Modern Quantum Mechanics

Solutions Manual

J. J. Sakurai

Late, University of California, Los Angeles

San Fu Tuan, Editor

University of Hawaii, Manoa

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Chapter 1

1. $[AB,CD] = ABCD - CDAB = ABCD + ACBD - ACBD - ACDB + ACDB + CADB - CADB - CDAB = A\{C,B\}D - AC\{D,B\} + \{C,A\}DB - C\{D,A\}B$.

2. (a) $X = a_o + \Sigma a_\ell \sigma_\ell$, $tr(X) = 2a_o$ because $tr(\sigma_\ell) = 0$. Next evaluate $tr(\sigma_k X) = tr(\sum_\ell a_\ell \sigma_k \sigma_\ell) = \sum_\ell a_\ell 2\delta_{\ell k} = 2a_k$ (where we have used $tr(\sigma_i \sigma_j) = tr(\frac{1}{2}(\sigma_i\sigma_j + \sigma_j\sigma_i)) = 2\delta_{ij}$). Hence $a_o = \frac{1}{2}\, tr(X)$, $a_k = \frac{1}{2}\, tr(\sigma_k X)$.

(b) $a_o = \frac{1}{2}(X_{11} + X_{22})$, while a_k can be explicitly evaluated from $a_k = \frac{1}{2}\, tr(\sigma_k X)$ with $X = [X_{ij}]$ and $i,j = 1,2$. The result is $a_1 = \frac{1}{2}(X_{12} + X_{21})$, $a_2 = \frac{i}{2}(-X_{21} + X_{12})$, and $a_3 = \frac{1}{2}(X_{11} - X_{22})$.

3.
$$\vec{\sigma}.\vec{a} = \sigma_x a_x + \sigma_y a_y + \sigma_z a_z = \begin{pmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{pmatrix},$$

$$\det\,(\vec{\sigma}.\vec{a}) = -|\vec{a}|^2.$$

Without loss of generality, choose $\hat{n}$ along positive z-direction, then $\exp(\pm i\vec{\sigma}.\hat{n}\phi/2) = \underline{1}\cos\phi/2 \pm i\sigma_z \sin\phi/2$, and if B is defined to be $B \equiv \cos\phi/2 + i\sin\phi/2$, then

$$\exp(i\sigma_z\phi/2)\vec{\sigma}.\vec{a}\,\exp(-i\sigma_z\phi/2) = \begin{pmatrix} a_z B^* B & (a_x - ia_y)B^2 \\ (a_x + ia_y)B^{*2} & -a_z B^* B \end{pmatrix}.$$

Since $B^*B = \cos^2\phi/2 + \sin^2\phi/2 = 1$, $\det\,[\exp(i\sigma_z\phi/2)\vec{\sigma}.\vec{a} \times \exp(-i\sigma_z\phi/2)] = -(a_z{}^2 + a_x{}^2 + a_y{}^2) = -|\vec{a}|^2$, that is determinant is invariant under specified operation. Next we note

$$\vec{\sigma}\cdot\vec{a}' = \begin{pmatrix} a'_z & a'_x - ia'_y \\ a'_x + ia'_y & -a'_z \end{pmatrix} =$$

$$= \begin{pmatrix} a_z & (a_x - ia_y)(\cos\phi + i\sin\phi) \\ (a_x + ia_y)(\cos\phi - i\sin\phi) & -a_z \end{pmatrix}$$

hence $a'_z = a_z$, $a'_x = a_x\cos\phi + a_y\sin\phi$, $a'_y = a_y\cos\phi - a_x\sin\phi$. This is a counter-clockwise rotation about z-axis through angle ϕ in x-y plane.

4. (a) Note $\mathrm{tr}(XY) = \sum_{a'} \langle a'|XY|a'\rangle = \sum_{a',a''} \langle a'|X|a''\rangle\langle a''|Y|a'\rangle$ (by

作业 closure property) $= \sum_{a',a''} \langle a''|Y|a'\rangle\langle a'|X|a''\rangle$ (by rearrangement) $=$

$\sum_{a''} \langle a''|YX|a''\rangle$. Since a'' is a dummy summation variable, relabel $a'' = a'$,

hence $\mathrm{tr}(XY) = \mathrm{tr}(YX)$.

(b) $\langle (XY)^\dagger a'|a''\rangle = \langle a'|[(XY)^\dagger]^\dagger|a''\rangle = \langle a'|XY|a''\rangle = \langle X^\dagger a'|Y|a''\rangle$

$= \langle Y^\dagger X^\dagger a'|a''\rangle$. Therefore $(XY)^\dagger = Y^\dagger X^\dagger$.

(c) Take $\exp[if(A)]|\alpha\rangle = (1 + if(A) - \frac{[f(A)]^2}{2!} + \ldots\ldots)|\alpha\rangle$

$= (1 + if(\alpha) - \frac{[f(\alpha)]^2}{2!} + \ldots\ldots\ldots)|\alpha\rangle = \exp[if(\alpha)]|\alpha\rangle$, where we

assume that $A|\alpha\rangle = \alpha|\alpha\rangle$. Therefore $\exp[if(A)] =$

$\sum_\alpha \exp[if(\alpha)]|\alpha\rangle\langle\alpha|$, where closure property of the complete set

$\{|\alpha\rangle\}$ has been used.

(d) $\sum_{a'} \psi^*_{a'}(\vec{x}')\psi_{a'}(\vec{x}'') = \sum_{a'} \langle\vec{x}'|a'\rangle^*\langle\vec{x}''|a'\rangle = \sum_{a'} \langle a'|\vec{x}'\rangle \times$

$\langle\vec{x}''|a'\rangle = \sum_{a'} \langle\vec{x}''|a'\rangle\langle a'|\vec{x}'\rangle = \langle\vec{x}''|\vec{x}'\rangle$.

5. (a) $|\alpha\rangle\langle\beta| = \sum_{a'}\sum_{a''} |a'\rangle\langle a'|\alpha\rangle\langle\beta|a''\rangle\langle a''| = \sum_{a'}\sum_{a''} |a'\rangle\langle a''| \times$

$(\langle a'|\alpha\rangle\langle a''|\beta\rangle^*)$. Hence $|\alpha\rangle\langle\beta| = [\langle a^{(i)}|\alpha\rangle\langle a^{(j)}|\beta\rangle^*]$, where expression inside square bracket is the (i,j) matrix element.

(b) $|\alpha\rangle = |s_z = \hbar/2\rangle = |+\rangle$, $|\beta\rangle = |s_x = \hbar/2\rangle = \frac{1}{2^{1/2}}[|+\rangle + |-\rangle]$.

Hence

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

$$= 1/\sqrt{2}\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$$

6. Given $A|i\rangle = a_i|i\rangle$ and $A|j\rangle = a_j|j\rangle$. The normalized state vector $|i\rangle + |j\rangle$ is of form $|\psi\rangle = \frac{1}{2^{1/2}}[|i\rangle + |j\rangle]$. Hence $A|\psi\rangle = (1/\sqrt{2})[a_i|i\rangle + a_j|j\rangle]$ where a_i, a_j are real numbers if A is Hermitian; but for $a_i \neq a_j$ clearly r.h.s. is a state vector distinct from $|\psi\rangle$. However under the condition that $|i\rangle$ and $|j\rangle$ <u>are degenerate</u> (i.e. $a_i = a_j = a$), then $A|\psi\rangle = a[(1/\sqrt{2})(|i\rangle + |j\rangle)] = a|\psi\rangle$ and $|\psi\rangle$ or $|i\rangle + |j\rangle$ is also an eigenket of A.

7. (a) Let $|\xi\rangle \in \{|a'\rangle\}$ and $A|a'\rangle = a'|a'\rangle$. Then since $\prod_{a'}(A - a')|\xi\rangle$ is a product <u>over all eigenvalues</u>, and $|\xi\rangle = \sum_{a'}|a'\rangle\langle a'|\xi\rangle$ must therefore satisfy $\prod_{a'}(A-a')|\xi\rangle = 0$. Hence $\prod_{a'}(A-a')$ is the null operator.

(b) $\prod_{a''\neq a'}\frac{(A-a'')}{(a'-a'')}|a'\rangle = \prod_{a''\neq a'}\frac{(a'-a'')}{(a'-a'')}|a'\rangle = |a'\rangle$.

Hence $\theta|\xi\rangle = \prod_{a''\neq a'}\frac{(A-a'')}{(a'-a'')}|\xi\rangle = |a'\rangle\langle a'|\xi\rangle$. The operator therefore projects out of ket $|\xi\rangle$, its $|a'\rangle$ component.

(c) Let $A = S_z$, than $\prod_{a'} (S_z - a') = (S_z - \hbar/2)(S_z + \hbar/2)$. Hence evidently $\prod_{a'=\pm\hbar/2} (S_z - a')|\pm\rangle = 0$. This verifies (a) above. For case (b) we have $\theta_+ = (S_z+\hbar/2)/\hbar$, $\theta_- = -(S_z-\hbar/2)/\hbar$ and $S_z = \hbar/2(|+\rangle\langle+|-|-\rangle \times \langle-|)$ while ket $|\xi\rangle = |+\rangle\langle+|\xi\rangle + |-\rangle\langle-|\xi\rangle$. Hence $\theta_+|\xi\rangle = \langle+|\xi\rangle|+\rangle$ and $\theta_-|\xi\rangle = \langle-|\xi\rangle|-\rangle$ and $\theta_\pm$ are the projection operators of $|\xi\rangle$ to $|\pm\rangle$ states.

8. The orthonormality property is $\langle+|+\rangle = \langle-|-\rangle = 1$, $\langle+|-\rangle = \langle-|+\rangle = 0$. Hence using the explicit representations of S_i in terms of linear combinations of bra-ket products, we obtain by elementary calculation $[S_i,S_j] = i\varepsilon_{ijk}\hbar S_k$ and $\{S_i,S_j\} = (\hbar^2/2)\delta_{ij}$.

9. Let $\hat{n} = n_x\hat{i} + n_y\hat{j} + n_z\hat{k}$, then $n_x = \sin\beta\cos\alpha$, $n_y = \sin\beta\sin\alpha$, $n_z = \cos\beta$ and $\vec{S}.\hat{n} = \sin\beta\cos\alpha\ S_x + \sin\beta\sin\alpha\ S_y + \cos\beta\ S_z$. Also due to completeness property of the ket space $|\vec{S}.\hat{n};+\rangle = a|+\rangle + b|-\rangle$ where $|a|^2 + |b|^2 = 1$ (normalization). Therefore the relation $\vec{S}.\hat{n}|\vec{S}.\hat{n};+\rangle = (\hbar/2)|\vec{S}.\hat{n};+\rangle$ [taking advantage of explicit representations $S_x = \frac{\hbar}{2}(|+\rangle \times \langle-| + |-\rangle\langle+|)$, $S_y = \frac{i\hbar}{2}(-|+\rangle\langle-| + |-\rangle\langle+|)$, $S_z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|)$] leads to :-

$$(\sin\beta\cos\alpha - i\sin\beta\sin\alpha)b + \cos\beta\ a = a \tag{1a}$$

$$(\sin\beta\cos\alpha + i\sin\beta\sin\alpha)a - \cos\beta\ b = b \tag{1b}$$

Together with the normalization condition $|a|^2 + |b|^2 = 1$, we find $a = \cos(\beta/2)e^{i\theta_a}$ and $b = \sin(\beta/2)e^{i\theta_b}$. From equation (1a) we have

$a = \dfrac{\sin\beta\ e^{-i\alpha}b}{(1-\cos\beta)}$, hence $e^{i(\theta_b-\theta_a)} = e^{i\alpha}$. Choose $\theta_a = 0$, then $\theta_b = \alpha$, and $|\vec{S}.\hat{n};+\rangle = \cos(\beta/2)|+\rangle + \sin(\beta/2)e^{i\alpha}|-\rangle$.

10. $H = a(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|)$. Let $|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, $\langle 1| = (1,0)$ and $\langle 2| = (0,1)$, H can be explicitly written using outer product of matrices as

$$H = a\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}.$$

The eigenvalues and corresponding eigenkets are obtained from $(H - \lambda I)X = 0$ where $X = \begin{pmatrix}x_1\\x_2\end{pmatrix}$ are eigenvectors and λ are corresponding eigenvalues determined from secular equation $\det(H - \lambda I) = 0$. This leads to $\lambda = \pm\sqrt{2}a$ and $x_2 = (\pm\sqrt{2} - 1)x_1$, hence $X = x_1\begin{pmatrix}1\\ \pm\sqrt{2} - 1\end{pmatrix}$ and by normalization of X we have $x_1 = \dfrac{1}{\sqrt{2(2\mp\sqrt{2})}}$. Thus eigenvectors and eigenvalues are

$$|\psi_1\rangle = \frac{|1\rangle + (\sqrt{2} - 1)|2\rangle}{\sqrt{2(2 - \sqrt{2})}}, \quad \lambda = \sqrt{2}a$$

$$|\psi_2\rangle = \frac{|1\rangle - (\sqrt{2} + 1)|2\rangle}{\sqrt{2(2 + \sqrt{2})}}, \quad \lambda = -\sqrt{2}a$$

11. Rewrite H as $H = \frac{1}{2}(H_{11} + H_{22})(|1\rangle\langle 1| + |2\rangle\langle 2|) + \frac{1}{2}(H_{11} - H_{22})(|1\rangle \times \langle 1| - |2\rangle\langle 2|) + H_{12}(|1\rangle\langle 2| + |2\rangle\langle 1|)$, where the three operator terms on r.h.s. behave like I, S_z, and S_x respectively. Note that $\frac{1}{2}(H_{11} + H_{22})$ is simply the "center of gravity" of the two levels. Because the identity operator I remains the same under any change of basis, we ignore the $\frac{1}{2}(H_{11} + H_{22})$ term for the moment. Compare now with the spin $\frac{1}{2}$ problem [problem 9 above]. $\vec{S}.\hat{n} = \frac{\hbar}{2} n_x(|+\rangle\langle -| + |-\rangle\langle +|) + \frac{\hbar}{2} n_y(-i|+\rangle \times \langle -| + i|-\rangle\langle +|) + \frac{\hbar}{2} n_z(|+\rangle\langle +| - |-\rangle\langle -|)$. The analogy is: $(\hbar/2)n_x \to H_{12}$,

$\frac{\hbar}{2}n_y \to 0$ ($\alpha=0$), $\frac{\hbar}{2}n_z \to \frac{1}{2}(H_{11}-H_{22})$. So one of the energy eigenkets is $\cos(\beta/2)|1\rangle + \sin(\beta/2)|2\rangle$ where β, analogous to $\tan^{-1}(n_x/n_z)$, is given by $\beta = \tan^{-1}\left[\frac{2H_{12}}{(H_{11}-H_{22})}\right]$.

The other energy eigenket can be written down by the orthogonality requirement (or by letting $\beta \to \beta+\pi$) as $-\sin(\beta/2)|1\rangle + \cos(\beta/2)|2\rangle$. The energy eigenvalues can be obtained by diagonalizing

$$\begin{pmatrix} \frac{1}{2}(H_{11}-H_{22}) & H_{12} \\ H_{12} & -\frac{1}{2}(H_{11}-H_{22}) \end{pmatrix}.$$

But they can also be obtained by comparing with the spin $\frac{1}{2}$ problem:

$$\left(\frac{\hbar}{2}n_x\right)^2 + \left(\frac{\hbar}{2}n_z\right)^2 = \hbar^2/4 \to \text{eigenvalue } \hbar/2,$$

so by analogy the eigenvalue in our case is $[\frac{1}{4}(H_{11}-H_{22})^2 + H_{12}^2]^{\frac{1}{2}}$. We must still add to this the center of gravity energy. The final answer is

$$\tfrac{1}{2}(H_{11}+H_{22}) \pm [\tfrac{1}{4}(H_{11}-H_{22})^2 + H_{12}^2]^{\frac{1}{2}}$$

where $\pm$ is the analogue of parallel (anti-parallel) spin direction to $\hat{n}$. For $H_{12} = 0$, we get $\beta = 0$ or π. The eigenvalues are $\frac{1}{2}(H_{11}+H_{22}) \pm \frac{1}{2}(H_{11}-H_{22}) = \left\{\begin{matrix} H_{11} \\ H_{22} \end{matrix}\right.$, a very reasonable result.

