1 Wave Function

$$\Psi_p = e^{i(2\pi x/\lambda - 2\pi t/T)}$$
$$= e^{i(kx-\omega t)}$$
$$= e^{\frac{i}{\hbar}(px-Et)}$$

$$\breve{p}\Psi_p = p\Psi_p = \hbar k \Psi_p \qquad \boxed{\breve{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}}$$

$$\breve{E}\Psi_p = E\Psi_p = \hbar\omega\Psi_p \qquad \boxed{\breve{E} = -\frac{\hbar}{i}\frac{\partial}{\partial t}}$$

- $|\boldsymbol{f}\rangle \equiv \int f(x)\,|x\rangle\,dx$
- $\langle \boldsymbol{x}|\boldsymbol{x'}\rangle \equiv \delta(x-x')$
- $\langle \boldsymbol{x}|\hat{\boldsymbol{x}}|\boldsymbol{x'}\rangle \equiv x\langle x|x'\rangle$

1. $\langle x|\hat{x}|f\rangle = xf(x)$

   $\boxed{\breve{x}\langle x|f\rangle \equiv x\langle x|f\rangle}$

2. $\langle \boldsymbol{x}|\hat{\boldsymbol{p}}|\boldsymbol{x'}\rangle \equiv \frac{\hbar}{i}\delta'(x-x')$

   $= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle$

3. $\langle x|\hat{p}|f\rangle = \int f(x')\,\delta'(x-x')\,dx'$

   $\boxed{\breve{p}\langle x|f\rangle \equiv \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|f\rangle}$

1.1 Schrodinger Ψ

$$\boxed{\breve{E}|\Psi\rangle = \widehat{H}|\Psi\rangle} = (\widehat{T}+\widehat{V})|\Psi\rangle$$

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \left[\frac{\hat{p}^2}{2m} + V(\hat{x},t)\right]|\Psi\rangle$$

$$\boxed{-\breve{E}\langle\Psi| = \langle\Psi|\hat{H}}$$

$$\boxed{\breve{E}\langle x|\Psi\rangle = \breve{H}\Psi} = (\breve{T}+\breve{V})\Psi = \left[\frac{\breve{p}^2}{2m} + V(\vec{\mathbf{r}},t)\right]\Psi$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(\vec{\mathbf{r}},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\breve{\mathbf{r}},t)\right]\Psi(\vec{\mathbf{r}},t)}$$

$$\boxed{-\breve{E}\langle\Psi|x\rangle = \breve{H}\Psi^*}$$

<u>If $V = V(x)$</u>

$\Psi(x,t) = \psi(x)\phi(t) \;\Rightarrow$

- $E_n\phi_n(t) = i\hbar\frac{\partial}{\partial t}\phi_n(t) \;\Rightarrow\; \boxed{\phi_n(t) = e^{-\frac{i}{\hbar}E_n t}}$
- $\boxed{E_n\psi_n(x) = \left(\frac{-\hbar^2}{2m}\partial_x^2 + V(x)\right)\psi_n(x)}$
  - ψ can be lin. sum of real or complex, so choose real ψ
- Linear :
$$\boxed{\begin{aligned}\Psi(x,t) &= \sum_n \psi_n(x)\,e^{-\frac{i}{\hbar}E_n t}c_n \\ &= \sum_n \langle x|n\rangle e^{-\frac{i}{\hbar}E_n t}\langle n|\Psi\rangle \\ &= \int_{x'}\langle x|\left[\sum_n |n\rangle e^{-\frac{i}{\hbar}E_n t}\langle n|\right]|x'\rangle\Psi(x')\,dx' \\ &= \int_{x'} U(x,t;x',0)\,\Psi(x')\,dx'\end{aligned}}$$
- $\sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2 = 0 \;\Rightarrow$ measuring stationary state, Ψ_n, returns one E_n (determinate state)

1.2 Usage

- $\langle f|g\rangle = \int_{-\infty}^{\infty} f(x)^* g(x)\ dx$
- $\langle f|g\rangle_{ab} = \int_a^b f(x)^* g(x)\ dx$
- $|f\rangle = \int f(x')|x'\rangle dx' \ \sim\ f(x) \equiv \langle x|f\rangle$
- $\langle f| = \int f(x)^* [...]\ dx$
- $\langle f|f\rangle = \int_a^b |f|^2 dx < \infty \ \Rightarrow\ f \in L_{2(a,b)}$ $\qquad \left(\int_a^b |f|^p\, dx < \infty \ \Rightarrow\ f \in L_{p(a,b)}\right)$

$$\langle x|\Psi\rangle = \Psi = \begin{cases} \displaystyle\sum_n c_n f_n \\ \displaystyle\int_n c_n f_n\ dn \end{cases}, \qquad \langle f_m|f_n\rangle = \begin{cases} \delta_{mn} \\ \delta_{(m-n)} \end{cases}, \qquad \text{(see Born int.)} \quad |c_n|^2 = \begin{cases} P(n) \\ \text{PDF}_{(n)} \end{cases}$$

$$\Rightarrow \boxed{c_n = \langle f_n|\Psi\rangle}$$

$\forall\{f_n\} \in L_2$:

$$|\Psi\rangle = \begin{cases} \displaystyle\sum_n c_n|f_n\rangle = \sum_n \langle f_n|\Psi\rangle\ |f_n\rangle = \left(\sum_n |f_n\rangle\langle f_n|\right)|\Psi\rangle = |\Psi\rangle \\ \displaystyle\int_n c_n|f_n\rangle\ dn = \int_n \langle f_n|\Psi\rangle|f_n\rangle\ dn = \left(\int_n |f_n\rangle\langle f_n|\ dn\right)|\Psi\rangle = |\Psi\rangle \end{cases}$$

$\breve{x}\Psi_y = x\Psi_y = y\Psi_y$ $\Rightarrow \boxed{\Psi_y = \delta_{(x-y)} = \langle x\|y\rangle}$	$\langle x\|\hat{p}\|p\rangle = \int \langle x\|\hat{p}\|x'\rangle\langle x'\|p\rangle\, dx'$ $p\langle x\|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x\|p\rangle$ $\langle x\|\hat{p}\|p\rangle = \breve{p}\Psi_p = p\Psi_p$ $\Rightarrow \boxed{\Psi_p = Ae^{\frac{i}{\hbar}px} = \langle x\|p\rangle}$	$\langle x\|\hat{H}\|n\rangle = E_n\langle x\|n\rangle$ $\breve{H}\Psi_n = E_n\Psi_n$ (See Potential Examples)
$\Psi_{(x,t)} = \int_{-\infty}^{\infty} \Psi_y c_{y(t)}\ dy$ $= \int_{-\infty}^{\infty} \delta_{(x-y)}\Psi_{(y,t)}\ dy$	$\Psi_{(x,t)} = \int_{-\infty}^{\infty} \Psi_p \phi_{(E_p,t)} c_p\ dp$ $= \int_{-\infty}^{\infty} \frac{e^{\frac{i}{\hbar}px}}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}\Phi_{(p,0)}\ dp$	$\Psi_{(x,t)} = \int_{-\infty}^{\infty} \Psi_n \phi_{(E_n,t)} c_n\ dn$ $= \int_{-\infty}^{\infty} \Psi_n e^{\frac{-i}{\hbar}E_n t} c_n\ dn$
$c_x(t) = \langle \Psi_x\|\Psi_{(x,t)}\rangle = \langle x\|\Psi\rangle$ $\Psi_{(x,t)} = \int_{-\infty}^{\infty} \delta_{(x-y)}\Psi_{(y,t)}\ dy$	$c_p(t) = \langle \Psi_p\|\Psi_{(x,t)}\rangle = \langle p\|\Psi\rangle$ $\boxed{\Phi_{(p,t)} = \int_{-\infty}^{\infty} \frac{e^{\frac{-i}{\hbar}px}}{\sqrt{2\pi\hbar}}\Psi_{(x,t)}\ dx}$	$c_n(t) = \langle \Psi_n\|\Psi_{(x,t)}\rangle = \langle n\|\Psi\rangle$ $\Psi_{(n,t)} = \int_{-\infty}^{\infty} \Psi_n^* \Psi_{(x,t)}\ dx$

$\boxed{\text{Born Interpretation: PDF}(x) = |\Psi(x)|^2 = \Psi^*\Psi}$

$\underline{P_{(a<x<b)} = \int_a^b |\Psi|^2 dx \equiv \langle\Psi|\Psi\rangle_{ab}}$

– $\boxed{\langle\Psi|\Psi\rangle = 1}$ (physical, bound states only)

- $\Psi(\pm\infty) = 0$
- $\text{Min}(V) \le E_\Psi \in \mathbb{R}$
- $\langle\Psi_n|\Psi_n\rangle \to \infty \;\Rightarrow\; \Psi_n$ not PHYSICAL sol. but $\Psi = \int c_n\Psi_n$ can if $\langle\Psi|\Psi\rangle = 1$

Boundary Conditions:

- $\Psi(x)$ isn't always cont. (see extra)
- $\frac{\partial\Psi(x)}{\partial x}$ is cont. except at $V = \infty$

$$\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} E\Psi dx = \int_{-\epsilon}^{\epsilon}\widehat{H}\Psi dx \;\Rightarrow$$

$$\lim_{\epsilon\to 0}\frac{\hbar^2}{2m}\Delta\left(\frac{d\Psi}{dx}\right) = \int_{-\epsilon}^{\epsilon} V\Psi dx$$

- $E[f(x)] = \int_{-\infty}^{\infty} f(x)\ \text{PDF}(x)\ dx = \int_{-\infty}^{\infty} f(x)\ |\Psi(x)|^2\ dx = \int_{-\infty}^{\infty}\Psi(x)^* f(x)\Psi(x)\ dx = \boxed{\langle\Psi|f\Psi\rangle \equiv \langle f(x)\rangle}$
- $\displaystyle\int_x \Psi^*\Psi\ dx = \int_x \left(\int_n c_n^*(t)\Psi_n^*(x)\ dn\right)\left(\int_{n'} c_{n'}(t)\Psi_{n'}(x)\ dn'\right)\ dx$

$$= \int_n c_n^*(t)\int_{n'} c_{n'}(t)\ \delta(n-n')\ dn'\ dn = \int_n |c_n(t)|^2\ dn \;\Rightarrow\; \boxed{\text{PDF}(n) = |c_n|^2 = c_n^* c_n}$$

$\underline{\text{Adjoint (herm. adj./herm. conj.)}: \left\{A^\dagger : \langle f|Af\rangle = \langle A^\dagger f|f\rangle\right\}} \;\Rightarrow\; \langle h|\hat{A}g\rangle = \langle\hat{A}^\dagger h|g\rangle$ (let $f{=}h{+}g,\ f{=}h{+}ig$)

$\underline{\text{Hermitian Operator: } \left\{A : \hat{A}^\dagger = \hat{A}\right\}}$

- $\boxed{\exists\{\Psi_n\}:\ \hat{A}\Psi_n(x) = a_n\Psi_n(x)}$ (spectral theorem)
- $\langle a\rangle = a \in \mathbb{R} \;\Rightarrow\; \hat{A}$ can be an observable
- $\boxed{\langle\Psi_m|\Psi_n\rangle \in \{\delta_{mn},\ \delta(m-n)\}}$
- $\boxed{\text{Axiom: } \{\Psi_n\} \text{ for } \hat{A} \text{ are complete}}$

Non-degenerate: $(m \ne n),\ (a_m \ne a_n) \;\Rightarrow\; \langle\Psi_m|\Psi_n\rangle \in \{\delta_{mn},\ \delta(m-n)\}$

Degenerate: $(m \ne n),\ (a_m = a_n),\ (\Psi_m \ne \Psi_n), \langle\Psi_m|\Psi_n\rangle \ne 0 \;\Rightarrow$ Use Gram-Schmidt to find orthogonal $\langle\Psi'_m|\Psi'_n\rangle = \langle a\Psi_m + b\Psi_n|\ c\Psi_m + d\Psi_n\rangle = 0$

$\underline{\text{Expectation: } E[\hat{A}(x,p)]}$

- $\displaystyle\int_{-\infty}^{\infty}\hat{A}(x,p)^*\ \Psi^*\Psi\ dx = \langle\hat{A}\Psi|\Psi\rangle = \boxed{\langle\Psi|\hat{A}\Psi\rangle \equiv \langle\hat{A}(x,p)\rangle}$ (won't work if $\int A\ |\Psi|^2\ dx$)

$$\langle\Psi|\hat{A}\Psi\rangle = \int_{-\infty}^{\infty}\Psi^*\hat{A}\Psi\ dx = \int_{-\infty}^{\infty}\left(\int_n c_n^*\Psi_n^*\ dn\right)\left(\int_{n'} c_{n'}\hat{A}\Psi_{n'}\ dn'\right)\ dx$$

$$= \int_n a_n|c_n|^2\ dn = E[a] \equiv \langle a\rangle$$

$c_n = \text{PDF}(n)$ (see above and Momentum Space)

$$\boxed{\langle a\rangle = \langle\Psi|\hat{A}\Psi\rangle = \langle\Psi|\hat{A}|\Psi\rangle = \langle A\rangle}$$

- $\boxed{\langle\sigma_a^2\rangle = \langle a^2\rangle - \langle a\rangle^2} \;\Rightarrow\; \sigma_A^2 = 0$ for Ψ_n (determinate state)

Matrix Operators:

Given complete $\{e_n\}$: $\langle e_m|e_n\rangle = \delta_{mn}$

1.) $\boxed{Q^{(e)}_{mn} \equiv \left\langle e_m \middle| \widehat{Q}(x,p) \middle| e_n \right\rangle}$

$$|\beta\rangle = \widehat{Q}|\alpha\rangle = \sum_m |e_m\rangle \left[\begin{array}{c} \langle e_m|\beta\rangle = \langle e_m|\widehat{Q}|\alpha\rangle \\ \sum_n b_n \langle e_m|e_n\rangle = \sum_n a_n \boxed{\langle e_m|\widehat{Q}|e_n\rangle} \\ \boxed{b_m = \sum_n \left(Q^{(e)}_m\right)_n a_n} \end{array}\right] = \begin{array}{r} \sum_m b_m|e_m\rangle = \sum_{n,m}\langle e_n|\alpha\rangle\ Q^{(e)}_{mn}|e_m\rangle \\ = \sum_{n,m} Q^{(e)}_{mn}|e_m\rangle\langle e_n|\alpha\rangle \\ \Rightarrow \boxed{\widehat{Q} = \sum_{m,n} Q^{(e)}_{mn}|e_m\rangle\langle e_n|} \end{array}$$

2.) Find $\widehat{Q}$ as a matrix

$$\begin{array}{l} |f\rangle = \sum_n c^{(e)}_n[f]\ \left|e_n\right\rangle \\ \quad\downarrow \\ f(x) = \sum_n c^{(e)}_n[f]\ e_n(x) \end{array} = \begin{pmatrix} \vdots \\ c_n[f] \\ \vdots \end{pmatrix}^{(e)} \cdot \begin{pmatrix} \vdots \\ e_n(x) \\ \vdots \end{pmatrix} \equiv \boxed{\begin{array}{c} \vec{c}^{\ (e)}[f] \cdot \vec{e}(x) \\ \int_n c^{(e)}[f](n) \cdot e(n,x)\ dn \end{array}}\ ,\quad \boxed{c^{(e)}_n[f] = \langle e_n|f\rangle}$$

$$\begin{aligned} &\widehat{Q}|f\rangle \\ &= \Big(\sum_{m,n'} Q^{(e)}_{mn'}|e_m\rangle\langle e_{n'}|\Big)\sum_n c^{(e)}_n|e_n\rangle \\ &= \sum_{m,n}\Big(\sum_{n'} Q^{(e)}_{mn'}\ c^{(e)}_n\langle e_{n'}|e_n\rangle\Big)|e_m\rangle \\ &= \sum_m\Big(\sum_n \left(Q^{(e)}_m\right)_n c^{(e)}_n\Big)|e_m\rangle \end{aligned}$$

$$\boxed{\begin{array}{l} \widehat{Q}\left[\begin{pmatrix} | \\ c \\ | \end{pmatrix}^{(e)} \cdot \begin{pmatrix} | \\ e \\ | \end{pmatrix}\right] = \left[\begin{pmatrix} & \vdots & \\ - & Q_m & - \\ & \vdots & \end{pmatrix}^{(e)} \begin{pmatrix} | \\ c \\ | \end{pmatrix}^{(e)}\right] \cdot \begin{pmatrix} | \\ e \\ | \end{pmatrix} \\ \widehat{Q}\ |f\rangle = \boxed{\widehat{Q}\ \left[\ \vec{c}^{\ (e)}[f] \cdot \vec{e}\ \right] = \left[\ \overline{Q}^{(e)}\ \vec{c}^{\ (e)}[f]\right] \cdot \vec{e}} \\ \qquad \langle x|\widehat{Q}|f\rangle = \int_m \left[\overline{Q}^{(\delta)} f\right](m) \cdot \delta(x-m)\ dm \\ \text{e.g.} \\ \qquad\qquad = \int_m \left[\int_n Q^{(\delta)}_m(n) \cdot f(n)\ dn\right] \delta(x-m)\ dm = \widehat{Q}f(x) \end{array}}$$

3.) Terms

Diagonalizable: $A \equiv PDP^{-1}$

Conj. Transpose, †: $A^\dagger \equiv A^{T*} = A^{*T}$

Hermitian, H: $H = H^\dagger$

$H = UDU^{-1} = UDU^\dagger$ (spectral theorem)

Unitary, U: $U :\ UU^\dagger = U^\dagger U = 1$

$\exists H :\ U = e^{iH} = (U')e^{iD}(U')^\dagger$

Hermitian Operator $\sim$ Hermitian Matrix

$\langle Qx|y\rangle = \langle x|Qy\rangle$ (if inf. size then must be in Hilbert Space)

(draw it out)

$\rightarrow\ (\overline{Q}x)^{*T} \cdot y_m|e_m\rangle = y_m x^{*T} \cdot (\overline{Q}^*_m)$

$= x^{*T} \cdot \overline{Q}^{*T} y_m|e_m\rangle$

$= x^{*T} \cdot \overline{Q} y_m|e_m\rangle$

$\rightarrow\ \overline{Q}^\dagger \equiv \overline{Q}^{*T} = \overline{Q}$ ☑

4.) Eigenvalue Equation

General Case:

$$\widehat{Q}|q_i\rangle = q_i|q_i\rangle$$

$$|q_i\rangle = \sum c_n^{(e)}{}_{[q_i]}\big|e_n\big\rangle$$

$$\boxed{\begin{aligned}\overline{Q}^{(e)} &= UDU^\dagger \qquad \text{(Spectral Theorem)}\\ &= \begin{pmatrix} | & | & \\ \vec{c}_{[q_0]} & \vec{c}_{[q_1]} & \dots \\ | & | & \end{pmatrix}^{(e)} \begin{pmatrix} q_0 & 0 & \dots \\ 0 & q_1 & \dots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} - & \vec{c}^{\,*}{}_{[q_0]} & - \\ - & \vec{c}^{\,*}{}_{[q_1]} & - \\ & \vdots & \end{pmatrix}^{(e)} \\ &\text{where } \langle \vec{c}_m|\vec{c}_n\rangle = \delta_{mn} \ \text{ since } \ Q^\dagger Q = QQ^\dagger \quad \text{(normal)}\end{aligned}}$$

$$\begin{aligned} q_i|q_i\rangle &= \widehat{Q}|q_i\rangle \\ \Big[q_i\ \vec{c}^{\,(e)}{}_{[q_i]}\Big]\cdot\vec{e}(x) &= \Big[\ \overline{Q}^{(e)}\ \vec{c}^{\,(e)}{}_{[q_i]}\Big]\cdot\vec{e}(x) \\ &\Downarrow^* \\ q_i\ \vec{c}^{\,(e)}{}_{[q_i]} &= \overline{Q}^{(e)}\ \vec{c}^{\,(e)}{}_{[q_i]} \end{aligned}$$

$$\begin{aligned} {}^*\forall n \qquad (qc)_n\ |e_n(x)\rangle &= (Qc)_n\ |e_n(x)\rangle \\ \langle e_n(x)|(qc)_n|e_n(x)\rangle &= \langle e_n(x)|(Qc)_n|e_n(x)\rangle \\ (qc)_n &= (Qc)_n \end{aligned}$$

$$q_i\begin{pmatrix} | \\ \vec{c}_{[q_i]} \\ | \end{pmatrix}^{(e)} = \begin{pmatrix} | & | & \\ \vec{c}_{[q_0]} & \vec{c}_{[q_1]} & \dots \\ | & | & \end{pmatrix}^{(e)} \begin{pmatrix} q_0 & 0 & \dots \\ 0 & q_1 & \dots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} - & \vec{c}^{\,*}{}_{[q_0]} & - \\ - & \vec{c}^{\,*}{}_{[q_1]} & - \\ & \vdots & \end{pmatrix}^{(e)} \begin{pmatrix} | \\ \vec{c}_{[q_i]} \\ | \end{pmatrix}^{(e)}$$

$$\boxed{\begin{aligned} &\underline{q_i\ ,\ \vec{c}^{\,(e)}{}_{[q_i]}}: \\ &\det\big(\overline{Q}^{(e)} - Iq_i\big) = 0 \end{aligned}}$$

Special Case:

$$|q_n\rangle = |e_n\rangle$$

$$\widehat{Q}|e_n\rangle = q_n|e_n\rangle$$

$$\begin{aligned} \widehat{Q}|a\rangle &= \sum_n \widehat{Q}|e_n\rangle\langle e_n|a\rangle \\ &= \Big(\sum_n q_n|e_n\rangle\langle e_n|\Big)|a\rangle \end{aligned} \Rightarrow \boxed{\widehat{Q} = \sum_n q_n|e_n\rangle\langle e_n|} \Rightarrow \boxed{\overline{Q}^{(e)} = \begin{pmatrix} q_0 & 0 & \dots \\ 0 & q_1 & \dots \\ \vdots & \vdots & q_i \end{pmatrix}}$$

$$Q^{(e)}_{mn} = q_n\delta_{mn}$$

$$\overline{Q}^{(e)} = \begin{pmatrix} q_0 & 0 & \dots \\ 0 & q_1 & \dots \\ \vdots & \vdots & \end{pmatrix}^{(e)} = \begin{pmatrix} 1 & 0 & \dots \\ 0 & 1 & \dots \\ \vdots & \vdots & \end{pmatrix}^{(e)} \begin{pmatrix} q_0 & 0 & \dots \\ 0 & q_1 & \dots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} 1 & 0 & \dots \\ 0 & 1 & \dots \\ \vdots & \vdots & \end{pmatrix}^{(e)}$$

$$\boxed{\vec{c}^{\,(e)}{}_{[q_i]} = \big(\dots\ 0\ 0\ 1_{(i)}\ 0\ 0\ \dots\big)^T}$$

5. Unitary Transformation and Trace

- $\boxed{|b_i\rangle = U|a_i\rangle \ \Leftrightarrow\ U = \sum |b_n\rangle\langle a_n|}$
- $\boxed{\overline{U}_{ij} = \langle a_i|U|a_j\rangle = \langle a_i|b_j\rangle}$
- $\boxed{\langle b_i|U\widehat{Q}U^\dagger|b_j\rangle = \langle a_i|\widehat{Q}|a_j\rangle}$
- $\boxed{\begin{aligned} (A)|a_i\rangle &= a_i|a_i\rangle \\ (UAU^\dagger)|b_i\rangle &= a_i|b_i\rangle \end{aligned}}$

- $\mathrm{Tr}(Q) = \sum\langle a_i|Q|a_i\rangle = \sum\langle b_i|Q|b_i\rangle$
- $\mathrm{Tr}(QP) = \mathrm{Tr}(PQ)$
- $\mathrm{Tr}(U^\dagger QU) = \mathrm{Tr}(Q)$
- $\mathrm{Tr}(\,|a_i\rangle\langle a_j|\,) = \delta_{ij}$
- $\mathrm{Tr}(\,|b_i\rangle\langle a_i|\,) = \langle a_i|b_i\rangle$

