Quantum 14

1a) $\hat{A}^\dagger = (\hat{A}^T)^*$

b) $\hat{A}^\dagger = \hat{A}$

$\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle \Rightarrow \langle\psi_n|\hat{A}|\psi_n\rangle = a_n$

$\langle\psi_n|\hat{A}^\dagger = a_n^* \Rightarrow \langle\psi_n|A^\dagger|\psi_n\rangle = \langle\psi_n|A|\psi_n\rangle = a_n^*$

$\Rightarrow a_n = a_n^* \quad \Rightarrow a_n$ is real

c) $|\psi\rangle = \sum_n c_n |n\rangle$ where $c_n = \langle n|\psi\rangle$

$\Rightarrow |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle = \left(\sum_n |n\rangle\langle n|\right)|\psi\rangle$

$\Rightarrow \sum_n |n\rangle\langle n| = 1$

2a) Eigenvalues of A and B can both be known exactly simultaneously

$[\hat{A}, \hat{B}] = 0$

b) $\Delta A = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}$

c) For compatible observables $\Delta A \Delta B = 0$ so observables can be known exactly

For incompatible observables both ΔA and ΔB are non-zero so neither can be known exactly.

3a) $|\Psi\rangle = \hat{A}|\Phi\rangle$

$|\Psi\rangle = \sum_n c_n|n\rangle \qquad |\Phi\rangle = \sum_n b_n|n\rangle$

$\Rightarrow \sum_n c_n|n\rangle = \sum_n b_n \hat{A}|n\rangle$

$\hat{A}|n\rangle = \sum_m a_{m,n}|m\rangle$

$\Rightarrow \sum_n c_n|n\rangle = \sum_{n,m} b_n a_{m,n}|m\rangle$

$= \sum_{n,m} a_{n,m} b_m |n\rangle$

$\Rightarrow c_n = \sum_m a_{n,m} b_m \Rightarrow \underline{c} = \underline{\underline{A}}\,\underline{b}$ with c, a and b as shown

4a) A fermion is a half-integer spin particle. In systems with multiple fermions the wavefunction must be antisymmetric on interchange of any 2 particles e.g $\psi_1(x_1)\psi_2(x_2) = -\psi_1(x_2)\psi_2(x_1)$

b) $\psi_{overall} = \psi_{spin}\,\psi_{spatial}$. $\psi_{overall}$ must be antisymmetric. If both particles are spin up, ψ_{spin} is symmetric meaning $\psi_{spatial}$ must be antisymmetric

$\psi_{spatial} = \phi_1(x_1)\,\phi_2(x_2)$ where x_1 describes position of particle 1

Antisymmetric $\Rightarrow \phi_1(x_1)\phi_2(x_2) = -\phi_1(x_2)\phi_2(x_1)$

If at same position $x_1 = x_2 \Rightarrow \phi_1(x_1)\phi_2(x_1) = -\phi_1(x_1)\phi_2(x_1)$
$\Rightarrow \phi_1(x_1)\phi_2(x_1) = 0 \Rightarrow$ Probability of being found at same position is 0

5a) $\langle \psi | \psi \rangle = \left(\frac{\sqrt{3}}{2} \langle \phi_0 | + \frac{1}{2} \langle \phi_1 | \right) \left(\frac{\sqrt{3}}{2} | \phi_0 \rangle + \frac{1}{2} | \phi_1 \rangle \right)$

$= \frac{3}{4} \langle \phi_0 | \phi_0 \rangle + \frac{\sqrt{3}}{4} \left(\langle \phi_0 | \phi_1 \rangle + \langle \phi_1 | \phi_0 \rangle \right) + \frac{1}{4} \langle \phi_1 | \phi_1 \rangle$