12. Here $\vec{S}\cdot\hat{n}|\hat{n};+\rangle = \frac{\hbar}{2}|\hat{n};+\rangle$ and $|\hat{n};+\rangle = \cos(\gamma/2)|+\rangle + \sin(\gamma/2)|-\rangle = \begin{pmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \end{pmatrix}$. It is easily seen that the eigenket of S_x belonging to eigenvalue $+\hbar/2$, is $\frac{1}{2^{\frac{1}{2}}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. Thus (a) probability of getting $+\hbar/2$ when S_x is measured is $\left|\frac{1}{2^{\frac{1}{2}}}(1,1)\begin{pmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \end{pmatrix}\right|^2 = \frac{1+\sin\gamma}{2}$. (b) $\langle S_x\rangle = \frac{\hbar}{2}(\cos\frac{\gamma}{2}, \sin\frac{\gamma}{2})\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \end{pmatrix} = \frac{\hbar}{2}\sin\gamma$. Hence $\langle(S_x-\langle S_x\rangle)^2\rangle = \langle S_x^2\rangle - \langle S_x\rangle^2 = \hbar^2/4 - (\hbar^2/4)\sin^2\gamma = (\hbar^2/4)\cos^2\gamma$. Answers are entirely reasonable for $\gamma = 0,\pi$ (parallel and anti-parallel to OZ), and for $\gamma = \pi/2$ (along OX).

13. Choosing the S_z diagonal basis, the first measurement corresponds to the operator $M(+) = |+\rangle\langle+|$. The second measurement is expressed by the operator $M(+;\hat{n}) = |+;\hat{n}\rangle\langle+;\hat{n}|$ where $|+;\hat{n}\rangle = \cos(\beta/2)|+\rangle + \sin(\beta/2)|-\rangle$ with $\alpha = 0$. Therefore

$$M(+;\hat{n}) = (\cos\tfrac{\beta}{2}|+\rangle + \sin\tfrac{\beta}{2}|-\rangle)(\cos\tfrac{\beta}{2}\langle+| + \sin\tfrac{\beta}{2}\langle-|)$$

$$= \cos^2(\beta/2)|+\rangle\langle+| + \cos\tfrac{\beta}{2}\sin\tfrac{\beta}{2}(|+\rangle\langle-| + |-\rangle\langle+|) + \sin^2(\beta/2)|-\rangle\langle-| .$$

The final measurement corresponds to the operator $M(-) = |-\rangle\langle-|$, and the total measurement $M_T = M(-)M(+;\hat{n})M(+) = |-\rangle\langle-|\{\cos^2(\beta/2)|+\rangle\langle+| + \cos\frac{\beta}{2}\sin\frac{\beta}{2}(|+\rangle\langle-| + |-\rangle\langle+|) + \sin^2(\beta/2)|-\rangle\langle-|\}|+\rangle\langle+| = \cos\frac{\beta}{2}\sin\frac{\beta}{2}|-\rangle\langle+|$. The intensity of the final $S_z = -\hbar/2$ beam, when the $S_z = \hbar/2$ beam surviving the first measurement is normalized to unity, is thus $\cos^2(\beta/2)\sin^2(\beta/2) = (\sin^2\beta)/4$. To maximize $S_z = -\hbar/2$ final beam, set $\beta = \pi/2$, i.e. along OX, and intensity is $\frac{1}{4}$.

14. (a) The eigenvalues and eigenvectors of 3×3 matrix representation

$$A = (1/\sqrt{2})\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

can be obtained by solving $\det[A - \lambda I] = 0$ and normalized eigenvectors $x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ where $[A-\lambda I]x = 0$ and $x_1^2+x_2^2+x_3^2 = 1$. The eigenvalues are +1, 0, -1 and the

and the corresponding eigenvectors are respectively

$$\tfrac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \quad (1/\sqrt{2})\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \ \tfrac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}.$$

There is no degeneracy. (b) These are the eigenvalues and eigenvectors of $J_x = \hbar A$ for a spin 1 particle.

15. Yes! Proof uses completeness and orthonormality of $\{|a',b'\rangle\}$, hence

$$[A,B] = \sum_{a',b'}\sum_{a'',b''}|a'',b''\rangle\langle a'',b''|(AB-BA)|a',b'\rangle\langle a',b'|;$$

but $(AB-BA)|a',b'\rangle = (a'b'-b'a')|a',b'\rangle = 0$, hence $[A,B] = 0$. An alternative a ,b' a',b'' ,u possible because

$\{|a',b'\rangle\}$ form a complete orthonormal set. Then $[A,B]|\alpha\rangle = 0$ because $[A,B]|a',b'\rangle = 0$, but since $|\alpha\rangle$ is arbitrary, $[A,B] = 0$ must hold as an <u>operator</u> equation.

16. $\{A,B\} = AB+BA = 0$. This implies that $\langle a''|\{A,B\}|a'\rangle = \langle a''|AB|a'\rangle + \langle a''|BA|a'\rangle = (a''+a')\langle a''|B|a'\rangle = 0$. In general $a''+a' \neq 0$, so $\langle a''|B|a'\rangle$ must vanish for $a'' = a'$ as well as $a'' \neq a'$, hence it is not possible to have a simultaneous eigenket of A and B. The "trivial" case is when $a''+a' = 0$, then $\langle a''|B|a'\rangle \neq 0$ necessarily, and simultaneous eigenket of A and B would appear to be possible. But note $A|a',b'\rangle = a'|a',b'\rangle$, $B|a',b'\rangle = b'|a',b'\rangle \rightarrow (AB+BA)|a',b'\rangle = (a'b' + b'a')|a',b'\rangle = 0$. Hence $a' = 0$, or $b' = 0$, or $a' = b' = 0$. Thus nontrivial simultaneous eigenkets are possible but at the cost that the eigenvalues of one or the other (or both) of operators A and B are zero.

17. No degeneracy implies $|n\rangle$ defined by $H|n\rangle = E_n|n\rangle$ is <u>unique</u>, i.e. only one energy eigenstate when E_n is given. Now $[A_1,H] = 0 \rightarrow [A_1, H]|n\rangle = 0$ or $H(A_1|n\rangle) = E_n(A_1|n\rangle)$, i.e. $A_1|n\rangle$ is an energy eigenket with eigenvalue E_n. The non-degeneracy assumption then implies $A_1|n\rangle$ is proportional to $|n\rangle$, viz. $A_1|n\rangle = a_1|n\rangle$ and likewise $A_2|n\rangle = a_2|n\rangle$. But we are given that $[A_1,A_2] \neq 0$, hence $A_1A_2|n\rangle \neq A_2A_1|n\rangle$ or $a_1a_2|n\rangle \neq a_2a_1|n\rangle$, and this is clearly impossible, hence energy eigenstates are, in general, degenerate. Note however this proof fails if $A_1|n\rangle = 0$ (or $A_2|n\rangle = 0$). For $H = \vec{p}^{\,2}/2m + V(r)$, L_x and L_z both commute with H and $[L_x,L_z] \neq 0$, so energy eigenstates are usually degenerate ($2\ell+1$ fold degeneracy). The exception is for S-state ($\ell=0$, $m_\ell = 0$) where $L_z|n,\ell=0,m_\ell=0\rangle = 0$, hence there need not be degeneracy in this case.

18. (a) This is solved in (1.4.56) and (1.4.57) of text. Basically we set $\lambda = -\langle\beta|\alpha\rangle/\langle\beta|\beta\rangle$ in $(\langle\alpha| + \lambda^*\langle\beta|)\cdot(|\alpha\rangle + \lambda|\beta\rangle) \geqslant 0$, and obtain Schwarz inequality

$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$.

(b) The generalized uncertainty relation (1.4.59) is $\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle\Delta A\Delta B\rangle|^2$ where according to (1.4.63) $|\langle\Delta A\Delta B\rangle|^2 = \frac{1}{4}|\langle [A,B]\rangle|^2 + \frac{1}{4}|\langle\{\Delta A,\Delta B\}\rangle|^2$. From (1.4.50) we know that $\Delta A = A - \langle A\rangle$ and $\Delta B = B - \langle B\rangle$ and $\Delta A|\alpha\rangle = \lambda\Delta B|\alpha\rangle$ as given. An elementary calculation leads to $[A,B] = [\Delta A,\Delta B]$, hence $\langle\alpha|[A,B]|\alpha\rangle = \langle\alpha| \times [\Delta A,\Delta B]|\alpha\rangle = \lambda^*\langle\alpha|\Delta B\Delta B|\alpha\rangle - \lambda\langle\alpha|\Delta B\Delta B|\alpha\rangle$. Choose next λ to be purely imaginary; $\langle\alpha|[A,B]|\alpha\rangle = -2\lambda\langle\alpha|(\Delta B)^2|\alpha\rangle$ while $\frac{1}{4}|\langle\alpha|[A,B]|\alpha\rangle|^2 = |\lambda|^2|\langle\alpha|(\Delta B)^2|\alpha\rangle|^2$. It is also evident that for λ imaginary $\langle\alpha|\{\Delta A,\Delta B\}|\alpha\rangle = 0$, therefore from (1.4.63) and the recognition that $\langle\alpha|(\Delta A)^2|\alpha\rangle\langle\alpha|(\Delta B)^2|\alpha\rangle = |\lambda|^2|\langle\alpha|(\Delta B)^2|\alpha\rangle|^2$, we have equality in the generalized uncertainty relation (1.4.59).

(c) Since $\Delta x = x - \langle x\rangle$, we may express $\langle x'|\Delta x|\alpha\rangle$ as $\int dx''\langle x'|x''\rangle\langle x''|\Delta x|\alpha\rangle = \int dx''\delta(x'-x'')x''\langle x''|\alpha\rangle - \int dx''\delta(x'-x'')\langle x\rangle\langle x''|\alpha\rangle$ where normalization $\langle x'|x''\rangle = \delta(x'-x'')$ is chosen. For $\Delta p = p - \langle p\rangle$ where $p = -i\hbar\frac{\partial}{\partial x}$, we have $\langle x'|\Delta p|\alpha\rangle = \int dx''\langle x'|x''\rangle\langle x''|\Delta p|\alpha\rangle$ and $\langle x''|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x''}\langle x''|\alpha\rangle$. Hence $\langle x'|\Delta p|\alpha\rangle = \int dx''\delta(x'-x'') \times (-i\hbar)\frac{\partial}{\partial x''}\langle x''|\alpha\rangle - \langle p\rangle\int dx''\delta(x'-x'')\langle x''|\alpha\rangle$. Use next explicit expression for $\langle x''|\alpha\rangle = (2\pi d^2)^{-1/4}\exp[\frac{i\langle p\rangle x''}{\hbar} - \frac{(x''-\langle x\rangle)^2}{4d^2}]$ in above integral forms for $\langle x'|\Delta x|\alpha\rangle$ and $\langle x'|\Delta p|\alpha\rangle$. We find

$$\langle x'|\Delta x|\alpha\rangle = \Lambda\langle x'|\Delta p|\alpha\rangle$$

where $\Lambda = -2id^2/\hbar$ an imaginary number.

9. (a) It is clear that $\langle\alpha|S_x|\alpha\rangle = \sum_{a''}\sum_{a'}\langle\alpha|a''\rangle\langle a''|S_x|a'\rangle\langle a'|\alpha\rangle = \sum_{a'}|\langle\alpha|a'\rangle|^2\langle a'|S_x|a'\rangle$ where $\{|a'\rangle\}$ is a complete set of base kets. Since $S_x = \frac{\hbar}{2}(|+\rangle\langle-|+|-\rangle\langle+|)$, evidently $S_x^2 = \frac{\hbar^2}{4}(|+\rangle\langle+|+|-\rangle\langle-|)$. Take $|\alpha\rangle = |+\rangle$ then $\langle+|S_x^2|+\rangle = \hbar^2/4$ and $\langle+|S_x|+\rangle = 0$. Therefore

$$\langle+|(\Delta S_x)^2|+\rangle = \langle+|S_x^2|+\rangle - \langle+|S_x|+\rangle^2 = \hbar^2/4.$$

Also from $S_y = \frac{i\hbar}{2}(-|+\rangle\langle-|+|-\rangle\langle+|)$, we have $S_y^2 = \frac{\hbar^2}{4}(|+\rangle\langle+|+|-\rangle\langle-|)$, hence it can be readily shown that $\langle+|S_y^2|+\rangle = \hbar^2/4$ and $\langle+|S_y|+\rangle = 0$. Therefore $\langle+|(\Delta S_y)^2|+\rangle$

x ... y ... $\hbar^2/16$. But $[S_x,S_y] = i\hbar S_z$ and thus $\langle+| \times$ $[S_x,S_y]|+\rangle = i\hbar\langle+|S_z|+\rangle = i\hbar^2/2$. The generalized uncertainty relation is therefore verified for the equality case.

(b) From $|\hat{n};+\rangle = \cos\frac{\beta}{2}|+\rangle + e^{i\alpha}\sin\frac{\beta}{2}|-\rangle$ it follows for $\beta = \pi/2$ and $\alpha = 0$ we have $|S_x;+\rangle = \frac{1}{2}^{\frac{1}{2}}(|+\rangle + |-\rangle)$. Simple calculations lead to $\langle S_x;+|S_x|S_x;+\rangle = \hbar/2$ and $\langle S_x;+|S_x^2|S_x;+\rangle = \hbar^2/4$, therefore $\langle S_x;+|(\Delta S_x)^2|S_x;+\rangle = 0$. Again $[S_x,S_y] = i\hbar S_z$, hence $\langle S_x;+|S_z|S_x;+\rangle = 0$ and $\langle S_x;+|(\Delta S_x)^2|S_x;+\rangle\langle S_x;+|(\Delta S_y)^2|S_x;+\rangle = \frac{1}{4}|\langle S_x;+| \times$ $[S_x,S_y]|S_x;+\rangle|^2$, both sides of generalized uncertainty relation being zero.

[Note explicit $\langle S_x;+|S_z|S_x;+\rangle = \frac{1}{2}^{\frac{1}{2}}(\langle+|+\langle-|)[\frac{\hbar}{2}(|+\rangle\langle+|-|-\rangle\langle-|)]\frac{1}{2}^{\frac{1}{2}}(|+\rangle+|-\rangle) = 0$ if we use systematically orthonormality conditions $\langle\pm|\pm\rangle = 1$, $\langle\pm|\mp\rangle = 0$.]

20. Take the normalized linear combination $|\ \rangle = \alpha|+\rangle + (1-\alpha^2)^{\frac{1}{2}}e^{i\beta}|-\rangle$, where α is rea and $|\alpha| \leq 1$. Than elementary calculations yield $\langle\ |(\Delta S_x)^2|\ \rangle = \frac{\hbar^2}{4}[1-4\alpha^2(1-\alpha^2)\times \cos^2\beta]$ and $\langle\ |(\Delta S_y)^2|\ \rangle = \frac{\hbar^2}{4}(1-4\alpha^2(1-\alpha^2)\sin^2\beta)$. The product

$$\langle\ |(\Delta S_x)^2|\ \rangle\langle\ |(\Delta S_y)^2|\ \rangle = \frac{\hbar^4}{16}\{1-4\alpha^2(1-\alpha^2)+4\alpha^4(1-\alpha^2)^2\sin^2 2\beta\}.$$

Maximum for $\sin^2 2\beta$ is when $\beta = \pi/4$, and r.h.s. becomes $\frac{\hbar^4}{16}[1-2\alpha^2(1-\alpha^2)]^2$. It is clear that $\alpha^2 = \frac{1}{2}$ is a minimum, and the maximum value $\hbar^4/16$ is reached when $\alpha^2 =$ 0, or $\alpha^2=1$. Hence the linear 'combination' that maximizes uncertainty product is $e^{i\pi/4}|-\rangle$ or $\pm|+\rangle$. That $\pm|+\rangle$ does not violate uncertainty relation has been proved in Problem 19(a) above. For the $e^{i\pi/4}|-\rangle$ case, we note that the phase f. tor $e^{i\pi/4}$ cancels out in the scalar product, and $\langle-|S_x|-\rangle = \langle-|S_y|-\rangle = 0$ while $\langle-|S_x^2|-\rangle = \langle-|S_y^2|-\rangle = \hbar^2/4$. Again $\langle-|[S_x,S_y]|-\rangle = \langle-|i\hbar S_z|-\rangle = i\hbar(-\hbar/2) = -i\hbar^2$ Hence explicitly we have $\langle-|(\Delta S_x)^2|-\rangle\langle-|(\Delta S_y)^2|-\rangle = \hbar^4/16 = \frac{1}{4}|\langle-|[S_x,S_y]|-\rangle|^2$, again no violation.