$\Phi(p,t)$ - Momentum Space (generalizable Born Interpretation):

$$\int_x \Psi^*\Psi dx = \int_x \int_p c_p^*(t)\Psi_p^*(x)dp \int_{p'} c_{p'}(t)\Psi_{p'}(x)dp'\ dx$$
$$= \int_p c_p^*(t) \int_{p'} c_{p'}(t) \int_x \Psi_p^*(x)\Psi_{p'}(x)dx\ dp'dp$$
$$= \int_p \Phi^* \int_{p'} \Phi'\ \delta(p-p')dp'dp$$
$$= \int_p \Phi^*\Phi\ dp \ \Rightarrow\ \boxed{\text{PDF}(p) = |\Phi|^2 = \Phi^*\Phi}$$

$$\boxed{\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle}$$

Anything in x-space can be done in p-space

(or generalize to any transform, c_n)

$$x\Phi = xe^{-\frac{i}{\hbar}px} = -\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi = \frac{\hbar}{i}\frac{\partial}{\partial(-p)}\Phi$$

- $\langle p|\hat{p}|p'\rangle \equiv p\langle p|p'\rangle \equiv p\,\delta(p-p')$

1. $\langle p|\hat{p}|f\rangle = pf(p) = \boxed{p\langle p|f\rangle \equiv \breve{p}\langle p|f\rangle}$
2. $\langle p|\hat{x}|p'\rangle = \iint \langle p|x\rangle\langle x|\hat{x}|x'\rangle\langle x'|p'\rangle\, dxdx'$
   $= \frac{1}{2\pi\hbar}\int xe^{\frac{i}{\hbar}x(p'-p)}dx$
   $= -\frac{\hbar}{i}\delta'(p-p') = -\frac{\hbar}{i}\frac{\partial}{\partial p}\langle p|p'\rangle$
3. $\langle p|\hat{x}|f\rangle = \int \langle p|\hat{x}|p'\rangle\langle p'|f\rangle\ dp'$
   $= \boxed{-\frac{\hbar}{i}\frac{\partial}{\partial p}\langle p|f\rangle \equiv \breve{x}\langle p|f\rangle}$

$\Rightarrow\ A(x,\hat{p}_x) \to A(\hat{x}_p, p)$

$\Rightarrow\ \boxed{\langle a\rangle = \big\langle \Phi \big| A(\hat{x}_p, p) \big| \Phi\big\rangle}$

Heisenberg Uncertainty Proof:

$$\langle f|g\rangle \equiv \Big\langle \big(\widehat{A} - \langle a\rangle\big)\Psi \Big| \big(\widehat{B} - \langle b\rangle\big)\Psi \Big\rangle$$
$$= \Big\langle \Psi \Big| \big(\widehat{A} - \langle a\rangle\big) \Big| \big(\widehat{B} - \langle b\rangle\big)\Psi \Big\rangle$$
$$= \big\langle \Psi|\widehat{A}(\widehat{B}\Psi)\big\rangle - \langle a\rangle\langle b\rangle = \big\langle \widehat{A}\widehat{B}\big\rangle - \langle a\rangle\langle b\rangle$$

$$\sigma_A^2\sigma_B^2 = \|(\widehat{A} - \langle a\rangle)\Psi\|^2\ \|(\widehat{B} - \langle b\rangle)\Psi\|^2$$
$$\equiv \langle f|f\rangle\langle g|g\rangle \geq \|\langle f|g\rangle\|^2 \qquad \text{(see Schwarz Ineq.)}$$
$$\geq\ \big[\text{Im}\big(\langle f|g\rangle\big)\big]^2\ =\ \left(\frac{1}{2i}\big[\langle f|g\rangle - \langle f|g\rangle^*\big]\right)^2$$
$$= \left(\frac{1}{2i}\langle \widehat{A}\widehat{B} - \widehat{B}\widehat{A}\rangle\right)^2 \equiv \boxed{\left(\frac{1}{2i}\Big\langle \big[\widehat{A}, \widehat{B}\big]\Big\rangle\right)^2}$$

Commutator

- $\big[\widehat{A}, \widehat{B}\big]f \equiv \widehat{A}(\widehat{B}f) - \widehat{B}(\widehat{A}f)$
- $\big[A, BC\big] = \big[A,B\big]C + B\big[A,C\big]$
- $\big[AB, C\big] = A\big[B,C\big] + \big[A,C\big]B$
- $\big[x, \hat{p}\big] = i\hbar$
- $\boxed{\sigma_A\sigma_B\ \geq\ \left\|\frac{1}{2i}\Big\langle\big[\widehat{A},\widehat{B}\big]\Big\rangle\right\|}$

$\Rightarrow \boxed{\Delta x\Delta p\ \geq\ \hbar/2}$

- $\boxed{\begin{array}{l}\big[\hat{p}, f(x)\big] = \hat{p}f(x) = \frac{\hbar}{i}\frac{\partial f}{\partial x} \\ \big[\hat{x}, g(p)\big] = \hat{x}g(p) = -\frac{\hbar}{i}\frac{\partial g}{\partial p}\end{array}}$

Commutator of Hermitian $\widehat{A}, \widehat{B}$

- $\big[A,B\big]^\dagger = -\big[A,B\big]$
- $\exists\Psi_n$ s.t. $\big(\widehat{A}\Psi_n = a\Psi_n\big)$, $\big(\widehat{B}\Psi_n = b\Psi_n\big)$

$\Leftrightarrow \big[\widehat{A},\widehat{B}\big] = 0$

$\Rightarrow \boxed{\sigma_A\sigma_B\ \geq\ 0\ \text{(Both can be measured concurrently)}}$

$\boxed{AB = BA}$

Anti-Hermitian Operators: $A^\dagger = -A$

- $\langle A\rangle = ai, \quad a \in \mathbb{R}$
- $\big[A,B\big]^\dagger = -\big[A,B\big]$

Operator Evolution (Heisenberg Equation)

$$\frac{d}{dt}\Big\langle \Psi(x,t)\Big|Q\Big|\Psi(x,t)\Big\rangle = \Big\langle \frac{\partial\Psi}{\partial t}\Big|Q\Big|\Psi\Big\rangle + \Big\langle \Psi\Big|\frac{\partial Q}{\partial t}\Big|\Psi\Big\rangle + \Big\langle \Psi\Big|Q\Big|\frac{\partial\Psi}{\partial t}\Big\rangle$$

$$\boxed{\begin{aligned} \tfrac{d}{dt}\langle Q\rangle &= \tfrac{1}{i\hbar}\Big\langle \big[\widehat{Q},\widehat{H}\big]\Big\rangle + \Big\langle \tfrac{\partial\widehat{Q}}{\partial t}\Big\rangle \\ i\hbar\tfrac{d}{dt}\langle Q\rangle &= \Big\langle \big[\widehat{Q},\widehat{H}\big]\Big\rangle + i\hbar\Big\langle \tfrac{\partial\widehat{Q}}{\partial t}\Big\rangle \end{aligned}}$$

(Q is conserved when this equals 0)

- Conservations: $\dfrac{d\langle\Psi|\Psi\rangle}{dt} = 0, \quad \dfrac{d\langle H\rangle}{dt} = 0$
- Ehrenfest's Theorem: $m\dfrac{d\langle x\rangle}{dt} = \langle p\rangle, \quad \dfrac{d\langle p\rangle}{dt} = -\Big\langle \dfrac{\partial V}{\partial x}\Big\rangle \;\Rightarrow$ other classical eq.
- Virial Theorem: $\frac{d}{dt}\langle xp\rangle = \frac{i}{\hbar}\big\langle [H,x]p + x[H,p]\big\rangle = \Big\langle \big[\frac{p^2}{2m},x\big]p + x\big[V,p\big]\Big\rangle$

$$= \tfrac{i}{\hbar}\big\langle \tfrac{1}{2m}p[p,x]p - \tfrac{1}{2m}[p,x]p^2 - x[p,V]\big\rangle$$

$$\boxed{\frac{d\langle xp\rangle}{dt} = 2\langle T\rangle - \Big\langle x\frac{\partial V}{\partial x}\Big\rangle} \to 0 = \tfrac{d}{dt}\Big\langle \Psi_n(x)\Big|Q_{(x,p)}\Big|\Psi_n(x)\Big\rangle \quad \text{(for stationary states)}$$

- Energy-Time Uncertainty: $(Q = Q(x,\hat{p}) \neq Q(x,\hat{p},t)) \;\Rightarrow\; \sigma_H\sigma_Q \geq \frac{\hbar}{2}\left|\frac{d\langle Q\rangle}{dt}\right|$

$$\Rightarrow \boxed{\begin{aligned} \sigma_Q \;\equiv\; \frac{d\langle Q\rangle}{dt}\Delta t \;&\approx\; \Delta\langle Q\rangle \\ \sigma_H\left(\frac{\sigma_Q}{|d\langle Q\rangle/dt|}\right) &\geq \frac{\hbar}{2} \\ \Delta E\Delta t &\geq \frac{\hbar}{2} \end{aligned}}$$

Δt is the amount of time it would take $\langle Q\rangle$ to change "appreciably", or one std. dev. at the constant rate $\frac{d}{dt}\langle Q\rangle$

Mass Lifetime:

$\Delta(mc^2)\Delta t \geq \frac{\hbar}{2}$ ☑

Orthogonal Time Example:

$\Psi(x,\tau) = \frac{\sqrt{2}}{2}(\Psi_1 e^{-\frac{i}{\hbar}E_1\tau} + \Psi_2 e^{-\frac{i}{\hbar}E_2\tau})$

$\Big\langle \Psi(x,0)\big|\Psi(x,\tau)\Big\rangle = 0 = \frac{1}{2}(e^{-\frac{i}{\hbar}E_1\tau} + e^{-\frac{i}{\hbar}E_2\tau})$

$\Rightarrow\; \tau\,\frac{E_2-E_1}{2} = \frac{\pi}{2}\,\hbar\,(\frac{1}{2}+n) \geq \frac{\hbar}{2}$ ☑

Translation Operator

$$f(x+\Delta x) \approx f(x) + \frac{df}{dx}\Delta x$$

$$= f(x) + f'(x)\Delta x + \frac{f''(x)}{2!}(\Delta x)^2 + ... = \left\{ \begin{array}{l} f(x') = \sum_n \frac{f^{(n)}(a)}{n!}(x'-a)^n \\ (x' = x+\Delta x),\ (a = x) \end{array} \right\}$$

$$= \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!}(\Delta x)^n \ = \ \sum_{n=0}^{\infty} \frac{(\Delta x \nabla)^n}{n!} f(x)$$

$$\boxed{f(x+\Delta x) = e^{\frac{i}{\hbar}(\Delta x)\check{p}}\ f(x)} \ \Leftrightarrow \ \boxed{f(x) = e^{\frac{i}{\hbar}x\check{p}}\ f(0)} \quad * \ \langle x | e^{\frac{i}{\hbar}x\hat{p}} | x' \rangle = e^{\frac{i}{\hbar}x\check{p}}\langle x | x' \rangle \ *$$

Time Translation :

$$f(t+\Delta t) \ = \ \underline{f(t) + f'(t)\Delta t} + ... \ = \ \sum_n \frac{(\Delta t)^n}{n!}\left(\frac{\partial}{\partial t}\right)^n f(t)$$

$$\langle x_N | \hat{U}_{(t)} | x_0 \rangle = \check{U}_{(x_N,\, t;\, x_0,\, 0)}$$

$$\langle x | \hat{U}_{(t)} | \Psi \rangle = \Psi_{(x,\,t)}$$

$$i\hbar\frac{\partial}{\partial t}\Psi = \check{H}_{(x,\,p,\,t)}\Psi$$

$$\frac{\partial f}{\partial t} = \left[\frac{-i\check{H}}{\hbar}\right] f$$

$$\frac{\partial^n f}{\partial t^n} \neq \left[\frac{-i\check{H}(t)}{\hbar}\right]^n f$$

$$\Rightarrow \left\{ \begin{array}{l} f(t_0+\Delta t) \ \approx \ e^{\frac{-i\Delta t}{\hbar}\check{H}(t_0)} f(t_0) \quad \text{(1st order)} \\ \boxed{\begin{array}{l} f(0+t) = \lim_{N\to\infty} \prod_{n=0}^{N-1} e^{\frac{-i}{\hbar}\check{H}(n\Delta t)\Delta t} f(0) \\ \qquad \sim\neq e^{\frac{-i}{\hbar}\int \check{H}(t)\, dt} f(0) \quad \left(\begin{array}{c}\text{since } 0 \neq \\ [H(t_0), H(t_1)]\end{array}\right) \end{array}} \end{array} \right.$$

Pictures: $\big\langle Q \big\rangle_{(t)} = \langle \Psi_{(x,t)} \,|\, Q_{(x,p,t)} \,|\, \Psi_{(x,t)} \rangle$

- $$\boxed{\text{Schrodinger Picture: } \big\langle Q \big\rangle_{(t)} = \Big\langle e^{\frac{-i}{\hbar}t\widehat{H}}\,\Psi_{(t=0)} \Big| \ Q_{(x,p,t)} \ \Big| e^{\frac{-i}{\hbar}t\widehat{H}}\,\Psi_{(t=0)} \Big\rangle}$$

$$Q = Q(x,p) \ \Rightarrow \ \big\langle Q \big\rangle_{(t)} = \Big\langle \sum e^{\frac{-i}{\hbar}E_n t} c_n \Psi_{n(x)} \Big| \ Q \ \Big| \sum e^{\frac{-i}{\hbar}E_n t} c_n \Psi_{n(x)} \Big\rangle \quad \text{(nice for stationary states)}$$

- $$\boxed{\text{Heisenberg Picture: } \big\langle Q \big\rangle_{(t)} = \Big\langle \Psi_{(t=0)} \Big| e^{\frac{i}{\hbar}t\widehat{H}}\, Q\, e^{\frac{-i}{\hbar}t\widehat{H}} \Big| \Psi_{(t=0)} \Big\rangle}$$

- $$\boxed{\text{Dirac Picture: } \big\langle Q \big\rangle_{(t)} = \Big\langle e^{\frac{-i}{\hbar}\int \widehat{H}_1(t)dt}\,\Psi_{(t=0)} \Big| e^{\frac{i}{\hbar}t\widehat{H}_0}\, Q\, e^{\frac{-i}{\hbar}t\widehat{H}_0} \Big| \ e^{\frac{-i}{\hbar}\int \widehat{H}_1(t)dt}\,\Psi_{(t=0)} \Big\rangle}$$

$$\big\langle Q \big\rangle_{(t+\Delta t)} \ = \ \big\langle Q \big\rangle_{(t)} + \tfrac{d\langle Q \rangle}{dt}\Delta t + ... \quad \Rightarrow$$

A 1st order approximation of $\big\langle Q \big\rangle_{(t+\Delta t)}$ should yield $\frac{d\langle Q \rangle}{dt} = \frac{1}{i\hbar}\Big\langle \big[Q, H\big] \Big\rangle + \frac{\partial Q}{\partial t}$

Schrodinger Picture

1.) $i\hbar\frac{\partial}{\partial t}\langle Q_S\rangle = \langle[Q_S, H_S]\rangle$

4.) $|\Psi_{S(t)}\rangle = U_{S(t,t_0)}|\Psi_{S(t_0)}\rangle$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}|\Psi_S\rangle = H_S\Psi_S = [H_S^0 + H^1_{S(t)}]|\Psi_S\rangle$$

$$= \sum E_n|n_S^0\rangle e^{-\frac{i}{\hbar}E_n t}\langle n^1_{S(t)}|\Psi(0)\rangle$$
$$+\sum |n_S^0\rangle e^{-\frac{i}{\hbar}E_n t}\cdot i\hbar\frac{\partial}{\partial t}\langle n^1_{S(t)}|\Psi(0)\rangle$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}U^0_{S(t,t_0)} = H_S^0 U^0_{S(t,t_0)}$$

$$\Rightarrow\ U^0_{S(t,t_0)} = e^{-\frac{i}{\hbar}H_S^0(t-t_0)}$$

Heisenberg Picture

1.) $Q_{H(t)}\ \equiv\ U_S^\dagger Q_S U_S$ $\qquad \begin{array}{c} H_S \neq H_S(t) \\ \Downarrow \\ H_H = H_S \end{array}$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}Q_H = [Q_H, H_H]$$

2.) $U_H\ \equiv\ U^\dagger_{S(t,t_0)}U_{S(t,t_0)} = \mathbb{I}$

3.) $|q_{H(t)}\rangle\ \equiv\ U^\dagger_{S(t,t_0)}|q_S\rangle$

$$\Rightarrow\ Q_H|q_{H(t)}\rangle = q|q_{H(t)}\rangle$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}|q_{H(t)}\rangle = -H_S|q_{H(t)}\rangle$$

4.) $|\Psi_H\rangle\ \equiv\ U^\dagger_{S(t,t_0)}|\Psi_{S(t)}\rangle = |\Psi_{S(t_0)}\rangle$

$$=\ U_{H(t,t_0)}|\Psi_{H(t_0)}\rangle$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}|\Psi_H\rangle = 0$$

Dirac/Interaction Picture (see transition amplitude)

1.) $Q_{I(t)}\ \equiv\ U_S^{0\dagger}Q_S U_S^0$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}Q_I = \left[Q_I, H_I^0\right] \qquad (H_S^0 = H_I^0\ \text{ see Heis. pic.})$$

2.) $U_{I(t,t_0)}\ \equiv\ U_S^{0\dagger}{}_{(t,t_0)}U_{S(t,t_0)}$

3.) $|q_{I(t)}\rangle\ \equiv\ U_S^{0\dagger}{}_{(t,t_0)}|q_S\rangle$

$$\Rightarrow\ Q_I|q_{I(t)}\rangle = q|q_{I(t)}\rangle$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}|q_{I(t)}\rangle = -H_S^0|q_{I(t)}\rangle$$

4.) $|\Psi_{I(t)}\rangle\ \equiv\ U_S^{0\dagger}{}_{(t,t_0)}|\Psi_{S(t)}\rangle$

$$=\ U_{I(t,t_0)}|\Psi_{I(t_0)}\rangle \qquad (\text{since } |\Psi_I(t_0)\rangle = |\Psi_S(t_0)\rangle)$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}|\Psi_I\rangle = U_S^{0\dagger}H^1_{S(t)}U_S^0|\Psi_I\rangle = H_I^1|\Psi_I\rangle$$

$$\Rightarrow\ i\hbar\frac{\partial}{\partial t}U_{I(t,t_0)} = H^1_{I(t)}U_{I(t,t_0)}$$

$$\Rightarrow\ U_{I(t,t_0)} = \mathbb{I} + \frac{1}{i\hbar}\int_{t_0}^t H^1_{I(t')}U_{I(t',t_0)}\,dt'$$

- $U_{I(t,t_0)} = \mathbb{I} + \frac{1}{i\hbar}\int_{t_0}^t H^1_{I(t')}U_{I(t',t_0)}\,dt'$

$$= \mathbb{I} + \mathcal{O}(H_I^1)$$
$$= \mathbb{I} + \frac{1}{i\hbar}\int_{t_0}^t H^1_{I(t')}\,dt' + \mathcal{O}([H_I^1]^2)$$
$$= \mathbb{I} + \frac{1}{i\hbar}\int_{t_0}^t H^1_{I(t')}\,dt'$$
$$+\left(\frac{1}{i\hbar}\right)^2\int_{t_0}^t\int_{t_0}^{t'} H^1_{I(t')}H^1_{I(t'')}\,dt''dt' + \ldots$$

- $U_{S(t,t_0)} = U_S^0 + \frac{1}{i\hbar}\int_{t_0}^t U_S^0 H^1_{I(t')}\,dt' + \left(\frac{1}{i\hbar}\right)^2\int_{t_0}^t\int_{t_0}^{t'} U_S^0 H^1_{I(t')}H^1_{I(t'')}\,dt''dt' + \ldots$

$$= U^0{}_{(t,t_0)}$$
$$+\frac{1}{i\hbar}\int_{t_0}^t U^0{}_{(t,t_0)}U^{0\dagger}{}_{(t',t_0)}H^1 U^0{}_{(t',t_0)}\,dt'$$
$$+\left(\frac{1}{i\hbar}\right)^2\int_{t_0}^t\int_{t_0}^{t'} U^0{}_{(t,t_0)}U^{0\dagger}{}_{(t',t_0)}H^1 U^0{}_{(t',t_0)}U^{0\dagger}{}_{(t'',t_0)}H^1 U^0{}_{(t'',t_0)}\,dt''dt' + \ldots$$

Infinitismal t Path Integral

$$S[x(t)] = \int_0^t \mathcal{L}(x,\dot{x})\,dt \;\rightarrow\; \mathcal{L}\delta t = \left[\tfrac{1}{2}m\left(\tfrac{x_1-x_0}{\delta t}\right)^2 - V\left(\tfrac{x_1+x_0}{2}, t_0+\tfrac{\delta t}{2}\right)\right]\delta t$$

$$\langle x|\hat{U}(\epsilon)|\Psi\rangle = \int \langle x|\hat{U}(\epsilon)|x'\rangle\langle x'|\Psi(x,t)\rangle\,dx' = \int \breve{U}(x,t+\epsilon;\,x',t)\Psi(x',t)\,dx' = \Psi(x,t+\epsilon)$$

- $$\begin{aligned}
\breve{U}(x_1,\epsilon;\,x_0,0) &= Ae^{\frac{i}{\hbar}S} = Ae^{\frac{i}{\hbar}\mathcal{L}\epsilon} \\
&= A\exp\left\{\tfrac{i}{\hbar}\left[\tfrac{1}{2}m\tfrac{(x_1-x_0)^2}{\epsilon} - \epsilon V\left(\tfrac{x_1+x_0}{2}, 0+\tfrac{\epsilon}{2}\right)\right]\right\} \\
(\eta = x_0 - x_1) \quad &= A\exp\left\{\tfrac{i}{\hbar}\left[\tfrac{1}{2}m\tfrac{\eta^2}{\epsilon}\right]\right\}\exp\left\{-\tfrac{i}{\hbar}\epsilon V(x_1+\tfrac{\eta}{2}, 0+\tfrac{\epsilon}{2})\right\} \\
&\approx A\exp\left\{\tfrac{i}{\hbar}\left[\tfrac{1}{2}m\tfrac{\eta^2}{\epsilon}\right]\right\}\exp\left\{-\tfrac{i}{\hbar}\epsilon V(x_1,0)\right\} \\
&\approx A\exp\left\{\tfrac{i}{\hbar}\left[\tfrac{1}{2}m\tfrac{\eta^2}{\epsilon}\right]\right\}\left[1-\tfrac{i}{\hbar}\epsilon V(x_1,0)\right]
\end{aligned}$$

$\frac{\eta^2}{\epsilon} \lesssim \pi$ Explanation

The integral involving $\breve{U}$ is over all η. The phase of the complex exponential will vary/oscillate too wildly and destructively interfere if η^2/ϵ were to grow too big, so $\eta^2 \sim \epsilon$ is all that matters. This means the integral is over $\sqrt{\epsilon}$, not ϵ. Because of this (somehow, Bibl. given), using a finite difference formula for derivatives is legitimate in this case, though not in general.

$$\begin{aligned}
\Psi(x,\epsilon) &= \int_{-\infty}^{\infty} \breve{U}(x,\epsilon;\,x',0)\Psi(x',0)\,dx' \\
&= A\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}S}\Psi(x',0)\,dx' \\
&= A\int_{-\infty}^{\infty} \exp\left\{\tfrac{i}{\hbar}\left[\tfrac{1}{2}m\tfrac{(x-x')^2}{\epsilon} - \epsilon V\left(\tfrac{x+x'}{2}, 0+\tfrac{\epsilon}{2}\right)\right]\right\}\Psi(x',0)\,dx' \\
&= A\int_{-\infty}^{\infty} \exp\left\{\tfrac{i}{\hbar}\left[\tfrac{1}{2}m\tfrac{\eta^2}{\epsilon} - \epsilon V\left(\tfrac{x+\eta/2}{2}, 0+\tfrac{\epsilon}{2}\right)\right]\right\}\Psi(x+\eta,0)\,d\eta \\
&\approx A\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\left[\frac{1}{2}m\frac{\eta^2}{\epsilon}\right]}\left[1-\tfrac{i}{\hbar}\epsilon V(x,0)\right]\left[\Psi(x,0)+\eta\Psi'(x,0)+\tfrac{\eta^2}{2}\Psi''(x,0)\right]d\eta \\
&\approx A\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\left[\frac{1}{2}m\frac{\eta^2}{\epsilon}\right]}\left[\left(1-\tfrac{i}{\hbar}\epsilon V(x,0)\right)\Psi(x,0)+\cancel{\eta\Psi'(x,0)}+\tfrac{\eta^2}{2}\Psi''(x,0)\right]d\eta \\
&= \cancel{A\sqrt{\tfrac{2\hbar\epsilon\pi}{-im}}}\left[\left(1-\tfrac{i}{\hbar}\epsilon V(x,0)\right)+\tfrac{1}{2}\cdot\tfrac{2\hbar\epsilon}{-im}\cdot\tfrac{1}{2}\tfrac{\partial^2}{\partial x^2}\right]\Psi(x,0) \\
&= \Psi(x,0) - \tfrac{i}{\hbar}\epsilon\breve{H}\Psi(x,0)
\end{aligned}$$

$$\boxed{i\hbar\,\frac{\Psi(x,\epsilon)-\Psi(x,0)}{\epsilon-0} = \breve{H}\Psi(x,0)}$$