$\langle \phi_n | \phi_m \rangle = \delta_{n,m}$

$\Rightarrow \langle \psi | \psi \rangle = \frac{3}{4} + \frac{1}{4} = 1$

b.i) $E_0 : \quad p(E_0) = \left(\frac{\sqrt{3}}{2} \right)^2 = \frac{3}{4}$

$E_1 : \quad p(E_1) = \left(\frac{1}{2} \right)^2 = \frac{1}{4}$

ii) $\langle E \rangle = \frac{3}{4} E_0 + \frac{1}{4} E_1$ eigenstate orthogonal so no cross terms

6a) $\hat{S}_x | \uparrow \rangle_x = \frac{\hbar}{2} \quad \Rightarrow \quad | \uparrow \rangle_x = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad | \downarrow \rangle_x = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

b) $\hat{S}_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \hat{S}_x \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

± eigenvalues

c) Singlet $\psi_{singlet} = \frac{1}{\sqrt{2}} \left(| \uparrow \rangle_1 | \downarrow \rangle_2 - | \downarrow \rangle_1 | \uparrow \rangle_2 \right)$

Triplet $\psi = \begin{cases} | \uparrow \rangle_1 | \uparrow \rangle_2 \\ \frac{1}{\sqrt{2}} \left(| \uparrow \rangle_1 | \downarrow \rangle_2 + | \downarrow \rangle_1 | \uparrow \rangle_2 \right) \\ | \downarrow \rangle_1 | \downarrow \rangle_2 \end{cases}$

7a) $|\psi\rangle = \sum_m d_m |\chi_m\rangle = \sum_n c_n |\psi_n\rangle$

Take $\langle \chi_m|$

$$d_m = \sum_n c_n \langle \chi_m | \psi_n \rangle$$

$$= \sum_n \langle \chi_m | \psi_n \rangle c_n = \sum_n S_{m,n} c_n$$

$\Rightarrow \underline{d} = \underline{S}\, \underline{c}$

b) $\hat{A}|\chi_n\rangle = \cancel{A_{n,\chi}|\chi_n\rangle}\ A_{\chi,m}|\chi_m\rangle$

$\hat{A}|\psi_n\rangle = \cancel{A_{n,\psi}|\psi_n\rangle}\ A_{\psi,n}|\psi_n\rangle$

$\hat{A}|\chi_m\rangle = \hat{A}\sum_n |\psi_n\rangle\langle\psi_n|\chi_m\rangle = \cancel{\hat{A}} \sum_n (S_{mn})^{\dagger} \hat{A}|\psi_n\rangle$

$\Rightarrow A_{\chi,m}|\chi_m\rangle = \sum_n \cancel{(S_{mn})^{\dagger}} A_{\psi,n}|\psi_n\rangle (S_{mn})^{\dagger}$

Take $\langle \chi_p|$

$A_{\chi,p} = \cancel{\#} \sum_n \cancel{(S_{pn})^{\dagger}} A_{\psi,n} \langle \chi_p|\psi_n\rangle (S_{pn})^{\dagger} \quad m \to p$

$A_{\chi,m} = \sum_n A_{\psi n} \cancel{\#} S_{mn} S_{nm}^{\dagger} \qquad S^{\dagger} = S^{-1}$

$\Rightarrow A_{\chi} = S A_{\psi} \cancel{A} S^{-1}$

c) $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\Rightarrow \hat{H} = \frac{\gamma\hbar}{2}\left[\begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix} + \begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix} + \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix}\right]$$

$$= \frac{\gamma\hbar}{2}\begin{pmatrix} c & a-ib \\ a+ib & -c \end{pmatrix}$$

7d) $S_{mn} = \langle x_m | \psi_n \rangle$ from 7a

$$\Rightarrow S = \begin{pmatrix} \langle + | \alpha \rangle & \langle + | \beta \rangle \\ \langle - | \alpha \rangle & \langle - | \beta \rangle \end{pmatrix}$$

$$\langle + | = \frac{1}{\sqrt{2}}(\langle \alpha | - i \langle \beta |) \qquad \langle - | = \frac{1}{\sqrt{2}}(\langle \alpha | + i \langle \beta |)$$