21. This is the rigid wall potential ("one-dimensional box"), c.f. (A.2.3) and (A.2.4) of Appendix A. The wave functions and energy eigenstates are $\psi_E(x) = \sqrt{2/a}\,\sin(n\pi x/a)$, n=1,2,3,...., and $E = \hbar^2 n^2\pi^2/2ma^2$, n=1 is ground state n>1 are the excited states. Next note that

$$\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2,\quad \langle(\Delta p)^2\rangle = \langle p^2\rangle - \langle p\rangle^2$$

where $p = \frac{\hbar\partial}{i\partial x}$ and $p^2 = -\hbar^2\partial^2/\partial x^2$. For rigid wall potential, we have

$$\langle x^2\rangle = \frac{2}{a}\int_0^a x^2\sin^2(n\pi x/a)\,dx = 2a^2\left[\frac{1}{6} - \frac{1}{4n^2\pi^2}\right] = a^2[1/3 - 1/2n^2\pi^2]$$

$$\langle x\rangle = \frac{2}{a}\int_0^a x\sin^2(n\pi x/a)\,dx = a/2$$

$$\langle p^2\rangle = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)(-\hbar^2\partial^2/\partial x^2)\sin\left(\frac{n\pi x}{a}\right)dx = \frac{\hbar^2}{a^2}(n\pi)^2$$

$$\langle p\rangle = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\left(\frac{\hbar\partial}{i\partial x}\right)\sin\left(\frac{n\pi x}{a}\right)dx = 0\ .$$

Therefore the uncertainty product $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{a^2}{2}[1/6 - 1/n^2\pi^2]\frac{\hbar^2}{a^2}(n\pi)^2 = \frac{\hbar^2}{2}[(n\pi)^2/6 - 1]$; for ground state n=1, for excited states n>1.

22. Assume that the ice pick is equivalent to a mass point m attached to a light rod of length L the other end of which is balanced on a fixed hard surface. For small angle θ departure of pick from vertical, the torque equation is $mL^2d^2\theta/dt^2 = mg\theta L$, and solution $\theta(t) = ae^{\sqrt{g/L}\,t} + be^{-\sqrt{g/L}\,t}$. The uncertainty relation at t=0 with $\Delta x \cong L\theta = (a+b)L$, $\Delta p \cong Lm d\theta/dt = \sqrt{g/L}(a-b)Lm = m\sqrt{gL}(a-b)$ is $\Delta x\Delta p = \hbar/2$ (best we can do and realized for Gaussian packet). Now $\Delta x\Delta p = \hbar/2$ implies $a^2 = b^2 + \hbar/(2m[gL^3]^{1/2})$. The displacement at later time t is minimized by making a and b as small as possible. So set $a = \pm\sqrt{\hbar/(2m[gL^3]^{1/2})}$, b = 0 (actually irrelevant for $t >> \sqrt{L/g}$). Displacement becomes noticeable when θ becomes as large as $\theta_f = \pi/100 \cong 2^o$. We have $\theta_f = ae^{\sqrt{g/L}\,t_f}$ and taking for definiteness $a = +\sqrt{\hbar/(2m[gL^3]^{1/2})}$, $t_f = \sqrt{L/g}[\ \ln\theta_f + \frac{1}{2}\ln(\frac{2m[gL^3]^{1/2}}{\hbar})]$. Use L = 10 cm, m = 100 gm, and g = 980 cm/sec^2, we have t_f = 3.4 sec. Actually this number is very insensitive

to m and θ_f. For any reasonable value, we get $t_f \sim 3$ sec.

23. (a) The characteristic equation $\det[B-\lambda I] = 0$, leads to $(\lambda-b)^2(\lambda+b) = 0$. Hence $\lambda = \pm b$ and $\lambda=b$ is a two-fold degenerate eigenvalue.

(b) Straightforward matrix multiplication gives

$$AB = \begin{pmatrix} ab & 0 & 0 \\ 0 & 0 & iab \\ 0 & -iab & 0 \end{pmatrix} = BA, \text{ hence } [A,B] = 0$$

(c) The eigenvectors (eigenkets) of B, together with $[A,B] = 0$, yield simultaneous eigenvectors of A and B. Let λ_i be eigenvalues of B, and corresponding eigenvectors are

$$u^i = \begin{pmatrix} u^i_1 \\ u^i_2 \\ u^i_3 \end{pmatrix}, \text{ where } Bu^i = \lambda_i u^i, \ i=1,2,3.$$

For $\lambda_1=b$, we have $bu^1_1 = bu^1_1$, $ibu^1_2 = bu^1_3$, and $iu^1_2 = u^1_3$. Choose $u^1_1 = 1$, $u^1_2 = u^1_3 = 0$ than

$$u^1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle.$$

For the degenerate $\lambda_2=b$, we have $bu^2_1 = bu^2_1$ and $iu^2_2 = u^2_3$. But u^2 must be orthogonal to u^1, hence $u^2_1 = 0$. Therefore we choose $u^2_1 = 0$, $u^2_2 = 1$, $u^2_3 = i$, and the normalized

$$u^2 = \frac{1}{2^{1/2}}\begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix} = \frac{1}{2^{1/2}}(|2\rangle + i|3\rangle), \text{ where } |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

For nondegenerate $\lambda_3 = -b$, again u^3 must be orthogonal to u^1 and u^2, therefore $u^3_1 = 0$ and relation $iu^3_2 = -u^3_3$ can be satisfied by choosing $u^3_2 = 1$, $u^3_3 = -i$. Together with normalization we have

$$u^3 = \frac{1}{2^{1/2}}\begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix} = \frac{1}{2^{1/2}}(|2\rangle - i|3\rangle).$$

In this new set $u^i (i=1,2,3)$, evidently $Au^1=au^1$, $Au^2 = -au^2$, $Au^3 = -au^3$, and there is two fold-degeneracy w.r.t. eigenvalue $-a$ of operator A.

24. (a) The rotation matrix [c.f. (3.2.44)] acting on a two-component spinor can be written as $\exp[-i\vec{\sigma}\cdot\hat{n}\theta/2] = \underline{1}\cos\frac{\theta}{2} - i\vec{\sigma}\cdot\hat{n}\sin\frac{\theta}{2}$. For clockwise rotation about x-axis through $-\pi/2$, we have $\theta = -\pi/2$, hence $\exp[-i\vec{\sigma}\cdot\hat{n}\theta/2] = \frac{1}{2^{1/2}}(1+i\sigma_x)$.

(b) If we transform from base kets in S_z representation to eigenkets of S_y as base kets, i.e. rotate by angle $-\pi/2$ about x-axis, S_z is transformed into

$$\frac{\hbar}{2}(1/\sqrt{2})(1-i\sigma_x)\sigma_z(1/\sqrt{2})(1+i\sigma_x) = -\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

[This can be seen by noting that if $\{|c\rangle\}$ is S_y basis while $\{|b\rangle\}$ is S_z basis, than transformation is

$$\langle c''|S_z|c'\rangle = \sum_{b',b''}\langle c''|b'\rangle\langle b'|S_z|b''\rangle\langle b''|c'\rangle.]$$

25. Given $\langle b'|A|b''\rangle$ is real. Take another basis $\{|c\rangle\}$, then $|c'\rangle = \sum_{b'}|b'\rangle\langle b'|c'\rangle$, hence $\langle c'|A|c''\rangle = (\sum_{b'}\langle c'|b'\rangle\langle b'|)A(\sum_{b''}\langle b''|c''\rangle|b''\rangle) = \sum_{b',b''}\langle c'|b'\rangle\langle b''|c''\rangle \times \langle b'|A|b''\rangle$. It is not necessary that $\langle c'|b'\rangle$ and $\langle b''|c''\rangle$ be real. Take the S_y and S_z cases of problem 24 above. Here $|b'\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |+\rangle$ while $|b''\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |-\rangle$ for S_z and $|c'\rangle = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} = |S_y;+\rangle$ while for S_y $|c''\rangle = \begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix} = |S_y;-\rangle$. Hence $\langle c'|b'\rangle = 1/\sqrt{2} = \langle c''|b'\rangle$, but $\langle c''|b''\rangle = i/\sqrt{2} = -\langle c'|b''\rangle$ are imaginary.

26. From problems 9 and 19, we have $|S_x;+\rangle = \frac{1}{2^{1/2}}(|+\rangle+|-\rangle)$, i.e. $\alpha = 0$, $\beta = \pi/2$ in $|\vec{S}\cdot\hat{n};+\rangle$. Now $|S_x;-\rangle$ corresponds to axis of quantization in the $-x$ direction, i.e. $\alpha=\pi, \beta = \pi/2$, hence $|S_x;-\rangle = \frac{1}{2^{1/2}}(|+\rangle-|-\rangle)$. Let $U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}$ be the transformation matrix between S_z diagonal basis and S_x diagonal basis, i.e.

$$\begin{pmatrix} |S_x;+\rangle \\ |S_x;-\rangle \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} |+\rangle \\ |-\rangle \end{pmatrix} = U|r\rangle$$

than evidently $U_{11} = U_{12} = 1/\sqrt{2}$ while $U_{21} = 1/\sqrt{2}$ and $U_{22} = -1/\sqrt{2}$. Take $|S_x;+\rangle$

$= U_{11}|+\rangle + U_{12}|-\rangle = \sum_a \langle a|S_x;+\rangle|a\rangle$ while $|S_x;-\rangle = U_{21}|+\rangle + U_{22}|-\rangle = \sum_b \langle b|S_x;-\rangle|b\rangle$ with a,b = +,−. Take the general form $U = \sum_r |b^{(r)}\rangle\langle a^{(r)}|$, than $U|r\rangle = \sum_r |b^{(r)}\rangle \times \langle a^{(r)}|r\rangle$. Identify $|a\rangle$ or $|b\rangle$ with $|b^{(r)}\rangle$ and $\langle a^{(r)}|r\rangle$ with $\langle a|S_x;+\rangle$ or $\langle b|S_x;-\rangle$, we see that U can indeed be expressed as $U = \sum_r |b^{(r)}\rangle\langle a^{(r)}|$.

27. (a) Matrix element $\langle b''|f(A)|b'\rangle = \sum_{a'} \langle b''|f(A)|a'\rangle\langle a'|b'\rangle = \sum_{a'} f(a')\langle b''|a'\rangle\langle a'|b'\rangle$ where $\langle a'|b'\rangle$ (likewise $\langle b''|a'\rangle$) is an element of the transformation matrix from the a' basis to the b' basis. (b) The matrix element $\langle \vec{p}''|F(\vec{r})|\vec{p}'\rangle = \int d\vec{r}' F(\vec{r}') \times \langle \vec{p}''|\vec{r}'\rangle\langle \vec{r}'|\vec{p}'\rangle$. Note that $\langle \vec{r}'|\vec{p}'\rangle = [1/(2\pi\hbar)^{3/2}]e^{i\vec{p}\cdot\vec{r}'/\hbar}$, this implies that

$$\langle \vec{p}''|F(\vec{r})|\vec{p}'\rangle = [1/(2\pi\hbar)^3]\int d\vec{r}' F(\vec{r}')e^{i(\vec{p}'-\vec{p}'')\cdot\vec{r}'/\hbar}.$$

Suppose $F(\vec{r})$ is spherically symmetric $= F(r)$, than (choosing z-axis along $\vec{p}'-\vec{p}''$)

$$\langle \vec{p}''|F(r)|\vec{p}'\rangle = \frac{2\pi}{(2\pi\hbar)^3}\int_{-1}^{+1} d(\cos\theta)\int_0^\infty r'^2 dr' F(r')e^{iqr'\cos\theta/\hbar}$$

where $q = |\vec{p}'-\vec{p}''|$. Integrate out the $\cos\theta$ integration on r.h.s. we have

$$\langle \vec{p}''|F(r)|\vec{p}'\rangle = \frac{1}{2\pi^2\hbar^2 q}\int_0^\infty r'\sin(qr'/\hbar)F(r')\,dr'$$

28. (a) $[x,F(p_x)]_{cl} = \frac{\partial x}{\partial x}\frac{\partial F}{\partial p_x} - \frac{\partial x}{\partial p_x}\frac{\partial F}{\partial x}$, but $\partial x/\partial p_x = 0$, hence $[x,F(p_x)]_{cl} = \partial F/\partial p_x$.

(b) Now $[x,F(p_x)]_{QM} = i\hbar[x,F(p_x)]_{cl}$, hence

$$[x,\exp(ip_x a/\hbar)]_{QM} = i\hbar\frac{\partial}{\partial p_x}\exp(ip_x a/\hbar) = -a\exp(ip_x a/\hbar).$$

(c) Using (b) we have

$$[x,\exp(ip_x a/\hbar)]|x'\rangle = -a\exp(ip_x a/\hbar)|x'\rangle.$$

Hence $x\exp(ip_x a/\hbar)|x'\rangle - \exp(ip_x a/\hbar)x|x'\rangle = -a\exp(ip_x a/\hbar)|x'\rangle$, and thence $x[\exp(ip_x a/\hbar)|x'\rangle] = (x'-a)[\exp(ip_x a/\hbar)|x'\rangle]$. This eigenvalue equation implies that $\exp(ip_x a/\hbar)|x'\rangle$ is an eigenstate of coordinate operator x, with corresponding eigenvalue $(x'-a)$.

29. (a) We assume that $G(\vec{p})$ and $F(\vec{x})$ can be expressed as a power series

$$G(\vec{p}) = \sum_{n,m,\ell} a_{nm\ell}\,p_i^n p_j^m p_k^\ell\ ,\quad F(\vec{x}) = \sum_{n,m,\ell} b_{nm\ell}\,x_i^n x_j^m x_k^\ell.$$

An elementary calculation yields $[x_i, p_i^n p_j^m p_k^\ell] = ni\hbar p_i^{n-1} p_j^m p_k^\ell$ (use $[x_i, ABC] = [x_i,A]BC + A[x_i,B]C + (AB)[x_i,C]$) and $[p_i, x_i^n x_j^m x_k^\ell] = -ni\hbar x_i^{n-1} x_j^m x_k^\ell$, where the relationships $[x_i,p_i^n] = ni\hbar p_i^{n-1}$ and $[p_i,x_i^n] = -ni\hbar x_i^{n-1}$ can be easily proved by mathematical induction. Using the series form for $G(\vec{p})$ and $F(\vec{x})$ we get at once $[x_i,G(\vec{p})] = i\hbar\partial G/\partial p_i$ and $[p_i,F(\vec{x})] = -i\hbar\partial F/\partial x_i$.

(b) $[x^2,p^2] = [x^2,pp] = [x^2,p]p + p[x^2,p]$, but from (a) $[p,x^2] = -2i\hbar x$, so $[x^2,p^2] = 2i\hbar xp + 2i\hbar px = 2i\hbar\{x,p\}$. The classical P.B. for $[x^2,p^2]$ is evaluated via $[x^2,p^2]_{cl} = \frac{\partial x^2}{\partial x}\frac{\partial p^2}{\partial p} - \frac{\partial x^2}{\partial p}\frac{\partial p^2}{\partial x} = 2x(2p) = 4xp$. Since in the classical limit $\{x,p\} = 2xp$, we have $[x^2,p^2]_{QM} = i\hbar[x^2,p^2]_{cl}$.

30. (a) $[x_i,T(\vec{\ell})] = i\hbar\partial T(\vec{\ell})/\partial p_i = i\hbar\frac{\partial}{\partial p_i}\exp(-i\vec{p}.\vec{\ell}/\hbar) = i\hbar(-i\ell_i/\hbar)\exp(-i\vec{p}.\vec{\ell}/\hbar) = \ell_i T(\vec{\ell})$. (b) Noting that $\langle x_i\rangle = \langle\alpha|x_i|\alpha\rangle$ where $|\alpha\rangle$ is a general state ket, take expression $\langle\alpha|T^\dagger(\vec{\ell})[x_i,T(\vec{\ell})]|\alpha\rangle = \langle\alpha|T^\dagger(\vec{\ell})\ell_i T(\vec{\ell})|\alpha\rangle = \ell_i$. But we note that $\langle\alpha|T^\dagger(\vec{\ell})[x_i,T(\vec{\ell})]|\alpha\rangle = \langle\alpha|T^\dagger x_i T|\alpha\rangle - \langle\alpha|T^\dagger T x_i|\alpha\rangle$, hence

$$\langle x_i\rangle_{translated} = \langle x_i\rangle + \ell_i, \text{ and therefore } \langle\vec{x}\rangle_{translated} = \langle\vec{x}\rangle + \vec{\ell}\,.$$

31. Given $[\vec{x},T(d\vec{x}')] = d\vec{x}'$ or $\vec{x}T(d\vec{x}') = d\vec{x}' + T(d\vec{x}')\vec{x}$ and $[\vec{p},T(d\vec{x}')] = 0$ or $\vec{p}T(d\vec{x}') = T(d\vec{x}')\vec{p}$, we study $\langle\alpha|T^\dagger(d\vec{x}')\vec{x}T(d\vec{x}')|\alpha\rangle$ substituting as we did in problem 30. We find $\langle\vec{x}\rangle_{translated} = \langle\alpha|T^\dagger(d\vec{x}')(d\vec{x}' + T(d\vec{x}')\vec{x})|\alpha\rangle$. Now $T^\dagger(d\vec{x}') = 1 + i\vec{K}.d\vec{x}'$, hence $T^\dagger(d\vec{x}')d\vec{x}' = d\vec{x}'$ to first order in small quantity $d\vec{x}'$. Hence $\langle\vec{x}\rangle_{translated} = d\vec{x}' + \langle\vec{x}\rangle$. Using $\vec{p}T(d\vec{x}') = T(d\vec{x}')\vec{p}$, we find $\langle\vec{p}\rangle_{translated} = \langle\alpha|T^\dagger(d\vec{x}')\vec{p}T(d\vec{x}')\times|\alpha\rangle = \langle\alpha|T^\dagger(d\vec{x}')T(d\vec{x}')\vec{p}|\alpha\rangle = \langle\alpha|\vec{p}|\alpha\rangle = \langle\vec{p}\rangle$. Hence $\langle\vec{p}\rangle_{translated} = \langle\vec{p}\rangle$.