Finite t, Free Particle Propagator

$$S[x(t)] = \int_0^t \mathcal{L}(x,\dot{x})\,dt = \lim_{N\to\infty} \sum_{n=0}^{N-1} \left[\tfrac{1}{2} m \left(\tfrac{x_{n+1}-x_n}{\delta t}\right)^2\right] \delta t$$

$$\langle x_N|\hat{U}(t)|\Psi(0)\rangle = \int \langle x_N|\hat{U}(t)|x_0\rangle \Psi(x_0,0)\ dx_0 = \int \breve{U}(x_N,t;\,x_0,0)\Psi(x_0,0)\ dx_0 = \Psi(x_N,t)$$

$$\Rightarrow\ \ \langle x_N|\hat{U}(t)|x_0\rangle = \langle x_N|e^{-\frac{i}{\hbar}Ht} e^{\frac{i}{\hbar}Ht_0}|x_0\rangle = \langle x_N, t_N\,|\,x_0, t_0\rangle$$

$$\langle x_N|\hat{U}(t)|x_0\rangle = \lim_{N\to\infty} \langle x_N|\hat{U}^N(\epsilon)|x_0\rangle = \lim_{N\to\infty} \langle x_N|\hat{U}(\epsilon)\ldots\hat{U}(\epsilon)\hat{U}(\epsilon)|x_0\rangle$$

$$= \lim_{N\to\infty} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle x_N|\hat{U}(\epsilon)|x_{N-1}\rangle \ldots \langle x_2|\hat{U}(\epsilon)|x_1\rangle\langle x_1|\hat{U}(\epsilon)|x_0\rangle\ dx_1\,dx_2\ldots dx_{N-1}$$

$$\breve{U}(x_N,t;\,x_0,0) = \int_{x_0}^{x_N} Ae^{\frac{i}{\hbar}S}\,\mathcal{D}[x(t)]$$

$$= \lim_{N\to\infty} A\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\left[\frac{1}{2}m\frac{(x_1-x_0)^2}{\epsilon}+\frac{1}{2}m\frac{(x_2-x_1)^2}{\epsilon}+\frac{1}{2}m\frac{(x_3-x_2)^2}{\epsilon}+\ldots\right]} dx_1\,dx_2\ldots dx_{N-1}$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \int\cdots\int_{-\infty}^{\infty} e^{-\frac{(y_1-y_0)^2}{i}-\frac{(y_2-y_1)^2}{i}}\ dy_1\,e^{\left[-\frac{(y_3-y_2)^2}{i}\cdots\right]}\,dy_2\ldots$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \int\cdots\int_{-\infty}^{\infty} e^{-\frac{y_1^2+y_1^2-2y_1(y_2+y_0)+y_2^2+y_0^2}{i}}\ dy_1\ldots$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \int\cdots\int_{-\infty}^{\infty} e^{-\frac{1}{i}\left(2\left[y_1^2-y_1(y_0+y_2)+\frac{(y_0+y_2)^2}{4}\right]-\frac{(y_2+y_0)^2}{2}+y_2^2+y_0^2\right)}\ dy_1\ldots$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \int\cdots\int_{-\infty}^{\infty} e^{-\frac{2}{i}\left[y_1-\cancel{\frac{y_2+y_0}{2}}\right]^2}\ dy_1\,e^{-\frac{(y_2-y_0)^2}{2i}}\ e^{-\frac{(y_3-y_2)^2}{i}\cdots}\ dy_2\,e^{[\ldots]}\ldots$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \int\ldots\sqrt{\tfrac{\pi i}{2}}\int_{-\infty}^{\infty} e^{-\frac{(y_2-y_0)^2}{2i}}\ e^{-\frac{(y_3-y_2)^2}{i}\cdots}\ dy_2\ldots$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \int\ldots\sqrt{\tfrac{(\pi i)^2}{3}}\int_{-\infty}^{\infty} e^{-\frac{(y_3-y_0)^2}{3i}}\ e^{-\frac{(y_4-y_3)^2}{i}\cdots}\ dy_3\ldots$$

$$= \lim_{N\to\infty} A\sqrt{\tfrac{2\hbar\epsilon}{m}}^{N-1} \sqrt{\tfrac{(\pi i)^{N-1}}{N}}\ e^{-\frac{(y_N-y_0)^2}{Ni}} \ \ = \lim_{N\to\infty} A\cancel{\sqrt{\tfrac{2\hbar\epsilon\pi}{-im}}^N}\sqrt{\tfrac{-im}{2\hbar\epsilon N\pi}}\ e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_N-x_0)^2}{N\epsilon}}$$

$$\boxed{\text{Free Particle}:\ \ \breve{U}(x_N,t;\,x_0,0) = \sqrt{\tfrac{-im}{2\hbar t\pi}}\ e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_N-x_0)^2}{t}}}$$

$$\boxed{\int_{x_0}^{x_N}\mathcal{D}[x(t)] = \lim_{N\to\infty}\sqrt{\tfrac{-im}{2\hbar\epsilon\pi}}\int_{-\infty}^{\infty}\sqrt{\tfrac{-im}{2\hbar\epsilon\pi}}\,dx_1\cdots\int_{-\infty}^{\infty}\sqrt{\tfrac{-im}{2\hbar\epsilon\pi}}\,dx_{N-1}}$$

All Paths Explanation

$$S[x] = S[x_{cl}] + \cancel{S'[x_{cl}]}\eta + \mathcal{O}(\eta^2)$$

1^{st} order variation of S from x_{cl} equals 0. This means propagator integrand for paths near x_{cl} will have about the same phase, and will add constructively. Paths very different from x_{cl} (like those with faster than light motion) will vary in action, and because $\hbar$ is so small their phases will vary wildly, meaning the sum will destructively interfere. The result is that only paths near the classical path will be important, with $S[x]/\hbar \lesssim \pi$.

Action-Energy Relationship

$$S(x_{cl} + \Delta x_{cl}, \dot{x} + \Delta \dot{x}_{cl}, \tau + \Delta\tau) = S_{cl} + \Delta S_{cl}$$

$$= \int_0^{\tau+\Delta\tau} \mathcal{L}\big(x_{cl} + \Delta x_{cl}, \dot{x}_{cl} + \Delta\dot{x}_{cl}, t\big)\, dt$$

$$dS = \tfrac{\partial S}{\partial \tau} d\tau + \Big[\tfrac{\partial S}{\partial x} dx + \tfrac{\partial S}{\partial \dot{x}} d\dot{x} = \int (dL) dt\Big] \qquad (\eta = dx,\ \eta(0) = 0)$$

$$\Delta S_{cl} = \mathcal{L}(\tau)\,\Delta\tau + \int_0^\tau \tfrac{\partial \mathcal{L}}{\partial x}\Big|_{cl}\, \eta + \tfrac{\partial \mathcal{L}}{\partial \dot{x}}\Big|_{cl}\, \dot{\eta}\, dt$$

$$= \mathcal{L}(\tau)\,\Delta\tau + \int_0^\tau \cancel{\Big[\tfrac{\partial \mathcal{L}}{\partial x} - \tfrac{d}{dt}\tfrac{\partial \mathcal{L}}{\partial \dot{x}}\Big]_{cl}}\eta + \tfrac{d}{dt}\Big[\tfrac{\partial \mathcal{L}}{\partial \dot{x}_{cl}}\eta\Big]\, dt$$

$$= \Big[\mathcal{L} + \tfrac{\partial \mathcal{L}}{\partial \dot{x}}\dot{x}\Big]_{cl,\tau}\, \Delta\tau$$

$$\boxed{\Delta S_{cl} = -H(t_f)\,\Delta t_f}$$

(Time-Independent) Hamiltonian-Lagrangian Propagator Relationship / Finite Path Integral

$$\breve{U}(x_N, t; x_0, 0) = \langle x_N | e^{-\frac{i}{\hbar}Ht} | x_0 \rangle = \langle x_N | [e^{-\frac{i}{\hbar}H\frac{t}{N}}]^N | x_0 \rangle = \lim_{N\to\infty} \langle x_N | [e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(\hat{x})\epsilon}]^N | x_0 \rangle \qquad \text{(not trivial)}$$

$$= \lim_{N\to\infty} \int_{x\ldots} \langle x_N | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(\hat{x})\epsilon} | x_{N-1} \rangle \ldots \langle x_1 | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(\hat{x})\epsilon} | x_0 \rangle\, dx \ldots$$

$$= \lim_{N\to\infty} \int_{x\ldots} \ldots \Big[\underbrace{\int \langle x_1 | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\epsilon} | p \rangle \langle p | x_0 \rangle\, dp}_{\text{free part. prop.}}\, e^{-\frac{i}{\hbar}V(x_0)\epsilon} \Big] dx \ldots$$

$$1. = \lim_{N\to\infty} \int_{x\ldots} \ldots \Big[\int \frac{e^{\frac{i}{\hbar}p(x_1 - x_0)}}{2\pi\hbar} e^{-\frac{i}{\hbar}\frac{p^2}{2m}\epsilon} e^{-\frac{i}{\hbar}V(x_0)\epsilon}\, dp \Big] dx \ldots = \boxed{\int e^{\frac{i}{\hbar}\int p\dot{x} - H(x,p)\, dt}\, [\mathcal{D}x\mathcal{D}p] \qquad \text{(Phase Space)}}$$

$$2. = \lim_{N\to\infty} \int_{x\ldots} \ldots \Big[\sqrt{\tfrac{-im}{2\pi\hbar\epsilon}}\, e^{\frac{im(x_1 - x_0)^2}{\epsilon}}\, e^{-\frac{i}{\hbar}V(x_0)\epsilon} \Big] dx \cdots = \lim_{N\to\infty} \int_{x\ldots} \ldots \sqrt{\tfrac{-im}{2\pi\hbar\epsilon}}\, e^{\frac{i}{\hbar}\mathcal{L}\epsilon}\, dx_1 \ldots$$

$$= \boxed{\int_{x_0}^{x_N} e^{\frac{i}{\hbar}S}\, [\mathcal{D}x] = \int_{x_0}^{x_N} e^{\frac{i}{\hbar}\int \mathcal{L}\, dt}\, [\mathcal{D}x] \qquad \text{(Configuration Space)}} \qquad \text{(above is only integrable if } p \text{ is quadratic in } H)$$

Trace of Propagator

$$G(t) = \int \langle x | e^{-\frac{i}{\hbar}Ht} | x \rangle\, d^3x$$

$$= \sum_n \int \langle x | n \rangle e^{-\frac{i}{\hbar}E_n t} \langle n | x \rangle\, dx$$

$$G(t) = \sum_n e^{-\frac{i}{\hbar}E_n t} \sim \sum_n e^{-\beta E_n} = Z(\beta)$$

1.3 Extra

$L_2 \subset$ Hilbert Space = complete inner product space

$\rho(x,t) \equiv \|\Psi\|^2 \quad , \quad P_a^b(t) = \int_a^b \rho\, dx \quad , \quad P(t) = P_{-\infty}^{\infty}(t) \quad , \quad \Psi = \sqrt{\rho}\, e^{\frac{i}{\hbar}S}$ e.g., $e^{\frac{i}{\hbar}(p\cdot x - Et)}$

- $$\begin{aligned} \breve{E}\rho &= \breve{E}(\Psi^*\Psi) = \Psi^*(\breve{E}\Psi) + \Psi(\breve{E}\Psi^*) \\ &= \Psi^*(\breve{H}\Psi) - \Psi(\breve{H}\Psi^*) \\ &= \Psi^*(\tfrac{p^2}{2m} + V)\Psi - \Psi(\tfrac{p^2}{2m} + V)\Psi^* \\ -\tfrac{\hbar}{i}\tfrac{\partial\rho}{\partial t} &= \tfrac{\hbar}{i}\nabla\cdot\left(\Psi^*\tfrac{p}{2m}\Psi - \Psi\tfrac{p}{2m}\Psi^*\right) \end{aligned}$$

  (Probability Current)

  $$\begin{aligned} \tfrac{\partial\rho}{\partial t} &= -\nabla\cdot J = -\nabla\cdot\left(\Psi^*\tfrac{p}{2m}\Psi - \Psi\tfrac{p}{2m}\Psi^*\right) \\ &= -\nabla\cdot\tfrac{\rho\nabla S}{m} \quad \left(\text{e.g., } \nabla S = p\right) \end{aligned}$$

  $$\left[\tfrac{d}{dt}P_a^b = J(a,t) - J(b,t)\right], \quad \left[\int J\, dV = \langle\Psi|\tfrac{p}{m}|\Psi\rangle = \tfrac{\langle p\rangle}{m}\right]$$

- $(V \in \mathbb{R}) \quad \Rightarrow \quad \frac{d}{dt}P = 0 \quad \Rightarrow \quad P(t) \equiv 1$

  $(V = V_0 - i\Gamma) \quad \Rightarrow \quad \frac{d}{dt}P = \frac{-2\Gamma}{\hbar}P \quad \Rightarrow \quad P(t) = e^{-2(\Gamma/\hbar)t}$

- $\langle\Psi_n|\Psi_n\rangle\ ,\ \langle\Psi_m|\Psi_m\rangle = 1 \ \Rightarrow\ \frac{d}{dt}\langle\Psi_n|\Psi_m\rangle = 0$

Schwarz Inequality:
$$\left\|\int_a^b f^* g\ dx\right\|^2 \leq \left\|\int_a^b f^* f\ dx\right\| \left\|\int_a^b g^* g\ dx\right\|$$
$$\|\langle f|g\rangle_{ab}\|^2 \leq \|\langle f|f\rangle_{ab}\|\, \|\langle g|g\rangle_{ab}\|$$

$$\Big[V(x) = V(-x)\Big] \ \Rightarrow\ \Big[\Psi(x) \Rightarrow \Psi(-x)\Big] \ \Rightarrow\ \Big[\Psi(-x) = \Psi(x)\Big] \ \cup\ \Big[\Psi(-x) = -\Psi(x)\Big]$$

Discontinuity in Ψ means the possiblity of $\sigma_p \to \infty$

Prob 3.29: $\Psi(x,0) = \begin{cases} \frac{1}{\sqrt{2n\lambda}} e^{2\pi i x/\lambda}, & -n\lambda < x < n\lambda \\ 0 & \text{else} \end{cases}$

$\sigma_p \to \infty$ because the integral of $\delta^2(x)$ is infinite

$$\int_{-\infty}^{\infty} f(x)D_1(x)dx = \int_{-\infty}^{\infty} f(x)D_2(x)dx \ \Rightarrow\ \delta(cx) = \frac{1}{|c|}\delta(x)$$

$$\delta(x - x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x')}dx' \ \Rightarrow\ F[\delta(x)] = \frac{1}{2\pi}$$

$$\delta'(x - x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} ike^{ik(x-x')}dx' \ \Rightarrow\ \int \delta'(x - x')f(x')dx' = f'(x)$$

Poisson Brackets

$$\{f,g\} = \sum_i \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i}\frac{\partial f}{\partial p_i}$$

$$\{\omega(q,p,t), H\} = \sum_i \frac{\partial \omega}{\partial q_i}\dot{q} + \dot{p}\frac{\partial \omega}{\partial p_i} = \dot{\omega} - \frac{\partial \omega}{\partial t}$$

Hamilton Eq. : $\dot{q} = \{q, H\},\ \dot{p} = \{p, H\}$

Canonical Transforms

$$\begin{matrix} q \to \bar{q}(q,p) \\ p \to \bar{p}(q,p) \end{matrix} \quad \text{s.t.} \quad \begin{matrix} \{\bar{q}_i, \bar{q}_j\} = 0 = \{\bar{p}_i, \bar{p}_j\} \\ \{\bar{q}_i, \bar{p}_j\} = \delta_{ij} \end{matrix} \quad \left(\begin{matrix}\text{Point Transforms} \\ \bar{q}(q) \text{ are canonical.}\end{matrix}\right)$$

$$\Rightarrow \begin{matrix} \dot{\bar{q}} = \frac{\partial H}{\partial \bar{p}} \\ \dot{\bar{p}} = -\frac{\partial H}{\partial \bar{q}} \end{matrix} \quad , \quad \{f,g\}_{q,p} = \{f,g\}_{\bar{q},\bar{p}}$$

Generator of Transformation

1. $\delta H = 0$

2. $\bar{q}_i = q_i + \delta q_i \quad , \quad \bar{p}_i = p_i + \delta p_i$

$$\begin{aligned} &\equiv q_i + \epsilon_\lambda \frac{\partial g}{\partial p_i} && \equiv p_i - \epsilon_\lambda \frac{\partial g}{\partial q_i} \\ &= q_i + \epsilon_\lambda\{q_i, g\} && = p_i + \epsilon_\lambda\{p_i, g\} \end{aligned}$$

3. $\Rightarrow\ \delta f = \epsilon_\lambda\{f,g\}\ \to\ \frac{\partial f}{\partial \lambda} = \{f,g\}$

$$\delta H = \epsilon_\lambda\{H,g\}$$

$$\Rightarrow \boxed{\frac{\partial H}{\partial \lambda} = 0 = \frac{dg}{dt}}$$

(e.g. $g = p$ or $g = l_z$)

$$g = l_z$$

$$\Rightarrow \begin{matrix} \delta x = -\epsilon y = -(\delta\theta) y \\ \delta y = \epsilon x = (\delta\theta) x \end{matrix}$$

$$\Rightarrow \boxed{\begin{matrix} \frac{\partial x}{\partial \theta} = -y \\ \frac{\partial y}{\partial \theta} = x \end{matrix}}$$

Tensors and Tensor Operators

rank-2 Tensor : $|t^{(2)}\rangle = \sum_{i=1}^{3}\sum_{j=1}^{3} t_{ij}|i\rangle|j\rangle = \sum_{i=1}^{3}\sum_{j=1}^{3} |ij\rangle\langle ij|t^{(2)}\rangle$

rank-2 Carte. Tens. Oper., T_{ij} : Set of $3^{n=2}$ Operators

rank-k Spher. Tens. Oper., T_k^q : Set of $2k+1$ Operators s.t. $U[R]T_k^q U^\dagger[R] = \sum_{q'=-k}^{k} D^k_{q'q} T_k^{q'}$

$$\begin{aligned} \Rightarrow UT_k^q U^\dagger U|jm\rangle &= \sum_{q'}\sum_{m'} D^k_{q'q} D^j_{m'm} T^k_{q'}|jm'\rangle \\ \sim\ U|kq\rangle|jm\rangle &= \sum_{q'}\sum_{m'} D^k_{q'q} D^j_{m'm} |kq'\rangle|jm'\rangle \end{aligned}$$

(CG coeff.)

Wigner-Eckhart : $\langle \alpha_2 j_2 m_2 | T_k^q | \alpha_1 j_1 m_1\rangle = \langle \alpha_2 j_2 | T_k | \alpha_1 j_1\rangle \cdot \langle j_2 m_2 | kq, j_1 m_1\rangle$

Functions

Associated Legendre Functions: $P_l^m \equiv \sqrt{1-x^2}^{\ |m|}\left(\frac{d}{dx}\right)^{|m|} P_l(x)$ (not a polynomial if odd)

Legendre Polynomials: $P_l(x) \equiv \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2 - l)^l$

Associated Laguerre Polynomials: $L \equiv$

Laguerre Polynomials: $L_\equiv$

2 Simple 1D Potentials

2.1 Infinite Square Well (1-D)

$$\boldsymbol{V(x)} = \begin{cases} \mathbf{0} & \boldsymbol{0 < x < a} \\ \infty & \text{otherwise} \end{cases}$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin k_n x$$

$$k_n = \frac{2\pi}{\lambda} = \frac{2\pi}{2a/n} = \frac{n\pi}{a} \qquad \forall n = 1, 2, 3, ... \qquad \boxed{!!\ \hat{p}\Psi_n \neq p\Psi_n\ !!}$$

wave isn't infinite

$$E_n = \frac{p^2}{2m} = \frac{\hbar^2 k_n^2}{2m}$$

2.1.1 3-D Rectangular Box

$$\Psi_{n_x n_y n_z}(x, y, z) = \Psi_{n_x}(x)\Psi_{n_y}(y)\Psi_{n_z}(z) = \sqrt{\frac{8}{a_x a_y a_z}}(\sin k_{n_x} x)(\sin k_{n_y} y)(\sin k_{n_z} z)$$

$$k_{n_i} = \frac{n_i \pi}{a_i} \qquad \forall n_x, n_y, n_z = 1, 2, 3, ...$$

$$E_{n_x n_y n_z} = \frac{\hbar^2}{2m}(k_{n_x}^2 + k_{n_y}^2 + k_{n_z}^2)$$

2.2 Harmonic Oscillator (1-D): $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$

$$\begin{aligned}\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 &= \frac{1}{2m}\left(p^2 + m^2\omega^2x^2\right)\\ &= \frac{1}{2m}\left(-ip + m\omega x\right)\left(ip + m\omega x\right) \sim E \sim \hbar\omega\end{aligned} \quad \Rightarrow \quad \boxed{a = a_- = \frac{1}{\sqrt{2m}}\frac{1}{\sqrt{\hbar\omega}}\left(i\hat{p} + m\omega x\right)}$$

$$\boxed{\begin{aligned}aa^\dagger &= \frac{H}{\hbar\omega} + \frac{1}{2}\\ aa^\dagger|n\rangle &= (\frac{E_n}{\hbar\omega} + \frac{1}{2})|n\rangle\end{aligned}}\ ,\ \boxed{\begin{aligned}a^\dagger a &= \frac{H}{\hbar\omega} - \frac{1}{2}\\ a^\dagger a|n\rangle &= (\frac{E_n}{\hbar\omega} - \frac{1}{2})|n\rangle\end{aligned}} \ \rightarrow\ \boxed{\left[a, a^\dagger\right] = 1} \ \leftarrow\ \boxed{\begin{aligned}H &= \hbar\omega(a^\dagger a + \tfrac{1}{2})\\ &= \hbar\omega(aa^\dagger - \tfrac{1}{2})\end{aligned}}$$

or $\left[H, a_\pm\right] = (\pm\hbar\omega)a_\pm$

$$\begin{aligned}(aa^\dagger)a\Psi_n &= a(a^\dagger a)\Psi_n\\ \left(\frac{H}{\hbar\omega} + \frac{1}{2}\right)a\Psi_n &= a\left(\frac{H}{\hbar\omega} - \frac{1}{2}\right)\Psi_n\\ \left(\frac{E_{an}}{\hbar\omega} + \frac{1}{2}\right)a\Psi_n &= \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)a\Psi_n\\ E_{an}(a\Psi_n) &= (E_n - \hbar\omega)(a\Psi_n)\\ &\Downarrow\\ E_{n-1}|n-1\rangle &= (E_n - \hbar\omega)|n-1\rangle\end{aligned}$$

$$\begin{aligned}(a^\dagger a)a^\dagger|n\rangle &= a^\dagger(aa^\dagger)|n\rangle\\ \left(\frac{H}{\hbar\omega} - \frac{1}{2}\right)a^\dagger|n\rangle &= a^\dagger\left(\frac{H}{\hbar\omega} + \frac{1}{2}\right)|n\rangle\\ \left(\frac{E_{a^\dagger n}}{\hbar\omega} - \frac{1}{2}\right)\cancel{c_n}|a^\dagger n\rangle &= \left(\frac{E_n}{\hbar\omega} + \frac{1}{2}\right)\cancel{c_n}|a^\dagger(n)\rangle\\ E_{a^\dagger n}|a^\dagger n\rangle &= (E_n + \hbar\omega)|a^\dagger(n)\rangle\\ &\Downarrow\\ E_{n+1}|n+1\rangle &= (E_n + \hbar\omega)|n+1\rangle\end{aligned}$$

