Quantum Final Exam Study Guide

* **Basics from previous exams:**

- Definition of a ket: $|\alpha\rangle = c_i |a_i\rangle$

  $a_i|\alpha\rangle = A|\alpha\rangle$

- Definition of an operator: $\hat{A} = |a\rangle\langle b|$

- Projection Operator/Completeness Relation: $\sum_i \Lambda_i = \sum_i |a_i\rangle\langle a_i| = 1$

  * sum to integral if a_i is continuous basis set

- To get the matrix elements of an operator: $A \rightarrow \sum_{m,n} |m\rangle\langle m|A|n\rangle\langle n|$

- Schwartz Inequality: $\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$

- Expectation value: $\langle\hat{A}\rangle = \langle\alpha|A|\alpha\rangle$

- RMS / Avg value: $\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$

  $\hookrightarrow \Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle\mathbb{I}$ (Dispersion Operator)

- Uncertainty Relation: $\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$

- Important Commutation Relations include:

  $[x_i, x_j] = 0 = [p_i, p_j]$ $\qquad$ $S_i = \frac{\hbar}{2}\sigma_i$ $\qquad$ $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $\quad$ $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

  $[x_i, p_j] = i\hbar\delta_{ij}$ $\qquad$ $[\sigma_i, \sigma_j] = \sigma_k$ $\qquad$ $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

  $[x, F(p)] = i\hbar\frac{\partial F}{\partial p}$

  $[p, G(x)] = -i\hbar\frac{\partial G}{\partial x}$

  $[A, H] = -i\hbar\frac{\partial A}{\partial t}$ (Heisenberg eqn of motion)

- Two pictures: Schrödinger Picture $\rightarrow$ state vectors evolve in time, operators const.

  Heisenberg Picture $\rightarrow$ eigenkets + operators evolve; state vectors cons

Basics (cont.)

* For functions of continuous variables

  - Definition of wave function: $\psi_a(x') = \langle x'|a\rangle$

    $\varphi_b(p') = \langle p'|b\rangle$

$$\Rightarrow \langle\beta|\alpha\rangle = \int dx' \langle\beta|x'\rangle\langle x'|\alpha\rangle = \int dx' \psi_b^*(x')\psi_a(x')$$

$$= \int dp' \langle\beta|p'\rangle\langle p'|\alpha\rangle = \int dp' \varphi_b^*(p')\varphi_a(p')$$

$$\langle\beta|A|\alpha\rangle = \int dx''\int dx' \langle\beta|x''\rangle\langle x''|A|x'\rangle\langle x'|\alpha\rangle$$

$$= \int dp''\int dp' \langle\beta|p''\rangle\langle p''|A|p'\rangle\langle p'|\alpha\rangle$$

$\rightarrow$ rewrite $\hat{A}$ in terms of x or p to solve

$$\langle\alpha|\alpha\rangle = \int dx' \langle\alpha|x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx' |\psi_a(x')|^2$$

$$= 1$$ $\rightarrow$ Normalization condition + PDF generator

$$\Rightarrow \langle x'|\hat{p}|p'\rangle = i\hbar\frac{\partial}{\partial x}\langle x'|p'\rangle \quad \Rightarrow \hat{p} = i\hbar\frac{\partial}{\partial x}$$

$$\Rightarrow \langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[\frac{ip'x'}{\hbar}\right]$$

* Translation operators obey the following properties

  ① Unitary

Important Derivations

① Angular Momentum

*Remember that: $J \rightarrow$ Arbitrary angular momentum (often refers to total)

$S \rightarrow$ Spin angular momentum

$L \rightarrow$ orbital angular momentum

Total Angular momentum operator: $\tilde{J}^2 = \tilde{J} \cdot \tilde{J}$
$= J_x^2 + J_y^2 + J_z^2$

Commutation Relations: $[\tilde{J}^2, \tilde{J}_z] = 0$ $\qquad [\hat{J}_i, \hat{J}_j] = i\hbar \epsilon_{ijk} J_k$

$[\hat{J}^2, \hat{J}_y] = 0$

$[\tilde{J}^2, \hat{J}_x] = 0$

*Following our approach from SHO, we define ladder operators

$\Rightarrow J_\pm = J_x \pm i J_y$

$\hookrightarrow [J^2, J_\pm] = 0$

$[J_z, J_\pm] = \hbar J_\pm$

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

$J_\pm^n |a, b\rangle = b \pm n\hbar |a, b \pm n\hbar\rangle$

*Since $\tilde{J}^2$ and $\tilde{J}_z$ commute, we might simultaneous eigenkets such

$\tilde{J}^2 |a, b\rangle = a$ $\quad$ and $\quad$ $\tilde{J}_z |a, b\rangle = b$

$\rightarrow$ Relationship b/w $\tilde{J}^2$ and J_z implies max value for b

*Individually, $\quad \langle a, b| J_- J_+ |a, b\rangle \geq 0$

$\langle a, b| J_+ J_- |a, b\rangle \geq 0$

$\Rightarrow \langle a, b| J_+ J_- + J_- J_+ |a, b \geq 0$

$= \langle a, b| 2(J^2 - J_z^2) |a, b\rangle \geq 0$

$\hookrightarrow a \geq b^2$

Derivations (cont)

* We can show that J_z is incremented in terms of $\hbar$ by:

$$J_z(J_\pm|a,b\rangle) = (J_\pm J_z + \hbar J_\pm)|a,b\rangle$$
$$= J_\pm(J_z + \hbar \mathbb{I})|a,b\rangle$$
$$= J_\pm(b+\hbar)|a,b\rangle$$
$$= (b+\hbar)(J_\pm|a,b\rangle)$$

* Note: Acting $J_\pm|a,b\rangle = c_\pm|a, b+\hbar\rangle$

Interpretation: $J_\pm$ increments eigenvalue of angular momentum

* To find extremum values, act raising/lowering operators on max/min states

$$J_+|a,b_{max}\rangle = 0$$
$$J_-J_+|a,b_{max}\rangle = 0$$
$$(J^2 - J_z^2 - \hbar J_z)|a,b_{max}\rangle = 0$$

*assuming a non-zero ket

$$a - b_{max}^2 - \hbar b_{max} = 0$$
$$a = b_{max}(b_{max}+\hbar)$$

* let $b_{max} = j\hbar$

$$a = j(j+1)\hbar^2$$

$\Rightarrow j(j+1)$ are eigenvalues of J^2

$$J_-|a,b_{min}\rangle = 0$$
$$J_+J_-|a,b_{min}\rangle = 0$$
$$(J^2 - J_z^2 + \hbar J_z)|a,b_{min}\rangle = 0$$
$$\hookrightarrow a - b_{min}^2 + \hbar b_{min} = 0$$
$$a = b_{min}(b_{min} - \hbar)$$

$$b_{max}(b_{max}+h) = b_{min}(b_{min}-\hbar)$$
$$\Rightarrow b_{max} = -b_{min}$$

Derivations (cont.)

$\Rightarrow$ This implies $b_{max} = b_{min} + \hbar$

$\hookrightarrow J_+^n |a, b_{min}\rangle = J_+^n |a, -b_{max}\rangle$

$\Rightarrow b_{max} = \frac{n\hbar}{2}$; since $n \in \mathbb{Z}$, b must be an integer or ½-integer

* But what about $c_\pm$?

$\Rightarrow J_\pm |a,b\rangle = c_\pm |a, b\pm\hbar\rangle$

$\rightarrow$ Starting w/ J_+

$\langle a,b| J_+^\dagger J_+ |a,b\rangle = |c_+|^2 \cancel{\langle a, b+\hbar | a, b+\hbar\rangle}^{1}$

$\Rightarrow |c_+|^2 = \hbar^2[j(j+1)] - b^2 - \hbar b$

*if $b = m\hbar$

$|c_+|^2 = \hbar^2[j(j+1)] - m^2\hbar^2 - \hbar^2 m$

$c_+ = \hbar\sqrt{j(j+1) - m^2 - m}$

$= \hbar\sqrt{(j-m)(j+m+1)}$

$\rightarrow$ Now w/ J_-

$|c_-|^2 \cancel{\langle a, b-\hbar | a, b-\hbar\rangle}^{1} = \langle a,b| J_-^\dagger J_- |a,b\rangle$

$= \hbar^2[j(j+1)] - b^2 + \hbar b$

$= \hbar^2[j(j+1)] - m^2\hbar^2 + \hbar^2 m$

$c_- = \hbar\sqrt{j(j+1) - m^2 + m}$

$= \hbar\sqrt{(j+m)(j-m-1)}$

Derivations (cont.)