32. Use of $\langle x'|\alpha\rangle = \frac{1}{d^{1/2}\pi^{1/4}}\exp(ikx' - x'^2/2d^2)$, we find by elementary calculation

$$\frac{\partial}{\partial x'}\langle x'|\alpha\rangle = \frac{1}{d^{1/2}\pi^{1/4}}(ik - x'/d^2)\exp(ikx' - x'^2/2d^2),\quad \frac{\partial}{\partial x'}\left(\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right) = \frac{\partial^2}{\partial x'^2}(\langle x'|\alpha\rangle)$$

$$= \frac{1}{d^{1/2}\pi^{1/4}}\left[-k^2 - \frac{1}{d^2} - \frac{2ikx'}{d^2} + x'^2/d^4\right]\exp(ikx' - x'^2/2d^2).$$

(a) $\langle p\rangle = \int_{-\infty}^{+\infty}\langle\alpha|x'\rangle[-i\hbar\frac{\partial}{\partial x'}]\langle x'|\alpha\rangle dx' = \frac{-i\hbar}{d\pi^{1/2}}\int_{-\infty}^{+\infty}\exp(-x'^2/d^2)(ik-x'/d^2)dx'$.

The odd term of integrand vanishes, and $\langle p\rangle = [\hbar k/d\pi^{1/2}]\int_{-\infty}^{+\infty}\exp(-x'^2/d^2)dx' = \frac{\hbar k d\pi^{1/2}}{d\pi^{1/2}}$

$= \hbar k$. Likewise $\langle p^2\rangle = \int_{-\infty}^{+\infty}\langle\alpha|x'\rangle p^2\langle x'|\alpha\rangle dx' = \int_{-\infty}^{+\infty}\langle\alpha|x'\rangle(-\hbar^2)\frac{\partial^2}{\partial x'^2}\langle x'|\alpha\rangle dx' =$

$= -\frac{\hbar^2}{d\pi^{1/2}}\int_{-\infty}^{+\infty}\exp(-x^2/d^2)[x^2/d^4 - k^2 - 1/d^2 - 2ikx/d^2]dx = \hbar^2/2d^2 + \hbar^2k^2$, again dropping odd terms in integrand.

(b) $\langle p|\alpha\rangle = \frac{d^{1/2}}{\hbar^{1/2}\pi^{1/4}}\exp[-(p-\hbar k)^2d^2/2\hbar^2]$. The expectation value $\langle p\rangle$ using momentum space wave function is then

$$\langle p\rangle = \int_{-\infty}^{+\infty}\langle\alpha|p\rangle p\langle p|\alpha\rangle dp = \frac{d}{\hbar\pi^{1/2}}\int_{-\infty}^{+\infty}p\ \exp[-(p-\hbar k)^2d^2/\hbar^2]dp.$$

Change variable to $q = p-\hbar k$, we have $\langle p\rangle = (d/\hbar\pi^{1/2})\int_{-\infty}^{+\infty}(q+\hbar k)\exp[-q^2d^2/\hbar^2]dq$, and dropping the odd integration contribution

$$\langle p\rangle = (d/\hbar\pi^{1/2})\hbar k\ (\hbar\pi^{1/2}/d) = \hbar k.$$

Similarly

$$\langle p^2\rangle = \int_{-\infty}^{+\infty}(d/\hbar\pi^{1/2})p^2\exp[-(p-\hbar k)^2d^2/\hbar^2]dp$$

and changing variable to $q = p-\hbar k$ (hence $p^2 = q^2 + 2q\hbar k + \hbar^2k^2$), we have

$$\langle p^2\rangle = (d/\hbar\pi^{1/2})\int_{-\infty}^{+\infty}(q^2+2\hbar kq+\hbar^2k^2)\exp[-q^2d^2/\hbar^2]dq$$

$$= (d/\hbar\pi^{1/2})[\hbar^3\sqrt{\pi}/2d^3 + \hbar\sqrt{\pi}\ \hbar^2k^2/d] = \hbar^2/2d^2 + \hbar^2k^2.$$

33. (a) To prove (i) $\langle p'|x|\alpha\rangle = i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle$, let us note that

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

$$= [1/(2\pi\hbar)]\int dx'x'e^{-ix'\cdot(p'-p'')/\hbar}.$$

But $\delta(p'-p'') = [1/(2\pi\hbar)]\int dx'e^{-ix'\cdot(p'-p'')/\hbar}$, so $\frac{\partial}{\partial p'}\delta(p'-p'') = \int\frac{dx'}{(2\pi\hbar)}\frac{x'}{\hbar i}e^{-\frac{ix'\cdot(p'-p'')}{\hbar}}$,

hence $\langle p'|x|p''\rangle = i\hbar\frac{\partial}{\partial p'}\delta(p'-p'')$. Express now $\langle p'|x|\alpha\rangle = \int dp''\langle p'|x|p''\rangle\langle p''|\alpha\rangle =$ $\int dp''i\hbar\frac{\partial}{\partial p'}\delta(p'-p'')\langle p''|\alpha\rangle = i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle$.

For (ii) we perform an analogous procedure. Write

$$\langle\beta|x|\alpha\rangle = \int dp'\langle\beta|p'\rangle\langle p'|x|\alpha\rangle = \int dp'\langle\beta|p'\rangle i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle$$

$$= \int dp'\phi^*_\beta(p')i\hbar\frac{\partial}{\partial p'}\phi_\alpha(p').$$

(b) Consider momentum eigenket with eigenvalue p'. Then $p|p'\rangle = p'|p'\rangle$. Now consider the ket $|p',\Xi\rangle = \exp[ix\Xi/\hbar]|p'\rangle$. Is this a momentum eigenket and if yes what is the value? To see this let's operate with p, than

$$p|p',\Xi\rangle = p(\exp[ix\Xi/\hbar])|p'\rangle = \{\exp(ix\Xi/\hbar)p + [p, \exp(ix\Xi/\hbar)]\}|p'\rangle$$

and $[p, \exp(ix\Xi/\hbar)] = -i\hbar\partial(\exp[ix\Xi/\hbar])/\partial x = -i\hbar(i\Xi/\hbar)\exp[ix\Xi/\hbar]$. So $p|p',\Xi\rangle=$ $\exp(ix\Xi/\hbar)p'|p'\rangle + \Xi\exp(ix\Xi/\hbar)|p'\rangle = (p' + \Xi)\exp(ix\Xi/\hbar)|p'\rangle = (p' + \Xi)|p',\Xi\rangle$. Hence $|p',\Xi\rangle$ is eigenket of p with eigenvalue $p' + \Xi$ and operator $\exp(ix\Xi/\hbar)$ is momentum translation operator and x is the generator of momentum translations.

Chapter 2

1. Hamiltonian $H = \omega S_z$. The Heisenberg equations of motion are:

$$\dot{S}_x = (1/i\hbar)[S_x, H] = (\omega/i\hbar)[S_x, S_z] = -\omega S_y$$

$$\dot{S}_y = (1/i\hbar)[S_y, H] = (\omega/i\hbar)[S_y, S_z] = +\omega S_x$$

$$\dot{S}_z = 0.$$

Hence $\dot{S}_x + i\dot{S}_y = -\omega S_y + i\omega S_x = i\omega(S_x+iS_y)$ and $\dot{S}_x - i\dot{S}_y = -\omega S_y - i\omega S_x = -i\omega(S_x-iS_y)$, so $(S_x \pm iS_y)_t = (S_x \pm iS_y)_{t=o}\, e^{\pm i\omega t}$ and we have finally $S_x(t) = S_x(0)\cos\omega t - S_y(0)\sin\omega t$, $S_y(t) = S_y(0)\cos\omega t + S_x(0)\sin\omega t$, $S_z(t) = S_z(0)$.

2. The Hamiltonian is obviously not Hermitian. Physically, the particle can go from state 2 to state 1 but not from state 1 to state 2. Because H is not Hermitian the time evolution operator is not unitary. Since unitarity is important for probability conservation, we suspect that probability conservation is violated.

To illustrate this point, set $H_{11} = H_{22} = 0$ for simplicity. For the time evolution operator we get, as usual, $\mathcal{U}(t,t_o=0) = \lim_{N\to\infty} (1-itH/\hbar N)^N$ where $\mathcal{U}$ is actually not unitary. But $H^2 = H_{12}^2\, |1\rangle\langle 2|1\rangle\langle 2| = 0$, hence $H^n = 0$ for $n > 1$. This means that $\mathcal{U}(t,t_o=0) = 1 - (itH_{12}/\hbar)|1\rangle\langle 2|$ even for a finite time interval. Now the most general initial state is $c_1|1\rangle + c_2|2\rangle$. At a later time we have $[1 - (itH_{12}/\hbar)|1\rangle\langle 2|](c_1|1\rangle + c_2|2\rangle) = c_1|1\rangle + c_2|2\rangle - (itH_{12}/\hbar)c_2|1\rangle$. Hence the probability for being found in $|1\rangle$ is $|c_1-(itH_{12}/\hbar)c_2|^2$ and the probability for being found in $|2\rangle$ is $|c_2|^2$. But the total probability is $|c_1|^2 - 2\,\mathrm{Im}(c_1c_2^*)H_{12}t/\hbar + |c_2|^2H_{12}^2t^2/\hbar^2 + |c_2|^2 \neq |c_1|^2 + |c_2|^2$ in general, and in fact $\langle\alpha, t_o=0|\alpha, t_o=0\rangle \neq \langle\alpha, t_o=0; t|\alpha, t_o=0; t\rangle$, so probability conservation is violated!

3. At time $t = 0$, $\hat{n} = \sin\beta\,\hat{x} + \cos\beta\,\hat{z}$, and $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, and $\vec{S}\cdot\hat{n} = \frac{\hbar}{2}(\sin\beta\,\sigma_x + \cos\beta\,\sigma_z)$. The eigenvalue equation at $t = 0$ $\vec{S}\cdot\hat{n}|\psi\rangle = \frac{\hbar}{2}|\psi\rangle$ where $|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ leads to

$a\cos\beta + b\sin\beta = a$, and a normalized eigenstate of form

$$\frac{(1+\cos\beta)^{\frac{1}{2}}}{2^{\frac{1}{2}}}\begin{pmatrix} 1 \\ \cdots \\ \sin\beta/(1+\cos\beta) \end{pmatrix}. \qquad (1)$$

The Hamiltonian $H = -\vec{\mu}_s\cdot\vec{B} = (g_s\mu_B/2)\sigma_z B$ is that under consideration.

(a) The time dependence of $\psi(t)$ is governed by $H|\psi\rangle = i\hbar\partial/\partial t|\psi\rangle$ or

$$-i\omega\begin{pmatrix} A(t) \\ -B(t) \end{pmatrix} = \partial/\partial t\begin{pmatrix} A(t) \\ B(t) \end{pmatrix} \qquad (2)$$

where $\omega = g_s\mu_B B/2\hbar$. This leads to two equations $-i\omega A(t) = \partial/\partial t[A(t)]$ and $+i\omega B(t) = \partial/\partial t\,[B(t)]$, thus $A(t) = A(0)e^{-i\omega t}$ and $B(t) = B(0)e^{+i\omega t}$. Compare with (1) above, we have

$$\psi(t) = \begin{pmatrix} [(1+\cos\beta)^{\frac{1}{2}}/2^{\frac{1}{2}}]e^{-i\omega t} \\ [\sin\beta/2^{\frac{1}{2}}(1+\cos\beta)^{\frac{1}{2}}]e^{+i\omega t} \end{pmatrix}. \qquad (3)$$

Next we express $|\psi(t)\rangle$ in the $|s_x;\pm\rangle$ basis as $\alpha_1|s_x;+\rangle + \alpha_2|s_x;-\rangle$ where $|s_x;\pm\rangle$ are given explicitly by (1.4.17a) and $\alpha_1 = \frac{1}{\sqrt{2}}(1,1)\begin{pmatrix} Ae^{-i\omega t} \\ Be^{+i\omega t} \end{pmatrix} = (1/\sqrt{2})Ae^{-i\omega t} + (1/\sqrt{2})Be^{i\omega t}$ and $\alpha_2 = \frac{1}{\sqrt{2}}(1,-1)\begin{pmatrix} Ae^{-i\omega t} \\ Be^{+i\omega t} \end{pmatrix} = (1/\sqrt{2})Ae^{-i\omega t} - (1/\sqrt{2})Be^{+i\omega t}$ (for short we have written $A(0) = A$ and $B(0) = B$). Hence probability of finding the electron in $s_x = \hbar/2$ state is $\alpha_1^*\alpha_1 = \frac{1}{2}[A^2+B^2+AB(e^{2i\omega t} + e^{-2i\omega t})] = \frac{1}{2}(1+\sin\beta\cos 2\omega t)$.

(b) $\langle s_x \rangle = \langle\psi(t)|s_x|\psi(t)\rangle = (A^*(t), B^*(t))\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} A(t) \\ B(t) \end{pmatrix} = \frac{\hbar}{2}(A^*(t)B(t) + B^*(t)A(t)) = (\hbar/2)\sin\beta\cos 2\omega t$.

(c) In case (i) $\beta\to 0$, $\alpha_1^*\alpha_1 = \frac{1}{2}$ and $\langle s_x \rangle = 0$; in case (ii) $\alpha_1^*\alpha_1 = \frac{1}{2}(1+\cos 2\omega t) = \cos^2\omega t$ while $\langle s_x \rangle \to \hbar(\cos^2\omega t - \frac{1}{2})$. These answers are eminently sensible since for $\beta \to 0$ $\hat{n}$ is along the z-axis, hence there is equal probability of being found in $|s_x;+\rangle$ (i.e. $\alpha_1^*\alpha_1$) and in $|s_x;-\rangle$ (i.e. $\alpha_2^*\alpha_2$) - both being $\frac{1}{2}$. Yet $\langle s_x \rangle$

$= 0$ as the classical analogue would also be reasonable for an electron pointed spin-wise in the z-direction. For $\beta = \pi/2$ (i.e. $\hat{n}$ along OX), at $t=0$ $a_1^* a_1 = 1$, and $\langle s_x \rangle = \hbar/2$ are entirely reasonable in terms of initial state requirements.

4. First work out $x(t)$ and $p(t)$ in the Heisenberg picture. Evidently $\dot{x} = (1/i\hbar)[x, p^2/2m] = p/m$, and $\dot{p} = (1/i\hbar)[p, p^2/2m] = 0$. So $p(t) = p(0)$ and is independent of time, while $x(t) = x(0) + (p(0)/m)t$. Hence $[x(t), x(0)] = (t/m)[x(0), p(0)] = i\hbar t/m$.