(Why ladders):

(use induction)

$$\boxed{\left[\frac{H}{\hbar\omega}, a_\pm\right] = (\pm1)a_\pm} \ \Rightarrow\ \left[\frac{H}{\hbar\omega}, a_\pm^m\right] = (\pm1)ma_\pm$$

$$\boxed{\frac{H}{\hbar\omega}|n\rangle = \frac{E_n}{\hbar\omega}|n\rangle = c_n|n\rangle} \ \Rightarrow\ \frac{H}{\hbar\omega}a_\pm^m|n\rangle = (\pm1\cdot m + c_n)|n\rangle$$

$$\begin{aligned}Ha_\pm^m|n\rangle &= \hbar\omega(c_n \pm m)a_\pm^m|n\rangle\\ *\ Ha_\pm^n|0\rangle &= \hbar\omega(c_0 \pm n)a_\pm^n|0\rangle\ *\\ &= E_{n0}\cdot a_\pm^n|0\rangle\end{aligned}$$

$E_n \geq \mathrm{Min}(V) \ \Rightarrow\ a\Psi_0 = 0$ (else is un-normalizable)

$$\begin{aligned}0 &= (ip + m\omega x)\Psi_0\\ \hbar\frac{d}{dx}\Psi_0 &= -m\omega x\Psi_0\end{aligned}$$

$$\boxed{\begin{aligned}\Psi_0 &= Ae^{-\frac{m\omega}{\hbar}\frac{x^2}{2}}\\ A &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\\ \frac{1}{\sigma^2} &= \frac{m\omega}{\hbar}\end{aligned}}$$

$$\begin{aligned}a^\dagger a|0\rangle &= \left(\frac{E_0}{\hbar\omega} - \frac{1}{2}\right)|0\rangle = 0\\ E_0|0\rangle &= \frac{1}{2}\hbar\omega|0\rangle \quad (c_0 = \tfrac{1}{2})\end{aligned}$$

$$aa^\dagger|a_+^n(0)\rangle = \left(\frac{\hbar\omega(n+1/2)}{\hbar\omega} + \frac{1}{2}\right)|a_+^n(0)\rangle$$

$$\boxed{aa^\dagger|a_+^n(0)\rangle = (n+1)|a_+^n(0)\rangle}$$

- $\langle a_+^n(0)|aa^\dagger|a_+^n(0)\rangle = n+1$
- $a^\dagger|a_+^n(0)\rangle = \sqrt{n+1}\ |a_+^{n+1}(0)\rangle$
- $a|a_+^{n+1}(0)\rangle = \sqrt{n+1}|a_+^n(0)\rangle\ **$

$$a^\dagger a|n,0\rangle = \left(\frac{\hbar\omega(n+1/2)}{\hbar\omega} - \frac{1}{2}\right)|n,0\rangle$$

$$\boxed{a^\dagger a|a_+^n(0)\rangle = n|a_+^n(0)\rangle}$$

$$\begin{aligned}\frac{H}{\hbar\omega}|a_+^n(0)\rangle &= \underline{(\tfrac{1}{2} + n)}|a_+^n(0)\rangle = \underline{c\circ a_+^n(0)}|a_+^n(0)\rangle\\ \frac{H}{\hbar\omega}a_\pm^m|a_+^n(0)\rangle &= \underline{(\tfrac{1}{2} + n \pm m)}a_\pm^m|a_+^n(0)\rangle\\ \frac{H}{\hbar\omega}|a_+^{n\pm m}(0)\rangle &= \underline{(c\circ a_+^{n\pm m}(0))}|a_+^{n\pm m}(0)\rangle\end{aligned} \ \rightarrow\ \begin{aligned}c_n &= \tfrac{1}{2} + n\\ a_+^n(0) &= n\\ a_\pm(n) &= n \pm 1\end{aligned} \ \rightarrow\ \begin{aligned}&\boxed{E_n = \hbar\omega(\tfrac{1}{2} + n)}\\ &\boxed{\begin{aligned}a|n\rangle &= \sqrt{n}|n-1\rangle\\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle\end{aligned}}\\ &\boxed{\Psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\Psi_0}\end{aligned}$$

2.2.1 Position/Momentum Operators

$$\boxed{x = \frac{1}{2}\frac{\sqrt{2m}\sqrt{\hbar\omega}}{m\omega}(a + a^\dagger)} \qquad \boxed{\hat{p} = \frac{1}{2}\frac{\sqrt{2m}\sqrt{\hbar\omega}}{i}(a - a^\dagger)}$$

Show Virial Theorem Works

$$\boldsymbol{2\langle T\rangle = N\langle V\rangle}$$

$$\begin{aligned} E_n &= 2\langle V\rangle_n \\ &= 2\langle\Psi_n|V|\Psi_n\rangle \\ &= 2\left\langle\Psi_n\left|\tfrac{1}{2}mw^2\tfrac{2m\hbar\omega}{(2m\omega)^2}(a+a^\dagger)^2\right|\Psi_n\right\rangle \\ &= \tfrac{2m^2\hbar\omega^3}{(2m\omega)^2}\left(0 + \left\langle\Psi_n\left|(aa^\dagger + a^\dagger a)\right|\Psi_n\right\rangle + 0\right) \end{aligned}$$

$$E_n = (n + 1/2)\hbar\omega \quad ☑$$

Heisenberg Picture

$$\tfrac{da_\pm}{dt} = \mp i\omega a_\pm$$

$$\Rightarrow \qquad a_\pm(t) = a_\pm(0)e^{\mp i\omega t}$$

$$x(t) \pm \tfrac{ip(t)}{m\omega} = x(0)e^{\mp i\omega t} \pm \tfrac{ip(0)}{m\omega}e^{\mp i\omega t}$$

$$x(t) = x(0)\cos\omega t + \tfrac{p(0)}{m\omega}\sin\omega t$$

$$\tfrac{p(t)}{m\omega} = -x(0)\sin\omega t + \tfrac{p(0)}{m\omega}\cos\omega t$$

Test the Uncertainty Principle

$$\sigma_x\sigma_p \ge \tfrac{1}{2}\left|\left\langle [x,p]\right\rangle\right|$$

$$\begin{aligned} xp - px &= \tfrac{2m\hbar\omega}{4m\omega i}\begin{pmatrix} a^2 - aa^\dagger + a^\dagger a - (a^\dagger)^2 \\ -a^2 + a^\dagger a - aa^\dagger + (a^\dagger)^2\end{pmatrix} \\ &= \tfrac{\hbar}{i}(a^\dagger a - aa^\dagger) = i\hbar(n + 1 - n) \\ &\Rightarrow \ \sigma_x\sigma_p \ge \frac{\hbar}{2} \quad ☑ \end{aligned}$$

$$\begin{aligned} \sigma_x^2 &= \langle x^2\rangle - \langle x\rangle^2 & \sigma_p^2 &= \langle p^2\rangle - \langle p\rangle^2 \\ &= \tfrac{2m\hbar\omega}{4m^2\omega^2}\begin{bmatrix}\langle(a+a^\dagger)^2\rangle \\ -\langle a+a^\dagger\rangle^2\end{bmatrix} & &= \tfrac{2m\hbar\omega}{-4}\begin{bmatrix}\langle(a-a^\dagger)^2\rangle \\ -\langle a-a^\dagger\rangle^2\end{bmatrix} \\ &= \tfrac{\hbar}{2m\omega}\langle aa^\dagger + a^\dagger a\rangle & &= \tfrac{\hbar m\omega}{2}\langle aa^\dagger + a^\dagger a\rangle \\ &= \tfrac{\hbar}{m\omega}(n + \tfrac{1}{2}) & &= \hbar m\omega(n + \tfrac{1}{2}) \end{aligned}$$

$$\Rightarrow \ \sigma_x\sigma_p = \hbar(n + \tfrac{1}{2}) \ge \tfrac{\hbar}{2} \quad ☑$$

2.2.2 Analytic Method

$$\boldsymbol{\Psi_n = A\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\xi^2/2}}$$

$$A = \left(\tfrac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\xi = \sqrt{\tfrac{m\omega}{\hbar}}x$$

Hermite Polynomials:

$$H_n(x) = (-1)^n\ e^{-x^2}\left(\frac{d}{dx}\right)^n e^{x^2}$$

$$e^{-z^2+2zx} = \sum_{n=0}^{\infty}\frac{z^n}{n!}H_n(x)$$

2.2.3 Coherent States

$$\boldsymbol{a|\alpha\rangle = \alpha|\alpha\rangle}$$

$$\boxed{\sigma_x\sigma_p = \frac{\hbar}{2}}$$

$$\langle\alpha|\alpha\rangle = \langle\alpha| \begin{pmatrix} \sum_{n=0}^{\infty}\langle\Psi_n|\alpha\rangle\ |\Psi_n\rangle = \\ \sum_{n=0}^{\infty}\left\langle \frac{(a^\dagger)^n}{\sqrt{n!}}\Psi_0 \middle| \alpha \right\rangle\ |\Psi_n\rangle = \\ \sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\langle\Psi_0|\alpha\rangle\ |\Psi_n\rangle \end{pmatrix} \Rightarrow \boxed{\Big|\alpha\Big\rangle = e^{-\alpha^2/2}\ \sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\ |\Psi_n\rangle} \to \Big|\alpha{=}0\Big\rangle = |\Psi_0\rangle$$

$$= \langle\Psi_0|\alpha\rangle^2\sum_{n=0}^{\infty}\frac{(\alpha^2)^n}{n!}\ \langle\Psi_n|\Psi_n\rangle$$

$$= \langle\Psi_0|\alpha\rangle^2\ e^{\alpha^2} = 1$$

$$a|\alpha_{(x,t)}\rangle = e^{-\frac{\alpha^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\ e^{\frac{-i}{\hbar}E_n t}a|\Psi_n\rangle$$

$$= e^{-\frac{\alpha^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\ e^{\frac{-i}{\hbar}\hbar\omega(\frac{1}{2}+n)t}\sqrt{n}|\Psi_{n-1}\rangle$$

$$= \left(\alpha e^{\frac{-i}{\hbar}\hbar\omega t}\right)e^{-\frac{\alpha^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\ e^{\frac{-i}{\hbar}\hbar\omega(\frac{1}{2}+n)t}|\Psi_n\rangle$$

$$\boxed{a|\alpha_{(x,t)}\rangle = \left(\alpha e^{-i\omega t}\right)|\alpha_{(x,t)}\rangle}$$

$|\alpha\rangle$ are obviously not orthogonal. They are an overcomplete basis.

2.2.4 3-D Harmonic Potential

$$\boldsymbol{V(r) = \frac{1}{2}kr^2}$$

$$\boxed{\begin{array}{c} \text{(Isotropic)} \\ E_{n_x n_y n_z} = \hbar\omega\left(n_x+n_y+n_z+\tfrac{3}{2}\right) = \hbar\omega\left(n+\tfrac{3}{2}\right) \quad l = n-2k \in \{n, n-2, ..., 0\} \end{array}}$$

2.3 Free Particle (1-D)

$$\boldsymbol{V(x) = 0}$$

$$\Psi_{(x,t)} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi_{(x,0)} e^{\frac{i}{\hbar}[px - E(p)t]}\, dp \qquad \langle x|U_{(t)}|\Psi\rangle = \iint \langle x|p\rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}\langle p|x'\rangle\, dp\, \langle x'|\Psi\rangle\, dx'$$

$$= \int \langle x|p\rangle e^{-\frac{i}{\hbar}E(p)t}\langle p|\Psi\rangle\, dp \qquad = \iint_{-\infty}^{\infty} \tfrac{1}{2\pi\hbar} e^{-\frac{i}{\hbar}\left[\frac{p^2 t}{2m} - p(x-x')\right]}\, dp\, \Psi_{(x',0)}\, dx'$$

$$\Phi_{(x,t)} = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi_{(x,0)} e^{\frac{-i}{\hbar}[px + E(p)t]}\, dx \qquad = \int \sqrt{\tfrac{-im}{2\pi\hbar t}}\, e^{\frac{im(x-x')^2}{2\hbar t}}\, \Psi_{(x',0)}\, dx'$$

($E < 0 \to \Psi = e^{\pm kx}$ is possible and also not normalizable, but solution above is already a complete set)

- $E(p) = \frac{p^2}{2m}$
- $v_{\text{wave}} = \boxed{v_{\text{phase}} = \frac{\omega(k)}{k}} = \frac{E}{p} = \frac{v_{\text{classical}}}{2}$
- $v_{\text{particle}} \approx \boxed{v_{\text{group}} = \frac{d\omega(k)}{dk}} = 2v_{\text{wave}} \quad \left(\begin{array}{c}\text{dispersion}\\ \text{relation}\end{array}\right)$

Heisenberg Pic. Free Particle

$$x_H(t) = x_H(0) + \frac{p_H(0)}{m}t$$

$$\left[x_H(0),\ x_H(t)\right] = \left[x_H(0), \frac{p_H(0)}{m}t\right] = \frac{i\hbar t}{m}$$

$$\boxed{\sigma_{x_t}\sigma_{x_0} \geq \frac{\hbar t}{2m}}$$

2.4 Delta Potential (1-D)

Potential Well: $\boldsymbol{V(x) = -\alpha\delta(x)}$ ($\alpha \to -\alpha$ for potential wall)

Bound State ($E < 0$) [only for Well]:

$$\Psi = \sqrt{k}e^{k|x|} = \begin{cases} \sqrt{k}e^{kx} & x \leq 0 \\ \sqrt{k}e^{-kx} & x \geq 0 \end{cases}$$

$$k = \frac{m\alpha}{\hbar^2}$$

$$E = -\frac{(\hbar k)^2}{2m}$$

Scattering State ($E > 0$) [for both]:

$$\Psi = \begin{cases} Ae^{iKx} + Be^{-iKx} & x < 0 \\ Fe^{iKx} & x > 0 \end{cases}$$

$$E = \frac{(\hbar K)^2}{2m}\ , \qquad \beta \equiv \frac{k}{K} = \frac{m\alpha/\hbar^2}{K}$$

$$B = \frac{i\beta}{1 - i\beta}A\ , \qquad F = \frac{1}{1 - i\beta}A$$

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2}\ , \qquad T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}$$

Can't normalize. All free particles have ranges of p and thus E, so R and T are approx. in the vicinity of E.

2.5 Finite Square Potential (1-D)

2.5.1 Potential Well $\quad V(x) = \begin{cases} -V_0 & -a < x < a \\ 0 & \text{otherwise} \end{cases}$

($V_0 \to -V_0$ for wall and do cases for $E > V_0, E = V_0, E < V_0$, and change to $\sinh, \cosh$ **if needed)**

$$k\,;K: \quad E = \tfrac{-(\hbar k)^2}{2m} = \tfrac{(\hbar K)^2}{2m}$$

$$l: \quad E + V_0 = \tfrac{(\hbar l)^2}{2m}$$

$$\upsilon: \quad V_0 = \tfrac{\hbar^2 \upsilon^2}{2m} = \tfrac{\hbar^2 (l^2+k^2)}{2m} = \tfrac{\hbar^2 (l^2-K^2)}{2m}$$

$$\frac{k_a}{l_a} \equiv \sqrt{\frac{(ka)^2}{(la)^2}} = \sqrt{\frac{(la)^2+(ka)^2}{(la)^2} - 1}$$

$$\boxed{\frac{k_a}{l_a} \equiv \sqrt{\left(\frac{\upsilon_a}{l_a}\right)^2 - 1}}\;, \quad \upsilon_a^2 = \begin{cases} l_a^2 + k_a^2 \\ l_a^2 - K_a^2 \end{cases}$$

Bound State $\;(E_n < 0)$ [only for well]:

$$\Psi_{\text{even}}(x) = \begin{cases} \Psi(-x) & x < 0 \\ D\cos(lx) & 0 < x < a \\ Fe^{-kx} & a < x \end{cases}$$

- $F = D\cos(la)e^{ka}$
- $\frac{-(\partial_x \Psi)(a)}{\Psi(a)} = k = l\tan(la) \;\Rightarrow$

  $\tan(l_a) = \sqrt{(\upsilon_a/l_a)^2 - 1}$

  big $\upsilon_a \;\to\; l \approx_< \frac{n\pi}{2a} \;\to\; E_n + V_0 = \frac{\hbar^2 l^2}{2m}$; n odd
- $\boxed{n_{\max} = \left\lfloor \frac{\upsilon_a}{\pi} \right\rfloor + 1}$

$$\Psi_{\text{odd}}(x) = \begin{cases} -\Psi(-x) & x < 0 \\ C\sin(lx) & 0 < x < a \\ Fe^{-kx} & a < x \end{cases}$$

- $F = D\sin(la)e^{ka}$
- $\frac{-(\partial_x \Psi)(a)}{\Psi(a)} = k = -l\cot(la) \;\Rightarrow$

  $-\cot(l_a) = \sqrt{(\upsilon_a/l_a)^2 - 1}$

  big $\upsilon_a \;\to\; l \approx_< \frac{n\pi}{2a} \;\to\; E_n + V_0 = \frac{\hbar^2 l^2}{2m}$; n even
- $\boxed{n_{\max} = \left\lfloor \frac{\upsilon_a + \frac{\pi}{2}}{\pi} \right\rfloor}$

Scattering State $\;(E > 0)$ [for both]:

$$\Psi = \begin{cases} Ae^{iKx} + Be^{-iKx} & x < -a \\ C\sin lx + D\cos lx & -a < x < a \\ Fe^{iKx} & a < x \end{cases}$$

$$\frac{d\Psi}{dx} = \begin{cases} iKAe^{iKx} - iKBe^{-iKx} & x < -a \\ lC\cos lx - lD\sin lx & -a < x < a \\ iKFe^{iKx} & a < x \end{cases}$$

$$B = i\sin(2l_a)\left(\tfrac{l_a^2 - K_a^2}{2K_a l_a}\right)\; F$$

$$F = \frac{e^{-2iK_a}}{\cos(2l_a) - i\left(\frac{l_a^2+K_a^2}{2K_a l_a}\right)\sin(2l_a)}\; A$$

(Can't normalize. See delta potential.)

$$T^{-1} = 1 + \left(\tfrac{l_a^2 - K_a^2}{2K_a l_a}\right)^2\; \sin^2(2l_a)$$

$$= 1 + \frac{V_0^2}{4E(E+V_0)}\; \sin^2\left(2a\sqrt{\frac{E+V_0}{\hbar^2/2m}}\right)$$

(full transmission at inf. sqr. well $E_n + V_0 = \frac{\hbar^2 l^2}{2m}$; $l = \frac{n\pi}{2a}$)

3 2D and 3D Schrodinger Equation

General dimensions, D

$$\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right)R(r) = \left[\frac{\partial^2}{\partial r^2} + \frac{D-1}{r}\frac{\partial}{\partial r}\right]R(r)$$

$$= \left[\frac{\partial^2}{\partial r^2} + \frac{D-1}{r}\frac{\partial}{\partial r}\right]r^n u(r)$$

$$= \left[\frac{\partial^2}{\partial r^2} + \frac{D-1+2n}{r}\frac{\partial}{\partial r} + \frac{2n(2D-4+2n)}{4r^2}\right]u$$

$$= \left[\frac{\partial^2}{\partial r^2} - \frac{(D-1)(D-3)}{4r^2}\right]u \qquad (n = \tfrac{1-D}{2}, \cancel{0, 2-D})$$

$$R(r) = u(r)/\sqrt{r}^{D-1} \;\sim\; e^{\frac{i}{\hbar}p_r r}/\sqrt{r}^{D-1}$$

$$L^2 \sim \hbar^2 \;\;,\quad \hat{p}_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{D-1}{2r}\right) \;\;,\quad \hat{p'}_r = \frac{\hbar}{i}\frac{\partial}{\partial r}$$

$$ER(r) = \left[\frac{\hat{p}_r^2}{2M} + V(r) + \frac{L^2 - \hbar^2(D-1)^2/4}{2(Mr^2)}\right]R(r)$$

$$Eu(r) = \left[\frac{\hat{p'}_r^2}{2M} + V(r) + \frac{L^2 - \hbar^2(D-1)(D-3)/4}{2(Mr^2)}\right]u(r)$$

3.1 2D Schrodinger

If $V = V(\rho)$

$\Psi(\vec{\mathbf{r}}) = R_m(\rho)\Phi_m(\phi) \;\Rightarrow$

$$ER = \left[\frac{-\hbar^2}{2M}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + V(\rho) + \frac{\hbar^2 m^2}{2M\rho^2}\right]R$$

$$\boxed{Eu = \frac{-\hbar^2}{2M}\frac{\partial^2 u}{\partial\rho^2} + \left[V(\rho) + \frac{\hbar^2(m^2+1/4)}{2M\rho^2}\right]u}$$

$$Eu\Phi = \left[\frac{\hat{p'}_\rho^2}{2M} + V(\rho) + \frac{\hat{L}_z^2 + \hbar^2/4}{2(M\rho^2)}\right]u\Phi$$

- $R_m(\rho) = u_m(\rho)/\sqrt{\rho} \qquad \left(\int \Psi r\, dr d\phi = 1\right)$
- $\Phi_m(\phi) = e^{im\phi}$
- $L_z = (\vec{r}\times\vec{p})_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$

3.2 3D Schrodinger

<u>If $V = V(r)$</u>

$$\Psi(\vec{\mathbf{r}}) = R_l(r)Y_l^m(\theta,\phi) = R_l(r)\Theta_l^m(\theta)\Phi_m(\phi) \;\Rightarrow$$

$$ER = \left[\frac{-\hbar^2}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r) + \frac{\hbar^2 l(l+1)}{2Mr^2}\right]R$$

$$\boxed{Eu = \frac{-\hbar^2}{2M}\frac{\partial^2 u}{\partial r^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2Mr^2}\right]u}$$

$$Eu\Theta = \left[\frac{\hat{p'}_r^2}{2M} + V(r) + \frac{\hat{L}^2}{2(Mr^2)}\right]u\Theta$$

- $R_l(r) = u_l(r)/r \qquad \left(\int \Psi r^2 \sin\theta\, dr d\theta d\phi = 1\right)$
- $\Phi_m(\phi) = e^{im\phi}$
- $\Theta_l^m(\theta) = AP_l^m(\cos\theta)$
  - $A = \epsilon\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}, \quad \epsilon = \begin{cases}(-1)^m & (m\ge 0)\\ 1 & (m\le 0)\end{cases}$
  - $P_l^m(x) =$ Assoc. Legendre Func. (see extra)
- $l \in \mathbb{N}_0,\ m \in \{-l, ..., -1, 0, 1, ..., l\}$
- $\widehat{L}_i = (\vec{r}\times\vec{p})_i$

$$\langle u|\nabla_r^2 u\rangle = \langle \nabla_r^2 u|u\rangle \;\Rightarrow\; \left[u^*\frac{\partial u}{\partial r} - u\frac{\partial u^*}{\partial r}\right]_0^\infty \begin{matrix}\leftarrow 1.)\\ \leftarrow 2.)\end{matrix} = 0$$

1.) $\int_0^\infty u^2\,dr = 1 \;\Rightarrow\; \boxed{u(\infty) = 0 \text{ or } e^{ir}}$

2.) $\boxed{u(0) = c = 0}$ $\left\{c \neq 0 \rightarrow \begin{matrix}\Psi_{l=0}(r) \sim \frac{c}{r}\\ \nabla^2(\frac{1}{r}) \sim \delta^3(r)\end{matrix} \rightarrow \begin{matrix}H\Psi \neq E\Psi\\ \text{if } V(r) \neq \delta^3(r)\end{matrix}\right\}$

$V \sim r^{-2<a},\ l \neq 0:\ \lim_{r\to 0} u'' \sim \frac{l(l+1)}{r^2}u,\ u \sim r^{l+1}$

$V \sim r^{-2<a<-1},\ E > 0:\ \lim_{r\to\infty} p_r^2 u \sim Eu,\ u \sim e^{\pm ikr}$

$V \sim r^{-1\le a},\ E > 0:\ u \gtrsim re^{\pm ikr}$

Sim for $E < 0$: $u \sim e^{\pm kr}$ or $re^{\pm kr}$ etc.