② Orbital Angular Momentum

* We define orbital angular momentum operator $\tilde{L}$ as:

$$\tilde{L} = \tilde{\hat{X}} \times \tilde{\hat{P}} \xrightarrow{\text{via cross-product}} \begin{aligned} \tilde{L}_x &= \tilde{y}\tilde{p}_z - \tilde{z}\tilde{p}_y \\ \tilde{L}_y &= \tilde{z}\tilde{p}_x - \hat{x}\tilde{p}_z \\ \tilde{L}_z &= \hat{x}\tilde{p}_y - \tilde{y}\tilde{p}_x \end{aligned}$$

$$\Rightarrow [\tilde{L}_i, \tilde{L}_j] = i\hbar \tilde{L}_k$$

* Using the infinitesimal rotation operators, we can generate wavefuntions in position basis

$$\mathcal{D}(\delta\varphi, \hat{z})|x', y', z\rangle = (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi L_z)|x', y', z'\rangle$$

$$= (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[xp_y - yp_x])|x', y', z'\rangle$$

$$= (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[p_y x - p_x y])|x', y', z\rangle \quad \text{b/c } [x_i, p_j] = i\hbar\delta_{ij}$$

* But when distributed, these are translation operators

$$= |x' - y\delta\varphi, y' + x\delta\varphi, z'\rangle$$

* Note, this matches what we expect from applying rotation matrix on our position operator

* We define our wavefunction as:

$$\varphi(\vec{r}) = \langle x', y', z' | \varphi\rangle \quad , \quad |\varphi\rangle = (\mathbb{I} - \tfrac{i}{\hbar}L_z\delta\varphi)|\alpha\rangle$$

$$= \langle r, \theta, \varphi | \varphi\rangle$$

$$= \langle r, \theta, \varphi | \mathbb{I} - \tfrac{i}{\hbar}L_z\delta\varphi|\alpha\rangle = \langle r, \theta, \varphi - \delta\varphi|\alpha\rangle$$

* Taylor expansion about $\delta\varphi = 0$ yields

$$= \langle r, \theta, \varphi|\alpha\rangle - \delta\varphi \frac{\partial}{\partial\varphi}\langle r, \theta, \varphi|\alpha\rangle$$

$$\Rightarrow \quad -i\hbar\frac{\partial}{\partial\varphi}\langle r, \theta, \varphi|\alpha\rangle = \langle r, \theta, \varphi|\tilde{L}_z|\alpha\rangle$$

$$\hookrightarrow \; -i\hbar\frac{\partial}{\partial\varphi} = L_z$$

Derivations (cont.)

* To derive other operators in Cartesian system, apply infinitesimal rotation operator to cartesian vector, then convert to spherical using δx_i and form matching. Taylor expand $\langle r, \theta, \varphi | L_i | \alpha \rangle$ about $\delta \varphi_i = 0$ and derive form of operator

Results: $\tilde{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$

$$\tilde{L}_x = -i\hbar\left(-\sin\varphi \frac{\partial}{\partial\theta} - \cot\theta \cos\varphi \frac{\partial}{\partial\varphi}\right)$$

$$\tilde{L}_y = -i\hbar\left(\cos\varphi \frac{\partial}{\partial\theta} - \cot \sin\varphi \frac{\partial}{\partial\varphi}\right)$$

* To derive Spherical Harmonics, we focus on L_z component

$$\Rightarrow L_z |l, m\rangle = m\hbar |l, m\rangle$$

$$\langle \hat{n} | L_z | l, m\rangle = m\hbar \langle \hat{n} | l, m\rangle$$

$$= i\hbar \frac{\partial}{\partial\varphi} Y_l^m(\theta, \varphi) = m\hbar Y_l^m(\theta, \varphi)$$

* Solving the above differential equation by separation of variables yields

$$\Phi(\varphi) \propto e^{+im\varphi}$$

* If we define the orbital angular momentum operators as:

$$L_\pm = L_x \pm i L_y$$

$$= -i\hbar e^{\pm i\varphi}\left(\pm i \frac{\partial}{\partial\theta} - \cot \frac{\partial}{\partial\varphi}\right)$$

then

$$L_+ |l, l\rangle = 0$$

$$\langle \hat{n} | L_+ | l, l\rangle = -i\hbar \, e^{i\varphi} \left(i \frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\theta}\right) Y_l^l(\theta, \varphi)$$

$$= 0$$

* Solving the above differential equation via separation of variables + $\Phi = e^{im\varphi}$

$$\Rightarrow Y_l^l(\theta, \varphi) = \Theta(\theta)\Phi(\varphi) = c_l e^{im\varphi} \sin^l(\theta)$$

Derivations (cont.)

* Normalization via

$$\langle l', m' | l, m \rangle = \langle l' m' | \theta, \varphi \rangle \langle \theta, \varphi | l, m \rangle$$
$$= \int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \, |Y_l^m|^2$$

$$\Rightarrow \quad c_l = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)(2l)!}{4\pi}}$$

③ Spherical Harmonic + The Rotation Operator

$\Rightarrow$ We want: $|\hat{n}\rangle = \mathcal{D}(\alpha, \beta, \gamma) |\hat{z}\rangle$
$$= \mathcal{D}(\varphi, \theta, \gamma) |\hat{z}\rangle$$

$$\hookrightarrow \quad \langle l', m' | \hat{n} \rangle = \sum_{l,m} \langle l', m' | \mathcal{D}(\varphi, \theta, \gamma) | l, m \rangle \langle l, m | \hat{z} \rangle$$

* $l = l'$ or total $\vec{L}$ changes

$$= \sum_m \langle l, m' | \mathcal{D}(\varphi, \theta, \gamma) | l, m \rangle \langle l, m | \hat{z} \rangle$$

$$= (Y_l^m)^* (\theta, \varphi) \, (Y_l^0)(\theta, \varphi)$$

$$=$$

$$J_\pm = J_x \pm iJ_y$$

$$\Rightarrow J_-J_+ = (J_x - iJ_y)(J_x + iJ_y)$$
$$= J_x^2 - iJ_yJ_x + iJ_xJ_y - i^2 J_y$$
$$= J_x^2 + J_y^2 + i(J_xJ_y - J_yJ_x)$$
$$= J^2 - J_z^2 + i[J_x, J_y]$$
$$= J^2 - J_z^2 + i(i\hbar J_z)$$
$$= J^2 - J_z^2 - \hbar J_z$$

* To derive L_x operator form

$$\mathcal{D}(\delta\varphi, \hat{x})|x', y', z'\rangle = (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi L_x)|x', y', z'\rangle$$
$$= (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[yp_z - zp_y])|x', y', z'\rangle$$
$$= (\mathbb{I} - \tfrac{i}{\hbar}\delta\varphi[p_zy - p_yz])|x', y', z'\rangle$$
$$= |x', y' - \delta\varphi z', z' + \delta\varphi y'\rangle$$