5. $[H, x] = [p^2/2m + V(x), x] = -i\hbar p/m$, therefore $[[H,x], x] = -\hbar^2/m$. Take the expectation value of $[[H,x], x]$ w.r.t. an energy eigenket $|a''\rangle$, we have

$$\langle a''|Hxx|a''\rangle - 2\langle a''|xHx|a''\rangle + \langle a''|xxH|a''\rangle = -\hbar^2/m. \tag{1}$$

Use next $H|a''\rangle = E_{a''}|a''\rangle$ and $\langle a''|H = E_{a''}\langle a''|$, (1) becomes

$$E_{a''}\langle a''|xx|a''\rangle - 2\langle a''|xHx|a''\rangle + E_{a''}\langle a''|xx|a''\rangle = -\hbar^2/m \tag{2a}$$

$$\text{or} \quad - E_{a''}\langle a''|xx|a''\rangle + \langle a''|xHx|a''\rangle = \hbar^2/2m \tag{2b}$$

Now using closure property, we have $\langle a''|xHx|a''\rangle = \sum_{a'} \langle a''|xH|a'\rangle\langle a'|x|a''\rangle = \sum_{a'} E_{a'}\langle a''|x|a'\rangle\langle a'|x|a''\rangle = \sum_{a'} E_{a'}|\langle a''|x|a'\rangle|^2$ and $\langle a''|xx|a''\rangle = \sum_{a'}\langle a''|x|a'\rangle\langle a'|x|a''\rangle = \sum_{a'}|\langle a''|x|a'\rangle|^2$. Equation (2b) becomes

$$\sum_{a'}|\langle a''|x|a'\rangle|^2 \, (E_{a'} - E_{a''}) = \hbar^2/2m. \tag{3}$$

6. Let $H = \vec{p}^2/2m + V(\vec{x})$, and we compute $[\vec{x}\cdot\vec{p}, H]$ through the following steps. $[\vec{x}\cdot\vec{p}, H] = [\vec{x}\cdot\vec{p}, \vec{p}^2/2m + V(\vec{x})] = (1/2m)[\vec{x}\cdot\vec{p}, \vec{p}^2] + [\vec{x}\cdot\vec{p}, V(\vec{x})] = (1/2m) \sum_{i,j} [x_i p_i, p_j p_j] + \sum_i [x_i p_i, V(\vec{x})] = (1/2m) \sum_{i,j} (x_i[p_i, p_j p_j] + [x_i, p_j p_j]p_i) + \sum_i (x_i[p_i, V(\vec{x})] + [x_i, V(\vec{x})]p_i) = (1/2m) \sum_{i,j} [x_i, p_j p_j]p_i + \sum_i x_i[p_i, V(\vec{x})] = (1/2m) \sum_{i,j}([x_i, p_j]p_j p_i + p_j[x_i, p_j]p_i) + \sum_i x_i[p_i, V(\vec{x})] = (1/2m) \sum_{i,j} (i\hbar\delta_{ij}p_j p_i + p_j(i\hbar\delta_{ij})p_i) + \sum_i x_i(-i\hbar\partial V/\partial x_i) = i\hbar\,[\vec{p}^2/m - \vec{x}\cdot\vec{\nabla}V(\vec{x})]$. Hence $\langle[\vec{x}\cdot\vec{p}, H]\rangle =$

$= i\hbar\ [\langle\vec{p}^2\rangle/m - \langle\vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle] = i\hbar\ d/dt\ \langle\vec{x}\cdot\vec{p}\rangle$ (using Heisenberg equation of motion for $\vec{x}\cdot\vec{p}$). The condition for quantum mechanical analogue of the virial theorem is $d/dt\ \langle\vec{x}\cdot\vec{p}\rangle = 0$, i.e. the expectation value of $\vec{x}\cdot\vec{p}$ for a stationary state is independent of t.

7. To compute $\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$, first note that state ket is fixed in the Heisenberg picture, hence $\langle x(t)\rangle = \langle t=0|x(t)|t=0\rangle = 0$ because $\langle x(0)\rangle = \langle p(0)\rangle = 0$ and $x(t) = x(0) + (p(0)/m)t$ from problem 4 above. Next we compute

$$[x(t)]^2 = [x(0)]^2 + (t/m)[x(0)p(0)+p(0)x(0)] + (t^2/m^2)[p(0)]^2.$$

Because $\langle x(0)\rangle = \langle p(0)\rangle = 0$, hence $\Delta x = x(0) - \langle x(0)\rangle = x(0)$ while $\Delta p = p(0) - \langle p(0)\rangle = p(0)$. From problem 18(b) of Chapter 1, the minimum uncertainty wave packet satisfies $x(0)|t=0\rangle = \lambda p(0)|t=0\rangle$ where λ is a purely imaginary number. It is then evident that $\langle(x(0)p(0) + p(0)x(0))\rangle = (1/\lambda)\langle x(0)x(0)\rangle + (1/\lambda^*)\langle x^2(0)\rangle = 0$. So $\langle(\Delta x)^2\rangle_t = \langle x^2\rangle_t = \langle t=0|(x(0))^2|t=0\rangle + (t^2/m^2)\langle t=0|(p(0))^2|t=0\rangle = \langle(\Delta x)^2\rangle_{t=0} + (t^2/m^2)\langle(\Delta p)^2\rangle_{t=0} = \langle(\Delta x)^2\rangle_{t=0} + (\hbar^2 t^2/4m^2\langle(\Delta x)^2\rangle_{t=0})$. This agrees with expansion of wave packet calculated using wave mechanics.

8. (a) $H = |a'\rangle\delta\langle a''| + |a''\rangle\delta\langle a'| = \delta\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ as is evident since $\langle a'|H|a'\rangle = \langle a''|H|a''\rangle = 0$, while $\langle a'|H|a''\rangle = \langle a''|H|a'\rangle = \delta$. Now $H|\psi\rangle = E|\psi\rangle$ and the secular equation is $\det[H - E\underline{1}] = 0$, i.e. $E = \pm\delta$ are the energy eigenvalues. The corresponding eigenkets satisfy (with $|\psi\rangle = \begin{pmatrix}A\\ B\end{pmatrix}$)

$$\begin{pmatrix}0 & \delta\\ \delta & 0\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix} = \pm\delta\begin{pmatrix}A\\ B\end{pmatrix}, \text{ and } |A|^2 + |B|^2 = 1 \text{ (normalization)}.$$

Obviously $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$ for $E = +\delta$ and $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$ for $E = -\delta$ are appropriate eigenket solutions.

(b) As a function of time we write $|\psi(t)\rangle = \begin{pmatrix}A(t)\\ B(t)\end{pmatrix}$, and $H|\psi(t)\rangle = i\hbar d/dt|\psi(t)\rangle$

reads $\begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix}\begin{pmatrix} A(t) \\ B(t) \end{pmatrix} = i\hbar d/dt \begin{pmatrix} A(t) \\ B(t) \end{pmatrix}$ or $\delta B(t) = i\hbar dA(t)/dt$ and $\delta A(t) = i\hbar dB(t)/dt$. Thus $A(t) = -(\hbar/\delta)^2 d^2A(t)/dt^2$ and $B(t) = -(\hbar/\delta)^2 d^2B(t)/dt^2$, and $A(t) = A_1\cos\omega t + A_2\sin\omega t$, $B(t) = B_1\cos\omega t + B_2\sin\omega t$ are the simple harmonic solutions with $\omega = \delta/\hbar$. It is evident that $|a'\rangle = |\psi(t=0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ hence $A_1 = 1$, $B_1 = 0$ and from normalization $B_2 = 1$, $A_2 = 0$. So $|\psi(t)\rangle = \begin{pmatrix} \cos\omega t \\ \sin\omega t \end{pmatrix}$.

(c) We need to evaluate $|\langle a''|\psi(t)\rangle|^2$ where $\langle a''| = (0,1)$. Evidently probability is $\sin^2\omega t$.

(d) The Hamiltonian $H = \delta\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = J_x$ for a spin ½ system if $\delta = \hbar/2$, hence $|\psi(t)\rangle = \begin{pmatrix} \cos\omega t \\ \sin\omega t \end{pmatrix}$ describes the evolution of a spinor in time, initially in state $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and hence an eigenstate of $J_z = \frac{\hbar}{2}\sigma_z$.

9. (a) Let the normalized energy eigenkets be written as $|E\rangle = |R\rangle\langle R|E\rangle + |L\rangle\langle L|E\rangle$. Now $H|E\rangle = E|E\rangle$ therefore $\Delta(|L\rangle\langle R| + |R\rangle\langle L|)|E\rangle = E|E\rangle$ or $\Delta(|L\rangle\langle R|E\rangle + |R\rangle\langle L|E\rangle) = E(|R\rangle\langle R|E\rangle + |L\rangle\langle L|E\rangle)$. Due to the linear independence of $|L\rangle$ and $|R\rangle$, we have $\Delta\langle R|E\rangle = E\langle L|E\rangle$ and $\Delta\langle L|E\rangle = E\langle R|E\rangle$. Now due to normalization condition $|\langle R|E\rangle|^2 + |\langle L|E\rangle|^2 = 1$, we have $\Delta^2 = E^2$ or $\Delta = \pm E$ (these define the two level system eigenvalues). Take $\Delta = +E$, and $\langle R|E\rangle = \langle L|E\rangle = 1/\sqrt{2}$, than $|+E\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle)$; for $\Delta = -E$, take $\langle R|E\rangle = -\langle L|E\rangle = 1/\sqrt{2}$ and $|-E\rangle = \frac{1}{\sqrt{2}}(|R\rangle - |L\rangle)$.

(b) Suppose at $t=0$, $|\alpha\rangle = |R\rangle\langle R|\alpha\rangle + |L\rangle\langle L|\alpha\rangle \equiv |\alpha, t=t_0=0\rangle$. The evolution of state vector $|\alpha, t_0=0; t\rangle$ is such that $e^{-iHt/\hbar}|\alpha\rangle = |\alpha, t_0=0; t\rangle$. From part (a) we have $|R\rangle = \frac{1}{\sqrt{2}}(|+E\rangle + |-E\rangle)$ and $|L\rangle = \frac{1}{\sqrt{2}}(|+E\rangle - |-E\rangle)$, therefore

$$e^{-iHt/\hbar}|\alpha\rangle = e^{-iHt/\hbar}(\langle R|\alpha\rangle|R\rangle + \langle L|\alpha\rangle|L\rangle)$$
$$= \frac{1}{\sqrt{2}}\langle R|\alpha\rangle e^{-iHt/\hbar}(|+E\rangle + |-E\rangle) + \frac{1}{\sqrt{2}}\langle L|\alpha\rangle\, e^{-iHt/\hbar}(|+E\rangle - |-E\rangle). \qquad (1)$$

But $e^{-iHt/\hbar}|\pm E\rangle = e^{\mp i\Delta t/\hbar}|\pm E\rangle$, hence from (1) we have

$$|\alpha,\ t_o=0;\ t\rangle = e^{-iHt/\hbar}|\alpha\rangle = \frac{1}{\sqrt{2}}\langle R|\alpha\rangle(e^{-i\Delta t/\hbar}|+E\rangle + e^{i\Delta t/\hbar}|-E\rangle) + \frac{1}{\sqrt{2}}\langle L|\alpha\rangle(e^{-i\Delta t/\hbar}|+E\rangle - e^{i\Delta t/\hbar}|-E\rangle). \tag{2}$$

Rearrange r.h.s. of (2) back to the $\{|R\rangle, |L\rangle\}$ basis, we have

$$|\alpha,\ t_o=0;\ t\rangle = (\langle R|\alpha\rangle\cos\Delta t/\hbar - i\langle L|\alpha\rangle\sin\Delta t/\hbar)|R\rangle + (\langle L|\alpha\rangle\cos\Delta t/\hbar - i\langle R|\alpha\rangle\sin\Delta t/\hbar)|L\rangle \tag{3}$$

(c) Suppose at $t=0$, $|\alpha\rangle = |R\rangle$ with certainty, than from (3) we have $\langle L|\alpha\rangle = 0$ and $\langle R|\alpha\rangle = 1$ (normalization). We need the development of $|L\rangle$ as a function of time, this corresponds to $|\alpha,t_o=0;t\rangle = \cos\Delta t/\hbar|R\rangle - i\sin\Delta t/\hbar|L\rangle$ and $\langle L|\alpha,t_o=0;t\rangle = -i\sin\Delta t/\hbar$. The transition probability is $|\langle L|\alpha,t_o=0;t\rangle|^2 = \sin^2\Delta t/\hbar$.

(d) In the Schrödinger picture the base kets $|R\rangle$ and $|L\rangle$ remain stationary in time and the state vector obeys $i\hbar\ \partial/\partial t|\alpha,t_o=0;\ t\rangle = H|\alpha,t_o=0;\ t\rangle$. Write $|\alpha,t_o=0;\ t\rangle = \alpha_R(t)|R\rangle + \alpha_L(t)|L\rangle$ and using $H = \Delta(|L\rangle\langle R|+|R\rangle\langle L|)$, the Schrödinger equation leads to coupled equations $i\hbar d\alpha_R(t)/dt = \Delta\alpha_L(t)$ and $i\hbar d\alpha_L(t)/dt = \Delta\alpha_R(t)$ where $\alpha_R(t) = \langle R|\alpha,t_o=0;\ t\rangle$ and $\alpha_L(t) = \langle L|\alpha\ ,t_o=0;\ t\rangle$. Solutions of the coupled equations can be obtained by noting that $d^2/dt^2[\alpha_{R,L}(t)] + (\Delta^2/\hbar^2)\alpha_{R,L}(t) = 0$, hence

$$\alpha_L(t) = A\cos\Delta t/\hbar + B\sin\Delta t/\hbar,\quad \alpha_R(t) = C\cos\Delta t/\hbar + D\sin\Delta t/\hbar \tag{4}$$

At $t = 0$ $|\alpha\rangle = \langle R|\alpha\rangle|R\rangle + \langle L|\alpha\rangle|L\rangle = \alpha_R(0)|R\rangle + \alpha_L(0)|L\rangle$, hence $\alpha_R(0) = C = \langle R|\alpha\rangle$ and $\alpha_L(0) = A = \langle L|\alpha\rangle$. Next the normalization condition at t, with $t_o=0$ $\langle\alpha,t_o=0;\ t|\alpha,t_o=0;\ t\rangle = 1$ give

$$\cos^2\Delta t/\hbar + (\langle R|\alpha\rangle^* D + D^*\langle R|\alpha\rangle + \langle L|\alpha\rangle^* B + B^*\langle L|\alpha\rangle)\cos\Delta t/\hbar\ \sin\Delta t/\hbar + (|D|^2 + |B|^2)\sin^2\Delta t/\hbar = 1. \tag{5}$$

Solution of (5) is possible with $D = -i\langle L|\alpha\rangle$ and $B = -i\langle R|\alpha\rangle$, hence (4) for $\alpha_L(t)$ and $\alpha_R(t)$ gives the coefficients of $|L\rangle$ and $|R\rangle$ in (3) of (b).

(e) The lack of Hermiticity here is same as in problem 2, replacing $H = H_{12}|1\rangle\langle 2|$

by $H = \Delta|L\rangle\langle R|$. We find again $H^n = 0$ for $n>1$, and $U(t,t_o=0) = 1 - it\Delta/\hbar\ |L\rangle\langle R|$ even for a finite time interval. The initial state is $\langle R|\alpha\rangle|R\rangle + \langle L|\alpha\rangle|L\rangle$; at a later time t we have $(1 - it\Delta/\hbar\ |L\rangle\langle R|)(\langle R|\alpha\rangle|R\rangle + \langle L|\alpha\rangle|L\rangle)$, hence probability for being found in $|L\rangle$ is $|\langle L|\alpha\rangle - (it\Delta/\hbar)\langle R|\alpha\rangle|^2$ and in $|R\rangle$ is $|\langle R|\alpha\rangle|^2$, but $|\langle L|\alpha\rangle - (it\Delta/\hbar)\langle R|\alpha\rangle|^2 + |\langle R|\alpha\rangle|^2 \neq |\langle L|\alpha\rangle|^2 + |\langle R|\alpha\rangle|^2$. Thus probability conservation is violated.

10. $H = p^2/2m + \frac{1}{2} m\omega^2x^2$ for the one dimensional simple harmonic oscillator.

(a) In the Heisenberg picture, the operators x and p obey the Heisenberg equations of motion: $dp/dt = (1/i\hbar)[p, H] = -m\omega^2x$, $dx/dt = (1/i\hbar)[x, H] = p/m$. This implies $\ddot{x} = -\omega^2x$ and $\ddot{p} = -\omega^2p$ with the initial conditions $x(0) = x_o$ and $p(0) = p_o$ $\dot{x}(0) = p_o/m$ and $\dot{p}(0) = -m\omega^2x_o$. The solutions are $x(t) = x_o\cos\omega t + (p_o/m\omega)\sin\omega t$, $p(t) = p_o\cos\omega t - m\omega x_o\sin\omega t$ which give $H = p^2(t)/2m + \frac{1}{2} m\omega^2x^2(t) = p_o^2/2m + \frac{1}{2} m\omega^2x_o^2$, i.e. H is time independent. Dynamical variables x and p are time-dependent in the Heisenberg picture. At $t = 0$, the Heisenberg and Schrödinger pictures coincide, thus $x_H(0) = x_S(0) = x_o$ (with $x_S(t) = x_S(0)$) and $p_H(0) = p_S(0) = p_o$ (with $p_S(t) = p_S(0)$) and we note the time-independence of dynamical variables in the Schrödinger picture.

The relationship between the Heisenberg and Schrödinger pictures is $x_H(t) = e^{iHt/\hbar}x_Se^{-iHt/\hbar}$ with $x_S = x_o$ and $p_H(t) = e^{iHt/\hbar}p_Se^{-iHt/\hbar}$ with $p_S = p_o$. Using (2.3.48) - (2.3.50), one knows $x_H(t) = x_o\cos\omega t + (p_o/m\omega)\sin\omega t$. Also

$$e^{iHt/\hbar}p_oe^{-iHt/\hbar} = p_o + (it/\hbar)[H,p_o] + (i^2t^2/2!\hbar^2)[H,[H,p_o]] + (i^3t^3/3!\hbar^3)[H,[H,[H,p_o]]] + \ldots = p_o - \frac{(t^2\omega^2)}{2!}p_o - tm\omega^2x_o + \frac{t^3m\omega^4x_o}{3!} + \ldots\ldots$$

where we have used $[H, x_o] = -i\hbar p_o/m$, $[H, p_o] = i\hbar m\omega^2x_o$. This implies that $p_H(t) = p_o\cos\omega t - m\omega x_o\sin\omega t$.