3.2.1 3D Free Particle, $V = 0$

$$-\frac{\hbar^2}{2M}\left[\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2}\right]u = \frac{\hbar^2 k^2}{2M}u \quad\Rightarrow\quad \left[\frac{\partial^2}{\partial\rho^2} + \frac{l(l+1)}{\rho^2}\right]|l\rangle = |l\rangle$$

$$a_l \equiv \frac{\partial}{\partial\rho} + \frac{l+1}{\rho} \qquad a_l^\dagger = -\frac{\partial}{\partial\rho} + \frac{l+1}{\rho}$$

$$a_l a_l^\dagger|l\rangle = |l\rangle \qquad a_l^\dagger a_l|l\rangle = a_{l+1}a_{l+1}^\dagger|l\rangle$$

$$a_l^\dagger|l\rangle = e^{i\theta_l}|a_l^\dagger(l)\rangle$$

$$a_l^\dagger\left(a_l a_l^\dagger\right)|l\rangle = \underline{a_l^\dagger|l\rangle}$$

$$\left(a_l^\dagger a_l\right)\underline{a_l^\dagger|l\rangle} = \left(a_{l+1}a_{l+1}^\dagger\right)\underline{a_l^\dagger|l\rangle}$$

$$\underline{a_l^\dagger|l\rangle} = \cancel{e^{i\theta_l}}\,|l+1\rangle$$

$$\boxed{\begin{matrix}\text{Bessel}:\ r\underline{R_0^B} = u_0^B \sim \sin(\rho) = \sin(kr)\\ \text{~~Neumann~~}:\ r\underline{R_0^N} = u_0^N \sim -\cos(\rho)\end{matrix}}$$

$$\cancel{e^{i\theta_l}}\frac{\rho}{k}R_{l+1} = a_l^\dagger(\tfrac{\rho}{k}R_l) = \left(-\frac{\partial}{\partial\rho} + \frac{l+1}{\rho}\right)(\tfrac{\rho}{k}R_l)$$

$$R_{l+1} = \left(-\frac{\partial}{\partial\rho} + \frac{l}{\rho}\right)R_l = -\rho^l\frac{\partial}{\partial\rho}\left(\rho^{-l}R_l\right)$$

$$\frac{R_l}{\rho^l} = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\frac{R_{l-1}}{\rho^{l-1}} = \left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^l R_0$$

$$\boxed{R_l = C_l(-\rho)^l\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^l R_0}$$

<u>Infinite Spherical Well</u>: $V(r) = \begin{cases}0 & r \le a\\ \infty & r > a\end{cases}$, $\quad E_n = \frac{\hbar^2 k_n^2}{2m}$

<u>Bessel</u>: $R_l^B(\rho) = C_l(-\rho)^l\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^l R_0^B(\rho)$, $\quad R_0^B(\rho) \sim k_n\sin(\rho)/\rho = \sin(k_n r)/r$ $\;\Rightarrow\;$ $\beta_l^n \equiv k_n a:\ R_l^B(\beta_l^n) = 0$, $\quad \beta_0^n = \frac{n\pi}{a}\cdot a$

3.2.2 Hydrogen Atom, $V = -\frac{ke^2}{r}$

$$Eu = \left(\frac{\hat{p}_r^2}{2m} + V(r) + \frac{\hat{L}^2}{2(mr^2)} \right) u \qquad u(r) = rR(r)$$

$$\boxed{Eu = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u + \left[-\frac{ke^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right] u}$$

$$\boxed{\Psi_{nlm}(\vec{\mathbf{r}}) = R_{nl}(r)\ Y_l^m(\theta,\phi) = R_{nl}(r)\ \Theta_l^m(\theta)\ \Phi_m(\phi)}$$

- $\Phi_m(\phi) = e^{im\phi}$
- $\Theta_l^m(\theta) = AP_l^m(\cos\theta)$
  - $A = \epsilon\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}$, $\quad \epsilon = \begin{cases} (-1)^m & (m \geq 0) \\ 1 & (m \leq 0) \end{cases}$
  - $P_l^m(x)$ Assoc. Legendre Func. (see extra)
- $R_{nl}(r) = \frac{B}{r}\rho^{l+1}e^{-\rho}\nu(\rho)$
  - $\rho = k_n r$, $\quad k_n = \frac{1}{a_0 n}$ (fine structure below)
  - $\nu(\rho) = L_{n-l-1}^{2l+1}(2\rho)$ Assoc. Laguerre Pol. (see extra)
  - $B = \sqrt{2k_n\ \frac{(n-l-1)!}{2n[(n+l)!]^3}}\ 2^{l+1}$

$$\boxed{\alpha \equiv \frac{kqq}{\hbar c} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \approx \frac{1}{137}} \qquad \boxed{a_0 \equiv \frac{\hbar^2}{m(kqq)} = \frac{4\pi\epsilon_0\hbar^2}{me^2}}$$

$$\boxed{E_n = -\frac{\hbar^2 k_n^2}{2m} = -\frac{\hbar^2}{2ma_0^2}\frac{1}{n^2} = -\frac{1}{2}\alpha^2\left(mc^2\right)\frac{1}{n^2} \approx -13.6\ \frac{1}{n^2}\ [\text{eV}]}$$

$$\boxed{\frac{1}{\lambda} = \frac{\alpha^2\left(mc^2\right)}{2hc}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = R\left(\tfrac{1}{n_f^2} - \tfrac{1}{n_i^2}\right) \ , \quad R = 1.097\ \text{E7}\ [\text{m}^{-1}]}$$

<u>Quantum Numbers - n, l, m</u>:

- $\Big(n \in \{1,2,3,...\}\Big)$, $\Big(l \in \{0,1,2,...,n-1\}\Big)$, $\Big(m \in \{-l,...,-1,0,1,...,l\}\Big)$
  - <u>Degeneracy is n^2</u>

<u>(outdated) Bohr Model</u>:

- $L = (\bar{r})(\bar{p}) = (a_0 n^2)(\hbar k_n) = n\hbar$ (not correct!!)
- Electrons don't radiate about the nucleus
- Energy diff. follows Rydberg formula

4 Spin and L

4.1 Hydrogen Atom

Angular Momentum :

$\boxed{\widehat{L}_i \equiv (\vec{r} \times \vec{p})_i}$, $\boxed{L_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi}}$

$\boxed{\widehat{L}_\pm \equiv \widehat{L}_x \pm i\widehat{L}_y}$

$\boxed{\widehat{L}^2 \equiv L_x^2 + L_y^2 + L_z^2}$

$\boxed{L_\pm L_\mp = \widehat{L}^2 - L_z^2 \pm \hbar L_z}$

Commutation Relations:

$\boxed{\big[\hat{x}, L_y\big] = i\hbar\hat{z}}$, $\boxed{\big[p_x, L_y\big] = i\hbar p_z}$, $\boxed{\big[L_x, L_y\big] = i\hbar L_z}$

$\boxed{\big[L^2, L_i\big] = \big[H, L_i\big] = \big[H, L^2\big] = 0}$ (can measure concurrently)

$$\rightarrow \begin{matrix} \boxed{L_z Y_{m'} = \hbar m' Y_{m'}} \\ \boxed{L^2 Y_{m'} = \hbar^2 \lambda_{m'} Y_{m'}} \end{matrix} \Rightarrow \begin{matrix} \langle L^2 - L_z^2\rangle = \langle L_x^2 + L_y^2\rangle \geq 0 \\ \bullet\ \sqrt{\lambda_{m'}} \geq\ m' \geq -\sqrt{\lambda_{m'}} \end{matrix}$$

Let $(L_\pm)^n Y_\mu \equiv |m\rangle$ (see harm. osc. for why ladders)

$$\boxed{\big[\tfrac{L_z}{\hbar}, L_\pm\big] = (\pm 1)L_\pm} \Rightarrow \big[\tfrac{L_z}{\hbar}, (L_\pm)^n\big] = \pm n (L_\pm)^n \Rightarrow \begin{matrix} L_z\big[(L_\pm)^n Y_\mu\big] = (\mu \pm n)\hbar\big[(L_\pm)^n Y_\mu\big] \\ \bullet\ L_z|m\rangle = (\mu \pm n)\hbar|m\rangle \end{matrix}$$

$$\boxed{\big[L^2, L_\pm\big] = 0} \Rightarrow \big[L^2, (L_\pm)^n\big] = 0 \Rightarrow \begin{matrix} L^2\big[(L_\pm)^n Y_\mu\big] = \lambda_\mu\big[(L_\pm)^n Y_\mu\big] \\ \bullet\ L^2|m\rangle = \lambda_\mu|m\rangle \end{matrix}$$

Then $\left(\sqrt{\lambda_\mu}\ \geq\ (\mu \pm n)\ \geq\ -\sqrt{\lambda_\mu}\right) \Rightarrow$ **Let** (else un-normalizable solution)

$\underline{L_+|m_t\rangle = 0}$, $L_z|m_t\rangle = \hbar l$,

$L^2|m_t\rangle = \lambda\hbar^2$, $L^2 = L_- L_+ + L_z^2 + \hbar L_z$

- $L^2|m_t\rangle = \hbar^2 l(l+1)|m_t\rangle = \lambda\hbar^2|m_t\rangle$

$\underline{L_-|m_b\rangle = 0}$, $L_z|m_b\rangle = \hbar l'$,

$L^2|m_b\rangle = \lambda\hbar^2$, $L^2 = L_+ L_- + L_z^2 - \hbar L_z$

- $L^2|m_b\rangle = \hbar^2 l'(l'-1)|m_b\rangle = \lambda\hbar^2|m_b\rangle$

$$\big[\lambda = l'(l'-1) = l(l+1)\big] \Rightarrow \big[l' = -l\big] \Rightarrow \begin{bmatrix} L_z|m_t\rangle = \hbar l\,|m_t\rangle \\ L_z|m_b\rangle = -\hbar l\,|m_b\rangle \end{bmatrix}$$ (Spherical Harmonics do not allow half-integer l)

Schrodinger Y_l^m:

$$\boxed{\begin{array}{c|l} l \in \{0, 1, 2, ...\} & L_z\big|Y_l^m\big\rangle = \hbar m\big|Y_l^m\big\rangle = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\big|Y_l^m\big\rangle \\ & L^2\big|Y_l^m\big\rangle = \hbar^2 l(l+1)\big|Y_l^m\big\rangle \\ m \in \{-l, -l+1, ..., l-1, l\} & L_\pm\big|Y_l^m\big\rangle = \hbar\sqrt{l(l+1) - m(m\pm 1)}\ \big|Y_l^m\big\rangle \end{array}}$$

4.2 Generalized

Angular Momentum:

$\widehat{J}_i \equiv ???$ $\boxed{J^2 \equiv J_x^2 + J_y^2 + J_z^2}$

$\boxed{J_\pm \equiv J_x \pm iJ_y}$ $\boxed{J_\pm J_\mp = J^2 - J_z^2 \pm \hbar J_z}$

Commutation Relations:

$\boxed{\left[J_i, J_j\right] = i\hbar J_k\ \epsilon_{ij}} \Leftrightarrow \boxed{J \times J = i\hbar J}$

$\boxed{\left[J^2, J_z\right] = 0} = \left[H, J_z\right]$ (if spher. symm.)

General:

$$\boxed{\begin{array}{c|l} & J_z\big|jm\big\rangle = \hbar m\big|jm\big\rangle \\ j \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, ...\right\} & J^2\big|jm\big\rangle = \hbar^2 j(j+1)\big|jm\big\rangle \\ m \in \{-j, -j+1, ..., j-1, j\} & J_\pm\big|jm\big\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\ \big|jm\big\rangle \\ & J_x\big|jm\big\rangle = \frac{J_+ + J_-}{2}\big|jm\big\rangle \end{array}}$$

Generator of Rotations:

$$U[R(\theta)] = e^{-\frac{i}{\hbar}\theta\hat{\theta}\cdot L} = \lim_{N\to\infty}\left[I - \frac{i}{\hbar}\frac{\theta}{N}\hat{\theta}\cdot L\right]^N \Leftrightarrow \boxed{U[R(\epsilon_z\hat{z})] = I - \frac{i}{\hbar}\epsilon_z L_z}$$

1.) $U[R(\epsilon_z\hat{z})]|x, y\rangle \equiv |x - \epsilon_z y, \epsilon_z x + y\rangle$

$\Rightarrow \langle x, y|U[R(\epsilon_z\hat{z})]|\Psi\rangle = \Psi(x + \epsilon_z y, \epsilon_z x - y)$

$\Rightarrow \underline{\langle x, y|L_z|\Psi\rangle = (XP_y - YP_x)\Psi(x, y)}$

or 2.) $U^\dagger XU \equiv X - \epsilon_z Y \Rightarrow [X, L_z] = -i\hbar Y$

$U^\dagger P_y U \equiv \epsilon_z P_x + P_y \Rightarrow [P_y, L_z] = i\hbar P_x$

$U^\dagger YU,\ U^\dagger P_x U, \Rightarrow \ldots$

$\Rightarrow \underline{L_z = XP_y - YP_x}$

Consistency Check: $U\left[R(-\epsilon_z\hat{z})\right]T(-\epsilon_x\hat{x} - \epsilon_y\hat{y})U\left[R(\epsilon_z\hat{z})\right]T(\epsilon_x\hat{x} + \epsilon_y\hat{y}) = T(-\epsilon_y\epsilon_z\hat{x} + \epsilon_x\epsilon_z\hat{y})$

$?U\left[R(-\epsilon_y\hat{y})\right]U\left[R(-\epsilon_x\hat{x})\right]U\left[R(\epsilon_y\hat{y})\right]U\left[R(\epsilon_x\hat{x})\right] = I + \frac{i}{\hbar}\epsilon_x\epsilon_y L_z = U\left[R(-\epsilon_x\epsilon_y\hat{z})\right]$

$(L_z = xp_y - yp_x)$

Tensors and Tensor Operators

rank-2 Tensor:

$$|t^{(2)}\rangle = \sum_{i=1}^{3}\sum_{j=1}^{3} t_{ij}\,|i\rangle|j\rangle$$

$$= \sum_{i=1}^{3}\sum_{j=1}^{3} |ij\rangle\langle ij|t^{(2)}\rangle$$

rank-2 Cartesian Tens. Oper., T_{ij} :

Set of $3^{n=2}$ Operators

rank-k Spherical Tensor Operator, T_k^q :

Set of $2k+1$ Operators s.t.

$$U[R]T_k^q U^\dagger[R] = \sum_{q'=-k}^{k} D^k_{q'q}T_k^{q'}$$

$\downarrow$

$$UT_k^q U^\dagger U|jm\rangle = \sum_{q'}\sum_{m'} D^k_{q'q}D^j_{m'm}T^k_{q'}|jm'\rangle$$

$$\sim\ U|kq\rangle|jm\rangle = \sum_{q'}\sum_{m'} D^k_{q'q}D^j_{m'm}|kq'\rangle|jm'\rangle$$

- $T_1^{\pm 1} = \mp\frac{V_x \pm iV_y}{\sqrt{2}}$
  $T_1^0 = V_z$

Wigner-Eckhart: $\langle\alpha_2 j_2 m_2|T_k^q|\alpha_1 j_1 m_1\rangle = \langle\alpha_2 j_2|T_k|\alpha_1 j_1\rangle \cdot \langle j_2 m_2|kq; j_1 m_1\rangle$

(CG coeff.)

4.3 1 Particle w/ Spin, $s = \frac{1}{2}$

*Find the Eigenvectors, e_i , of S_z and S^2 in the form of $|\chi\rangle = \begin{pmatrix} \cos\frac{\theta}{2}\, e^{i\phi_1} \\ \sin\frac{\theta}{2}\, e^{i\phi_2} \end{pmatrix} = e^{i\gamma} \begin{pmatrix} \cos\frac{\theta}{2}\, e^{-i\phi} \\ \sin\frac{\theta}{2}\, e^{i\phi} \end{pmatrix}$ $\quad \gamma = \frac{\phi_1+\phi_2}{2}$, $\phi = \frac{\phi_2-\phi_1}{2}$

$$* \boxed{ e_i \in \left\{ \; |\tfrac{1}{2}\ \tfrac{1}{2}\rangle \equiv |\uparrow\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |\tfrac{1}{2}\ \tfrac{-1}{2}\rangle \equiv |\downarrow\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \; \right\} }$$

$$\left. \begin{aligned} S^2|\uparrow\rangle &= \frac{3\hbar^2}{4}|\uparrow\rangle \\ S^2|\downarrow\rangle &= \frac{3\hbar^2}{4}|\downarrow\rangle \end{aligned} \right\} \Rightarrow \begin{aligned} S^2 &= \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{3\hbar^2}{4}\sigma_0 = * \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{3\hbar^2}{4} & 0 \\ 0 & \frac{3\hbar^2}{4} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{T*} \\ &= \tfrac{3\hbar^2}{4}\mathbb{I} \qquad \big(\text{only for } s = 1/2 \text{ systems}\big) \end{aligned}$$

$$\left. \begin{aligned} S_-|\uparrow\rangle &= \hbar|\downarrow\rangle \\ S_+|\downarrow\rangle &= \hbar|\uparrow\rangle \\ S_+|\uparrow\rangle &= S_-|\downarrow\rangle = 0 \end{aligned} \right\} \Rightarrow \begin{aligned} S_+ &= \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & S_- &= \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ &= \hbar|\uparrow\rangle\langle\downarrow| & &= \hbar|\downarrow\rangle\langle\uparrow| \end{aligned} \quad \text{(can't measure)}$$

$$\left. \begin{aligned} S_z|\uparrow\rangle &= \frac{\hbar}{2}|\uparrow\rangle \\ S_z|\downarrow\rangle &= -\frac{\hbar}{2}|\downarrow\rangle \end{aligned} \right\} \Rightarrow \begin{aligned} S_z &= \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z = * \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{T*} \\ &= \tfrac{\hbar}{2}|\uparrow\rangle\langle\uparrow| - \tfrac{\hbar}{2}|\downarrow\rangle\langle\downarrow| \end{aligned}$$

$$\left. \begin{aligned} S_x &= \frac{1}{2}(S_+ + S_-) \\ S_y &= \frac{1}{2i}(S_+ - S_-) \end{aligned} \right\} \Rightarrow \begin{aligned} S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y \\ \boxed{\{S_i, S_j\} = \tfrac{\hbar^2}{2}\delta_{ij}} \qquad \big(\text{only for } s = 1/2 \text{ systems}\big) \end{aligned}$$

<u>General Direction, $\hat{n}$</u>

$$\begin{aligned} \hat{n}\cdot\vec{S} &= (\cos\phi\sin\theta)S_x + (\sin\phi\sin\theta)S_y + (\cos\theta)S_z \\ &= \frac{\hbar}{2}\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \end{aligned}$$

$$\hat{n}\cdot\vec{S}\,|\chi_\pm\rangle = \pm\tfrac{\hbar}{2}\,|\chi_\pm\rangle$$

$$\boxed{ |\chi_+\rangle = e^{i\gamma}\begin{bmatrix} \cos\frac{\theta}{2}\, e^{-i\phi/2} \\ \sin\frac{\theta}{2}\, e^{i\phi/2} \end{bmatrix} \;,\; |\chi_-\rangle = e^{i\gamma}\begin{bmatrix} -\sin\frac{\theta}{2}\, e^{-i\phi/2} \\ \cos\frac{\theta}{2}\, e^{i\phi/2} \end{bmatrix} }$$

Properties of Pauli Matrices, σ_i

- $\sigma_i^2 = I = (\hat{n}\cdot\sigma)^2 \;\Leftarrow\; (\hat{n}\cdot\sigma)^2 - I^2 = (\hat{n}\cdot\sigma + I)(\hat{n}\cdot\sigma - I) = 0 = (\hat{n}\cdot S + \frac{\hbar}{2})(\hat{n}\cdot S - \frac{\hbar}{2})$
- $\sigma_i\sigma_j = i\sigma_k = -\sigma_j\sigma_i \;\Rightarrow\; \left[\frac{\sigma_i}{2}, \frac{\sigma_j}{2}\right] = i\frac{\sigma_k}{2} \qquad (i \neq j)$
- $(A\cdot\sigma)(B\cdot\sigma) = A\cdot B + i(A\times B)\cdot\sigma \qquad \big(\text{if } [A_i,\sigma_i] = 0 = [B_i,\sigma_i]\big)$
- $\mathrm{Tr}\ \sigma_i = 0 \;\Rightarrow\; \mathrm{Tr}(\sigma_\alpha\sigma_\beta) = 2\delta_{\alpha\beta} \qquad \alpha \in (0,x,y,z)$
- $\sum c_\alpha\sigma_\alpha = 0 \to c_\alpha = 0 \;\Rightarrow\; M_{2\times 2} = \sum \frac{1}{2}\mathrm{Tr}(M\sigma_\alpha)\sigma_\alpha$
- Rotate $\hat{k}$ to $\hat{n}$ by angle θ, $\hat{\theta} = (-\sin\phi, \cos\phi, 0) = \hat{k}\times\hat{n}$ $\qquad U[R(\theta)] = e^{-i\frac{\theta}{2}\hat{\theta}\cdot\sigma} = I\cos\frac{\theta}{2} - i\big(\hat{\theta}\cdot\sigma\big)\sin\frac{\theta}{2} = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{-i\phi} \\ \sin\frac{\theta}{2}e^{i\phi} & \cos\frac{\theta}{2} \end{bmatrix}$
- Rotate about $\hat{n}$ by angle ϵ, $\hat{n} = (n_x, n_y, n_z)$ $\qquad U[R(\psi)] = I\cos\frac{\psi}{2} - i\big(\hat{n}\cdot\sigma\big)\sin\frac{\psi}{2} = \begin{bmatrix} \cos\frac{\psi}{2} - in_z\sin\frac{\psi}{2} & (-in_x - n_y)\sin\frac{\psi}{2} \\ (-in_x + n_y)\sin\frac{\psi}{2} & \cos\frac{\psi}{2} + in_z\sin\frac{\psi}{2} \end{bmatrix}$

4.4 2 Objects w/ Spin

Objects could be orbital momentum, another particle spin, etc.

4.4.1 2 Objects w/ Spin $\frac{1}{2}$: $\quad \frac{1}{2}\otimes\frac{1}{2} = 1 \oplus 0 \;\Rightarrow\; (2s_1+1)(2s_2+1) = \sum_{s=|s_1-s_2|}^{s_1+s_2} 2s+1$

*Find Eigenvectors, e_i , of $(S^{(1,2)})_z$ and $(S^{(1,2)})^2$ in the form of $|\chi_i\chi_j\rangle$ (using $(S^{(1,2)})_\pm$)

$$\boxed{\chi_i\chi_j \to |\chi_i\chi_j\rangle \equiv |\chi_i\rangle|\chi_j\rangle \equiv |\chi_i\rangle\otimes|\chi_j\rangle}$$

Choose $|\chi_i\rangle \equiv S_z$-Eigenvector w/ Spin $\frac{1}{2}$ (e.g, $|\frac{1}{2}\frac{-1}{2}\rangle = \binom{0}{1}$, as opposed to $\binom{.6}{.8}$)

$$S^{(i)} \equiv \begin{pmatrix} S_x^{(i)} \\ S_y^{(i)} \\ S_z^{(i)} \end{pmatrix}$$

- $S_z^{(2)}S_x^{(1)}\Big(|\chi_1\rangle\otimes|\chi_2\rangle\Big) = \Big(S_x^{(1)}|\chi_1\rangle\Big)\otimes\Big(S_z^{(2)}|\chi_2\rangle\Big)$
- $S^{(i)}\cdot S^{(j)} \equiv \underline{S_x^{(i)}S_x^{(j)} + S_y^{(i)}S_y^{(j)}} + S_z^{(i)}S_z^{(j)}$

$$= S_z^{(i)}S_z^{(j)} + \underline{\tfrac{1}{2}S_+^{(i)}S_-^{(j)} + \tfrac{1}{2}S_-^{(i)}S_+^{(j)}}$$

$$(S^{(i)})^2 \equiv S^{(i)}\cdot S^{(i)}$$

$$S^{(1,2)} \equiv \big(S^{(1)} + S^{(2)}\big) \equiv \begin{pmatrix} S_x^{(1)} + S_x^{(2)} \\ S_y^{(1)} + S_y^{(2)} \\ S_z^{(1)} + S_z^{(2)} \end{pmatrix}$$

- $\big(S^{(1,2)}\big)^2 = \big(S^{(1)} + S^{(2)}\big)\cdot\big(S^{(1)} + S^{(2)}\big)$

1. $\left(S^{(1,2)}\right)_z$

$$\left(S^{(1,2)}\right)_z \chi_1\chi_2 = \left(S_z^{(1)} + S_z^{(2)}\right)|\chi_1\rangle|\chi_2\rangle$$

$$= S_z^{(1)}|\chi_1\rangle \otimes |\chi_2\rangle + |\chi_1\rangle \otimes S_z^{(2)}|\chi_2\rangle$$

$$\left(S^{(1,2)}\right)_z |\chi_1\chi_2\rangle = \hbar(m_1+m_2)\ |\chi_1\chi_2\rangle$$

$$\Rightarrow\ \underline{e_i = a_i|\uparrow\uparrow\rangle + b_i|\uparrow\downarrow\rangle + c_i|\downarrow\uparrow\rangle + d_i|\downarrow\downarrow\rangle}$$

$$\begin{aligned}
|\uparrow\uparrow\rangle &= |\tfrac{1}{2}\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}\tfrac{1}{2}\rangle \\
|\uparrow\downarrow\rangle &= |\tfrac{1}{2}\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}\tfrac{-1}{2}\rangle \\
|\downarrow\uparrow\rangle &= |\tfrac{1}{2}\tfrac{-1}{2}\rangle \otimes |\tfrac{1}{2}\tfrac{1}{2}\rangle \\
|\downarrow\downarrow\rangle &= |\tfrac{1}{2}\tfrac{-1}{2}\rangle \otimes |\tfrac{1}{2}\tfrac{-1}{2}\rangle
\end{aligned}$$

2. Use $\left(S^{(1,2)}\right)_\pm$ on $|\uparrow\rangle \otimes |\uparrow\rangle$ to GUESS e_i from "nice" bevahior

$$\begin{aligned}
S_-\ |\uparrow\uparrow\rangle &= \tfrac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\
S_-\left[\tfrac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)\right] &= |\downarrow\downarrow\rangle \\
S_-\ |\downarrow\downarrow\rangle &= 0
\end{aligned}$$

S_+ works too

If $\frac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$ then maybe $\frac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$ works (try $S_\pm$ on it).