* In spherical:

$$x = r\sin\theta\cos\varphi \longrightarrow \delta x = r\cos\theta\,\delta\theta\cos\varphi + r\sin\theta\sin\varphi\,\delta\varphi$$
$$y = r\sin\theta\sin\varphi \longrightarrow \delta y = r\sin\theta\cos\varphi\,\delta\varphi + r\cos\theta\,\delta\theta\sin\varphi$$
$$z = r\cos\theta \longrightarrow \delta z = -r\sin\theta\,\delta\theta$$

$$\Rightarrow y'\delta\varphi_x = r\sin\theta\sin\varphi\,\delta\varphi_x = -r\sin\theta\,\delta\theta$$
$$\hookrightarrow \delta\theta = -\sin\varphi\,\delta\varphi_x$$

$$\delta x = 0 = r\cos\theta\cos\varphi\,\delta\theta - r\sin\theta\sin\varphi\,\delta\varphi$$
$$\cos\theta\cos\varphi\,\delta\theta = \sin\theta\sin\varphi\,\delta\varphi$$
$$\cot\theta\cot\varphi\,\delta\theta = \delta\varphi$$
$$-\cot\theta\cos\varphi\,\delta\varphi_x = \delta\varphi$$

$$\Rightarrow |x', y' - \delta\varphi_x z', z' + \delta\varphi_x y'\rangle = |r, \theta + \delta\theta, \varphi - \delta\varphi\rangle$$
$$= |r, \theta + \sin\varphi\,\delta\varphi_x, \varphi - \cot\theta\cos\varphi\,\delta\varphi_x\rangle$$

* Now, Taylor expand about $\delta\varphi_x$

$$\langle r, \theta, \varphi|\mathbb{I} - \tfrac{i}{\hbar}L_x\delta\varphi_x|\alpha\rangle = \langle r, \theta + \sin\varphi\,\delta\varphi_x, \varphi - \cot\theta\cos\varphi\,\delta\varphi_x|\alpha\rangle$$

36. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for −8/15 read $-\sqrt{8/15}$.

Notation:

	J J …	
	M M …	
m_1 m_2		
m_1 m_2	Coefficients	
⋮ ⋮		

1/2×1/2

M	m_1	m_2	J=1	J=0
+1	+1/2	+1/2	1	
0	+1/2	−1/2	1/2	1/2
0	−1/2	+1/2	1/2	−1/2
−1	−1/2	−1/2	1	

1×1/2

M	m_1	m_2	J=3/2	J=1/2
+3/2	+1	+1/2	1	
+1/2	+1	−1/2	1/3	2/3
+1/2	0	+1/2	2/3	−1/3
−1/2	0	−1/2	2/3	1/3
−1/2	−1	+1/2	1/3	−2/3
−3/2	−1	−1/2	1	

2×1/2

M	m_1	m_2	J=5/2	J=3/2
+5/2	+2	+1/2	1	
+3/2	+2	−1/2	1/5	4/5
+3/2	+1	+1/2	4/5	−1/5
+1/2	+1	−1/2	2/5	3/5
+1/2	0	+1/2	3/5	−2/5
−1/2	0	−1/2	3/5	2/5
−1/2	−1	+1/2	2/5	−3/5
−3/2	−1	−1/2	4/5	1/5
−3/2	−2	+1/2	1/5	−4/5
−5/2	−2	−1/2	1	

3/2×1/2

M	m_1	m_2	J=2	J=1
+2	+3/2	+1/2	1	
+1	+3/2	−1/2	1/4	3/4
+1	+1/2	+1/2	3/4	−1/4
0	+1/2	−1/2	1/2	1/2
0	−1/2	+1/2	1/2	−1/2
−1	−1/2	−1/2	3/4	1/4
−1	−3/2	+1/2	1/4	−3/4
−2	−3/2	−1/2	1	

2×1

M	m_1	m_2	J=3	J=2	J=1
+3	+2	+1	1		
+2	+2	0	1/3	2/3	
+2	+1	+1	2/3	−1/3	
+1	+2	−1	1/15	1/3	3/5
+1	+1	0	8/15	1/6	−3/10
+1	0	+1	2/5	−1/2	1/10
0	+1	−1	1/5	1/2	3/10
0	0	0	3/5	0	−2/5
0	−1	+1	1/5	−1/2	3/10
−1	0	−1	2/5	1/2	1/10
−1	−1	0	8/15	−1/6	−3/10
−1	−2	+1	1/15	−1/3	3/5
−2	−1	−1	2/3	1/3	
−2	−2	0	1/3	−2/3	
−3	−2	−1	1		

1×1

M	m_1	m_2	J=2	J=1	J=0
+2	+1	+1	1		
+1	+1	0	1/2	1/2	
+1	0	+1	1/2	−1/2	
0	+1	−1	1/6	1/2	1/3
0	0	0	2/3	0	−1/3
0	−1	+1	1/6	−1/2	1/3
−1	0	−1	1/2	1/2	
−1	−1	0	1/2	−1/2	
−2	−1	−1	1		

3/2×1

M	m_1	m_2	J=5/2	J=3/2	J=1/2
+5/2	+3/2	+1	1		
+3/2	+3/2	0	2/5	3/5	
+3/2	+1/2	+1	3/5	−2/5	
+1/2	+3/2	−1	1/10	2/5	1/2
+1/2	+1/2	0	3/5	1/15	−1/3
+1/2	−1/2	+1	3/10	−8/15	1/6
−1/2	+1/2	−1	3/10	8/15	1/6
−1/2	−1/2	0	3/5	−1/15	−1/3
−1/2	−3/2	+1	1/10	−2/5	1/2
−3/2	−1/2	−1	3/5	2/5	
−3/2	−3/2	0	2/5	−3/5	
−5/2	−3/2	−1	1		

$$Y_1^0=\sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1=-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0=\sqrt{\frac{5}{4\pi}}\Big(\frac{3}{2}\cos^2\theta-\frac{1}{2}\Big)$$

$$Y_2^1=-\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2=\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

$$Y_\ell^{-m}=(-1)^m Y_\ell^{m*}$$

$$d^{\ell}_{m,0}=\sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^m\,e^{-im\phi}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

$$d^j_{m',m}=(-1)^{m-m'}d^j_{m,m'}=d^j_{-m,-m'}$$

2×3/2

M	m_1	m_2	J=7/2	J=5/2	J=3/2	J=1/2
+7/2	+2	+3/2	1			
+5/2	+2	+1/2	3/7	4/7		
+5/2	+1	+3/2	4/7	−3/7		
+3/2	+2	−1/2	1/7	16/35	2/5	
+3/2	+1	+1/2	4/7	1/35	−2/5	
+3/2	0	+3/2	2/7	−18/35	1/5	
+1/2	+2	−3/2	1/35	6/35	2/5	2/5
+1/2	+1	−1/2	12/35	5/14	0	−3/10
+1/2	0	+1/2	18/35	−3/35	−1/5	1/5
+1/2	−1	+3/2	4/35	−27/70	2/5	−1/10
−1/2	+1	−3/2	4/35	27/70	2/5	1/10
−1/2	0	−1/2	18/35	3/35	−1/5	−1/5
−1/2	−1	+1/2	12/35	−5/14	0	3/10
−1/2	−2	+3/2	1/35	−6/35	2/5	−2/5
−3/2	0	−3/2	2/7	18/35	1/5	
−3/2	−1	−1/2	4/7	−1/35	−2/5	
−3/2	−2	+1/2	1/7	−16/35	2/5	
−5/2	−1	−3/2	4/7	3/7		
−5/2	−2	−1/2	3/7	−4/7		
−7/2	−2	−3/2	1			

3/2×3/2

M	m_1	m_2	J=3	J=2	J=1	J=0
+3	+3/2	+3/2	1			
+2	+3/2	+1/2	1/2	1/2		
+2	+1/2	+3/2	1/2	−1/2		
+1	+3/2	−1/2	1/5	1/2	3/10	
+1	+1/2	+1/2	3/5	0	−2/5	
+1	−1/2	+3/2	1/5	−1/2	3/10	
0	+3/2	−3/2	1/20	1/4	9/20	1/4
0	+1/2	−1/2	9/20	1/4	−1/20	−1/4
0	−1/2	+1/2	9/20	−1/4	−1/20	1/4
0	−3/2	+3/2	1/20	−1/4	9/20	−1/4
−1	+1/2	−3/2	1/5	1/2	3/10	
−1	−1/2	−1/2	3/5	0	−2/5	
−1	−3/2	+1/2	1/5	−1/2	3/10	
−2	−1/2	−3/2	1/2	1/2		
−2	−3/2	−1/2	1/2	−1/2		
−3	−3/2	−3/2	1			