$$\Rightarrow S_{yz} = \begin{pmatrix} 1/\sqrt{2} & -i/\sqrt{2} \\ \frac{1}{\sqrt{2}} & i/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

e) $H^{(y)} = S H S^{-1}$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \frac{\gamma\hbar}{2} \begin{pmatrix} c & a-ib \\ a+ib & -c \end{pmatrix} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$= \frac{\gamma\hbar}{4} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} c+ia+b & c-ia-b \\ a+ib-ic & a+ib+ic \end{pmatrix}$$

$$= \frac{\gamma\hbar}{4} \begin{pmatrix} c+b+ia-ia+b-c & c-ia-b-ia+b+c \\ c+ia+b+ia-b+c & c-ia-b+ia-b-c \end{pmatrix}$$

$$= \frac{\gamma\hbar}{4} \begin{pmatrix} 2b & 2c-2ia \\ 2c+2ia & -2b \end{pmatrix} = \frac{\gamma\hbar}{2} \begin{pmatrix} b & c-ia \\ c+ia & -b \end{pmatrix}$$

f) $\det(H^{(y)} - \lambda I) = 0 \Rightarrow \begin{vmatrix} \frac{\gamma\hbar}{2} b - \lambda & \frac{\gamma\hbar}{2}(c-ia) \\ \frac{\gamma\hbar}{2}(c+ia) & -\frac{\gamma\hbar}{2} b - \lambda \end{vmatrix} = 0$

$$(b - \tfrac{2}{\gamma\hbar}\lambda)(-b - \tfrac{2}{\gamma\hbar}\lambda) - (c-ia)(c+ia) = 0$$

$$-b^2 + \frac{4}{\gamma^2\hbar^2}\lambda^2 - c^2 - a^2 = 0$$

$$\lambda^2 = \frac{\gamma^2\hbar^2}{4}(a^2+b^2+c^2) \qquad \lambda_y = \pm \frac{\gamma\hbar}{2}\sqrt{a^2+b^2+c^2}$$

Same as eigenvalues of $H^{(z)}$

g) $\langle S_z \rangle = \langle \psi_0 | S_z | \psi_0 \rangle$

$$|\psi_0\rangle^{(y)} = \left(\sqrt{\frac{1+b}{2}}\right) \frac{1}{\sqrt{2}} (|\alpha\rangle + i|\beta\rangle) + \left(\frac{ia-c}{\sqrt{2(1+b)}}\right) \frac{1}{\sqrt{2}} (|\alpha\rangle - i|\beta\rangle)$$

$$= \frac{1}{2}\left(\sqrt{1+b} + \frac{ia-c}{\sqrt{1+b}}\right)|\alpha\rangle + \frac{i}{2}\underbrace{\left(\sqrt{1+b} + \frac{c-ia}{\sqrt{1+b}}\right)}_{i\sqrt{1+b} + \frac{ic+a}{\sqrt{1+b}}}|\beta\rangle$$

$$\Rightarrow \langle S_z \rangle = \frac{\hbar}{2}\,\frac{1}{4}\left(\sqrt{1+b}\;\frac{+ia-c}{\sqrt{1+b}}\right)\left(\sqrt{1+b}\;\frac{-ia-c}{\sqrt{1+b}}\right)$$

$$-\frac{\hbar}{2}\,\frac{1}{4}\left(i\sqrt{1+b}\;\frac{+ic+a}{\sqrt{1+b}}\right)\left(-i\sqrt{1+b}\;\frac{-ic+a}{\sqrt{1+b}}\right)$$

$$= \frac{\hbar}{8}\left(1+b-2c+\frac{c^2}{1+b}+\frac{a^2}{1+b}\right)-\frac{\hbar}{8}\left(1+b+2c+\frac{c^2}{1+b}+\frac{a^2}{1+b}\right)$$

$$= -\frac{4c\hbar}{8} = -\frac{\hbar c}{2}$$

8a) We write Hamiltonian as $H_0 + \lambda H_1$ where $\lambda H_1 = H'$ and λ is small