Guess for $\{e_i\}$:

$$\begin{aligned}
|1\ 1\rangle &\equiv |\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle &&= |\uparrow\uparrow\rangle \\
|1\ 0\rangle &\equiv \tfrac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{-1}{2}\rangle + |\tfrac{1}{2}\tfrac{-1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle\right) &&= \tfrac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\
|1\ \text{-}1\rangle &\equiv |\tfrac{1}{2}\tfrac{-1}{2}\rangle|\tfrac{1}{2}\tfrac{-1}{2}\rangle &&= |\downarrow\downarrow\rangle \\
|0\ 0\rangle &\equiv \tfrac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{-1}{2}\rangle - |\tfrac{1}{2}\tfrac{-1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle\right) &&= \tfrac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)
\end{aligned}$$

3. Check if the guesses are eigenvectors of $\left(S^{(1,2)}\right)^2$ [and do $\left(S^{(1,2)}\right)_z$ to see eigenvalues]

(work has been skipped, do it yourself, check answer below)

$$\begin{aligned}
S^2|1\ 1\rangle &= \hbar^2(1)(1+1)|1\ 1\rangle && (s=1) && S_z|1\ 1\rangle = \hbar(1)|1\ 1\rangle && (m=1) \\
S^2|1\ 0\rangle &= \hbar^2(1)(1+1)|1\ 0\rangle && (s=1) && S_z|1\ 0\rangle = \hbar(0)|1\ 0\rangle && (m=0) \\
S^2|1\ \text{-}1\rangle &= \hbar^2(1)(1+1)|1\ \text{-}1\rangle && (s=1) && S_z|1\ \text{-}1\rangle = \hbar(-1)|1\ \text{-}1\rangle && (m=-1) \\
S^2|0\ 0\rangle &= \hbar^2(0)(0+1)|0\ 0\rangle && (s=0) && S_z|0\ 0\rangle = \hbar(0)|0\ 0\rangle && (m=0) \quad ☑
\end{aligned}$$

$$* \quad \boxed{e_i \in \left\{\begin{array}{l}
\left.\begin{aligned}
|1\ 1\rangle &= 1 \leftarrow \cancel{e^{i\phi}}\ |\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle &&= |\uparrow\uparrow\rangle \\
|1\ 0\rangle &= \tfrac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{-1}{2}\rangle + |\tfrac{1}{2}\tfrac{-1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle\right) &&= \tfrac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\
|1\ \text{-}1\rangle &= |\tfrac{1}{2}\tfrac{-1}{2}\rangle|\tfrac{1}{2}\tfrac{-1}{2}\rangle &&= |\downarrow\downarrow\rangle
\end{aligned}\right\} \quad \text{Triplet}: \ s=1 \\[2ex]
\left.\begin{aligned}
|0\ 0\rangle &= \tfrac{1}{\sqrt{2}}\left(|\tfrac{1}{2}\tfrac{1}{2}\rangle|\tfrac{1}{2}\tfrac{-1}{2}\rangle - |\tfrac{1}{2}\tfrac{-1}{2}\rangle|\tfrac{1}{2}\tfrac{1}{2}\rangle\right) &&= \tfrac{\sqrt{2}}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)
\end{aligned}\right\} \quad \text{Singlet}: \ s=0
\end{array}\right.}$$

4.4.2 2 Objects w/ Any Spin: $j_1 \otimes j_2 = (j_1 + j_2) \oplus |j_1 - j_2| \;\Rightarrow\; (2j_1+1)(2j_2+1) = \sum_{j=|j_1-j_2|}^{j_1+j_2} 2j+1$

- $|\chi_1\rangle$ has spin, j_1; and $|\chi_2\rangle$ has spin, j_2
- $j_{\max} = j_2 + j_1$ and $j_{\min} = |j_2 - j_1|$
- Possible total $|j\ m\rangle$ must satisfy

  1.) $j_{\min} \leq j \leq j_{\max}$, **2.)** $-j \leq m \leq j$,

  3.) have integer differences

If j_1 and j_2 are known from the start,

$$\boxed{\begin{aligned} |j\ m\rangle &= \sum_{m_1,m_2} |j_1\ m_1\rangle \otimes |j_2\ m_2\rangle\ \langle j_1\ m_1| \otimes \langle j_2\ m_2| j\ m\rangle \\ &= \sum_{m_1,m_2} |j_1\ m_1\rangle \otimes |j_2\ m_2\rangle\ C^{j_1 j_2 j}_{m_1 m_2 m} \end{aligned}}$$

where the sum is over all poss. int. diff. values that satisfy

$m_1 + m_2 = m, \quad -j_1 \leq m_1 \leq j_1, \quad -j_2 \leq m_2 \leq j_2,$

and C are the corresponding Clebsh-Gordan coefficients, whose squared value is the probability of measuring the $\chi_1 \otimes \chi_2$ state represented by that term.

Possible Combined $|j\ m\rangle$

$$\begin{array}{l}
(2j_{\max}+1)\left\{\begin{array}{l} \big|j_{\max}\ \ j_{\max}\big\rangle = 1 \leftarrow \cancel{e^{i\phi}} \cdots \\ \big|j_{\max}\ \ j_{\max}{-}1\big\rangle \\ \quad\vdots \\ \big|j_{\max}\ \ {-j_{\max}}\big\rangle \end{array}\right. \\
(2j_{\max}-1)\left\{\begin{array}{l} \big|j_{\max}{-}1\ \ j_{\max}{-}1\big\rangle = 1 \cdot \ldots \\ \big|j_{\max}{-}1\ \ j_{\max}{-}2\big\rangle \\ \quad\vdots \end{array}\right. \\
\quad\vdots \\
(2j_{\min}+1)\left\{\begin{array}{l} \big|j_{\min}\ \ j_{\min}\big\rangle = 1 \cdot \ldots \\ J_-\big|j_{\min}\ \ j_{\min}\big\rangle \sim \ldots \\ \quad\vdots \\ \big|j_{\min}\ \ {-j_{\min}}\big\rangle \end{array}\right.
\end{array}$$

If the top state in a j-set (see box above) is known, applying the J_- lowering operator (and normalizing) provides the coefficients for the rest of the set of varying m. The coefficients for each top state of a set are (by convention) positive, real, and normalized to 1. This makes all of the coefficients real. For the top state of the initial $j_{\max}$-set, $|j_{\max}\ j_{\max}\rangle$, there is only one product-ket in the sum; its coefficient is thus set to 1. For an arbitrary set below the first, the top state has product-ket coefficients such that the state is orthogonal to all other previously determined states that have the same m. To reduce some work to solve for them, use

$$C^{j_1 j_2 j}_{m_1 m_2 m} = (-1)^{j_1+j_2-j} \cdot C^{j_1 j_2 j}_{-m_1 -m_2 -m}$$

$$\langle j_1\ m_1|\langle j_2\ m_2|j\ m\rangle = (-1)^{j_1+j_2-j} \cdot \langle j_1\ \ -m_1|\langle j_2\ \ -m_2|j\ \ -m\rangle$$

If m_1 and m_2 are also known from the start, then $m = m_1 + m_2$, and

$$\boxed{|j_1\ m_1\rangle \otimes |j_2\ m_2\rangle = \sum_j C^{j_1 j_2 j}_{m_1 m_2 m}\ |j\ \ {\scriptstyle (m_1+m_2)}\rangle}$$

where the sum is only over all possible s as satisfied above - **1.), 2.) and 3.)**. In this case, the total z-component, m, is known. The only unknown is the total spin, s, whose probability to be measured is C^2.

4.5 Electron in Magnetic Field

$\mu_{\text{clas.}} = IA = \frac{q}{2\pi r} v(\pi r^2) = \frac{q}{2\pi r}\frac{L}{mr}(\pi r^2) = \left(\frac{q}{2m}\right) L \;\rightarrow\; \frac{e\hbar}{2m}\cdot n$ (Bohr magneton)

$\mu_{\text{quan.}} = \left(\frac{g_e q}{2m}\right) S = \left(\frac{q}{m}\right) S = \gamma S$

$$\begin{aligned} \tau_\mu &= \mu \times B \\ F_\mu &= \nabla(\mu \cdot B) \end{aligned} \quad , \quad \begin{aligned} H &= -\mu \cdot B \\ &= -\gamma S \cdot B \end{aligned}$$

<u>Larmor Precession</u>

$$B = B_0 \hat{k}$$

$$\begin{aligned} H &= -\gamma B_0 S_z \\ &= -\gamma B_0 \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix} \end{aligned} \quad \Rightarrow$$

$$\begin{aligned} \chi(t) &= \cos(\alpha/2)\begin{pmatrix}1\\0\end{pmatrix} e^{-\frac{i}{\hbar}E_1 t} + \sin(\alpha/2)\begin{pmatrix}0\\1\end{pmatrix} e^{-\frac{i}{\hbar}E_2 t} \\ &= \begin{pmatrix} \cos(\alpha/2) e^{-\frac{i}{\hbar}E_1 t} \\ \sin(\alpha/2) e^{-\frac{i}{\hbar}E_2 t} \end{pmatrix} \end{aligned}$$

$$\begin{pmatrix} \langle S_x \rangle \\ \langle S_y \rangle \\ \langle S_z \rangle \end{pmatrix} = \begin{pmatrix} \frac{\hbar}{2}\sin(\alpha)\cos(\gamma B_0 t) \\ -\frac{\hbar}{2}\sin(\alpha)\sin(\gamma B_0 t) \\ \frac{\hbar}{2}\cos(\alpha) \end{pmatrix}$$ (torque from B with S leads to precession)

<u>Stern-Gerlach</u>

5 Bosons and Fermions

Distinguishable Particles: $\boxed{\psi(r_1, r_2) \equiv \psi_a(r_1)\psi_b(r_2)}$

Indistinguishable Particles:

$$\boxed{P_x f(x_1, x_2;\ y_1, y_2;\ \ldots) \ = \ \pm\ f(x_2, x_1;\ y_1, y_2;\ \ldots)} \quad , \quad \boxed{\iint |\Psi(x_1,x_2)|^2 dx_1 dx_2 = \iint \Pr(x_1,x_2) \frac{dx_1 dx_2}{2}}$$

Boson:
$\big(s \in \{0, 1, 2, \ldots\}\big)$

$$\psi_+(r_1, r_2) \equiv \frac{1}{\sqrt{2}}\Big[\psi_a(r_1)\psi_b(r_2) + \psi_a(r_2)\psi_b(r_1)\Big]$$

$$\boxed{\psi(r_1, r_2) = \psi(r_2, r_1)} \quad \rightarrow \quad \boxed{P_i\Psi = \Psi} \quad \text{(symmetric)}$$

Fermion:
$\big(s \in \{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\}\big)$

$$\psi_-(r_1, r_2) \equiv \frac{1}{\sqrt{2}}\Big[\psi_a(r_1)\psi_b(r_2) - \psi_a(r_2)\psi_b(r_1)\Big]$$

$$\boxed{\psi(r_1, r_2) = -\psi(r_2, r_1)} \quad \rightarrow \quad \boxed{P_i\Psi = -\Psi} \quad \text{(antisymmetric)}$$

5.1 Exchange Forces: $\Big\langle (x_1 - x_2)^2 \Big\rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$

Dist. Part. :	$\big\langle (\Delta x)^2 \big\rangle = \big\langle (\Delta x)^2 \big\rangle_d = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b$	
Symmetric:	$\big\langle (\Delta x)^2 \big\rangle = \big\langle (\Delta x)^2 \big\rangle_d - 2\ \big\| \langle \psi_b \| x \| \psi_a \rangle \big\|^2$	(attractive if overlap)
Antisymmetric:	$\big\langle (\Delta x)^2 \big\rangle = \big\langle (\Delta x)^2 \big\rangle_d + 2\ \big\| \langle \psi_b \| x \| \psi_a \rangle \big\|^2$	(repulsive if overlap)

- $\langle x_1 x_2 \rangle = \dfrac{1}{2}\displaystyle\int \Big[\psi_a(r_1)^*\psi_b(r_2)^* \pm \psi_b(r_1)^*\psi_a(r_2)^*\Big] x_1 x_2 \Big[\psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_1)\psi_a(r_2)\Big] dx_1 dx_2$

$$= \ \frac{1}{2}\langle x \rangle_a \langle x \rangle_b + \frac{1}{2}\langle x \rangle_b \langle x \rangle_a$$

$$\pm\ \frac{1}{2}\Big\langle \psi_b(r_1)\Big| x_1 \Big|\psi_a(r_1)\Big\rangle\Big\langle \psi_a(r_2)\Big| x_2 \Big|\psi_b(r_2)\Big\rangle \pm \frac{1}{2}\Big\langle \psi_a(r_1)\Big| x_1 \Big|\psi_b(r_1)\Big\rangle\Big\langle \psi_b(r_2)\Big| x_2 \Big|\psi_a(r_2)\Big\rangle$$

$$= \langle x \rangle_a \langle x \rangle_b \pm \Big\| \langle \psi_b | \, x \, | \psi_a \rangle \Big\|^2$$

Two Electrons:

$$\psi(r_1,r_2)\chi(m_1,m_2) = \begin{cases} \overset{\text{(singlet)}}{-\psi(r_1,r_2)\chi(m_2,m_1)} & \Rightarrow \ \begin{matrix}\chi \text{ is antisymmetric so} \\ \psi \text{ is symmetric}\end{matrix} \ \Rightarrow \ \text{Attractive (ground state)} \\[2ex] \overset{\text{(triplet)}}{-\psi(r_2,r_1)\chi(m_1,m_2)} & \Rightarrow \ \begin{matrix}\chi \text{ is symmetric so} \\ \psi \text{ is antisymmetric}\end{matrix} \ \Rightarrow \ \text{Repulsive} \end{cases}$$

5.2 Statistics

Sterling's Approx:

$$\log(z!) \approx z\log(z) - z \qquad z \gg 1 \;\text{ or }\; z = 0$$

$$\frac{d}{dz}\log(z!) \approx \log(z)$$

Lagrange Multiplier:

$$G(X,\alpha,\beta) = \log(Q_{(X)}) + \alpha f_1(X) + \beta f_2(X)$$

$$\frac{\partial G}{\partial \alpha}[Q_{\max}] = 0, \qquad \frac{\partial G}{\partial \beta}[Q_{\max}] = 0, \qquad \frac{\partial G}{\partial N_n}[Q_{\max}] = 0$$

$$\sum_n N_n = N \qquad\qquad \sum_n N_n E_n = E$$

$$f_1(X) = N - \sum_n N_n = 0 \qquad\qquad f_2(X) = E - \sum_n N_n E_n = 0$$

Let there be N_n particles in the E_n energy level having d_n degeneracies, and $Q(N_1, N_2, ...)$ be the number of possible configurations for such a state given $X = (N_1, N_2, ..., N_n)$.

Dist.

$$\begin{cases} \textbf{1.)}\ Q(X) = \prod_n \binom{N - N_1 - ... - N_{n-1}}{N_n} d_n^{N_n} \\ \qquad\qquad = N! \prod_n \frac{d_n^{N_n}}{N_n!} \\ \textbf{2.)}\ \log(Q) = \log(N!) + \sum_n N_n \log(d_n) - \log(N_n!) \end{cases}$$

$$\textbf{3.)}\ \frac{\partial G}{\partial N_n} \approx \log(d_n) - \log(N_n) - \alpha - \beta E_n = 0$$

$$\textbf{4.)}\ N_n = \frac{d_n}{e^{\beta E_n + \alpha}}$$

Fermion

$$\begin{cases} \textbf{1.)}\ Q(X) = \prod_n \binom{d_n}{N_n} \\ \textbf{2.)}\ \log(Q) = \sum_n \log(d_n!) - \log(N_n!) - \log[(d_n - N_n)!] \end{cases}$$

$$\textbf{3.)}\ \frac{\partial G}{\partial N_n} \approx -\log(N_n) + \log(d_n - N_n) - \alpha - \beta E_n = 0$$

$$\textbf{4.)}\ N_n = \frac{d_n}{e^{\beta E_n + \alpha} + 1}$$

Boson

$$\begin{cases} \textbf{1.)}\ Q(X) = \prod_n \binom{N_n + d_n - 1}{N_n} \\ \textbf{2.)}\ \log(Q) = \sum_n \log[(N_n + d_n - 1)!] - \log(N_n!) - \log[(d_n - 1)!] \end{cases}$$

$$\textbf{3.)}\ \frac{\partial G}{\partial N_n} \approx \log(N_n + d_n - 1) - \log(N_n) - \alpha - \beta E_n = 0$$

$$\textbf{4.)}\ N_n = \frac{d_n - 1}{e^{\beta E_n + \alpha} - 1} \approx \frac{d_n}{e^{\beta E_n + \alpha} - 1}$$

Given some substance in thermal equilibrium,

$$\beta = \frac{1}{k_b T} \qquad \mu(T) \equiv -\frac{\alpha}{k_b T}$$

where μ depends on the situation.

$$\frac{N_n}{d_n}: \qquad n(\epsilon) \quad = \quad \begin{cases} \frac{1}{e^{(\epsilon-\mu)/k_b T}} & \text{Maxwell-Boltzmann} \\ \frac{1}{e^{(\epsilon-\mu)/k_b T}+1} & \text{Fermi-Dirac} \\ \frac{1}{e^{(\epsilon-\mu)/k_b T}-1} & \text{Bose-Einstein} \end{cases}$$

6 Perturbation Theory

$$H^{(0)}\psi_n = E_n\psi_n$$
$$\downarrow$$
$$H\psi_n' = E_n'\psi_n'$$

$$\left[H^{(0)} + \lambda H^{(1)}\right]\left[\psi_n + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + ...\right] = \left[E_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...\right]\left[\psi_n + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + ...\right]$$

$$\begin{array}{ccc} \cancel{\lambda^0 H^{(0)}\psi_n} & & \cancel{\lambda^0 E_n\psi_n} \\ + \lambda^1(H^{(0)}\psi_n^{(1)} + H^{(1)}\psi_n) & & + \lambda^1(E_n\psi_n^{(1)} + E_n^{(1)}\psi_n) \\ & = & \\ + \lambda^2(H^{(0)}\psi_n^{(2)} + H^{(1)}\psi_n^{(1)}) & & + \lambda^2(E_n\psi_n^{(2)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(2)}\psi_n) \\ + ... & & + ... \end{array} \qquad {\scriptstyle (\lambda=1)}$$

6.1 Non-Degenerate Theory

$\underline{E_n^{(1)},\ \psi_n^{(1)}:}$

$$E_n\psi_n^{(1)} + E_n^{(1)}\psi_n = H^{(0)}\psi_n^{(1)} + H^{(1)}\psi_n$$

$$\langle\psi_m| \quad (-H^{(1)} + E_n^{(1)})|\psi_n\rangle = \langle\psi_m| \quad (H^{(0)} - E_n)|\psi_n^{(1)}\rangle = \sum c_i^{(1)}(E_i - E_n)\langle\psi_m|\psi_i\rangle$$

$$-\langle\psi_m|H^{(1)}|\psi_n\rangle + E_n^{(1)}\langle\psi_m|\psi_n\rangle = c_m^{(1)}(E_m - E_n)$$

$$\boxed{E_n^{(1)} = \langle\psi_n|H^{(1)}|\psi_n\rangle} \qquad \boxed{\psi_n^{(1)} = \sum_{m\neq n}\frac{\langle\psi_m|H^{(1)}|\psi_n\rangle}{E_n - E_m}\psi_m + (0)\psi_n}$$

$\underline{E_n^{(2)},\ |n^{(2)}\rangle:}$

$$\begin{aligned} -\langle m^{(0)}|H^{(1)}|n^{(1)}\rangle + E_n^{(1)}\langle m^{(0)}|n^{(1)}\rangle + E_n^{(2)}\langle m^{(0)}|n^{(0)}\rangle &= \langle m^{(0)}|H^{(0)} - E_n^{(0)}|n^{(2)}\rangle \\ &= c_m^{(2)}(E_m - E_n) \end{aligned}$$

$$\boxed{E_n^{(2)} = \sum_{m\neq n}\frac{\left|\langle m|H^{(1)}|n\rangle\right|^2}{E_n - E_m}} = \langle n|H^{(1)}|n^{(1)}\rangle \quad , \quad \boxed{|n^{(2)}\rangle = \sum_{m\neq n}\frac{\langle m|H^{(1)} - E_n^{(1)}|n^{(1)}\rangle}{E_n - E_m}\cdot|m\rangle}$$

$\underline{E_n^{(i+1)},\ |n^{(i+1)}\rangle:}$

$$E_n^{(i+1)} = \langle n|H^{(1)}|n^{(i)}\rangle$$

$$|n^{(i+1)}\rangle = \sum_{m\neq n}\frac{\langle m|H^{(1)}|n^{(i)}\rangle - \sum_{j=0}^{i}E_n^{(j+1)}\langle m|n^{(i-j)}\rangle}{E_n - E_m}\cdot|m\rangle$$

6.2 Degenerate Perturbation Theory (see Matrix Operators)

$$\Psi = \sum_i \left(c_i^{(\psi)}[\Psi]\right)\psi_i \equiv \sum_i c_i^{(\psi)}\psi_i = c_0^{(\psi)}\psi_0 + c_1^{(\psi)}\psi_1 + \ldots \quad , \quad \forall\psi_i:$$

- $H^{(0)}\psi_i = E_n\psi_i$ (ψ_n are degenerate eigenfunctions of $H^{(0)}$)
- $\langle\psi_i|\psi_j\rangle = \delta_{ij}$
- $\langle\psi_i|\hat{Q}|\psi_j\rangle \equiv Q_{ij}$

$$E_n\Psi^{(1)} + E^{(1)}\Psi = H^{(0)}\Psi^{(1)} + H^{(1)}\Psi \qquad \text{(first order)}$$

$$\begin{aligned}\cancel{E_n\langle\psi_i|\Psi^{(1)}\rangle} + E^{(1)}\langle\psi_i|\Psi\rangle &= \cancel{\langle H^{(0)}\psi_i|\Psi^{(1)}\rangle} + \langle\psi_i|H^{(1)}|\Psi\rangle \\ &= \langle\psi_i|H^{(1)}|c_0\psi_0 + c_1\psi_1 + \ldots\rangle \\ c_iE^{(1)} &= c_0\langle\psi_i|H^{(1)}|\psi_0\rangle + c_1\langle\psi_i|H^{(1)}|\psi_1\rangle + \ldots\end{aligned}$$

$$E^{(1)}\begin{pmatrix} c_0[\Psi] \\ c_1[\Psi] \\ \vdots \end{pmatrix}^{(\psi)} = \begin{pmatrix} H_{00}^{(1)} & H_{01}^{(1)} & \ldots \\ H_{10}^{(1)} & H_{11}^{(1)} & \ldots \\ \vdots & \vdots & \end{pmatrix}^{(\psi)} \begin{pmatrix} c_0[\Psi] \\ c_1[\Psi] \\ \vdots \end{pmatrix}^{(\psi)} \Rightarrow \boxed{\begin{array}{c}\text{(solve for } E^{(1)}, \vec{c}^{\,(\psi)}[\Psi])\\ \left\| \begin{matrix} H_{aa}^{(1)} - E^{(1)} & H_{ab}^{(1)} & \ldots \\ H_{ba}^{(1)} & H_{bb}^{(1)} - E^{(1)} & \ldots \\ \vdots & \vdots & \end{matrix} \right\| = 0\end{array}}$$

In general,

$$E_i^{(1)}\vec{c}^{\,(\psi)}[\Psi_i] \;=\; \overline{H^{(1)}}^{(\psi)}\;\vec{c}^{\,(\psi)}[\Psi_i] \qquad (i\text{th eigen-})$$

$$E_i^{(1)}\begin{pmatrix} | \\ \vec{c}\,[\Psi_i] \\ | \end{pmatrix}^{(\psi)} = \begin{pmatrix} | & | & \\ \vec{c}\,[\Psi_i] & \vec{c}\,[\Psi_i] & \ldots \\ | & | & \end{pmatrix}^{(\psi)} \begin{pmatrix} E_0^{(1)} & 0 & \ldots \\ 0 & E_1^{(1)} & \ldots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} - & \vec{c}^{\,*}[\Psi_i] & - \\ - & \vec{c}^{\,*}[\Psi_i] & - \\ & \vdots & \end{pmatrix}^{(\psi)} \begin{pmatrix} | \\ \vec{c}\,[\Psi_i] \\ | \end{pmatrix}^{(\psi)}$$

Instead of solving the characteristic polynomial, it would be wise to choose a basis $\{\psi\}$ such that $\vec{c}^{\,(\psi)}[\Psi_i] = (\ldots 0\ 0\ 1_{(i)}\ 0\ 0\ \ldots)^T \;\Leftrightarrow\; \Psi_i = \psi_i$, making $\overline{H^{(1)}}^{(\psi)}$ diagonal with eigenvalue entries. These are the energy eigenvalues, $E_i^{(1)} = \left(H^{(1)}\right)_{ii}^{(\psi)} = \langle\psi_i|H^{(1)}|\psi_i\rangle$, which is just like first-order non-Perturbation energy. This also means $|\psi_i\rangle$ are eigenfunctions of $H^{(1)}$ (see Matrix Operators).