2×2

M	m_1	m_2	J=4	J=3	J=2	J=1	J=0
+4	+2	+2	1				
+3	+2	+1	1/2	1/2			
+3	+1	+2	1/2	−1/2			
+2	+2	0	3/14	1/2	2/7		
+2	+1	+1	4/7	0	−3/7		
+2	0	+2	3/14	−1/2	2/7		
+1	+2	−1	1/14	3/10	3/7	1/5	
+1	+1	0	3/7	1/5	−1/14	−3/10	
+1	0	+1	3/7	−1/5	−1/14	3/10	
+1	−1	+2	1/14	−3/10	3/7	−1/5	
0	+2	−2	1/70	1/10	2/7	2/5	1/5
0	+1	−1	8/35	2/5	1/14	−1/10	−1/5
0	0	0	18/35	0	−2/7	0	1/5
0	−1	+1	8/35	−2/5	1/14	1/10	−1/5
0	−2	+2	1/70	−1/10	2/7	−2/5	1/5
−1	+1	−2	1/14	3/10	3/7	1/5	
−1	0	−1	3/7	1/5	−1/14	−3/10	
−1	−1	0	3/7	−1/5	−1/14	3/10	
−1	−2	+1	1/14	−3/10	3/7	−1/5	
−2	0	−2	3/14	1/2	2/7		
−2	−1	−1	4/7	0	−3/7		
−2	−2	0	3/14	−1/2	2/7		
−3	−1	−2	1/2	1/2			
−3	−2	−1	1/2	−1/2			
−4	−2	−2	1				

$$d^1_{0,0}=\cos\theta \qquad d^{1/2}_{1/2,1/2}=\cos\frac{\theta}{2} \qquad d^1_{1,1}=\frac{1+\cos\theta}{2}$$

$$d^{1/2}_{1/2,-1/2}=-\sin\frac{\theta}{2} \qquad d^1_{1,0}=-\frac{\sin\theta}{\sqrt{2}}$$

$$d^1_{1,-1}=\frac{1-\cos\theta}{2}$$

$$d^{3/2}_{3/2,3/2}=\frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,1/2}=-\sqrt{3}\frac{1+\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^2_{2,2}=\Big(\frac{1+\cos\theta}{2}\Big)^2$$

$$d^{3/2}_{3/2,-1/2}=\sqrt{3}\frac{1-\cos\theta}{2}\cos\frac{\theta}{2} \qquad d^2_{2,1}=-\frac{1+\cos\theta}{2}\sin\theta$$

$$d^{3/2}_{3/2,-3/2}=-\frac{1-\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^2_{2,0}=\frac{\sqrt{6}}{4}\sin^2\theta \qquad d^2_{1,1}=\frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^{3/2}_{1/2,1/2}=\frac{3\cos\theta-1}{2}\cos\frac{\theta}{2} \qquad d^2_{2,-1}=-\frac{1-\cos\theta}{2}\sin\theta \qquad d^2_{1,0}=-\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^{3/2}_{1/2,-1/2}=-\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2} \qquad d^2_{2,-2}=\Big(\frac{1-\cos\theta}{2}\Big)^2 \qquad d^2_{1,-1}=\frac{1-\cos\theta}{2}(2\cos\theta+1) \qquad d^2_{0,0}=\Big(\frac{3}{2}\cos^2\theta-\frac{1}{2}\Big)$$

Figure 36.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974).

Quantum II Final Exam Study Guide

Basics

$|\alpha\rangle = \sum_i' c_i |a_i\rangle$ and $A|\alpha\rangle = a_i|\alpha\rangle$ (Definition of a ket)

$A = |a\rangle\langle b|$ (Definition of an operator)

$\sum_i' \Lambda_i = \sum_i' |a_i\rangle\langle a_i| = 1$ (Projection Operator/Completeness Relation)

*To get the matrix elements of an operator:

$$A \rightarrow \sum_{m,n}' |m\rangle\langle m|A|n\rangle\langle n|$$

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$ (Schwartz Inequality)

$\langle A\rangle = \langle\alpha|A|\alpha\rangle$ (Expectation Value)

$\Delta A = A - \langle A\rangle \mathbb{I}$ (Dispersion Operator)

$\hookrightarrow \langle(\Delta A)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$ (Avg value or RMS)

$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$ (Uncertainty Relation)

*Important Commutation relations include:

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

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

$[x, F(p)] = i\hbar\frac{\partial F}{\partial p}$

$[p, G(x)] = i\hbar\frac{\partial G}{\partial x}$

$[\sigma_i, \sigma_j] = \sigma_k$ where:

$\sigma_x = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix}$, $\sigma_y = \begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix}$, $\sigma_z = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}$

$[A, H] = -i\hbar\frac{\partial A}{\partial t}$ (Heisenberg Eqn of Motion)

*For functions of a continuous variable:

$\psi_a(x') = \langle x'|a\rangle$

$\varphi_b(p') = \langle p'|b\rangle$

$\langle\beta|\alpha\rangle = \int dx' \psi_\beta^*(x')\psi_\alpha(x')$

$= \int dp' \varphi_\beta^*(p')\varphi_\alpha(p')$

$p = i\hbar\,\partial/\partial x$

$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left[\frac{i}{\hbar}p'\cdot x'\right]$

Basics (cont.)

* Remember, for angular momentum:

  $J \rightarrow$ Arbitrary Angular Momentum (usually refers to total)

  $L \rightarrow$ Orbital Angular Momentum

  $S \rightarrow$ Spin Angular Momentum

* Important angular momentum formulas include:

$$J^2 = J \cdot J = J_x^2 + J_y^2 + J_z^2 \qquad J_\pm = J_x \pm i J_y$$

$$[J^2, J_i] = 0 \qquad [J^2, J_\pm] = 0 = [J_z, J_\pm]$$

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \qquad [J_+, J_-] = 2\hbar J_z$$

$\Rightarrow$ We often write simultaneous eigenkets of J^2, J_z as $|a,b\rangle$ such that:

$$J^2|a,b\rangle = a|a,b\rangle \qquad J_\pm |a,b\rangle = \sqrt{(j\pm m+1)(j\mp m)}\,\hbar\,|a, b+\hbar\rangle$$

$$J_z|a,b\rangle = b|a,b\rangle \qquad J_\pm^n |a,b\rangle = (b\pm n\hbar)|a, b\pm n\hbar\rangle$$

* When adding angular momentum, it is useful to use direct product notation:

$$|S_1, S_{1z}; S_2, S_{2z}\rangle = |S_1, S_{1z}\rangle \otimes |S_2, S_{2z}\rangle$$

$\Rightarrow$ Our total system operators now become:

$$J = J_1 + J_2 = J_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes J_2$$

$$J^2 = (J_1 + J_2)\cdot(J_1 - J_2) = J_1^2 + J_2^2 + 2 J_1 \cdot J_2$$

$$= J_{1z} + J_{2z} + \tfrac{1}{2}(J_{1+}J_{2-} + J_{1-}J_{2+})$$

* This flexibility allows us to use two sets of kets to describe the system:

$$|j_1, j_2; m_1, m_2\rangle \Longleftrightarrow |j_1, j_2; j, m\rangle$$

$$[J_1^2, J_2^2] = [J_{1z}, J_{2z}] = [J_{1i}, J_{2j}] = 0$$

* Use of the Clebsh - Gordon coefficients allow us to relate the two sets of kets to one another (see table)

  $\hookrightarrow$ If calculating by hand, equate states of degeneracy 1 (ie max or min J) and use ladder operators

Tensor Operators

* For Cartesian Tensors, we know they rotate like:

$$\text{Rank } 1 \rightarrow \quad V_i' = R_{ij} V_j$$

$$2 \rightarrow \quad W = \tilde{R}'\hat{R}\, v_i v_j$$

* Remember, we defined our rotation operator $R(\alpha,\beta,\gamma)$ as:

$$R(\alpha,\beta,\gamma)|j,m\rangle = \sum_{j',m'}' |j',m'\rangle\langle j',m'|R(\alpha,\beta,\gamma)|j,m\rangle$$

$$= \mathcal{D}^{(j)}_{mm'}|j',m'\rangle \quad \text{where } j=j' \text{ so } \vec{J} = \text{const.}$$