(b) At t=0, the general state vectors for both pictures are equal: $|\alpha\rangle_H = |\alpha\rangle_S =$

$|\alpha,t=0\rangle$, e.g. $|\alpha,t=0\rangle = \Sigma_n c_n(0)|n\rangle$. At $t\neq 0$, $|\alpha,t\rangle_H = |\alpha,t=0\rangle = \Sigma_n c_n(0)|n\rangle$ i.e. time independent, while $|\alpha,t\rangle_S = e^{-iHt/\hbar}|\alpha,t=0\rangle = \Sigma_n c_n(0)e^{-i\omega(n+\frac{1}{2})t}|n\rangle$ and is thus time dependent. (We have used $H = \hbar\omega(N+\frac{1}{2})$ which is time-independent in both pictures). We can recast $|\alpha,t\rangle_S$ as $|\alpha,t\rangle_S = \Sigma_n c_n(t)|n\rangle$ with $c_n(t) = c_n(0)e^{-i\omega(n+\frac{1}{2})t}$. Also note $i\hbar\partial/\partial t|\alpha,t\rangle_S = H|\alpha,t\rangle_S$ which is the Schrödinger equation for the Schrödinger state vector. <u>Remarks</u>: $c_n(t)$ can be determined in the two pictures by (a) $c_n(t) = \langle n|\alpha,t\rangle_S = c_n(0)e^{-i\omega(n+\frac{1}{2})t}$, the Schrödinger picture with <u>base kets $|n\rangle$ time independent</u>, and (b) $c_n(t) = \langle n,t|\alpha,t\rangle_H = \langle n|e^{-iHt/\hbar}|\alpha,t\rangle_H = c_n(0)e^{-i\omega(n+\frac{1}{2})t}$, the Heisenberg picture with <u>base kets $|n,t\rangle = e^{iHt/\hbar}|n\rangle$ which are time-dependent</u>.

11. For a one-dimensional SHO potential $H = p^2/2m + \frac{1}{2} m\omega^2x^2$, hence $\dot{x} = (1/i\hbar)[x,H] = p/m$, and $\dot{p} = (1/i\hbar)[p,H] = (1/i\hbar)(m\omega^2/2)[p,x^2] = (m\omega^2/2i\hbar)[-2i\hbar x] = -m\omega^2x$. Hence $\ddot{x} + \omega^2x = 0$, and solution is $x(t) = A\cos\omega t + B\sin\omega t$. At $t=0$, $x(0) = A$ while $\dot{x}(t) = -A\omega\cos\omega t + B\omega\cos\omega t$ leads to $\dot{x}(0) = B\omega$ and thus $p(0) = m\omega B$. Thus in the Heisenberg picture $x(t) = x(0)\cos\omega t + (p(0)/m\omega)\sin\omega t$.

Our state vector $|\alpha\rangle = e^{-ipa/\hbar}|0\rangle$ at $t=0$; for $t>0$ we have in the Heisenberg picture $\langle x(t)\rangle = \langle\alpha|x(t)|\alpha\rangle$. We note that

$$e^{ip(0)a/\hbar}x(0)e^{-ip(0)a/\hbar} = e^{ip(0)a/\hbar}([x(0),e^{-ip(0)a/\hbar}] + e^{-ip(0)a/\hbar}x(0))$$
$$= x(0) + a,$$

while $e^{ip(0)a/\hbar}p(0)e^{-ip(0)a/\hbar} = p(0)$. Hence

$$\langle x(t)\rangle = \langle\alpha|x(t)|\alpha\rangle = \langle 0|e^{ipa/\hbar}x(t)e^{-ipa/\hbar}|0\rangle$$
$$= \langle 0|e^{ip(0)a/\hbar}[x(0)\cos\omega t+(p(0)/m\omega)\sin\omega t]e^{-ipa/\hbar}|0\rangle.$$

Since $\langle 0|x(0)|0\rangle = \langle 0|p(0)|0\rangle = 0$, we obtain for $\langle x(t)\rangle = a\cos\omega t$.

12. (a) The wave function in problem 11 takes form $\langle x'|\alpha\rangle = \langle x'|e^{-ipa/\hbar}|0\rangle$. Since $e^{ipa/\hbar}|x'\rangle = |x'-a\rangle$(hence $\langle x'|e^{-ipa/\hbar} = \langle x'-a|$), we have $\langle x'|\alpha\rangle = \langle x'-a|0\rangle$. Hence $\langle x'|\alpha\rangle = \pi^{-\frac{1}{4}}x_0^{-\frac{1}{2}}\exp[-(x'-a)^2/2x_0^2]$.

(b) The ground state wave function is

$$\langle x'|0\rangle = \pi^{-1/4}\, x_0^{-1/2} \exp[-\frac{x'^2}{2x_0^2}] \; .$$

The probability of finding $|\alpha\rangle$ in the ground state is

$$P = \int\langle\alpha|x'\rangle\langle x'|0\rangle dx' = (1/\pi^{1/2}x_0)\int_{-\infty}^{\infty} \exp[-\{(x'-a)^2+x'^2\}/2x_0^2]\; dx' = e^{-a^2/2x_0^2}.$$

P is time independent and hence does not change for $t>0$.

13. (a) From the given information, we can write

$$x = \sqrt{\hbar/2m\omega}(a+a^\dagger),\; p = i\sqrt{\hbar m\omega/2}(a^\dagger-a) \tag{1}$$

$x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n}|n-1\rangle+\sqrt{n+1}|n+1\rangle)$ and $p|n\rangle = i\sqrt{\hbar m\omega/2}(\sqrt{n+1}|n+1\rangle-\sqrt{n}|n-1\rangle)$.

Remember also that $a^\dagger a = N$ where N is number operator and $N|n\rangle = n|n\rangle$ while $\langle m|n\rangle = \delta_{mn}$. Therefore $\langle m|x|n\rangle = \frac{1}{2}\sqrt{2\hbar/m\omega}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})$, likewise $\langle m|p|n\rangle = (m\omega i/2)\sqrt{2\hbar/m\omega}(\sqrt{n+1}\delta_{m,n+1}-\sqrt{n}\delta_{m,n-1})$. Computation of $\langle m|\{x,p\}|n\rangle = \langle m|xp|n\rangle + \langle m|px|n\rangle$ is obtained by using (1) and $\langle m|x = \sqrt{\hbar/2m\omega}(\sqrt{m}\langle m-1|+\sqrt{m+1}\langle m+1|)$ as well as $\langle m|p = -i\sqrt{\hbar m\omega/2}(\sqrt{m+1}\langle m+1|-\sqrt{m}\langle m-1|)$ [sign change comes from complex conjugation when passing to dual space]. The calculation is then straightforward leading to $\langle m|\{x,p\}|n\rangle = -i\hbar(\sqrt{n(m+1)}\delta_{m+1,n-1}-\sqrt{m(n+1)}\delta_{m-1,n+1})$. For $\langle m|x^2|n\rangle = \langle m|xx|n\rangle$, try evaluate the scalar product $\langle m|x$ and $x|n\rangle$, the answer is $\langle m|x^2|n\rangle = (\hbar/2m\omega)\{\sqrt{n(n-1)}\delta_{m,n-2}+(2n+1)\delta_{m,n}+\sqrt{(n+1)(n+2)}\delta_{m,n+2}\}$. Likewise $\langle m|p^2|n\rangle = \langle m|pp|n\rangle$ and we evaluate the scalar product $\langle m|p$ and $p|n\rangle$, the answer is $\langle m|p^2|n\rangle = -\frac{\hbar m\omega}{2}\{\sqrt{n(n-1)}\delta_{m,n-2}-(2n+1)\delta_{m,n}+\sqrt{(n+1)(n+2)}\delta_{m,n+2}\}$.

(b) Virial theorem states $\langle p^2/m\rangle = \langle\vec{x}\cdot\vec{\nabla}V\rangle$, hence in one dimension we have $\langle p^2/m\rangle = \langle x dV/dx\rangle$. For the SHO, $H = p^2/2m + V(x) = p^2/2m + \frac{1}{2}m\omega^2x^2$ therefore $x dV/dx = m\omega^2x^2$. Now $\langle p^2/m\rangle = \frac{1}{m}\langle n|p^2|n\rangle = \frac{\hbar\omega}{2}(2n+1) = \hbar\omega(n+\frac{1}{2})$, while $\langle x dV/dx\rangle = m\omega^2\langle x^2\rangle = \frac{m\omega^2\hbar}{2m\omega}(2n+1) = \hbar\omega(n+\frac{1}{2})$. Therefore the virial theorem is verified.

14. (a) $\langle x'|p'\rangle = (2\pi\hbar)^{-1/2}e^{ip'x'/\hbar}$ or $\langle p'|x'\rangle = (2\pi\hbar)^{-1/2}e^{-ip'x'/\hbar}$, hence $\langle p'|x|\alpha\rangle$

$= \int dx' \langle p'|x|x'\rangle\langle x'|\alpha\rangle = \int dx'\ x'\langle p'|x'\rangle\langle x'|\alpha\rangle$. Note that explicitly we have $i\hbar\partial/\partial p'[(2\pi\hbar)^{-\frac{1}{2}}e^{-ip'x'/\hbar}] = x'\langle p'|x'\rangle$. Hence $\langle p'|x|\alpha\rangle = \int dx' i\hbar\partial/\partial p'(\langle p'|x'\rangle\langle x'|\alpha\rangle)$ $= i\hbar\partial/\partial p'\ \langle p'|\alpha\rangle$ where we assume that differentiation and integration can be interchanged.

(b) For $H = p^2/2m + \frac{1}{2} m\omega^2x^2$, the state vector $|\ \rangle_S$ satisfies in Schrödinger picture

$$(p^2/2m + \tfrac{1}{2} m\omega^2x^2)|\ \rangle_S = i\hbar\partial/\partial t|\ \rangle_S\ . \tag{1}$$

In the momentum representation, we have

$$\langle p'|(p^2/2m + \tfrac{1}{2} m\omega^2x^2)|\ \rangle_S = i\hbar\partial/\partial t\ \langle p'|\ \rangle_S \tag{2}$$

and thus

$$\frac{p'^2}{2m}\langle p'|\ \rangle_S + \tfrac{1}{2} m\omega^2(-\hbar^2\partial^2/\partial p'^2)\langle p'|\ \rangle_S = i\hbar\partial/\partial t\ \langle p'|\ \rangle_S \tag{3}$$

where in (3) we have used identity $\langle p'|xx|\ \rangle_S = i\hbar\partial/\partial p'\ \langle p'|x|\ \rangle_S = -\hbar^2\frac{\partial^2}{\partial p'^2}\langle p'|\ \rangle_S$.

For the SHO problem there is a complete symmetry between x and p. So the energy eigenfunctions in momentum space must be of the form $e^{-p^2/2p_o^2}\ H_n(p/p_o)$ up to normalization ($p_o \equiv \sqrt{\hbar m\omega}$) in analogy with $e^{-x^2/2x_o^2}\ H_n(x/x_o)$ ($x_o = \sqrt{\hbar/m\omega}$) in position space.

15. From (2.3.45a), we have $x(t) = x(0)\cos\omega t + (p(0)/m\omega)\sin\omega t$, and $x(t)x(0) = [x(0)]^2\cos\omega t + (p(0)x(0)/m\omega)\sin\omega t$. Simple harmonic oscillator (SHO) ground state is from (2.3.30) $\langle x'|0\rangle = (1/\pi^{\frac{1}{4}}x_o^{\frac{1}{2}})\exp[-\frac{1}{2}(x'/x_o)^2]$, $x_o = \sqrt{\hbar/m\omega}$. Then

$$\begin{aligned} C(t) &= \langle 0|x(t)x(0)|0\rangle \\ &= \int\int\langle 0|x'\rangle\langle x'|[(x(0))^2\cos\omega t + (p(0)x(0)/m\omega)\sin\omega t]|x''\rangle\langle x''|0\rangle\ dx'dx'' \\ &= \int\langle 0|x'\rangle\langle x'|0\rangle x'^2\cos\omega t\ dx' + (\sin\omega t/m\omega)\langle 0|p(0)x(0)|0\rangle. \end{aligned}$$

The term $\langle 0|p(0)x(0)|0\rangle$ vanishes (c.f. problem 13 with m=n=0 or by explicit evaluation in $|x'\rangle$ representation). Hence C(t) is given by

$$C(t) = \cos\omega t \int_{-\infty}^{\infty}(x'^2/\pi^{\frac{1}{2}}x_o)\exp[-(x'/x_o)^2]\ dx' = (\hbar/2m\omega)\cos\omega t.$$

16. (a) Let linear combination be $|\alpha\rangle = a|0\rangle + b|1\rangle$. Then $\langle x\rangle = (a^*\langle 0|+b^*\langle 1|)x(a|0\rangle +b|1\rangle)$ or $x = a^*a\langle 0|x|0\rangle + a^*b\langle 0|x|1\rangle + b^*a\langle 1|x|0\rangle + b^*b\langle 1|x|1\rangle$. From problem 13 we have $\langle m|x|n\rangle = \frac{1}{2}\sqrt{2\hbar/m\omega}(\sqrt{n}\delta_{m,n-1}+\sqrt{n+1}\delta_{m,n+1})$, hence $\langle x\rangle = \frac{a^*b}{2}\sqrt{2\hbar/m\omega} + \frac{b^*a}{2}\sqrt{2\hbar/m\omega}$ or $\langle x\rangle = \frac{1}{2}\sqrt{2\hbar/m\omega}(a^*b+b^*a)$. Without loss of generality choose a,b to be real and normalized such that $a^2+b^2 = 1$, then $\langle x\rangle = \sqrt{2\hbar/m\omega}\,a\sqrt{1-a^2}$. Maximum of $\langle x\rangle$ then requires $d\langle x\rangle/da = 0$ or $a = +1/\sqrt{2}$ and likewise $b = +1/\sqrt{2}$. Hence $\langle x\rangle_{max} = \frac{1}{2}\sqrt{2\hbar/m\omega}$ and up to a common phase $|\alpha\rangle = \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$.

(b) The state vector in Schrödinger representation evolves for $t>0$ as $|\alpha,t_o;t\rangle = \mathcal{U}(t,t_o)|\alpha,t_o\rangle$ where $\mathcal{U}(t,t_o) = e^{-iH(t-t_o)/\hbar}$ and $H = p^2/2m + \frac{1}{2}m\omega^2x^2$ is independent of time. Taking $t_o=0$, we have $|\alpha,t\rangle = e^{-iHt/\hbar}(|0\rangle+|1\rangle)/\sqrt{2}$, but since $\{|n\rangle\}$ are energy eigenkets with energy eigenvalues $E_n = \hbar\omega(n+\frac{1}{2})$, we write $|\alpha,t\rangle = (e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle)/\sqrt{2}$ as the state vector for $t>0$ in the Schrödinger picture.

(i) In the Schrödinger picture

$$\langle\alpha,t|x|\alpha,t\rangle = \tfrac{1}{2}(e^{i\omega t/2}\langle 0|+e^{3i\omega t/2}\langle 1|)x(e^{-i\omega t/2}|0\rangle+e^{-3i\omega t/2}|1\rangle)$$
$$= \tfrac{1}{2}(\langle 0|x|0\rangle+e^{-i\omega t}\langle 0|x|1\rangle+e^{i\omega t}\langle 1|x|0\rangle+\langle 1|x|1\rangle)$$
$$= \tfrac{1}{2}(e^{-i\omega t}\tfrac{1}{2}\sqrt{2\hbar/m\omega} + e^{i\omega t}\tfrac{1}{2}\sqrt{2\hbar/m\omega}) = \tfrac{1}{2}\sqrt{2\hbar/m\omega}\cos\omega t.$$

(ii) In the Heisenberg picture $|\alpha\rangle = (|0\rangle+|1\rangle)/\sqrt{2}$, $x(t) = x(0)\cos\omega t+ \frac{p(0)}{m\omega}\sin\omega t$, hence $\langle x\rangle = \langle\alpha|x(t)|\alpha\rangle = \frac{1}{2}(\cos\omega t\langle 0|x(0)|0\rangle + \frac{\sin\omega t}{m\omega}\langle 0|p(0)|0\rangle + \cos\omega t\langle 0|x(0)|1\rangle + \frac{\sin\omega t}{m\omega}\langle 0|p(0)|1\rangle + \cos\omega t\langle 1|x(0)|0\rangle + \frac{\sin\omega t}{m\omega}\langle 1|p(0)|0\rangle + \cos\omega t\langle 1|x(0)|1\rangle + \frac{\sin\omega t}{m\omega}\langle 1|p(0)|1\rangle)$. The evaluation of $\langle n|x(0)|m\rangle$ and $\langle n|p(0)|m\rangle$ have been given in problem 13, and give for $\langle\alpha|x(t)|\alpha\rangle = \langle x(t)\rangle_H = \frac{1}{2}\sqrt{2\hbar/m\omega}\cos\omega t$ as in (i).