It is best to find a hermitian operator, $\hat{A}$, that commutes with $H^{(0)}$ and $H^{(1)}$, whose eigenvalues within the degenerate basis are unique. The corresponding eigenfunctions will be a basis that makes $H^{(1)}$ diagonal. This will also make them eigenfunctions of $H^{(1)}$.

1. $A = A^\dagger$
2. $[A, H^{(0)}] = 0 \;\rightarrow\; \left\{\exists\{\Psi\} \;\middle|\; (A\Psi_n = a_n\Psi_n),\ (H^{(0)}\Psi_n = E_n\Psi_n)\right\}$
3. $\{\psi\} \subset \{\Psi\}$ s.t $\forall\psi_i : \begin{cases} \left(H^{(0)}\psi_i = E_n\psi_i\right), & \leftarrow \text{degenerate} \\ (A\psi_i = a_i\psi_i|), & (\forall_{(i\neq j)}\ a_i \neq a_j) \end{cases}$
4. $[A, H^{(1)}] = 0 \;\Rightarrow\; 0 = \langle A\psi_i|H^{(1)}|\psi_j\rangle - \langle\psi_i|H^{(1)}|A\psi_j\rangle$
   $0 = (a_i - a_j)H_{ij}^{(1)}$
   $0 = H_{ij}^{(1)} \quad ☑$

6.3 Hydrogen Energy Corrections

6.3.1 Fine Structure - $\alpha^4 mc^2$

The Dirac Equation can derive the total fine structure correction with a α^4 order approx.

1. Relativistic, $\hat{\boldsymbol{p}}^4$

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2 = mc^2\sqrt{1 + \tfrac{p^2}{m^2c^2}} - mc^2$$

$$= mc^2\left[\frac{(\frac{1}{2})}{1!}\left(\frac{p^2}{m^2c^2}\right) + \frac{(\frac{1}{2})(1-\frac{1}{2})}{2!}\left(\frac{p^2}{m^2c^2}\right)^2 + ...\right]$$

$$= \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + ...$$

$$\downarrow$$

$$H_r^{(1)} = -\frac{p^4}{8m^3c^2}$$

(For some reason $\hat{p}^4$ needs to be hermitian to use perturbation theory. It only isn't when $l = 0$, while $\hat{p}^2$ always is hermitian. See Prob. 6.15)

L^2 and L_z should commute with p^4 because the perturbation is spherically symmetric, meaning l and m_l should be conserved (see Operator Evolution). Their eigenvalues are also distinct (taking the eigenfunctions of nlm_l together) within each set of n^2 degeneracies, so their eigenvectors and eigenvalues can be used. n, l and m_l the "good" numbers.

$$\langle r^{-1}\rangle = \frac{1}{n^2a_0^1}$$

$$\langle r^{-2}\rangle = \frac{1}{(l+1/2)n^3a_0^2}$$

$$\left\langle\psi_{nlm_l}|H_r^{(1)}|\psi_{nlm_l}\right\rangle = \frac{-1}{8m^3c^2}\langle\psi_{nlm_l}|p^4|\psi_{nlm_l}\rangle$$

$$= \frac{-1}{8m^3c^2}\langle p^2\psi_{nlm_l}|p^2|\psi_{nlm_l}\rangle$$

$$= \frac{-1}{8m^3c^2}\left\langle\left[2m(E_n - V)\right]^2\right\rangle$$

$$= \frac{-4m^2}{8m^3c^2}\langle E_n^2 - 2E_nV + V^2\rangle$$

$$= -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+1/2} - 3\right]$$

2. Spin-Orbit Coupling, $\boldsymbol{S_e}\cdot\boldsymbol{L_e}$

In the electron's frame of reference, the proton is spinning around it, creating a B-field affecting its magnetic dipole moment. The non-inertial reference frame requires multiplying by the Thomas procession correction, which in this case is $C_T = g_e - 1 = 1/2$. In the lab frame, the moving electron's magnetic dipole moment creates an electric dipole moment, which is affected by the proton charge. The latter is much harder to calculate.

$$
\begin{aligned}
H_{so}^{(1)} &= -C_T\ \mu_e \cdot B(L_e) \qquad \text{(See Electron in Magnetic Field)}\\
&= \tfrac{1}{2}\tfrac{qS}{m} \cdot \tfrac{k_\mu}{r^3}\int I d\vec{l} \times \vec{r} \qquad \left(\sim\ \tfrac{1}{2}\tfrac{qS}{m} \cdot \tfrac{k_\mu}{r^3}\int \tfrac{mqd\vec{v}\times\vec{r}}{m} \right)\\
&= \tfrac{1}{2}\tfrac{qS}{m} \cdot \tfrac{k_\epsilon}{c^2}\tfrac{2\pi}{r} I = \tfrac{1}{2}\tfrac{qS}{m} \cdot \tfrac{k_\epsilon}{c^2}\tfrac{2\pi}{r}\tfrac{q(L/mr)}{2\pi r}\\
&= \frac{kqq}{2m}\frac{1}{mc^2}\frac{S\cdot L}{r^3} = \frac{e^2}{8\pi\epsilon_0 m^2 c^2}\frac{S\cdot L}{r^3}
\end{aligned}
$$

$S \cdot L$ does not commute with L or S (meaning m_l and m_s are bad), but $[S\cdot L, S^2] = [S\cdot L, L^2] = 0$. The sum of the two, $J \equiv L + S$, and J^2 also commute with the perturbation. They are all conserved, and their unique eigenvalues per set of degeneracies - $l, s{=}1/2, j, m_j$ - are the “good” numbers (along with n).

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

$$
\langle r^{-3}\rangle = \frac{1}{l(l+1/2)(l+1)n^3a_0^3}
$$

(note: divergent at $l=0$)

$$
\begin{aligned}
\langle nljm_j|H_{so}^{(1)}|nljm_j\rangle &= \frac{kqq}{2m}\frac{1}{mc^2}\frac{\hbar^2[j(j+1)-l(l+1)-s(s+1)]}{2l(l+1/2)(l+1)n^3a_0^3}\\
&= \frac{kqq}{4mn^4}\frac{\hbar^2\alpha^3m^3c^3}{\hbar^3mc^2}\frac{n[j(j+1)-l(l+1)-s(s+1)]}{l(l+1/2)(l+1)}\\
&= \frac{kqq}{4\hbar cn^4}\frac{\alpha^3m^2c^4}{mc^2}\frac{n[j(j+1)-l(l+1)-s(s+1)]}{l(l+1/2)(l+1)}\\
&= \frac{E_n^2}{mc^2}\left\{\frac{n\left[j(j+1)-l(l+1)-3/4\right]}{l(l+1/2)(l+1)}\right\}
\end{aligned}
$$

3. Darwin Term (correction for $H_{so}^{(1)}$ when $l=0$) skipped

4. Total Correction

$$
\begin{aligned}
E_{fs}^{(1)} &= E_r^{(1)} + E_{so}^{(1)}\\
&= -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+\frac{1}{2}} - 3\right] + \frac{E_n^2}{mc^2}\left\{\frac{n\left[j(j+1)-l(l+1)-3/4\right]}{l(l+1/2)(l+1)}\right\}\\
&= \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right) \qquad (j{=}l\pm1/2)\\
&\downarrow\\
E_{nj} &= E_n + E_{fs}^{(1)}\\
&= E_n\left[1 - \frac{E_n}{2mc^2}\left(\frac{4n}{j+1/2} - 3\right)\right]\\
&= -\frac{\alpha^2mc^2}{2n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+1/2} - 3/4\right)\right]
\end{aligned}
$$

Fine structure splits the l energy degeneracies. However, since $j = l \pm 1/2$, there are still two j degeneracies if $n > 2$. Overall, the good numbers to use for stationary state solutions to the hydrogen atom w/ fine structure correction are $n, l, s{=}1/2, j, m_j$. Note, J^2, L^2, and S^2 always commute(?)

6.3.2 Zeeman Effect (Ext. B-Field)

$$\begin{aligned} H_B^{(1)} &= -(\mu_s + \mu_l) \cdot B_{\text{ext}} \qquad \text{(see Electron in Magnetic Field)} \\ &= -\left(\frac{g_e q}{2m} S + \frac{q}{2m} L\right) \cdot B_{\text{ext}} \\ &= \frac{e}{2m}(2S + L) \cdot B_{\text{ext}} \end{aligned}$$

Weak Zeeman ($B_{\text{ext}} \ll B_{\text{int}}$)

$$\begin{aligned} H_{WZ}^{(1)} &= \frac{e}{2m} B_{\text{ext}} \cdot (2S + L) \\ &= \frac{e}{2m} B_{\text{ext}} \cdot (J + S) \end{aligned}$$

Fine structure perturbation dominate the Zeeman perturbation, so the fine structure numbers are the good ones: $n, l, s{=}1/2, j$, and m_j. m_l and m_s can't be used for $\langle L \rangle$ or $\langle S \rangle$, so instead use the fact that the "vector" $J = L + S$ is conserved, so a **time-averaged** S-component to the J "vector" can be defined as $S_{\text{ave}} = \frac{S \cdot J}{J^2} J$, where $S \cdot J = \frac{1}{2}(J^2 + S^2 - L^2)$.

$$\begin{aligned} E_{\text{WZ}}^{(1)} &= \frac{e}{2m} B_{\text{ext}} \cdot \langle nljm_j | J + S_{\text{ave}} | nljm_j \rangle \\ &= \frac{e}{2m} B_{\text{ext}} \cdot \left\langle J \left(1 + \frac{S \cdot J}{J^2}\right) \right\rangle \\ &= \frac{e}{2m} B_{\text{ext}} \cdot \langle J \rangle \left(1 + \frac{j(j+1) - l(l+1) + 3/4}{2j(j+1)}\right) \\ &= \frac{e\hbar}{2m} B_{\text{ext}} m_j \left(1 + \frac{j(j+1) - l(l+1) + 3/4}{2j(j+1)}\right) \qquad \text{(let } B_{\text{ext}} \text{ be parallel to the z-axis)} \\ &= \mu_B B_{\text{ext}} m_j g_j \qquad \begin{array}{l} \mu_B\text{=Bohr magneton=}5.788 \times 10^{-5} \text{ ev/T} \\ g_j\text{=Lande g-factor} \end{array} \end{aligned}$$

Strong Zeeman ($B_{\text{ext}} \gg B_{\text{int}}$)

For a strong magnetic field parallel to the z-axis, m_l and m_s are stuck in the same place, making them and l conserved. The external torque, however, means that the total angular momentums, j and m_j are not. Though unneeded, obviously $s{=}1/2$.

$$\begin{aligned} E_{SZ}^{(1)} &= \frac{e}{2m} B_{\text{ext}} \langle 2S_z + L_z \rangle \\ &= \mu_B B_{\text{ext}} (2m_s + m_l) \end{aligned}$$

The spin-orbit correction must be changed with respect to the new good numbers, m_l and m_s. The relativistic correction uses the same numbers, so it stays the same.

$$E_{\text{so}}^{(1)} = \frac{e^2}{8\pi\epsilon_0 m^2c^2}\left\langle\frac{S_xL_x + S_yL_z + S_zL_z}{r^3}\right\rangle$$
$$= \frac{e^2}{8\pi\epsilon_0 m^2c^2}\frac{0+0+\hbar^2 m_s m_l}{l(l+1/2)(l+1)n^3a_0^3}$$
$$= \frac{kqq}{2m^2c^2}\frac{\hbar^2}{(\hbar/\alpha mc)^3n^3}\frac{m_sm_l}{l(l+1/2)(l+1)}$$
$$= \frac{kqq}{2\hbar c}\frac{\alpha^3m^2c^4}{4mc^2n^4}\frac{4nm_sm_l}{l(l+1/2)(l+1)}$$
$$= \frac{E_n^2}{2mc^2}\frac{4nm_sm_l}{l(l+1/2)(l+1)}$$

$\rightarrow$

$$E_{\text{fs}}^{(1)} = E_{\text{so}}^{(1)} + E_{\text{r}}^{(1)}$$
$$= \frac{E_n^2}{2mc^2}\frac{4nm_sm_l}{l(l+1/2)(l+1)} + \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{l+1/2}\right]$$
$$= \frac{4nE_n^2}{2mc^2}\left[\frac{m_sm_l}{l(l+1/2)(l+1)} + \frac{3}{4n} - \frac{1}{l+1/2}\right]$$
$$\downarrow$$
$$E_{nlm_lm_s} = E_n + E_{\text{SZ}}^{(1)} + E_{\text{fs}}^{(1)}$$

Intermediate Zeeman ($B_{\text{ext}} \sim B_{\text{int}}$)

There are no good numbers here (see Degenerate Perturbation Theory). The basis is chosen to be $|j\ m_j\rangle = \sum_i C_i|l\ m_l\rangle \otimes |s\ m_s\rangle$ (see 2 Objects w/ Any Spin), as it makes $\overline{H^{(1)}}^{(e)}$ easier (instead of using l, m_l, m_s).

1.) $\psi_i = |j\ m_j\rangle_i$

2.) $\Big(\langle l\ m_l|\langle s\ m_s|\Big)_x\Big(|l\ m_l\rangle|s\ m_s\rangle\Big)_y = \delta_{xy}$

3.) $Q_{rc}^{(\psi)} = \langle\psi_r|\hat{Q}|\psi_c\rangle$

4.) ψ_i s.t. $\begin{cases} 0 \le l < n \\ j_{(l\pm)} = l \pm 1/2, \\ 2l^2 < i \le 2(l{+}1)^2 \end{cases}$

$$\langle{\scriptstyle jm_j}|H_{fs}^{(1)}|{\scriptstyle jm_j}\rangle = \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+1/2}\right)$$
$$\equiv \gamma_n\left(3 - \frac{4n}{j+1/2}\right)$$

$$\langle{\scriptstyle jm_j}|H_{IZ}^{(1)}|{\scriptstyle jm_j}\rangle = \langle{\scriptstyle jm_j}|H_{IZ}^{(1)}\Big(C_i|{\scriptstyle lm_l}\rangle \otimes |{\scriptstyle sm_s}\rangle\Big)$$
$$= \mu_B B_{\text{ext}}(2m_s + m_l)C_i^2$$
$$\equiv \beta(2m_s + m_l)C_i^2$$

$$\overline{H^{(1)}}^{(jm_j)} = \overline{H_{fs}^{(1)}}^{(jm_j)} + \overline{H_{IZ}^{(1)}}^{(jm_j)}$$

See Griffith Prob. 6.25 for example with $n = 2$

6.3.3 Stark Effect (Small Ext. E-Field)

- $H^{(1)} = -p \cdot E = eE \cdot r$ (small r)
- $n = 1 \;\rightarrow\; H^{(1)} = 0$
- $n = 2 \;\rightarrow\; \begin{cases} H^{(1)} = 0 & m = \pm 1 \\ H^{(1)} = ke|E|a_0 & m = 0 \end{cases}$ (k is some constant)

6.3.4 Lamb Shift (quantitized E-field) - $\alpha^5 mc^2$ (skipped)

6.3.5 Hyperfine (Spin-Spin), $\boldsymbol{S_p} \cdot \boldsymbol{S_e}$ - $m/m_p\ \alpha^4 mc^2$

(Coupling between the electron magnetic moment and the magnetic field from the proton magnetic moment)

$$\mu_e = -\frac{g_e e}{2m_e} S_e = -\frac{e}{m_e} S_e, \qquad \mu_p = \frac{g_p e}{2m_p} S_p$$

$$B(\mu_p) = \frac{\mu_0}{4\pi r^3}[3(\vec{\mu_p} \cdot \hat{r})\hat{r} - \vec{\mu_p}] + \frac{2\mu_0}{3}\vec{\mu_p}\delta^3(r)$$

$$H_{hf}^{(1)} = -\mu_e \cdot B(\mu_p) = \ldots$$

$$\downarrow$$

$$E_{hf}^{(1)} = \left(\frac{e}{m_e}\right)\left(\frac{2\mu_0}{3}\frac{g_p e}{2m_p}\right)\langle S_e \cdot S_p \rangle \left|\psi_{nlm}(0)\right|^2$$

In the ground state, $\left|\psi_{100}(0)\right|^2 = 1/(\pi a_0^3)$. S_e^2, S_p^2, and the sum $S = S_e + S_p$ commute with $S_e \cdot S_p$, so s_e, s_p, m_s, s^2 are the good numbers. S_e and S_p do not, so m_{se} and m_{sp} are not good numbers.

$$\begin{aligned}
E_{hf}^{(1)} &= \left(\frac{e}{m_e}\right)\left(\frac{2}{3\epsilon_0 c^2}\frac{g_p e}{2m_p}\right)\frac{1}{2\pi a_0^3}\langle S^2 - S_e^2 - S_p^2 \rangle \\
&= \frac{g_p e^2}{4\pi\epsilon_0 c^2 m_p m_e}\frac{4\alpha^3 m_e^3 c^3 \hbar^2}{3\hbar^3}\left[\frac{s(s+1)}{2} - 3/4\right] \\
&= \frac{4}{3} g_p \frac{m_e}{m_p}\alpha^4 m_e c^2 \left[\frac{s(s+1)}{2} - 3/4\right] \\
&= \frac{4}{3} g_p \frac{m_e}{m_p}\alpha^4 m_e c^2 \cdot \begin{cases} \frac{1}{4} & s = 1 \ \text{(triplet)} \\ \frac{-3}{4} & s = 0 \ \text{(singlet)} \end{cases} \quad \rightarrow \quad \begin{array}{l} \Delta E = 5.88 \times 10^{-6}\ \text{eV} \\ \lambda = 21\ \text{cm}, \quad \nu = 1420\ \text{MHz} \end{array}
\end{aligned}$$

6.4 Transition Amplitude (See Pictures)

$$H(t) = H^0 + H^1(t)$$
$$\downarrow$$
$$U(t)|i^0\rangle = \sum_n |n^0\rangle e^{-\frac{i}{\hbar}E_n^0 t}\langle n^0|U_I|i^0\rangle$$
$$|\Psi(t)\rangle = \boxed{\sum_n |n^0\rangle e^{-\frac{i}{\hbar}E_n^0 t} d_n(t)}$$
$$\downarrow$$
$$0 = \langle f^0|i\hbar\tfrac{\partial}{\partial t} - H^0 - H^1(t)|\Psi(t)\rangle$$
$$= \sum_n \langle f^0|\left[i\hbar\dot{d}_n - H^1(t)\,d_n\right]|n^0\rangle e^{-\frac{i}{\hbar}E_n^0 t}$$
$$\downarrow$$
$$\dot{d}_f(t) = \sum_n \tfrac{1}{i\hbar}\langle f^0|H^1(t)|n^0\rangle\, e^{\frac{i}{\hbar}(E_f^0 - E_n^0)t}\, d_n(t)$$
$$= \sum_n \tfrac{1}{i\hbar}\langle f^0|H^1(t)|n^0\rangle\, e^{i\omega_{fn}t}\, d_n(t)$$

$$d_n(t) = d_n(0) + \int_0^t \dot{d}_n\, dt' :$$

- $d_n(0) \;=\; \delta_{ni}$ (if $|d_{n\neq i}(t)| \ll 1$) (0^{th} order)
- $\dot{d}_f(t) \;\approx\; \frac{1}{i\hbar}\langle f^0|H^1(t)|i^0\rangle\, e^{i\omega_{fi}t}$
- $\boxed{d_n(t) \;\approx\; \delta_{ni} + \frac{1}{i\hbar}\int_0^t \langle n^0|H^1(t')|i^0\rangle\, e^{i\omega_{ni}t'}\, dt'}$ $\left(\begin{smallmatrix}1^{\text{st}}\\ \text{order}\end{smallmatrix}\right)$
- $\dot{d}_f(t) \;\approx\; \frac{1}{i\hbar}\overline{H^1_{fi}}(t)\, e^{i\omega_{fi}t} + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t \sum_n \overline{H^1_{fn}}(t)\, e^{i\omega_{fn}t}\, \overline{H^1_{ni}}(t')\, e^{i\omega_{ni}t'}\, dt'$
- ...