⇒ Comparing this to our classical picture, we see:

$$\langle\alpha|V_i|\alpha\rangle \rightarrow \langle\alpha|\mathcal{D}^{+}(R)\,V\,\mathcal{D}(R)|\alpha\rangle = \sum_{ji}' R_i R_j \langle\alpha|V|\alpha\rangle$$

$$\text{where } \mathcal{D}(R) = \exp[\tfrac{i}{\hbar}(J\cdot\hat{n})\,\delta\varphi]$$

↳ $$\sum' R_{ij} V_j = \mathcal{D}^{+}(R)\, V_i\, \mathcal{D}(R)$$

* Applying our infinitesimal operator, we see

$$V_i' = V_i + \frac{\epsilon}{i\hbar}[V_i, \vec{J}\cdot\hat{n}] = \sum_j' R_{ij}(\hat{n},\epsilon)\, V_j$$

which allows us to deduce the commutation relation:

$$[V_i, J_j] = i\hbar\, \epsilon_{ijk} V_k$$

* A closer examination of rank two tensors reveals they can be decomposed as follows:

$$U_i V_j = \underbrace{\frac{U\cdot V}{3}\delta_{ij}}_{\substack{\text{scalar}\\ 1}} + \underbrace{\frac{U_iV_j - U_jV_i}{2}}_{\substack{\text{anti-symmetric}\\ \text{tensor}\\ 3}} + \underbrace{\left(\frac{U_iV_j + U_jV_i}{2} - \frac{U\cdot V}{3}\delta_{ij}\right)}_{\substack{\text{traceless symmetric tensor}\\ 5}}$$

⇒ The circled #'s represent the number of independent componets per term, which happen to match the multiplicity of states for $l=0,1,2,\ldots$ respectively

↳ Replacing $\hat{n}$ by $\vec{v}$ in our definition of spherical tensors, we see:

$$T_q^{(k)} = Y_{l=k}^{m=q}(\vec{v})$$

ex. $$Y_1^0 = \sqrt{\tfrac{3}{4}}\cos\theta = \sqrt{\tfrac{3}{4}}\, V_z$$

$$Y_1^{\pm1} = \sqrt{\tfrac{3}{8\pi}}\, e^{\pm i\varphi}\cos\theta = \sqrt{\tfrac{3}{2\pi}}\, V_x \pm iV_y$$

Tensor Operators (cont.)

* To derive the transformation properties, we return to our definition of the spherical harmonics

$$Y_\ell^m(\hat{n}) = \langle \hat{n} | \ell, m \rangle$$

⇒ Remembering $|n'\rangle = \mathcal{D}(R)|n\rangle \Leftrightarrow \langle n'| = \langle n| \mathcal{D}(R^{-1})$, we see our angular momentum kets transform as:

$$\mathcal{D}(R^{-1})|\ell, m\rangle = \sum_{m'} |\ell, m'\rangle\langle \ell, m'| \mathcal{D}(R^{-1})|\ell, m\rangle$$

$$= \sum_{m'} |\ell, m'\rangle \mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

* Applying $\langle n|$ to both sides of the equation

$$\langle n|\mathcal{D}(R^{-1})|\ell, m\rangle = \sum_{m'} \langle n|\ell, m'\rangle \mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

$$\langle n'|\ell, m\rangle = \sum_{m'} Y_\ell^{m'}(n) \mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

$$Y_\ell^m(n') = \sum_{m'} Y_\ell^{m'}(n) \mathcal{D}_{mm'}^{(\ell)}(R^{-1})$$

* Now switching to operator formulations:

$$\mathcal{D}^+(R)\, Y_\ell^m(v)\, \mathcal{D}(R) = \sum_{m'} Y_\ell^{m'}(v) \left[\mathcal{D}_{mm'}^{(\ell)}(R)\right]^*$$

* Finally moving to tensor notation:

$$\mathcal{D}^+(R)\, T_q^{(k)}\, \mathcal{D}(R) = \sum_{q'} T_{q'}^{(k)} \left[\mathcal{D}_{qq'}^{(k)}(R)\right]^*$$

* Applying this equation to an infinitesimal rotation:

$$[J\cdot n, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle k, q'| J\cdot n | k, q\rangle$$

⇒ Evaluating the above in the $z, \pm$ directions yields:

$$[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$$

$$[J_\pm, T_q^{(k)}] = \hbar \sqrt{(k \mp q)(k \pm q + 1)}\, T_{q\pm 1}^{(k)}$$

* We have a theorem that defines spherical tensors in terms of Cartesian tensors:

$$T_q^{(k)} = \sum_{q_1} \sum_{q_2} \underbrace{\langle k_1, k_2; q_1, q_2 | k_1, k_2; k, q\rangle}_{\text{CG coefficient (from table)}} X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \quad \text{(irreducable spherical tensors)}$$

Tensor Operators (cont.)

↳ To show our above formula transforms as a spherical tensor:

$$\mathcal{D}^{+}(R)\,T_q^{(k)}\,\mathcal{D}(R) = \sum_{q_1 q_2} \langle k_1 k_2; q_1 q_2 | k_1 k_2; k, q\rangle\, \mathcal{D}^{+}(R)\,X_{q_1}^{(k_1)}\,\mathcal{D}(R)\,\mathcal{D}^{+}(R)\,Z_{q_2}^{(k_2)}\,\mathcal{D}(R)$$

$$= \sum_{q_1}\sum_{q_2}\sum_{q_1'}\sum_{q_2'} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle\, X_{q_1'}^{(k_1)}\left[\mathcal{D}_{q_1 q_1'}^{(k_1)}(R)\right]^{*} Z_{q_2'}^{(k_2)}\left[\mathcal{D}_{q_2 q_2'}^{(k_2)}(R)\right]^{*}$$

*using $\mathcal{D}_{m_1 m_1'}^{(j_1)}(R)\,\mathcal{D}_{m_2 m_2'}^{(j_2)}(R) = \sum_{j}\sum_{m}\sum_{m'} \langle j_1 j_2, m_1 m_2 | j_1 j_2; j, m\rangle \langle j_1 j_2, m_1' m_2' | j_1 j_2; j, m'\rangle\, \mathcal{D}_{mm'}^{(j)}$

$$= \sum_{k''}\sum_{q_1}\sum_{q_2}\sum_{q_1'}\sum_{q_2'}\sum_{q'}\sum_{q''} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle \langle k_1 k_2, q_1 q_2 | k_1 k_2; k'' q'\rangle \langle k_1 k_2; q_1 q_2 | k_1 k_2; k'', q''\rangle$$
$$\cdot \left[\mathcal{D}_{q'q''}(R)\right]^{*} X_{q_1'}^{(k_1)}\, Z_{q_2'}^{(k_2)}$$

$$= \sum_{q'} T_{q'}^{(k)}\left[\mathcal{D}_{qq'}^{(k)}(R)\right]^{*}$$

*We can determine the matrix elements of a spherical tensor via Wigner-Eckart Theorem

⇒ Starting from $[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$

$$\langle \alpha', j', m' |\, J_z T_q^{(k)} - T_q^{(k)} J_z - \hbar q\, T_q^{(k)} \,| \alpha, j, m\rangle = 0$$

$$\langle \alpha', j', m' |\, m' T_q^{(k)} - T_q^{(k)} m - q\, T_q^{(k)} \,| \alpha, j, m\rangle = 0$$

↳ $m' = m + q$ where q is the ang. momentum added by spherical tensor

⇒ We apply the Wigner-Eckart Thm by noting $\langle \alpha', j' m' | T_q^{(k)} | \alpha, j m\rangle$ can be written in terms of a CG coefficient and a reduced matrix element

$$\langle \alpha' j' m' | T_q^{(k)} | \alpha j m\rangle = \langle j k; m q | j k; j' m'\rangle \frac{1}{\sqrt{2j+1}} \langle \alpha' j' \| T_q^{(k)} \| \alpha j\rangle$$

↳ Our general approach is to calculate the reduced matrix element in a simple case then use that result in our case of interest

ex.