(c) We evaluate $\langle(\Delta x)^2\rangle_t$ in the Schrödinger picture for definiteness. Here

$$\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2,$$

with $\langle x\rangle = \frac{\cos\omega t}{2}\sqrt{2\hbar/m\omega}$ from (b). Again $\langle\alpha,t|x^2|\alpha,t\rangle = \frac{1}{2}(\langle 0|x^2|0\rangle + e^{-i\omega t}\langle 0|x^2|1\rangle + e^{i\omega t}\langle 1|x^2|0\rangle + \langle 1|x^2|1\rangle)$. Use again the expression for $\langle m|x^2|n\rangle$ from problem 13, i.e. $\langle 0|x^2|0\rangle = \hbar/2m\omega$, $\langle 1|x^2|1\rangle = 3\hbar/2m\omega$, $\langle 0|x^2|1\rangle = \langle 1|x^2|0\rangle = 0$. Therefore $\langle x^2\rangle = \langle\alpha,t|x^2|\alpha,t\rangle = \frac{1}{2}(2\hbar/m\omega) = \hbar/m\omega$, and

$$\langle(\Delta x)^2\rangle = \frac{\hbar}{m\omega}(1-\cos^2\omega t/2).$$

17. If we work in the Schrödinger picture, than

$$\langle 0|e^{ikx}|0\rangle = \int_{-\infty}^{\infty}\psi_0^*(x)e^{ikx}\psi_0(x)dx$$

where $\psi_0(x) = (m\omega/\pi\hbar)^{\frac{1}{4}}\exp[-m\omega x^2/2\hbar]$. First we note from problem 13 that $\langle 0|x^2|0\rangle = \hbar/2m\omega$, therefore $\exp[-k^2\langle 0|x^2|0\rangle/2] \equiv \exp[-k^2\hbar/4m\omega]$. Now explicitly $\langle 0|e^{ikx}|0\rangle = (m\omega/\pi\hbar)^{\frac{1}{2}}\int_{-\infty}^{\infty}e^{ikx-m\omega x^2/\hbar}dx$, this can be evaluated by noting that $\int_{-\infty}^{\infty}e^{-(ax^2+bx+c)}dx = \sqrt{\pi/a}\; e^{(b^2-4ac)/4a}$. Hence $\langle 0|e^{ikx}|0\rangle = (m\omega/\pi\hbar)^{\frac{1}{2}}(\hbar\pi/m\omega)^{\frac{1}{2}}\; e^{-k^2\hbar/4m\omega} = \exp[-k^2\langle 0|x^2|0\rangle/2]$.

18. (a) Take $a|\lambda\rangle = \exp[-|\lambda|^2/2]\; a\,\exp[\lambda a^\dagger]\;|0\rangle = \exp[-|\lambda|^2/2]\; a\sum_{n=0}^{\infty}(\lambda^n/n!)(a^\dagger)^n|0\rangle$; but we know that $(a^\dagger)^k|n\rangle = \sqrt{(n+1)(n+2)\ldots\ldots(n+k)}\,|n+k\rangle$ hence $(a^\dagger)^k|0\rangle = \sqrt{k!}\,|k\rangle$ and $a(a^\dagger)^k|0\rangle = \sqrt{k!}\; a|k\rangle = \sqrt{k}\sqrt{k!}\,|k-1\rangle$. Thus $a|\lambda\rangle = e^{-|\lambda|^2/2}\sum_{n=1}^{\infty}\lambda^n\frac{\sqrt{n}\sqrt{n!}}{n!}|n-1\rangle =$

$= e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}\lambda^{n+1}(\sqrt{n+1}/\sqrt{(n+1)!})|n\rangle$. But $(n+1)!/(n+1) = n!$, hence

$$a|\lambda\rangle = e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}(\lambda^{n+1}/\sqrt{n!})|n\rangle = \lambda e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}(\lambda^n/\sqrt{n!})|n\rangle. \qquad (1)$$

The r.h.s. of (1) is $\lambda e^{-|\lambda|^2/2}e^{\lambda a^\dagger}|0\rangle$ by noting that $e^{\lambda a^\dagger}|0\rangle = \sum_{n=0}^{\infty}(\lambda a^\dagger)^n/n!\;|0\rangle = \sum_{n=0}^{\infty}\lambda^n|n\rangle/\sqrt{n!}$. Hence with $|\lambda\rangle = e^{-|\lambda|^2/2}e^{\lambda a^\dagger}|0\rangle$, we have indeed $a|\lambda\rangle = \lambda|\lambda\rangle$ with λ in general a complex number. For normalization we find

$$\langle\lambda|\lambda\rangle = e^{-|\lambda|^2}\langle 0|e^{\lambda^* a}e^{\lambda a^\dagger}|0\rangle = e^{-|\lambda|^2}\langle 0|e^{\lambda^* a}\sum_{n=0}^{\infty}\lambda^n|n\rangle/\sqrt{n!}$$
$$= e^{-|\lambda|^2}\langle 0|\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}(\lambda^n/\sqrt{n!})(\lambda^* a)^m/m!\;|n\rangle\;, \qquad (2)$$

but $a^m|n\rangle = \sqrt{n(n-1)\ldots\ldots(n-m+1)}\,|n-m\rangle$, hence (2) contributes by orthonormality of states only when $n-m = 0$, i.e.

$$\langle\lambda|\lambda\rangle = e^{-|\lambda|^2}\langle 0|\sum_{n=0}^{\infty}\frac{\lambda^n(\lambda^*)^n}{\sqrt{n!}(n!)}\sqrt{n!}|0\rangle = e^{-|\lambda|^2}e^{+|\lambda|^2} = 1.$$

Therefore $|\lambda\rangle$ is a normalized coherent state.

(b) $\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$, $x = \sqrt{\hbar/2m\omega}(a+a^\dagger)$, where $a|\lambda\rangle = \lambda|\lambda\rangle$ and $\langle\lambda|a^\dagger = \langle\lambda|\lambda^*$. So $\langle x\rangle = \langle\lambda|x|\lambda\rangle = \sqrt{\hbar/2m\omega}(\langle\lambda|(a+a^\dagger)|\lambda\rangle) = \sqrt{\hbar/2m\omega}(\lambda+\lambda^*)$, and $\langle x\rangle^2 = (\hbar/2m\omega)(\lambda^2+\lambda^{*2}+2\lambda\lambda^*) = (\hbar/2m\omega)(\lambda+\lambda^*)^2$. Now $x^2 = xx = (\hbar/2m\omega)[a^{\dagger 2}+a^2+aa^\dagger+a^\dagger a] = (\hbar/2m\omega)[a^{\dagger 2}+a^2+2a^\dagger a+1]$, hence $\langle x^2\rangle = (\hbar/2m\omega)[\lambda^{*2}+\lambda^2+2\lambda^*\lambda+1] = (\hbar/2m\omega)[(\lambda^*+\lambda)^2+1]$. Likewise $\langle p\rangle^2 = -(\hbar m\omega/2)[\lambda^*-\lambda]^2$ and $\langle p^2\rangle = (\hbar m\omega/2)[1-(\lambda^*-\lambda)^2]$, using $p = i\sqrt{\hbar m\omega/2}(a^\dagger-a)$. Hence $\langle(\Delta p)^2\rangle = \langle p^2\rangle - \langle p\rangle^2 = \hbar m\omega/2$ and $\langle(\Delta x)^2\rangle = \hbar/2m\omega$ and $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \hbar^2/4$.

(c) Write $|\lambda\rangle = e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}(\lambda^n/\sqrt{n!})|n\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle$, hence $f(n) = e^{-|\lambda|^2/2}(\frac{\lambda^n}{\sqrt{n!}})$.

Therefore $|f(n)|^2 = e^{-|\lambda|^2}|\lambda|^{2n}/n!$ and is a Poisson distribution

$$P(\lambda',n) = e^{-\lambda'}\lambda'^n/n!, \text{ where } \lambda' = |\lambda|^2.$$

Now $\Gamma(n+1) = n!$, hence $|f(n)|^2 = e^{-|\lambda|^2}|\lambda|^{2n}/\Gamma(n+1)$. The maximum value is obtained by noting that $\ln|f(n)|^2 = -|\lambda|^2 + n\ln[|\lambda|^2] - \ln\Gamma(n+1)$, and $\frac{\partial}{\partial n}\ln|f(n)|^2 = \ln|\lambda|^2 - \frac{\partial}{\partial n}\ln\Gamma(n+1) = 0$. The latter equation defines n_{max} where for large n, $\frac{\partial}{\partial n}\ln\Gamma(n+1) \sim \ln n$. Hence $n_{max} = |\lambda|^2$.

(d) The translation operator $e^{-ip\ell/\hbar}$ where p is momentum operator and ℓ just the displacement distance, can be rewritten as

$$e^{-ip\ell/\hbar} = e^{\ell\sqrt{m\omega/2\hbar}(a^\dagger-a)} = e^{\ell\sqrt{m\omega/2\hbar}a^\dagger}e^{-\ell\sqrt{m\omega/2\hbar}a}e^{-\frac{1}{2}(-\ell^2)(m\omega/2\hbar)[a^\dagger,a]}$$

$$= e^{-\frac{1}{2}(-\ell^2)(m\omega/2\hbar)[a^\dagger,a]}e^{\ell\sqrt{m\omega/2\hbar}a^\dagger}e^{-\ell\sqrt{m\omega/2\hbar}a} = e^{\frac{-\ell^2 m\omega}{4\hbar}}e^{\ell\sqrt{m\omega/2\hbar}a^\dagger}e^{-\ell\sqrt{m\omega/2\hbar}a}.$$

Note $e^{-\ell\sqrt{m\omega/2\hbar}a}|0\rangle = |0\rangle$; because $a|0\rangle = 0$. Hence

$$e^{-ip\ell/\hbar}|0\rangle = e^{-|\lambda|^2/2}e^{\lambda a^\dagger}|0\rangle, \text{ where } \lambda = \ell\sqrt{m\omega/2\hbar}$$

[We have used here the identity $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$, true for any pair of operators A and B that commute with $[A,B]$, c.f. R. J. Glauber, Phys. Rev. 84, 399 (1951).]

19. We know that $[a_\pm, a_\pm^\dagger] = 1$ and $[a_+, a_-] = [a_+^\dagger, a_-] = 0$ (since oscillators are independent), then $[J_z, J_+] = \frac{\hbar^2}{2}(a_+^\dagger a_+ a_+^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_- - a_+^\dagger a_- a_+^\dagger a_+ + a_+^\dagger a_- a_-^\dagger a_-) =$ $\frac{\hbar^2}{2}(a_+^\dagger a_+ a_+^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_- - a_+^\dagger a_-(a_+ a_+^\dagger - 1) + a_- a_-^\dagger a_+^\dagger a_-) = \frac{\hbar^2}{2}(a_+^\dagger a_+ - a_-^\dagger a_- - a_+^\dagger a_+ + 1$ $+ a_- a_-^\dagger) a_+^\dagger a_- = \frac{\hbar^2}{2}([a_-, a_-^\dagger] + 1) a_+^\dagger a_- = \frac{\hbar^2}{2}(2) a_+^\dagger a_- = \hbar J_+$. Similarly $[J_z, J_-] = -\hbar J_-$, and $\vec{J}^2 = J_x^2 + J_y^2 + J_z^2 = J_+ J_- - \hbar J_z + J_z^2$ is such that $[\vec{J}^2, J_z] = J_+ J_- J_z - \hbar J_z^2 + J_z^3$ $- J_z J_+ J_- + \hbar J_z^2 - J_z^3 = [J_+ J_-, J_z] = [J_+, J_z] J_- + J_+ [J_-, J_z] = -\hbar J_+ J_- + \hbar J_+ J_- = 0$. Explicitly $J_+ J_- - \hbar J_z + J_z^2 = \hbar^2 a_+^\dagger a_- a_-^\dagger a_+ - \frac{\hbar^2}{2}(a_+^\dagger a_+ - a_-^\dagger a_-) + \frac{\hbar^2}{4}(a_+^\dagger a_+ a_+^\dagger a_+ -$ $a_+^\dagger a_+ a_-^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_+ + a_-^\dagger a_- a_-^\dagger a_-) = \hbar^2 a_+^\dagger a_+ (1 + a_-^\dagger a_-) - \frac{\hbar^2}{2}(a_+^\dagger a_+ - a_-^\dagger a_-) + \frac{\hbar^2}{4}(a_+^\dagger a_+ a_+^\dagger a_+$ $-2 a_+^\dagger a_+ a_-^\dagger a_- + a_-^\dagger a_- a_-^\dagger a_-) = \frac{\hbar^2}{2} a_+^\dagger a_+ (1 + a_-^\dagger a_- + \tfrac{1}{2} a_+^\dagger a_+) + \frac{\hbar^2}{2} a_-^\dagger a_- (1 + \tfrac{1}{2} a_-^\dagger a_-) =$ $\frac{\hbar^2}{4} a_+^\dagger a_+ (a_+^\dagger a_+ + a_-^\dagger a_-) + \frac{\hbar^2}{2}(a_+^\dagger a_+ + a_-^\dagger a_-)(1 + \tfrac{1}{2} a_-^\dagger a_-) = \frac{\hbar^2}{2} N(a_+^\dagger a_+/2 + 1 + a_-^\dagger a_-/2) =$ $\frac{\hbar^2}{2} N(N/2 + 1)$.

20. In the region $x>0$, ψ obeys the same differential equation as the two-sided harmonic oscillator; however, the only acceptable solutions are those that vanish at the origin. Therefore, the eigenvalues are those of the ordinary harmonic oscillator belonging to wave functions of odd parity. Now the parity of the SHO wave functions alternates with increasing n, starting with an even-parity ground state. Hence,

$$E = (4n+3)\hbar\omega/2 = (4n+3)\hbar\sqrt{k/m}/2 \quad \text{with } n=0,1,2,\ldots\ldots$$

(a) Ground state energy $= 3\hbar\sqrt{k/m}/2$ for $n=0$.

(b) From (2.3.31), $\langle x'|1\rangle = \psi_1 = \frac{1}{\sqrt{2}\,x_0}\left(x' - x_0^2 \frac{d}{dx'}\right)(1/\pi^{1/4}\sqrt{x_0})\exp[-\tfrac{1}{2}(x'/x_0)^2]$ (where $x_0 \equiv \sqrt{\hbar/m\omega}$). Hence $\psi_1 = (2/\sqrt{2}\,x_0^{3/2}\pi^{1/4}) x' \exp[-\tfrac{1}{2}(x'/x_0)^2]$ and $\langle x^2\rangle =$ $(2/x_0^3\pi^{1/2})\int_0^\infty x'^4 \exp[-(x'/x_0)^2]dx' = (2\Gamma(5/2)/x_0^3\pi^{1/2}2)x_0^5 = \frac{3}{4}x_0^2 = \frac{3\hbar}{4m\omega}$.

21. The solution to the particle trapped between the rigid wall (one dimensic

$$\psi_n(x) = A_n \sin(n\pi x/L), \; n = 1,2,3,\ldots\ldots$$

Now, $P(x,t)dx = |\psi(x,t)|^2 dx$ is the probability that the particle describe the wave function $\psi(x,t)$ may be found between x and x+dx, therefore in or for the particle to be exactly at $x = L/2$ for $t=0$, $\psi(x,0) = a\delta(x-L/2)$ whe $a = 1$ via normalization.

The eigenvalues corresponding to $\psi_n(x)$ are $E_n = n^2\pi^2\hbar^2/2mL^2$, $n = 1,2,3,$ and by the expansion postulate

$$\psi(x,t) = \sum_n c_n e^{-iE_n t/\hbar}\psi_n(x),$$

the transition amplitude c_n is then given by

$$c_n = \int_0^L \psi_n^*(x)\psi(x,0)dx = \int_0^L A_n \sin(n\pi x/L)\delta(x-L/2)dx = A_n \sin(\tfrac{n\pi}{2}). \quad (3$$

Hence $c_n = (-1)^{\frac{n-1}{2}} A_n$ (for n odd) and $c_n = 0$ (for n even). Therefore (relativ probabilities are $P = |c_n|^2 = |A_n|^2 \delta_{n,odd}$, and (2) reads (using (3))

$$\psi(x,t) = \sum_{n\,odd} A_n^2 \exp[-i(n^2\pi^2/L^2)\hbar t/2m] \sin(n\pi x/L) \, (-1)^{\frac{n-1}{2}} \quad (4)$$

where in fact for normalized $\psi_n(x)$ in (1), $A_n = \sqrt{2/L}$ (independent of n).