<u>Interactive Picture Method</u>:

$$U_I(t,t_0) = \mathbb{I} + \frac{1}{i\hbar}\int_{t_0}^t H_I^1(t')\, dt' + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t \int_{t_0}^{t'} H_I^1(t') H_I^1(t'')\, dt'' dt' + \ldots$$

- $\langle f^0|U_I(t,t_0)|i^0\rangle \;=\; \langle f^0|e^{\frac{i}{\hbar}E_f^0(t-t_0)}\, U(t,t_0)|i^0\rangle$

$$\equiv\; d_f(t) = \boxed{\delta_{fi} + \frac{1}{i\hbar}\int_{t_0}^t \langle f^0|H^1(t')|i^0\rangle\, e^{i\omega_{fi}(t'-t_0)}\, dt'} \quad (1^{\text{st}}\text{ order})$$
$$+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t \int_{t_0}^{t'} \sum_n \langle f^0|H^1(t')|n^0\rangle\, e^{i\omega_{fn}(t'-t_0)}\, \langle n^0|H^1(t'')|i^0\rangle\, e^{i\omega_{ni}(t''-t_0)}\, dt'' dt' + \ldots$$

<u>Normal Schrodinger Propagator</u>:

$$U_S(t,t_0) = U^0(t,t_0) + \frac{1}{i\hbar}\int_{t_0}^t U^0(t,t_0)\, {U^0}^\dagger(t',t_0)\, H^1(t')\, U^0(t',t_0)\, dt'$$
$$+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t \int_{t_0}^{t'} U^0(t,t_0)\, {U^0}^\dagger(t',t_0)\, H^1(t')\, U^0(t',t_0) {U^0}^\dagger(t'',t_0)\, H^1(t'')\, U^0(t'',t_0)\, dt'' dt' + \ldots$$

- $\langle f^0|U(t,t_0)|i^0\rangle \;=\; \boxed{\delta_{fi}\, e^{-\frac{i}{\hbar}E_f^0(t-t_0)} + \frac{1}{i\hbar}\int_{t_0}^t e^{-\frac{i}{\hbar}E_f^0(t-t')}\langle f^0|H^1(t')|i^0\rangle e^{-\frac{i}{\hbar}E_i^0(t'-t_0)}\, dt'}$ (1^{st} order)

$$+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t \int_{t_0}^{t'} \sum_n e^{-\frac{i}{\hbar}E_f^0(t-t')}\langle f^0|H^1(t')|n^0\rangle e^{-\frac{i}{\hbar}E_n^0(t'-t'')}\langle n^0|H^1(t'')|i^0\rangle e^{-\frac{i}{\hbar}E_i^0(t''-t_0)}\, dt'' dt' + \ldots$$

6.5 Variation Principle - Approx. Ground State Energy

$$\begin{aligned}\psi = \sum c_n \psi_n \;\;\rightarrow\;\; E(\psi) > E_0 = E(\psi_0) \\ \psi \equiv f(b,x), \qquad \langle H \rangle = \langle T \rangle + \langle V \rangle\end{aligned} \quad \Rightarrow \quad \begin{aligned} &b_{\min} : \; \frac{d}{db}\langle H \rangle = 0 \\ &E_0 \approx \Big\langle f(b_{\min}, x) \Big| H \Big| f(b_{\min}, x) \Big\rangle\end{aligned}$$

6.6 Selection Rules - Orbital Transitions

Electric Dipole Approximation ONLY: $\lambda_\gamma \gg$ atom length $\rightarrow$ E, B feels homogenously oscillating to the atom

$\psi_{nlm} \rightarrow \psi_{n'l'm'}$:

- $\Delta m \in \{-1, \overset{?}{\emptyset}, 1\}$

  $s(\gamma) = 1 \;\;\rightarrow\;\; m_s(\gamma) \in \{-\hbar, \overset{?}{\emptyset}, \hbar\}$
  $E = E\hat{z} \;\;\rightarrow\;\; \Delta m = 0$

- $\Delta l = \pm 1$

  $1s \leftrightarrow 2p$
  Exception:$(2s \rightarrow 1s)$ through two-photon emission

- $\Delta j \in \{-1, 0, 1\}$
  Exception:$(j = 0 \rightarrow j = 0)$ not allowed

7 Blackbody Radiation

- Power Spectrum : $\quad I'(\omega) = \dfrac{\hbar^3 \omega^3}{h^2 c^2} \dfrac{1}{e^{\hbar\omega/k_b T} - 1} \;\; \left[\frac{I}{\Omega \cdot f}\right]$ $\qquad$ ($\mu = 0$ for photons since photon number isnt conserved)
- Stefan-Boltzmann Law : $\quad I = \dfrac{dP}{dA} \propto T^4$ $\qquad$!! important !!
- Wien's Displacement Law : $\quad \lambda_{\max} = \dfrac{2.9 \times 10^{-3}}{T}$ [m] $\qquad$ (mode of spectrum)

8 Adiabatic Theorem - Slow Changing of Potential

$$t = 0 \;\rightarrow\; \begin{array}{c} H_{(t=0)} = H^{(0)} \\ H_{(0)}|n\rangle = E_n|n\rangle \end{array} \qquad t = t \;\rightarrow\; \begin{array}{c} H = H^{(0)}{}_{(t)} \\ H_{(t)}|n_{(t)}\rangle = E_{n(t)}|n_{(t)}\rangle \end{array}$$

$$\boxed{\text{Dynamic Phase}: \; \theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'}$$

$$|\Psi_{m(t)}\rangle \equiv \sum_n |n_{(t)}\rangle\, e^{i\theta_n(t)}\, \langle n_{(t)}|m_{(0)}\rangle$$

$$\approx |m_{(t)}\rangle\, e^{i\theta_m(t)}\, e^{i\gamma_m(t)}$$

$$= |m_{(t)}\rangle\, e^{i\theta_m(t)}\, e^{\frac{i}{\hbar}\int A^m\cdot dR}$$

$$\sum_n \cancel{H|n\rangle e^{i\theta_n}} c_n = i\hbar \sum_n |\dot{n}\rangle\, e^{i\theta_n}\, c_n + \cancel{|n\rangle i\dot{\theta}_n e^{i\theta_n}} c_n + |n\rangle\, e^{i\theta_n}\, \dot{c}_n$$

$$\langle m|\dot{H}|n\rangle + \langle m|H|\dot{n}\rangle = \cancel{\langle m|\dot{E}_n|n\rangle} + \langle m|E_n|\dot{n}\rangle$$

$$\Downarrow$$

$$\boxed{\dot{c}_m = \frac{d}{dt}\langle m(t)|m(0)\rangle = -\langle m|\dot{m}\rangle\, c_m - \sum_{n\neq m} \frac{\langle m|\dot{H}|n\rangle}{E_n - E_m}\, e^{i(\theta_n - \theta_m)}\, \langle n|\Psi\rangle}$$

(not trivial)

$$\approx -\langle m_{(t)}|\dot{m}_{(t)}\rangle\, c_m \quad\Rightarrow\quad c_{m(t)} \approx c_{m(0)}\, e^{\frac{i}{\hbar} i\hbar \int \langle m|\dot{m}\rangle dt'}$$

$$c_{n(t)} \approx \delta_{nm}\, e^{i\gamma_m(t)} \qquad \boxed{\text{Berry Phase}: \; \gamma_m(t) = i\int_0^t \langle m(t')|\dot{m}(t')\rangle\, dt' \in \mathbb{R}}$$

Berry/Geometric Phase

$$\gamma_m(t) = i\int_0^t \langle m_{(t')}|\dot{m}_{(t')}\rangle\, dt' = \boxed{\frac{1}{\hbar}\int_{R_i}^{R_f} i\hbar\langle m|\nabla_R m\rangle \cdot dR}$$

$$\Rightarrow \frac{1}{\hbar}\oint i\hbar\langle m|\nabla_R m\rangle\cdot dR = \frac{1}{\hbar}\iint \nabla_R \times i\hbar\langle m|\nabla_R m\rangle \cdot da$$

$$\sim \quad \boxed{\frac{1}{\hbar}\oint A^m \cdot dR} \quad = \frac{1}{\hbar}\iint \nabla_R \times A^m \cdot da = \frac{1}{\hbar}\Phi_B^m$$

Aharanov-Bohm Effect:

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{(p - qA)^2}{2m} + V + \cancel{q\phi}\right]\Psi$$

$$\Rightarrow\; \Psi = e^{\frac{i}{\hbar}\int_{\mathcal{O}}^{r} qA\cdot dr'}\psi \;, \quad \breve{E}\psi = \breve{H}\psi$$

$$= \boxed{e^{ig}\psi}$$

$$\vec{A} = \frac{\Phi_B}{2\pi r}\hat{\phi} \;\Rightarrow\; \Delta g_{\text{closed}} = \frac{q}{\hbar}\oint \frac{\Phi_B}{2\pi r}\hat{\phi}\cdot r\,d\hat{\phi}$$

$$= \frac{q\Phi_B}{\hbar} = \gamma_m$$

Infinitismal Path Integral

R : Slow degree of freedom (nucleus)

r : Fast degree of freedom (electron)

$$\mathbb{I} = \int dR \sum_n |R, n(R)\rangle\langle R, n(R)|$$

$$\approx \int dR |R, n(R)\rangle\langle R, n(R)|$$

$$\langle\chi_{(\epsilon)}|e^{-\frac{i}{\hbar}H\epsilon}|\chi_{(0)}\rangle = \langle R_{(\epsilon)}|e^{-\frac{i}{\hbar}H_f\epsilon}|R_{(0)}\rangle\langle n_{(R(\epsilon))}|e^{-\frac{i}{\hbar}H_s\epsilon}|n_{(R(0))}\rangle$$

$$\breve{U}_{(R_1,\epsilon;\, R_0, 0)} = \sqrt{\frac{-im}{2\pi\hbar\epsilon}}\, e^{\frac{i}{\hbar}\mathcal{L}_s\epsilon}\, e^{-\frac{i}{\hbar}E_n(R_0)\epsilon}\langle n_{(R_1)}|n_{(R_0)}\rangle$$

$$\Psi_{(R_1,\epsilon)} = \langle\chi_{(\epsilon)}|\hat{U}_{(\epsilon)}|\Psi_{(R_0,0)}\rangle \approx \sqrt{\frac{-im}{2\pi\hbar\epsilon}}\int e^{\frac{i}{\hbar}\mathcal{L}_s\epsilon}\, e^{-\frac{i}{\hbar}E_n(R_1+\eta)\epsilon}\langle n_{(R_1)}|n_{(R_1+\eta)}\rangle\Psi_{(R_1+\eta,0)}\, d\eta \qquad (\eta = R_0 - R_1)$$

$$\approx \sqrt{\frac{-im}{2\pi\hbar\epsilon}}\int e^{\frac{i}{\hbar}\frac{m}{2}\frac{\eta^2}{\epsilon}}\left[1 - \frac{i}{\hbar}\epsilon(V_s + E_n)\right]\langle n(R_1)|\Big[|n(R_1)\rangle + \eta|\partial n(R_1)\rangle + \frac{\eta^2}{2}|\partial^2 n(R_1)\rangle\Big]\left[1 + \eta\frac{d}{dR} + \frac{\eta^2}{2}\frac{d^2}{dR^2}\right]\Psi_{(R_1,0)}\, d\eta$$

$$\approx \sqrt{\frac{-im}{2\pi\hbar\epsilon}}\int e^{\frac{i}{\hbar}\frac{m}{2}\frac{\eta^2}{\epsilon}}\left[1 - \frac{i}{\hbar}\epsilon V(R_1, 0) + \cancel{\eta(\ldots)} + \frac{\eta^2}{2}\frac{d^2}{dR^2} + \eta^2\langle n|\partial n\rangle\frac{d}{dR} + \frac{\eta^2}{2}\langle n|\partial^2 n\rangle\right]\Psi_{(R_1,0)}\, d\eta$$

$$\breve{E}|\Psi\rangle = \hat{H}|\Psi\rangle \;:\; \hat{H} = \frac{P_s^2}{2m} + V_s + \hat{H}_f$$

$$\breve{E}\Psi = \breve{H}\Psi \quad : \breve{H} = \frac{(P_s - A^n)^2}{2m} + V + \Phi^n$$

$$\boxed{\begin{array}{l} A^n = i\hbar\langle n|\partial n\rangle \\ \Phi^n = \frac{\hbar^2}{2m}\left[\langle\partial n|\partial n\rangle - \langle\partial n|n\rangle\langle n|\partial n\rangle\right] \end{array}}$$

$$\left(\begin{array}{c} \langle n|\partial n\rangle + \langle\partial n|n\rangle = 0 \\ A^n \text{ is added/subtracted in} \end{array}\right)$$

9 Integral Form

$$\psi(r) = \psi_0(r) + \int g(r - r_0)V(r_0)\psi(r_0)\ d^3r \qquad g(r) = -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}$$

$$= \psi_0 + \int gV\psi_{(r_0)}$$

$$= \psi_0 + \int gV\psi_0 + \int\int gVgV\psi_{(r_0)}$$

$$= \psi_0 + \int gV\psi_0 + \int\int gVgV\psi_0 + \int\int gVgVgV\psi_0 + ...$$

10 Klein-Gordon Equation (Spinless Free Particle)

$$(p^2c^2 + m^2c^4)\psi = E^2\psi$$

$$(-E^2 + p^2c^2 + m^2c^4)\psi = 0$$

$$\left[-(E/c)^2 + p^2 + (mc)^2\right]\psi = 0$$

$$\frac{[-(E/c)^2 + p^2 + (mc)^2]}{\hbar^2}\psi = 0$$

$$\left[\frac{1}{c^2}\frac{\partial}{\partial t}^2 - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0$$

$$\boxed{(-\Box^2 + \mu^2)\psi = 0}$$

11 Dirac Equation

$$\mu^2 = \Box^2 \qquad\qquad E^2 = p^2c^2 + m^2c^4 = H^2$$

$$\begin{aligned} m &= \sqrt{\nabla^2 - \partial_t^2} \\ &= A\partial_x + B\partial_y + C\partial_z + iD\partial_t \\ &= i\gamma^\mu\partial_\mu \end{aligned} \qquad \begin{aligned} \sqrt{p^2+m^2} &= \alpha\cdot p + \beta m \\ &= \alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z + \beta m \end{aligned}$$

$$\begin{aligned} \partial_x^2 + \partial_y^2 + \partial_z^2 - \frac{\partial}{\partial t}^2 &= (A\partial_x + B\partial_y + C\partial_z + iD\partial_t)^2 \\ &= A^2\partial_x^2 + B^2\partial_y^2 + C^2\partial_z^2 - D^2\partial_t^2 \\ &\quad + [AB+BA]\partial_x\partial_y + [AC+CA]\partial_x\partial_z + [BC+CB]\partial_y\partial_z \\ &\quad + [AD+DA]i\partial_x\partial_t + [BD+DB]i\partial_y\partial_t + [CD+DC]i\partial_z\partial_t \end{aligned}$$

$$D = \gamma^0, \qquad A = i\gamma^1 = i\beta\alpha_1, \qquad B = i\gamma^2 = i\beta\alpha_2, \qquad C = i\gamma^3 = i\beta\alpha_3$$

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \qquad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

$$\gamma^\mu = \left[\begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}\right] \quad \gamma^5 = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}$$

$$\boxed{\begin{aligned} &(i\hbar\gamma^\mu\partial_\mu - mc)\psi = 0 \\ &\qquad (i\not{\partial} - m)\psi = 0 \qquad \text{(natural units)} \end{aligned}} \qquad \boxed{\begin{aligned} &i\hbar\tfrac{\partial}{\partial t}\psi = (c\alpha\cdot p + \beta mc^2)\psi \\ &i\hbar\tfrac{\partial}{\partial t}\psi = (c\alpha\cdot(p-qA) + \beta mc^2 + q\phi)\psi \end{aligned}}$$

$$\begin{aligned} i\hbar\tfrac{\partial}{\partial t}\psi &= (c\alpha\cdot(p-qA) + \beta mc^2 + q\phi)\psi \\ &= (c\alpha\cdot\pi + \beta mc^2 + q\phi)\psi \end{aligned}$$

$$\begin{aligned} \psi(t) &= \psi(p)e^{i(p\cdot r - Et)} \\ \phi &= 0 \end{aligned} \quad \Rightarrow \quad E\psi = (\alpha\cdot\pi + \beta m)\psi$$

$$\begin{bmatrix} E-m & -\sigma\cdot\pi \\ -\sigma\cdot\pi & E+m \end{bmatrix}\begin{bmatrix} \psi_+ \\ \psi_- \end{bmatrix} = 0 \;\Leftrightarrow\; \begin{aligned} (E-m)\psi_+ &= (\sigma\cdot\pi)\,\psi_- \\ (E+m)\psi_- &= (\sigma\cdot\pi)\,\psi_+ \end{aligned}$$

$$(E-m)\psi_\pm = \tfrac{(\sigma\cdot\pi)(\sigma\cdot\pi)}{E+m}\psi_\pm$$

$$E_s\psi_\pm \approx \tfrac{(\sigma\cdot\pi)^2}{2m}\psi_\pm \qquad \begin{gathered}\text{(Pauli's Eq.)} \\ \text{($\sim$ to Schrodinger)}\end{gathered}$$

$$\boxed{\begin{gathered} \sigma\cdot A\sigma\cdot B = \\ A\cdot B + i\sigma\cdot(A\times B) \end{gathered}} = \tfrac{\sigma\cdot\pi\sigma\cdot\pi}{2m}\psi_\pm = \tfrac{\pi\cdot\pi + i\sigma\cdot(\pi\times\pi)}{2m}\psi_\pm$$

$$= \left[\tfrac{\pi^2}{2m} - \tfrac{q\hbar}{2m}\sigma\cdot B\right]\psi_\pm$$

$$\boxed{(g_e = 2)} \qquad = \left[\tfrac{\pi^2}{2m} - \tfrac{g_e q}{2m}S\cdot B\right]\psi_\pm$$

$$i\hbar\tfrac{\partial}{\partial t}\psi = (c\alpha\cdot p + \beta mc^2)\psi$$

$$\psi(t) = \psi(p)e^{i(p\cdot r - Et)} \;\Rightarrow\; E\psi = (\alpha\cdot p + \beta m)\psi$$

$$\begin{bmatrix} E-m & -\sigma\cdot p \\ -\sigma\cdot p & E+m \end{bmatrix}\begin{bmatrix} \psi_+ \\ \psi_- \end{bmatrix} = 0 \;\Leftrightarrow\; \begin{aligned} (E-m)\psi_+ &= (\sigma\cdot p)\,\psi_- \\ (E+m)\psi_- &= (\sigma\cdot p)\,\psi_+ \end{aligned}$$

$$\boxed{p = 0 \;\Rightarrow\; \begin{cases} \psi = \begin{bmatrix} \psi_+ \\ 0 \end{bmatrix}, & E = m \\ \psi = \begin{bmatrix} 0 \\ \psi_- \end{bmatrix}, & E = -m \end{cases}}$$

$$\psi_\pm = \tfrac{(\sigma\cdot p)^2}{E^2-m^2}\psi_\pm = \tfrac{p^2}{E^2-m^2}\psi_\pm \;\Rightarrow\; \boxed{E_\pm = \pm\sqrt{p^2+m^2}}$$

$$\boxed{\int \|\psi_+\|^2 + \|\psi_-\|^2 d^3r = 1}$$

Hydrogen Fine Structure

$$\begin{aligned} E\psi &= H\psi \\ E\psi &= (\alpha\cdot p + \beta m + q\phi)\psi \end{aligned} \quad \Rightarrow \quad \begin{aligned} (E-m-V)\psi_+ &= (\sigma\cdot p)\psi_- \\ (E+m-V)\psi_- &= (\sigma\cdot p)\psi_+ \end{aligned}$$

$$\begin{aligned}
(E-m-V)\psi_+ &= (\sigma\cdot p)\left(\tfrac{1}{E+m-V}\right)(\sigma\cdot p)\psi_+ \\
(E_s - V)\psi_+ &= \tfrac{1}{2m}(\sigma\cdot p)\left(1+\tfrac{E_S-V}{2m}\right)^{-1}(\sigma\cdot p)\psi_+ \\
&\approx \tfrac{p^2}{2m}\psi_+ \qquad (1^{\text{st}} \text{ order}, v^2) \\
&\approx \tfrac{p^2}{2m}\psi_+ - \tfrac{\sigma\cdot p}{(2m)^2}\left(E_S - V\right)(\sigma\cdot p)\psi_+ \qquad (2^{\text{nd}} \text{ order}, v^4) \\
&= \tfrac{p^2}{2m}\psi_+ - \tfrac{\sigma\cdot p}{(2m)^2}\Big[(\sigma\cdot p)\overbrace{(E_S - V)\psi_+}^{1^{\text{st}} \text{ order}} + [\cancel{E_S} - V, \sigma\cdot p]\,\psi_+\Big] \\
&\approx \left[\tfrac{p^2}{2m} - \tfrac{p^2}{(2m)^2}\tfrac{p^2}{2m} - \tfrac{(\sigma\cdot p)(\sigma\cdot[p,V])}{(2m)^2}\right]\psi_+ \\
E_S\psi_+ &= \left[\tfrac{p^2}{2m} + V - \tfrac{p^4}{8m^3} - \tfrac{i\sigma\cdot(p\times[p,V])}{4m^2} - \underbrace{\tfrac{p[p,V]}{4m^2}}_{\text{(isn't Hermitian)}}\right]\psi_+ = H\psi_+
\end{aligned}$$

$$\begin{aligned}
1 &= \int \|\psi_+\|^2 + \|\psi_-\|^2\, d^3r \\
&= \int \|\psi_+\|^2 + \|\tfrac{\sigma\cdot p}{E+m-V}\psi_+\|^2\, d^3r \\
&\approx \int \|\psi_+\|^2 + \|\tfrac{\sigma\cdot p}{2m}\psi_+\|^2\, d^3r \\
&= \int \psi_+^\dagger(1+\tfrac{p^2}{4m^2})\psi_+\, d^3r \\
&\approx \left\langle (1+\tfrac{p^2}{8m^2})\psi_+ \middle| (1+\tfrac{p^2}{8m^2})\psi_+ \right\rangle \\
&\equiv \langle\psi_S|\psi_S\rangle
\end{aligned}$$

$$\begin{aligned}
E_S\Big(1+\tfrac{p^2}{8m^2}\Big)^{-1}\psi_S &= H\left(1+\tfrac{p^2}{8m^2}\right)^{-1}\psi_S \\
E_S\psi_S &= \left(1+\tfrac{p^2}{8m^2}\right)H\left(1+\tfrac{p^2}{8m^2}\right)^{-1}\psi_S \\
&= \left(H + \tfrac{p^2 H}{8m^2}\right)\left(1 - \tfrac{p^2}{8m^2} + \mathcal{O}(p^4)\right)\psi_S \\
&\approx \left(H + \left[\tfrac{p^2}{8m^2}, H\right]\right)\psi_S \approx \left(H + \left[\tfrac{p^2}{8m^2}, V\right]\right)\psi_S \qquad (2^{\text{nd}} \text{ order}, v^4) \\
E_S\psi_S &= \left(\tfrac{p^2}{2m} + V - \tfrac{p^4}{8m^3} - \tfrac{i\sigma\cdot(p\times[p,V])}{4m^2} - \tfrac{p[p,V]}{4m^2} + \tfrac{[p,V]p + p[p,V]}{8m^2}\right)\psi_S \\
&= \left(\tfrac{p^2}{2m} + V - \tfrac{p^4}{8m^3} - \tfrac{i\sigma\cdot(p\times[p,V])}{4m^2} - \tfrac{[p,[p,V]]}{8m^2}\right)\psi_S \\
&= \boxed{(H_S + H_{\text{rel.}} + H_{\text{so}} + H_{\text{darwin}})\psi_S} \\
&= \left(\tfrac{p^2}{2m} + V - \tfrac{p^4}{8m^3} - \tfrac{1}{4m^2}\sigma\cdot(p\times\nabla V) + \overbrace{\tfrac{1}{8m^2}\nabla^2 V}^{\text{Darwin} \Rightarrow}\right)\psi_S \\
&= \left(\tfrac{p^2}{2m} + V - \tfrac{p^4}{8m^3} - \tfrac{1}{2m^2}S\cdot[\vec{p}\times\tfrac{qq\vec{r}}{4\pi r^3}] + \tfrac{1}{8m^2}[qq\delta^3(r)]\right)\psi_S \\
&= \left(\tfrac{p^2}{2m} + V - \tfrac{p^4}{8m^3} + \underbrace{\tfrac{e^2}{8\pi m^2}\tfrac{S\cdot L}{r^3}}_{l\neq 0} + \underbrace{\tfrac{e^2}{8m^2}\delta^3(r)}_{l=0}\right)\psi_S
\end{aligned}$$

$$\begin{aligned}
\overline{V(r)} &= V(r) + \sum_i \cancel{\overline{\tfrac{\partial V}{\partial r_i}\delta r_i}} \\
&\quad + \tfrac{1}{2!}\sum_{ij}\overline{\tfrac{\partial^2 V}{\partial r_i \partial r_j}\delta r_i \delta r_j} \\
&\quad + \mathcal{O}(\delta r^3) \\
&= \underline{V(r) + \tfrac{1}{2}(\delta r)^2\nabla^2 V} + .. \\
&\qquad (\delta r \sim \tfrac{\hbar}{mc})
\end{aligned}$$

Exact Energy Eigenvalues : $E_{nj} = mc^2\left[1 + \left(\dfrac{\alpha}{n-(j+1/2)+\sqrt{(j+1/2)^2-\alpha^2}}\right)^2\right]^{-1/2}$