b\rangle} = \langle a|V|b\rangle \to \eta_V\eta_b\eta_a^* \equiv 1$ for matrix element to be non-zero

$x, y, x \to -x, -y, -z \qquad r, \theta, \phi \to r, \pi-\theta, \phi+\pi$

$Y_{lm}(\pi-\theta,\phi+\pi) = (-1)^l Y_{lm}(\theta,\phi)$

Rotations

spin 1/2:

$e^{\frac{i\vec{S}\cdot\vec{n}\phi}{\hbar}} = \hat{I}\cos\frac{\phi}{2} + i\hat{\sigma}\cdot\hat{n}\sin\frac{\phi}{2}$

spin 1:

$$e^{\frac{i\theta S_y}{\hbar}} = \begin{pmatrix} \frac{1}{2}(1+\cos\theta) & \frac{1}{\sqrt{2}}\sin\theta & \frac{1}{2}(1-\cos\theta) \\ -\frac{1}{\sqrt{2}}\sin\theta & \cos\theta & \frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta) & -\frac{1}{\sqrt{2}}\sin\theta & \frac{1}{2}(1+\cos\theta) \end{pmatrix}$$

$$e^{\frac{i\theta S_z}{\hbar}} = \begin{pmatrix} e^{i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix}$$

Angular Momentum

$[\hat{J}_i,\hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k \qquad [\hat{J}^2,\hat{J}_k] = 0$

$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \qquad \hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-) \qquad \hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$

$\hat{J}_z|jm\rangle = \hbar m|jm\rangle \qquad \hat{J}^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle$

$\hat{J}_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}|jm\pm 1\rangle$

$[\hat{J}_z,\hat{J}_\pm] = \pm\hbar\hat{J}_\pm \qquad [\hat{J}_+,\hat{J}_-] = 2\hbar\hat{J}_z$

spin 1/2:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$[\sigma_i,\sigma_j] = 2i\epsilon_{ijk}\sigma_k \qquad \{\sigma_i,\sigma_j\} = 2\hat{I}\delta_{ij} \qquad \hat{S}_i = \frac{\hbar}{2}\sigma_i$

spin 1:

$$\hat{S}_x = \hbar\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \qquad \hat{S}_y = \hbar\begin{pmatrix} 0 & \frac{-i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & \frac{-i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}$$

$$\hat{S}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$\vec{\mu}_{orbital} = \frac{q}{2mc}\vec{L} \qquad \vec{\mu}_{spin} = \frac{gq}{2mc}\vec{S} \qquad H \to H_0 - \vec{\mu}\cdot\vec{B}$

Addition of Angular Momentum

$|jm\rangle = \sum_{m_1,m_2}|j_1m_1\rangle|j_2m_2\rangle\underbrace{\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array}\right)}_{CG\ coefficients}$

$\vec{J} = \vec{L} + \vec{S} \qquad |l-s| \leq j \leq l+s \qquad -j \leq m_j \leq j$

$\vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

$J^2 = J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+}$

$j \otimes \frac{1}{2}$:

$|j = l \pm \frac{1}{2}, m = m_l + m_s\rangle = \pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}|l, m-\frac{1}{2}\rangle|\frac{1}{2},\frac{1}{2}\rangle +$

$\sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}|l, m+\frac{1}{2}\rangle|\frac{1}{2}, -\frac{1}{2}\rangle$

$\vec{L}\cdot\vec{S}|jm\rangle = \begin{cases} \frac{\hbar^2}{2}l & j = l+\frac{1}{2} \\ \frac{-\hbar^2}{2}(l+1) & j = l-\frac{1}{2} \end{cases}$

$\frac{1}{2}\otimes\frac{1}{2}$:
$|11\rangle = |\frac{1}{2}\frac{1}{2}\rangle|\frac{1}{2}\frac{1}{2}\rangle$
$|10\rangle = \frac{1}{\sqrt{2}}\left(|\frac{1}{2}\frac{1}{2}\rangle|\frac{1}{2}-\frac{1}{2}\rangle + |\frac{1}{2}-\frac{1}{2}\rangle|\frac{1}{2}\frac{1}{2}\rangle\right)$
$|1-1\rangle = |\frac{1}{2}-\frac{1}{2}\rangle|\frac{1}{2}-\frac{1}{2}\rangle$
$|00\rangle = \frac{1}{\sqrt{2}}\left(|\frac{1}{2}\frac{1}{2}\rangle|\frac{1}{2}-\frac{1}{2}\rangle - |\frac{1}{2}-\frac{1}{2}\rangle|\frac{1}{2}\frac{1}{2}\rangle\right)$
option A: product basis - $J_1^2 \quad J_2^2 \quad J_{1z} \quad J_{2z}$
$|j_1m_1\rangle\otimes|j_2m_2\rangle = |j_1j_2;m_1m_2\rangle = |m_1m_2\rangle$
option B: total AM basis - $J_1^2 \quad J_2^2 \quad J^2 \quad J_z$
$|j_1j_2;jm\rangle = |jm\rangle$

Tensor Operators/Wigner Eckart The.