We can then use a series ~~a~~ expansion of the energy and wavefunct in terms of λ and corrections

$$E_n = E_n^{(0)} + \lambda E_n^{'(1)} + \lambda^2 E_n^{'(2)} + \dots$$

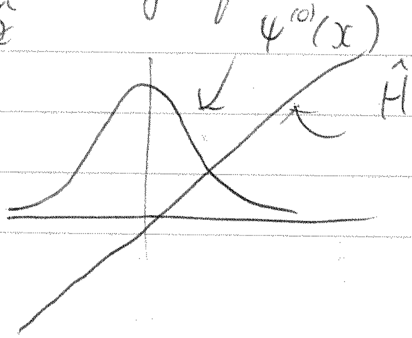
where $E_n^{(1)} = \lambda E_n^{'(1)}$

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \dots$$

Then using $\hat{H}\psi_n = E_n \psi_n$ with our power series expressions we can equate terms corresponding to each power of λ to get corrections. Looking at λ terms then taking $\langle \psi_n^{(0)} |$ of both sides will lead to expression for first order energy correction

$\psi_n^{(0)}$ is unperturbed wave function and H' is perturbing Hamiltonian

b) Take ground state of quantum harmonic oscillator and perturb with $\hat{H}' = a\hat{x}$



Since $\psi^{(0)}$ is even and H' is odd $\langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle = 0$
so 1st order energy correction is 0

In general, for wavefunctions and perturbations of opposite parity the 1st order correction is 0.

c) $\hat{H}|\psi_n\rangle = \left(\frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2}\right)|\psi_n\rangle$

$\langle \psi_m | \psi_n \rangle = \delta_{m,n}$

$\Rightarrow \langle \psi_m | \hat{H} | \psi_n \rangle = \frac{\hbar^2 n^2 \pi^2 \delta_{m,n}}{2ma^2} = \begin{cases} \frac{\hbar^2 m^2 \pi^2}{2ma^2} & \text{for } n=m \\ 0 & n \neq m \end{cases}$

↑ mass not index

$\Rightarrow H_{11} = \frac{\hbar^2\pi^2}{2ma^2}$ $H_{22} = \frac{4\hbar^2\pi^2}{2ma^2}$ $H_{33} = \frac{9\hbar^2\pi^2}{2ma^2}$ $H_{44} = \frac{16\hbar^2\pi^2}{2ma^2}$

all others 0

$$\Rightarrow H = \frac{\hbar^2\pi^2}{2ma^2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 16 \end{pmatrix}$$

d) $\langle \psi_m | x | \psi_n \rangle = \int_0^a \frac{2}{a}\sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right) x\,dx$

$= \frac{1}{a}\int_0^a x\left(\cos\left(\frac{(n-m)\pi x}{a}\right) - \cos\left(\frac{(n+m)\pi x}{a}\right)\right)dx$

$= \frac{1}{a}\left[\left(\frac{a}{(n-m)\pi}\right)^2\cos\left(\frac{(n-m)\pi x}{a}\right) - \left(\frac{a}{(n+m)\pi}\right)^2\cos\left(\frac{(n+m)\pi x}{a}\right)\right]_0^a$ for $n \neq m$

$= 0$ if $n+m$ is even

for $n=m$ $\frac{1}{a}\int_0^a x\left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right)dx$

$= \int_0^a 2\sin^2\left(\frac{n\pi x}{a}\right) x\,dx$ $= \frac{1}{a}\left[\frac{x^2}{2} - \left(\frac{a}{2n\pi}\right)^2\cos\left(\frac{2n\pi x}{a}\right)\right]_0^a$