$$\langle 3, 0 | T_0^{(2)} | 1, 0\rangle = \langle 1, 2; 0, 0 | 1, 2; 1, 0\rangle \langle 3 \| T^{(2)} \| 1\rangle$$

$$\int Y_3^0(\theta,\varphi)\, Y_2^0(\theta,\varphi)\, Y_1^0(\theta,\varphi)\, d\Omega = \langle 1, 2; 0, 0 | 1, 2; 1, 0\rangle \langle 3 \| T^{(2)} \| 1\rangle$$

↳ $\langle 3 \| T^{(2)} \| 1\rangle = \sqrt{\frac{3}{4\pi}}$

Perturbation Theory

* Perturbation theory is an approximation technique that allows us to solve non-idealized problems in quantum mechanics and other fields

* In the case of time-independent, non-degenerate perturbations:
  - ⇒ For a given Hamiltonian, we write it as:

$$H = H_0 + V, \quad \text{where the solutions to } H_0 \text{ are known, but not for } V$$

ex. Two State System

↳ $H = E_1^{(0)} |1^{(0)}\rangle\langle 1^{(0)}| + E_2^{(0)} |2^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{12} |1^{(0)}\rangle\langle 2^{(0)}| + \lambda V_{21} |2^{(0)}\rangle\langle 1^{(0)}|$

$$\doteq \begin{bmatrix} E_1 & \lambda V_{12} \\ \lambda V_{21} & E_2 \end{bmatrix}; \quad V_{12} = V_{21}, \quad V_{12}, V_{21} \in \mathbb{R} \text{ for Hermiticity}$$

⇒ From normal matrix operations, we see:

$$E_1 = \tfrac{1}{2}(E_1^{(0)} + E_2^{(0)}) + \sqrt{\tfrac{1}{4}(E_1^{(0)} - E_2^{(0)}) + \lambda^2 V_{12}^2}$$

$$E_2 = \tfrac{1}{2}(E_1^{(0)} + E_2^{(0)}) - \sqrt{\tfrac{1}{4}(E_1^{(0)} - E_2^{(0)}) + \lambda^2 V_{12}^2}$$

⇒ However, if we are unable to find an exact solution, we proceed as follows:

↳ We know: $H_0 |n\rangle = E_n^{(0)} |n\rangle$

$$(H_0 + \lambda V)|n\rangle = E_n |n\rangle$$

⇒ If we define $\Delta_n = E_n - E_n^{(0)}$

↳ $E_n^{(0)} - H_0 |n\rangle = \lambda V - \Delta_n |n\rangle$

$$\langle n^{(0)} | E_n^{(0)} - H_0 |n\rangle = \langle n^{(0)} | \lambda V - \Delta_n |n\rangle$$

$$0 = \langle n^{(0)} | \lambda V - \Delta_n |n\rangle$$

* Now defining the projection operator: $\varphi_n = \mathbb{I} - |n^{(0)}\rangle\langle n^{(0)}|$

$$= \sum_{k \neq n}' |k^{(0)}\rangle\langle k^{(0)}|$$

↳ $|n\rangle = \dfrac{1}{E_n^{(0)} - H_0} \varphi_n (\lambda V - \Delta_n)|n\rangle$

* but as $\lambda \to 0$, we must approach $H^{(0)}|n^{(0)}\rangle = E_n^{(0)}|n\rangle$

Perturbation Theory (cont.)

$\Rightarrow$ We redefine $|n\rangle$ as:

$$|n\rangle = c_n(\lambda)|n^{(0)}\rangle + \frac{1}{E_n^{(0)}-H_0}\varphi_n(\lambda V-\Delta_n)|n\rangle \,, \quad c_n(\lambda) = \langle n^{(0)}|n\rangle$$

*Note: Since we choose $\langle n^{(0)}|n\rangle = 1$, we must always normalize $|n\rangle$ after we solve for it

$\hookrightarrow$ $$\boxed{|n\rangle = |n^{(0)}\rangle + \frac{1}{E_n^{(0)}-H_0}\varphi_n(\lambda V-\Delta_n)|n\rangle}$$

*If we multiply both sides by $\langle n^{(0)}|$, we can extract Δ_n

$$\boxed{\Delta_n = \lambda\langle n^{(0)}|V|n\rangle}$$

*Now if we expand both $|n\rangle$ and Δ_n in power series:

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \dots$$

$$\Delta_n = \lambda\Delta_n^{(1)} + \lambda^2\Delta_n^{(2)} + \dots$$

*Substituting these into our above equations + matching powers of λ:

$$\Delta_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$$\Delta_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle = \sum_{k\neq n}' \frac{|V_{nk}|^2}{(E_n^{(0)}-E_k^{(0)})^2}$$

$$|n^{(1)}\rangle = \frac{1}{E_n^{(0)}-H_0}\varphi_n|n^{(0)}\rangle = \sum_{k\neq n}' \frac{V_{kn}}{E_n^{(0)}-E_k^{(0)}}|k^{(0)}\rangle$$

*Proceeding to the <u>time-independent, degenerate</u> perturbation case:

$\Rightarrow$ Simply put we must diagonalize the degenerate submatrix however possible

$\hookrightarrow$ For our degenerate energies, our eigenkets become:

$$|l^{(0)}\rangle = \sum_{m\in D}' |m^{(0)}\rangle\langle m^{(0)}|l^{(0)}\rangle$$

$\hookrightarrow$ To solve the eigenvalue equation ($H = H_0 + V$):

$$(E - H_0 - V)|l\rangle = 0$$

$\hookrightarrow$ We isolate the degenerate/non-degenerate spaces with:

$$\tilde{P}_0 = \sum_{k\in D}' |k^{(0)}\rangle\langle k^{(0)}| \qquad \tilde{P}_1 = \sum_{k\notin D}' |k^{(0)}\rangle\langle k^{(0)}| = \tilde{\mathbb{I}} - \tilde{P}_0$$

Perturbation Theory (cont.)

$\Rightarrow$ We can now rewrite the eigenvalue equation as:

$$(E-H_0-\lambda V)P_0|l\rangle + (E-H_0-\lambda V)P_1|l\rangle = 0$$

* Applying the projection operators to the above equation yields:

① $(E-H_0-\lambda V)\tilde{P}_0^2|l\rangle + (E-H_0-\lambda V)P_0P_1|l\rangle = 0$

* using $P_0P_0 = 1$, $P_0P_1 = 0$

$$(E-E_D^{(0)}-\lambda P_0 V)P_0|l\rangle - \lambda P_0 V P_1|l\rangle = 0$$

② $-\lambda P_1 V P_0|l\rangle + (E-H_0-\lambda P_1 V)P_1|l\rangle = 0$

* Solving the above system of equations yields:

$$|l\rangle = \lambda[E-H_0-\lambda P_1VP_1]^{-1}P_1VP_0|l\rangle$$

$\hookrightarrow P_1|l\rangle = \tilde{P}_1 \dfrac{\lambda}{E-H_0-\lambda P_1VP_1} P_1VP_0|l\rangle$

* expanding $|l\rangle$ as a power series and $\dfrac{1}{E-H_0-\lambda P_1VP_1} \approx \dfrac{1}{E-H_0} + \dfrac{\lambda P_1VP_1}{(E-H_0)^2} + \ldots$

$$\Rightarrow P_1|l^{(1)}\rangle = \sum_{k\notin D} \frac{V_{kl}}{E_D^{(0)}-E_k^{(0)}}|k^{(0)}\rangle$$

ex. Linear Stark Effect

* Our physical set-up is a hydrogen like atom in a uniform $\vec{E}$-field

$\hookrightarrow V = -ezE_0$; $n = N+l+1$, where $n\in\mathbb{Z}^+$, $l\in[0,n-1]$, $N\in\{0,\mathbb{Z}^+\}$

$\Rightarrow H|nlm\rangle = E_n|nlm\rangle$ $\qquad L_z|nlm\rangle = m\hbar|nlm\rangle$

$L^2|nlm\rangle = l(l+1)\hbar^2|nlm\rangle$ $\qquad \Pi|nlm\rangle = (-1)^l|nlm\rangle$ (Parity)