$T_q^{(k)}$ = spherical tensor of rank k, qth component
$\langle\alpha', j'm'|T_q^{(k)}|\alpha, jm\rangle = 0$ unless $m' = q+m$, $|k-j| \le j' \le k+j$

$$\langle\alpha'j'm'|T_q^{(k)}|\alpha jm\rangle = \underbrace{\langle jk;mq|jk;j'm'\rangle}_{CG\ coefficient}\overbrace{\frac{\langle\alpha'j'||T^{(k)}||\alpha j\rangle}{\sqrt{2j+1}}}^{reduced\ m.e}$$

Time Independent Perturbation Theory

$H = H_0 + \lambda V$ where $H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$
$E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$
$|n^{(1)}\rangle = \sum_{m\neq n}|m^{(0)}\rangle\frac{\langle m^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}$
$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle$

Degenerate Perturbation Theory

$H = H_0 + V$
$V_{ij} = \langle\psi_i|V|\psi_j\rangle$ $\qquad\psi_i = i^{th}$ degenerate state

$$[V_{ij}] = \begin{array}{c|cccc} & |\psi_1\rangle & |\psi_2\rangle & \dots & |\psi_n\rangle \\ \langle\psi_1| & & & & \\ \langle\psi_1| & & & & \\ \vdots & & & & \\ \langle\psi_1| & & & & \end{array}$$

1. Calculate $V|\psi_j\rangle$ for each j.
2. Calculate $\langle\psi_i|V|\psi_j\rangle$ and put them in the matrix.
3. Diagonalize matrix to get energy of perturbation.

Variational Principle

1. Choose $|\psi\rangle$ - a trial ket which depends on one or more parameters $(\lambda_1, \lambda_2, \dots)$
2. Compute $\frac{\langle\psi|H|\psi\rangle}{\langle\psi||\psi\rangle} \ge E_0$
3. Minimize with respect to $\lambda_1.\lambda_2, \dots$.
4. To get first excited state choose $|\psi_1\rangle$ such that $\langle\psi_1|\psi\rangle = 0$ and so on.

Time Dependent Perturbation Theory

$H = H_0 + \lambda V(t) \to |n(t)\rangle = \sum_n c_n(t)e^{-iE_n^{(0)}t/\hbar}|n^{(0)}\rangle$
i = initial state at t_0

$c_n^{(0)} = \delta_{ni} \qquad c_n^{(1)} = -\frac{i}{\hbar}\int_{t_0}^{t}dt'e^{i\frac{E_n^{(0)}-E_1^{(0)}}{\hbar}t'}\langle n^{(0)}|V(t')|i^{(0)}\rangle$
$P_{i\to n} = |c_n|^2 = |c_n^{(0)} + \lambda c_n^{(1)} + \lambda^2 c_n^{(2)} + \dots|$
Fermi Golden Rule: $\Gamma_{i\to n} = \frac{2\pi}{\hbar}|\langle n|V|i\rangle|^2\delta(E_n - E_i)$
assumes $V(t) = Ve^{i\omega t} + V^\dagger e^{-i\omega t}$

Radiation

Scattering

$\psi(\vec{r}) \to e^{ikz} + f_k(\theta,\phi)\frac{e^{ikr}}{r}$ $\qquad \frac{d\sigma}{d\Omega} = |f_k(\theta,\phi)|^2$
Born: $f(\theta) = \frac{-m}{2\pi\hbar^2}\int V(\vec{r}')e^{-i\vec{q}\cdot\vec{r}'}d^3\vec{r}' \to f(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty dr\, rV(r)\sin qr$
$\vec{q} = \vec{k}_f - \vec{k}_i$ $\qquad q = 2k\sin\frac{\theta}{2}$
Partial Waves:
$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]u_{kl}(r) = \frac{\hbar^2k^2}{2m}u_{kl}(r)$
as $r\to\infty$, $u_{kl}(r) \to$ free solution and $-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u = \frac{\hbar^2k^2}{2m}u \Rightarrow \frac{d^2u}{dr^2} + k^2u = 0$
so $u \sim \sin kr, \cos kr$ but there is a phase shift
$u_{kl}(r) \to C\sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \Rightarrow j_l(kr) \to \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right)$
$j_0(kr) = \frac{\sin kr}{kr}$ $\qquad n_0(kr) = \frac{-\cos kr}{kr}$
$\sigma_k = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$ s-wave $\to \sigma_k = \frac{4\pi}{k^2}\sin^2\delta_0$