$\cancel{\Rightarrow V_1 = \frac{q\mathcal{E}x}{a}}$

$\cancel{n \neq m}$ $n = m$ $\quad \langle \psi_n | x | \psi_n \rangle = \frac{a}{2} + \frac{1}{a} \overbrace{\left[-\left(\frac{a}{2\pi n}\right)^2 \cos\left(\frac{2n\pi x}{a}\right) \right]_0^a}^{0} = \frac{a}{2}$

$\cancel{\Rightarrow V_1 = q\mathcal{E}\left(\frac{a}{2} - \frac{1}{a}\left(\frac{a}{2\pi n}\right)^2 \cos x\right)}$

$\Rightarrow \quad V_{nn} = \frac{q\mathcal{E}a}{2}$

$\cancel{V_{13} = V_{31} = \frac{a}{4\pi^2}}$

$V_{12} = V_{21} = q\mathcal{E}\left(\frac{a}{\pi^2}\left(\cos(\pi) - \cos(0)\right) - \frac{a}{9\pi^2}\left(\cos(3\pi) - \cos(0)\right)\right)$

$= \frac{q\mathcal{E}a}{\pi^2}\left(-2 + \frac{2}{9}\right) = \frac{-16}{9}\frac{q\mathcal{E}a}{\pi^2}$

$V_{23} = V_{32} = \frac{q\mathcal{E}a}{\pi^2}\left(-2 + \frac{2}{25}\right) = \frac{-48}{25}\frac{q\mathcal{E}a}{\pi^2}$

$V_{34} = V_{43} = \frac{q\mathcal{E}a}{\pi^2}\left(-2 + \frac{2}{49}\right) = \frac{-96}{49}\frac{q\mathcal{E}a}{\pi^2}$

$V_{14} = V_{41} = \frac{q\mathcal{E}a}{\pi^2}\left(\frac{-2}{9} + \frac{2}{25}\right) = \frac{-32}{225}\frac{q\mathcal{E}a}{\pi^2}$

$$\Rightarrow V = q\mathcal{E}a \begin{pmatrix} \frac{1}{2} & \frac{-16}{9\pi^2} & 0 & \frac{-32}{225\pi^2} \\ \frac{-16}{9\pi^2} & \frac{1}{2} & \frac{-48}{25\pi^2} & 0 \\ 0 & \frac{-48}{25\pi^2} & \frac{1}{2} & \frac{-96}{49\pi^2} \\ \frac{-32}{225\pi^2} & 0 & \frac{-96}{49\pi^2} & \frac{1}{2} \end{pmatrix}$$

c) $E_n^{(1)} = \langle \psi_n^{(0)} | q\mathcal{E}x | \psi_n^{(0)} \rangle$

$\Rightarrow E_n^{(1)} = \frac{q\mathcal{E}a}{2}$ for all of first 4 state

(5)

f) $$E_1^{(2)} = \sum_{k \neq 1} \frac{|\langle \psi_k^{(0)} | V | \psi_1^{(0)} \rangle|^2}{E_1^{(0)} - E_k^{(0)}}$$

$$= \left(\frac{-16 q \varepsilon a}{9\pi^2}\right)^2 \frac{1}{E_1 - E_2} + 0 + \left(\frac{-32 q \varepsilon a}{225\pi^2}\right)^2 \frac{1}{E_1 - E_4}$$

$$= \frac{q^2 \varepsilon^2 a^2}{\pi^4}\left(\frac{256}{81} \times \frac{1}{\frac{-3\hbar^2\pi^2}{2ma^2}} + \frac{1024}{50625} \times \frac{1}{\frac{-15\hbar^2\pi^2}{2ma^2}}\right)$$

$$= -\frac{q^2 \varepsilon^2 a^4 m}{\hbar^2 \pi^6}\left(\frac{512}{243} + 2.697 \times 10^{-3}\right)$$