* Remember, in terms of spherical tensors: $z = \hat{T}_0^{(1)}$

$\hookrightarrow \langle n, l'm'|T_0^{(1)}|nlm\rangle \rightarrow m=m'$ b/c no addition of ang. momentum

$l'\in[l+1, |l-1|]$

* Notice that: $\Pi^\dagger z \Pi = -z$

$\hookrightarrow \langle odd|z|even\rangle = \langle odd|\Pi^\dagger\Pi z\Pi^\dagger\Pi|even\rangle$

$= \langle odd|z|even\rangle$

$\left.\begin{array}{l}\langle odd|z|odd\rangle = -\langle odd|z|odd\rangle \\ \langle even|z|even\rangle = -\langle even|z|even\rangle\end{array}\right\}$ must equal ⓪

$\Rightarrow$ From this we see $l' = l\pm1$ and that we can now write out the interaction matrix

Perturbation Theory (cont.)

ex. Linear Stark Effect (cont.)

$$\Rightarrow V \doteq \begin{bmatrix} 0 & \langle 200|V|210\rangle \\ \langle 210|V|200\rangle & 0 \end{bmatrix} = \begin{bmatrix} 0 & 3ea_0E_0 \\ 3ea_0E_0 & 0 \end{bmatrix} \quad \text{for } n=2,\ l=0,1$$

↳ via diagonalization:

$$|+\rangle = \frac{1}{\sqrt{2}}(|200\rangle + |210\rangle) \qquad \Delta_+^{(1)} = 3ea_0E_0$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|200\rangle - |210\rangle) \qquad \Delta_-^{(1)} = -3ea_0E_0$$

⇒ Further corrections to H-atom from perturbation theory include:

① "Relativistic Correction"

$$E = \sqrt{(pc)^2 + m^2c^4}$$

$$T = \sqrt{(pc)^2 + m^2c^4} - m_ec^2$$

$$= mc^2\left(1 + \frac{(pc)^2}{m^2c^4}\right)^{1/2} - m_ec^2$$

↳ $T \approx \frac{p^2}{2m} - \frac{p^4}{8m_e^3c^2}$ ⟵ becomes interaction term in perturbed Hamiltonian

$$\Rightarrow H = \frac{p^2}{2m} - \frac{e^2}{r} - \frac{p^4}{8m_e^3c^2}$$

* But since $[L, p^2] = 0$, we can proceed via non-degenerate P.T b/c perturbation doesn't break the degeneracy

↳ $\Delta_{nl}^{(1)} = \langle nlm|\frac{-p^4}{8m_e^3c^2}|nlm\rangle$

* but $\frac{1}{2mc^2}\left(\frac{p^2}{2m}\right)^2 = \frac{p^4}{8m_e^3c^2} = \frac{1}{2mc^2}\left(H_0 + \frac{e^2}{r}\right)^2$

$$= \left[\langle nlm|\frac{e^4}{r^2}|nlm\rangle + 2E_n^{(0)}\langle nlm|\frac{e^2}{r}|nlm\rangle + (E_n^{(0)})^2\right]\cdot\frac{1}{2mc^2}$$

$$= \frac{-1}{2}mc^2\alpha^4\left(\frac{-3}{4n^2} - \frac{1}{n^3(l+\frac{1}{2})}\right)$$

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

② Spin-Orbit Coupling

$\vec{B} = \frac{-\vec{v}}{c} \times \vec{E}$, $\vec{\mu} = \frac{e\vec{S}}{m_ec}$ ($\vec{S}$ = spin vector)

$$H_{LS} = -\vec{\mu}\cdot B$$

$$= \frac{eS}{m_ec}\left(\frac{v}{c} \times \frac{\vec{r}}{r}\frac{dV_c}{dr}\left(\frac{-1}{e}\right)\right) \qquad * V_c = \text{central potential}$$

$$= \frac{eS}{m_ec}\left[\frac{p}{m_ec} \times \frac{\vec{r}}{r}\frac{dV_c}{dr}\left(\frac{-1}{e}\right)\right] = \frac{1}{m_e^2c^2r}\frac{dV_c}{dr}\vec{L}\cdot\vec{S}$$

Perturbation Theory (cont.)

* Rewriting $L \cdot S$ as $J^2 = (L+S)^2$

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

* Introducing the spin-angular functions

$$\mathcal{Y}_{\ell}^{j=\ell+1/2} \equiv \frac{1}{\sqrt{2\ell+1}}\begin{bmatrix} \pm\sqrt{\ell \pm m + 1/2}\; Y_{\ell}^{m-1/2}(\theta,\varphi) \\ \sqrt{\ell \mp m + 1/2}\; Y_{\ell}^{m+1/2}(\theta,\varphi)\end{bmatrix}$$

* Note: $m = m_\ell + m_s$

$$= (\ )\, Y_\ell^m \chi^+ + (\ )\, Y_\ell^m \chi^-, \text{ where } \chi^\pm \text{ are spinor states}$$

$$\Rightarrow \Delta_{n\ell}^{(1)} = \frac{1}{2m_e^2c^2}\left\langle \frac{1}{r}\frac{dV_c}{dr}\right\rangle_{n\ell} \frac{\hbar}{2}\begin{Bmatrix} \ell \\ -\ell+1 \end{Bmatrix} \text{ for } \begin{matrix} j = \ell+1/2 \\ = \ell - 1/2 \end{matrix} \quad (\text{choose a } j)$$

where $\frac{1}{2}\int \mathcal{Y}^*(J^2 - L^2 - S^2)\mathcal{Y}\, d\Omega = \frac{\hbar^2}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right](\ )$ is used in the expectation value calculation

$$\Rightarrow \text{In H-atom: } V_c = \frac{e^2}{r} \rightarrow \left\langle \frac{1}{r}\frac{dV}{dr}\right\rangle = \left\langle \frac{e^2}{r^3}\right\rangle = \frac{-2m_e^3c^2\alpha^2}{n\ell(\ell+1)(\ell+1/2)\hbar^2}$$

* Now considering a <u>time-dependent</u> perturbation such that:

$$H = H_0 + V(t)$$

⇒ Note: Our normal time evolution operator $U(t,t_0) = \exp\left[\frac{-i}{\hbar}Ht\right]$ only works when H is time independent

⇒ We must develop the interaction picture

$$|\alpha\rangle = \sum_n{}' c(0)|n\rangle \; ; \quad c(0) = \langle n|\alpha\rangle|_{t=0}$$

$$|\alpha, t_0=0, t\rangle = \sum_n{}' c_n(t)\exp[-iE_nt/\hbar]|n\rangle \rightarrow c_n(t) \text{ only associated w/ } V$$

↳ $c_n \rightarrow 0$ yields normal evolution

$$\Rightarrow |\alpha, t_0; t\rangle_I = e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S \quad (\text{time evolve only unperturbed Hamiltonian})$$

* Operators now transform as: $\hat{A}_I = e^{+iH_0t/\hbar}\hat{A}_S e^{-iH_0t/\hbar}$

$$↳ i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle_I = i\hbar\frac{\partial}{\partial t}\left(e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S\right)$$

$$= i\hbar\frac{H_0}{-i\hbar}e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S + i\hbar e^{iH_0t/\hbar}\left(\frac{\partial}{\partial t}|\alpha, t_0; t\rangle_S\right)$$

$$= -H_0 e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S + e^{iH_0t/\hbar}(H_0 + V(t))|\alpha, t_0; t\rangle_S$$

$$= e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S$$

$$= V_I(t)|\alpha, t_0; t\rangle_I$$

Perturbation Theory (cont.)