$$= -2.11 \frac{q^2 \varepsilon^2 a^4 m}{\hbar^2 \pi^6}$$ ~~[illegible]~~

$$E_2^{(2)} = \left(\frac{-16 q \varepsilon a}{9\pi^2}\right)^2 \frac{1}{\frac{3\hbar^2\pi^2}{2ma^2}} + \left(\frac{-48 q \varepsilon a}{25\pi^2}\right)^2 \frac{1}{\frac{-5\hbar^2\pi^2}{2ma^2}}$$

$$= 0.632 \frac{q^2 \varepsilon^2 a^4 m}{\hbar^2 \pi^6}$$

Largest contributions from adjacent wavefunctions e.g ± 1

Higher energy wavefunctions give negative correction, lower order give positive correction

9a) $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \qquad [\hat{J}_i, \hat{J}_j] = i\hbar \varepsilon_{ijk} \hat{J}_k$

$$[\hat{J}_x, \hat{J}^2] = [\hat{J}_x, \hat{J}_x^2] + [\hat{J}_x, \hat{J}_y^2] + [J_x, J_z^2]$$

$$= 0 + [J_x, J_y]J_y + \hat{J}_y[\hat{J}_x, \hat{J}_y] + [J_x, J_z]J_z + J_z[J_x, J_z]$$

using formula given in paper

$$= i\hbar J_z J_y + i\hbar J_y J_z - i\hbar J_y J_z - i\hbar J_z J_y = 0$$

$[J_z, J_+] = [J_z, J_x] + i[J_z, J_y] = i\hbar J_y + \hbar J_x = \hbar J_+$

b) $\hat{J}_z(\hat{J}_+|j m_j\rangle) = ([J_z, J_+] + J_+ J_z)|j m_j\rangle$

$= (\hbar J_+ + J_+ \hbar m_j)|j m_j\rangle = \hbar(m_j+1)\, J_+|j m_j\rangle$

$\Rightarrow$ eigenvalue $(m_j+1)\hbar$ $\Rightarrow$ quantum number m_j+1

J_+ raise m_j by 1 but cannot have a state where $m_j > j$
$\Rightarrow J_+|j\, j\rangle = 0$

c) $\hat{J}^2 = (\underline{\hat{L}} + \underline{\hat{S}})^2 = \hat{L}^2 + \hat{S}^2 + 2\underline{\hat{L}}\cdot\underline{\hat{S}}$

$= \hat{L}^2 + \hat{S}^2 + 2L_x S_x + 2L_y S_y + 2L_z S_z$

$L_x = \frac{1}{2}(L_+ + L_-) \qquad L_y = \frac{1}{2i}(L_+ - L_-)$

$\Rightarrow \hat{J}^2 = L^2 + S^2 + \frac{2}{4}(L_+ + L_-)(S_+ + S_-) - \frac{1}{2}(L_+ - L_-)(S_+ - S_-) + 2L_z S_z$

$= L^2 + S^2 + \frac{1}{2}\left(\cancel{L_+S_+} + L_+S_- + L_-S_+ + \cancel{L_-S_-} - \cancel{L_+S_+} + L_+S_- + L_-S_+ - \cancel{L_-S_-}\right) + 2L_z$

$= \hat{L}^2 + \hat{S}^2 + \hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+ + 2\hat{L}_z\hat{S}_z$

d) $\hat{J}^2|l\,l, s\,s\rangle = (\hat{L}^2 + \hat{S}^2 + \hat{L}_+\hat{S}_- + \hat{L}_-\hat{S}_+ + 2\hat{L}_z\hat{S}_z)|l\,l, s\,s\rangle$

$= (\hbar^2 l(l+1) + \hbar^2 s(s+1) + 0 + 0 + 2\hbar^2 m_l m_s)|l\,l, s\,s\rangle$

0 as $S_+|s\,s\rangle = 0$ and $L_+|l\,l\rangle = 0$

$= \hbar^2(l(l+1) + s(s+1) + 2ls)|l\,l, s\,s\rangle$

$\Rightarrow$ Eigenvalue $\hbar^2(l(l+1) + s(s+1) + 2ls)$

e) $|\tfrac{1}{2}, -\tfrac{1}{2}\rangle = a|1\,{-1}, \tfrac{1}{2}\tfrac{1}{2}\rangle + b|1\,0, \tfrac{1}{2}, -\tfrac{1}{2}\rangle \qquad m_l + m_s = m_j = -\tfrac{1}{2}$

$a^2 + b^2 = 1$

$$J_-|\tfrac12,-\tfrac12\rangle = (L_- + S_-)\left(a|1\,-1,\tfrac12\,\tfrac12\rangle + b|1\,0,\tfrac12\,-\tfrac12\rangle\right)$$

$$= aL_-|1\,-1,\tfrac12\,\tfrac12\rangle + aS_-|1\,-1,\tfrac12\,\tfrac12\rangle + bL_-|1\,0,\tfrac12\,-\tfrac12\rangle + bS_-|1\,0,\tfrac12\,-\tfrac12\rangle$$

Use equation for raising ~~ladder~~ operators

$$\cancel{=0}$$

$$= \cancel{a\sqrt{2-0}\,|1\,0,\tfrac12\,\tfrac12\rangle} + a\sqrt{\tfrac34+\tfrac14}\,|1\,-1,\tfrac12\,-\tfrac12\rangle + b\sqrt{2-0}\,|1\,-1,\tfrac12\,-\tfrac12\rangle + 0$$

$$= \cancel{a\sqrt{\ }}\; a|1\,-1,\tfrac12\,-\tfrac12\rangle + b\sqrt{2}\,|1\,-1,\tfrac12\,-\tfrac12\rangle = 0$$

$$\Rightarrow a + \sqrt{2}\,b = 0 \quad \text{and} \quad a^2 + b^2 = 1$$

$$\Rightarrow (-\sqrt{2}\,b)^2 + b^2 = 1$$

$$2b^2 + b^2 = 1 \qquad b = \frac{1}{\sqrt3} \qquad \Rightarrow a = -\sqrt{\frac23}$$

$$|\tfrac12,-\tfrac12\rangle = -\sqrt{\frac23}\,|1\,-1,\tfrac12\,\tfrac12\rangle + \frac{1}{\sqrt2}\,|1\,0,\tfrac12\,-\tfrac12\rangle$$

10a) Let $\hat{H}$ have eigenvectors $|n\rangle$ with eigenvalues E_n such that $\hat{H}|n\rangle = E_n|n\rangle$

$$|\psi\rangle = \sum_n a_n|n\rangle$$ where ~~$\sum_n |a_n|^2 \neq 1$ to be normalized~~

$$\hat{H}|\psi\rangle = \sum_n a_n E_n|n\rangle \Rightarrow \langle\psi|\hat{H}|\psi\rangle = \sum_n |a_n|^2 E_n$$

$$\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2}$$

Since $E_n \geq E_0$ $\quad \dfrac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2} \geq E_0$ with equality for $|a_0| = 1$ and $a_n = 0$ otherwise

b) For a given Hamiltonian, we can compute $\frac{\langle \psi_{trial} | \hat{H} | \psi_{trial} \rangle}{\langle \psi_{trial} | \psi_{trial} \rangle}$ for a trial wave function. As this is $\geq E_0$ it gives us an upper bound on E_0. We can let $|\psi_{trial}\rangle$ be a function of various parameters which we can minimise over to get a better upper bound on E_0.