* we convert the above equation to a # by multiplying both sides by $\langle n|$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \langle n|\alpha, t_0; t\rangle_I = \langle n|V_I|\alpha, t_0; t\rangle_I$$

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m{}' \langle n|V_I|m\rangle\langle m|\alpha, t_0; t\rangle_I$$

$$= \sum_m{}' V_{nm}\, c_m(t)\, e^{i\omega_{nm}t}$$

* If we now expand c_n in a power series to develop perturbation theory

$$c_n(t) = c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \ldots$$

ex. Exact Solution to a 2 state problem

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|, \quad E_2 > E_1$$

$$V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1| \quad > \quad H \doteq \begin{bmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{bmatrix}$$

* From the above system we get the following differential equations:

$$i\hbar \frac{\partial}{\partial t} c_1(t) = V_{12}(t)\, e^{-i(E_2-E_1)t/\hbar}\, c_2(t) \qquad * \text{Assume } c_1(0) = 1$$

$$i\hbar \frac{\partial}{\partial t} c_2(t) = V_{21}(t)\, e^{+i(E_2-E_1)t/\hbar}\, c_1(t) \qquad c_2(0) = 0$$

$\Rightarrow$ we solve this system by taking the derivative of one equation and substituting it into the other, yielding:

$$|c_2(t)|^2 = \frac{\gamma^2/\hbar^2}{\gamma^2/\hbar^2 + (\omega-\omega_{21})^2}\sin^2\left[\left(\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4}\right)^{1/2} t\right]$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

* But we really want an approximation technique for this problem

$$\Rightarrow i\hbar \frac{dc_n^{(j)}}{dt} = \sum_m{}' V_{nm}\, e^{i\omega_{nm}t}\, c_m^{(j-1)}(t)$$

* We now must develop a proper time evolution operator

$\hookrightarrow |\alpha, t_0; t\rangle_I = U_I(t, t_0)|\alpha, t_0; t\rangle_I$

* if we take the time derivative of the above equation:

$$i\hbar \frac{\partial}{\partial t}\left(U_I(t,t_0)|\alpha, t_0; t\rangle_I\right) = V_I\, U_I(t,t_0)|\alpha, t_0; t\rangle_I$$

$$i\hbar \frac{\partial}{\partial t} U(t,t_0) = V_I\, U_I(t,t_0)$$

$$\hookrightarrow U_I(t,t_0) = \mathbb{I} - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\, U_I(t', t_0)\, dt'$$

* but since most problems aren't directly integrable, we approximate by

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

Quantom Qualifier Breakdown

January 2008
- Q1: Infinite Square Well, Schrödingers Eqn, Spin 1/2 Particles
- Q2: SHO, Expectation value, uncertainty relation
- Q3: Variational Principle
- Q4: Hermitian Operators, Probabilities,
- Q5: Infinite Square Well, Perturbation Theory
- Q6: Central Potential, Hydrogen Atom, Schrödingers Eqn

August 2008
- Q1: 3-D Spherical Well, Schrödingers Eqn
- Q2: Perturbation Theory, Degenerate Perturbation Theory
- Q3: SHO; Schrödinger Eqn, Ladder Operators
- Q4: Infinite Square Well, Probabilities, Perturbation Theory (Widening box)
- Q5: Time Evolution, Schrödinger Eqn
- Q6: Hydrogen Atom, Expectation value, Angular Momentum

January 2009
- Q1: Spin 1/2 Particles, Spinors, Expectation Value, probabilities
- Q2: Perturbation Theory
- Q3: 2-D well, Schrödinger Eqn,
- Q4: Angular Momentum, Clebsh-Gordon Coefficients, Spin Scattering?
- Q5: Probabilities, Time Evolution
- Q6: Hydrogen Atom, Angular Momentum

August 2009
- Q1: Step Potential, Schrödingers Eqn, Probability
- Q2: Variational Method, Expectation Value
- Q3: Eigenvalue/Eigenvectors, Perturbation Theory
- Q4: Central Potential, Angular Momentum
- Q5: Infinite Square Well, Identical Particles
- Q6: Spin 1/2 Particles, Time Evolution, Probabilities

January 2010

Q1: δ-Function Potential, Schrödinger Eqn, expectation value
Q2: Hydrogen Atom, Probability, Uncertainty principle
Q3: Time-Dependent Perturbation Theory,
Q4: Spin 1/2 Particles, Probability, Time Evolution
Q5: Two-level system, Coupling
Q6: Hyperfine Splitting, e^- & p^+ spin

August 2010

Q1: Step Potential, Zero-Potential, Probability
Q2: SHO, Ladder Operators, Uncertainty principle, multiple particles, degeneracy
Q3: Dirac Formalism, Matrix Mechanics
Q4: 3-D SHO, Perturbation Theory
Q5: Hydrogen Atom, Variational Method, Expectation value
Q6: Step Potential, Gamow Factor

August 2011

Q1: Completeness Relation, Probability, Time Evolution, Schrödinger Picture, Heisenberg Picture
Q2: SHO, Probability, Parity?
Q3: Angular Momentum, Probability
Q4: Spin System, Spin 1/2 Particles, Probability
Q5: Perturbation Theory, Infinite Square Well
Q6: Variational Method, SHO, Matrix Mechanics

January 2012

Q1: Stationary States, Time Evolution, Probability, Uncertainty principle
Q2: Dirac Notation, Hermitian Operators
Q3: SHO, Schrödinger Eqn, Expectation Value
Q4: Angular Momentum, Hydrogen Atom, Hyperfine splitting
Q5: Interaction Picture, Schrödinger Eqn
Q6: Perturbation Theory, SHO

August 2012

Q1: Matrix Manipulation, Time Evolution
Q2: Spin 1/2 Particles; Uncertainty Principle
Q3: Spin 1/2 Particles, Clebsh-Gordon Coefficients, Coupling
Q4: Hydrogen-like Atom, Perturbation Theory, Probability
Q5: SHO, Time-dependent Perturbation Theory
Q6: Time Evolution, Expectation Value

January 2013:

Q1: δ-Function Potential, Scattering, Schrödinger Eqn
Q2: Scattering, Born Approx,
Q3: Spin 1/2 Particles, Matrix Manipulation, Expectation value, Probability
Q4: SHO, Ladder operators
Q5: Infinite Square Well, Perturbation Theory,
Q6: 3-D Well, Schrödinger Eqn

August 2013:

Q1: Infinite Square Well, Schrödinger Eqn, Box Expansion
Q2: Angular Momentum, Ladder Operators,
Q3: Step Potential, Scattering, Schrödinger Eqn
Q4: Hydrogen Atom, Probabilities
Q5: Matrix Manipulation, Perturbation Theory
Q6: SHO, Perturbation Theory, Time Evolution, Time Dependent Perturbation Theory

January 2014:

Q1: Schrödinger Eqn, Angular Momentum, Perturbation Theory
Q2: Infinite Square Well, Schrödinger Eqn, Probability
Q3: Matrix Manipulation, Probability
Q4: Clebsh-Gordon Coefficients, Angular Momentum
Q5: Zeeman Splitting, Hydrogen Atom
Q6: SHO, Perturbation Theory

August 2014:

Q1: Schrödinger Eqn, Expectation Values, SHO, Uncertainty principle

Q2: Spin 1/2 Particles, Angular Momentum, Ladder Operators

Q3: SHO, Perturbation Theory, Probability

Q4: Identical Particles, Infinite Square Well, Spin 1/2 Particles

Q5: Angular Momentum, Expectation Value

Q6: Variational Method

January 2015:

Q1: SHO, Ladder operators

Q2: Hydrogen Atom, Angular Momentum, Time Evolution, Probability, Expectation Value

Q3: Step Potential, Schrödinger Eqn, Infinite Square Well

Q4: Matrix Manipulation, Time Evolution

Q5: Interaction Picture

Q6: 2-D Well, Perturbation Theory

August 2015:

Q1: Step Potential, Scattering, Probability Current

Q2: Confined Harmonic Oscillator, Angular Momentum

Q3: Matrix Manipulation

Q4: Infinite Square Well, Well Expansion, Probability

Q5: SHO, Perturbation Theory

Q6: Hydrogen Atom, Expectation Value, Probability

January 2016:

Q1: Clebsh-Gordon Coefficients, Spinor States, Probability

Q2: SHO, Perturbation Theory, Parity

Q3: Identical Particles, Infinite Square Well, Spin 1/2 Particles

Q4: Matrix Manipulation, Time Evolution

Q5: Spin 1/2 Particles, Spinor States, Time Evolution, Probability

Q6: Finite Square Well, Schrödinger Eqn, Scattering