c) i) $|\psi\rangle = |0\rangle + \beta|1\rangle$ $\qquad$ $|0\rangle$ and $|1\rangle$ are orthonormal

$$\langle \psi | \psi \rangle = 1 + \beta^2$$

$$\Rightarrow |\psi\rangle = \frac{1}{\sqrt{1+\beta^2}}\left(|0\rangle + \beta|1\rangle\right)$$

ii) $\langle H \rangle = \langle \psi | \hat{H} | \psi \rangle$

$$= \frac{1}{1+\beta^2}\left(\frac{\hbar\omega}{2} + \beta^2 \frac{3\hbar\omega}{2}\right)$$

$$= \frac{\hbar\omega}{2(1+\beta^2)}\left(1+3\beta^2\right)$$

iii) $\hat{V}_\varepsilon = q\varepsilon\hat{x}$

$$a_+ + a_- = \frac{2}{\sqrt{2}}\alpha\hat{x} \quad \Rightarrow \hat{x} = \frac{1}{\alpha\sqrt{2}}(a_+ + a_-)$$

$$\hat{V}_\varepsilon = \frac{q\varepsilon(\hat{a}_+ + \hat{a}_-)}{\alpha\sqrt{2}}$$

iv) $$\frac{\langle \hat{\psi} | \hat{H} | \hat{\psi} \rangle}{\langle \hat{\psi} | \hat{\psi} \rangle} = \frac{1}{1+\beta^2}\left(\langle 0| + \beta\langle 1|\right)\left(\hat{H}_0 + \frac{q\varepsilon}{\alpha\sqrt{2}}(a_+ + a_-)\right)\left(|0\rangle + \beta|1\rangle\right)$$

$$= \frac{1}{(1+\beta^2)}\left(\langle 0| + \beta\langle 1|\right)\left(E_0|0\rangle + \beta E_1|1\rangle + \frac{q\varepsilon}{\alpha\sqrt{2}}|1\rangle + \frac{\beta q\varepsilon}{\alpha}|2\rangle\right.$$

$$\cancel{= \frac{1}{1+\beta^2}\left(E_0 + \beta^2 E_1 + \frac{\beta q\varepsilon}{\alpha\sqrt{2}}\right.} \quad \left. + \frac{\beta q\varepsilon}{\alpha\sqrt{2}}|0\rangle\right)$$

$$= \frac{1}{1+\beta^2}\left(E_0 + \beta^2 E_1 + \frac{\beta q \varepsilon}{\alpha\sqrt{2}} + \frac{\beta q \varepsilon}{\alpha\sqrt{2}}\right)$$

$$= \frac{1}{1+\beta^2}\left(E_0 + \beta^2 E_1 + \frac{\sqrt{2}\beta q \varepsilon}{\alpha}\right)$$

$$\frac{\partial E_{trial}}{\partial \beta} = \frac{-2\beta}{(1+\beta^2)^2}\left(E_0 + \beta^2 E_1 + \frac{\sqrt{2} q}{\alpha}\varepsilon\beta\right) + \frac{1}{(1+\beta^2)}\left(2\beta E_1 + \frac{\sqrt{2} q}{\alpha}\varepsilon\right) = 0$$

$$\Rightarrow -2\beta(E_0 + \beta^2 E_1 + \gamma\beta) + (1+\beta^2)(2E_1\beta + \gamma) = 0$$

$$-2\beta E_0 - \cancel{2\beta^3 E_1} - 2\gamma\beta^2 + 2E_1\beta + \gamma + \cancel{2E_1\beta^3} + \beta^2\gamma = 0$$

$$\Rightarrow -\gamma\beta^2 + 2(E_1 - E_0)\beta + \gamma = 0$$

$$\Rightarrow \beta = \frac{-2(E_1-E_0) \pm \sqrt{4(E_1-E_0)^2 + 4\gamma}}{-2\gamma}$$

$$= \frac{E_1 - E_0}{\gamma} \pm \sqrt{\frac{(E_1-E_0)^2}{\gamma^2} + 1}$$

Take negative square root for smaller β which will give smaller energy

$$\Rightarrow \beta = \frac{E_1 - E_0}{\gamma} - \sqrt{\frac{(E_1-E_0)^2}{\gamma^2} + 1}$$