22. Our Schrödinger equation is $(-\hbar^2/2m)d^2\psi/dx^2 - v_o\delta(x)\psi = -E\psi$ (i.e. $E>0$ hence $-E<0$ is bound state energy). Integrate above equation from $-\epsilon$ to $+\epsilon$, and let $\epsilon \to 0$, we have

$$\frac{-\hbar^2}{2m}\left(d\psi/dx\big|_{x=\epsilon} - d\psi/dx\big|_{x=-\epsilon}\right) - v_o\psi(0) = 0. \quad (1)$$

For $x \neq 0$,

$$\frac{-\hbar^2}{2m} d^2\psi/dx^2 = -E\psi \quad (2)$$

with bound solutions $\psi(x>0) = A\exp[-(2mE/\hbar^2)^{\frac{1}{2}}x]$ and $\psi(x<0) = A\exp[+(2mE/\hbar^2)^{\frac{1}{2}}x]$ Substitute these solutions into (1), we have $(-\hbar^2/2m)[-(2mE/\hbar^2)^{\frac{1}{2}} - (2mE/\hbar^2)^{\frac{1}{2}}]$. $v_o = 0$ or $E = v_o^2 m/2\hbar^2$. This is an unique solution, no excited bound states a expected.

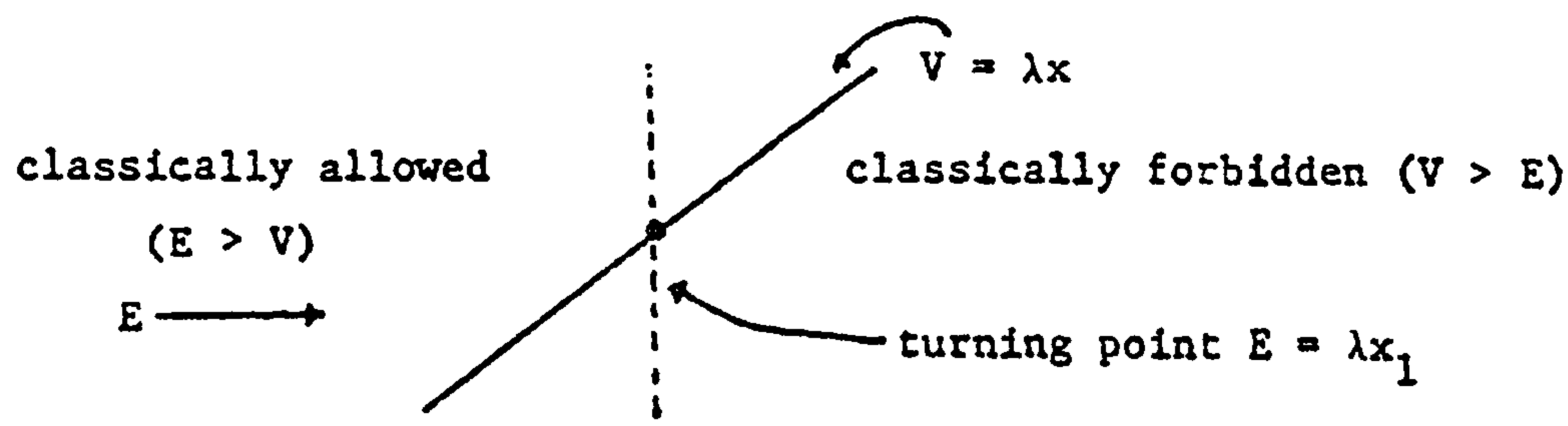
Using the result of problem 22, where $2mE/\hbar^2 = \lambda^2 m^2/\hbar^4$ in our notation, we have $\psi(x,t=0) = A\exp[-m\lambda|x|/\hbar^2]$. The normalization is then $2A^2 \int_0^\infty \exp[-2m\lambda x/\hbar^2]dx = 1$ or $2A^2[\hbar^2/2m\lambda] = 1$ and hence $A = (m\lambda/\hbar^2)^{1/2}$. From (2.5.7) and (2.5.16), we have

$$\psi(x,t>0) = \int_{-\infty}^{\infty} dx'\psi(x',0)K(x,x';t)$$

$$= (m\lambda/\hbar^2)^{1/2}(m/2\pi i\hbar t)^{1/2}\int_{-\infty}^{\infty} \exp[-m\lambda|x'|/\hbar^2]\exp[i(x-x')^2 m/2\hbar t]dx'$$

where we have used $\psi(x',0) = (m\lambda/\hbar^2)^{1/2}\exp[-m\lambda|x'|/\hbar^2]$.

(a)

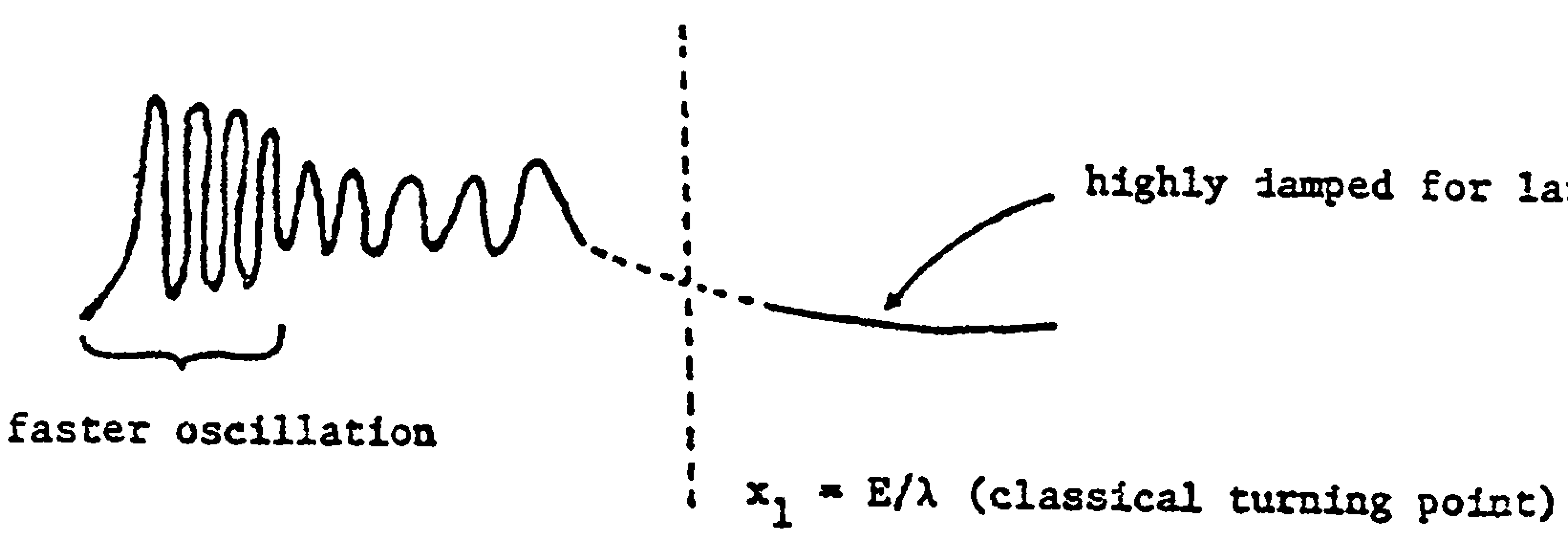


The energy spectrum is continuous. Aside from normalization, the wave functions are:-

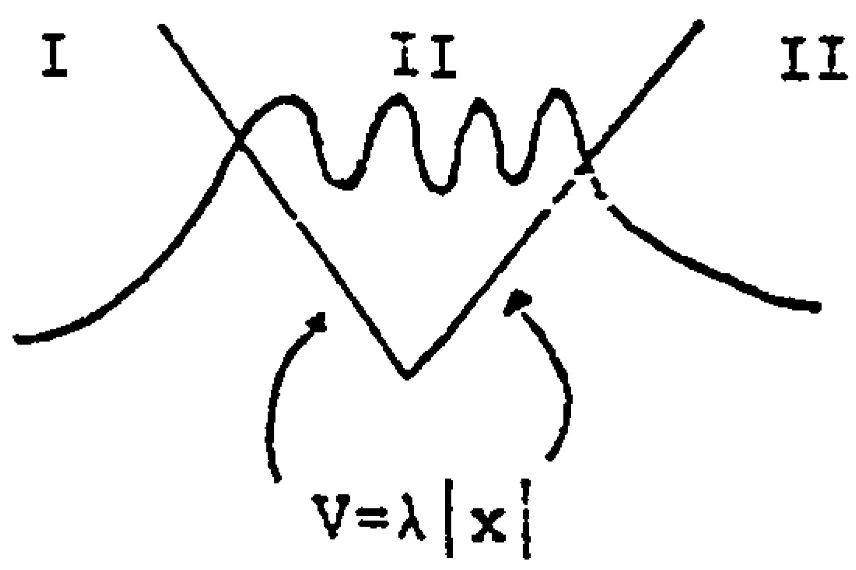
Classically allowed region: $\dfrac{1}{(E-\lambda x)^{1/4}}\, e^{\pm(i/\hbar)\int^x \sqrt{2m(E-\lambda x')}dx'}$

classically forbidden region: $\dfrac{1}{(\lambda x - E)^{1/4}}\, e^{-(1/\hbar)\int^x \sqrt{2m(\lambda x'-E)}dx'}$

These expressions are not valid near $x \approx x_1 = E/\lambda$ (classical turning point). The sketch of energy eigenfunction specified by E looks as follow



(b) The most important change is that the energy spectrum is now discrete, and the wave functions are:



Region I: $\frac{1}{(\lambda x-E)^{1/4}}\, e^{+(1/\hbar)\int^x \sqrt{2m(\lambda x'-E)}dx'}$

Region II: $\frac{1}{(E-\lambda x)^{1/4}} \left\{{\sin \atop \cos}\right\} \left(\frac{1}{\hbar} \int^x \sqrt{2m(E-\lambda x')}dx' \right)$

25. The electron is confined to the interior of a hollow cylindrical shell, where using cylindrical coordinates (ρ, θ, z) the boundary conditions are:-

$$\psi(\rho_a, \theta, z) = \psi(\rho_b, \theta, z) = \psi(\rho, \theta, 0) = \psi(\rho, \theta, L) = 0$$

(a) Inside the cylindrical shell, the Schrödinger equation in cylindrical coordinates reads

$$-\frac{\hbar^2}{2m_e}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\theta^2} + \frac{\partial^2\psi}{\partial z^2}\right] = E\psi = -|E|\psi \text{ (bound states).}$$

Using the method of separation of variables $\psi = R(\rho)Q(\theta)Z(z)$ and

$$\psi(\rho, \theta, z) = (AJ_m(\kappa\rho)+BN_m(\kappa\rho))(Ce^{im\theta}+De^{-im\theta})(Ee^{\alpha z}+Fe^{-\alpha z})$$

are the energy eigenfunctions where m is an integer (to preserve single-valued ψ), $\kappa \equiv \sqrt{\alpha^2 - 2m_e|E|/\hbar^2}$, and with $x = \kappa\rho$, $R(x) = AJ_m(x) + BN_m(x)$ satisfies Bessel equation

$$\frac{d^2R}{dx^2} + \frac{1}{x}\frac{dR}{dx} + (1-m^2/x^2)R = 0$$

Impose next the boundary conditions; $\psi(\rho, \theta, 0) = 0$ implies $E=-F$, hence $Z(z) = E(e^{\alpha z}-e^{-\alpha z}) = 2E\sinh\alpha z$. Now ψ will not vanish at $z = L$ unless α is complex, so write $\alpha = ik$ and $Z(z) = 2Ei\sin kz$, thence $Z(L) = 0$ if and only if $kL = \ell\pi$ (ℓ is non zero integer). Since $\alpha^2<0$, κ is also imaginary. Vanishing of solution at $\rho = \rho_a$ and $\rho = \rho_b$ leads to

$$AJ_m(\kappa\rho_a)+ BN_m(\kappa\rho_a) = 0, \quad AJ_m(\kappa\rho_b)+BN_m(\kappa\rho_b) = 0$$

and eliminating A/B we have $J_m(\kappa\rho_b)N_m(\kappa\rho_a) - N_m(\kappa\rho_b)J_m(\kappa\rho_a) = 0$. Now $\alpha^2 = -k^2 = -\ell^2\pi^2/L^2 = \kappa^2 + 2m|E|/\hbar^2$, therefore $E = (\hbar^2/2m_e)[\kappa^2 + \ell^2\pi^2/L^2]$. If we write $\kappa = k_{mn}$, the n^{th} root of the transcendental equation $J_m(k_{mn}\rho_b)N_m(k_{mn}\rho_a) - N_m(k_{mn}\rho_b)J_m(k_{mn}\rho_a) = 0$, than the energy can be written as

$$E_{\ell mn} = (\hbar^2/2m_e)[k_{mn}^2 + (\ell\pi/L)^2] \quad \begin{cases} \ell = 1,2,3,\ldots. \\ m = 0,1,2,\ldots. \end{cases}$$

(b) In the field free region between $\rho_a<\rho<\rho_b$ of cylindrical shell, we can have case (a) above with $\vec{A} = \phi = 0$ and $(-i\hbar\vec{\nabla})^2/2m\ \psi = E\psi$, or the gauge-invariant form (with $\phi = 0$) $\frac{1}{2m}(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A})^2\psi' = E\psi'$, $\psi' = e^{+ief/\hbar c}\psi$ and $\vec{A} = \vec{\nabla}f$ (with $\vec{\nabla}\times\vec{A} = \vec{B} = 0$). So to find solution with field coupling terms $(\vec{A}\neq 0)$, we find the solution ψ with $\vec{A} = 0$ and then multiply by phase factor $e^{+ief/\hbar c}$, where $f(\vec{r},t) = \int^r d\vec{r}'\cdot\vec{A}(\vec{r}',t)$. Let us choose a gauge in which $A_z = A_\rho = 0$, $A_\theta = (G/\rho)\hat{\theta}$ with G a constant. Then $d\vec{r}' = \rho' d\theta'\hat{\theta}$ and $f(\vec{r},t) = \int_0^\theta \rho' d\theta' G/\rho' = G\theta$, and $\psi' = e^{ie\theta G/\hbar c}\psi$. Now G can be determined using Stoke's theorem that $\int(\vec{\nabla}\times\vec{A})\cdot d\vec{S} = \int_C \vec{A}\cdot d\vec{\ell}$ where C is a closed contour inside cylindrical shell. We have $B\rho_a^2\pi = 2\pi G$, and hence

$$\psi' = e^{ie\theta B\rho_a^2/2\hbar c}\psi = e^{i\beta\theta}\psi \qquad (1)$$

It is evident that the solution ψ' (by symmetry) is of form $\psi' = R(\rho)e^{i\beta\theta}Q(\theta)Z(z)$. Except for $\tilde{Q}(\theta) = e^{i\beta\theta}Q(\theta)$, the forms of $R(\rho)$ and $Z(z)$ are the same as in part (a) of problem but with a different separation constant for $R(\rho)$. Now $Q''(\theta) + m^2Q(\theta) = 0$, hence $\tilde{Q}''(\theta) - 2i\beta\tilde{Q}' + (m^2-\beta^2)\tilde{Q} = 0$. The separated equation for R and $\tilde{Q}$ reads

$$\frac{\rho}{R}\frac{d}{d\rho}(\rho dR/d\rho) + \frac{1}{\tilde{Q}}\frac{d^2\tilde{Q}}{d\theta^2} - \frac{2i\beta}{\tilde{Q}}\frac{d\tilde{Q}}{d\theta} + \rho^2(k^2+2mE/\hbar^2) = 0.$$

Again as in part (a) we have $\kappa^2 = 2m_eE/\hbar^2 - k^2 = 2m_eE/\hbar^2 - \ell^2\pi^2/L^2$ or writing $\kappa = k_{\gamma n}$ with $\gamma^2 = m^2-\beta^2$, we have

$$E = \frac{\hbar^2}{2m_e}[k_{\gamma n}^2 + (\ell\pi/L)^2]$$

where $k_{\gamma n}$ is the n^{th} root of transcendental equation

$$0 = J_\gamma(k_{\gamma n}\rho_b)N_\gamma(k_{\gamma n}\rho_a) - N_\gamma(k_{\gamma n}\rho_b)J_\gamma(k_{\gamma n}\rho_a)$$

($N_\gamma \to J_{-\gamma}$ for γ not an integer). Note because γ depends on β (hence B), the energy eigenvalues are influenced by $\vec{B}$ even though the electron never "touches" the magnetic field.

(c) The ground state of B=0 case is

$$E_{101} = \frac{\hbar^2}{2m_e}[k_{01}^2 + \pi^2/L^2]$$

with $J_0(k_{01}\rho_b)N_0(k_{01}\rho_a) = N_0(k_{01}\rho_b)J_0(k_{01}\rho_a)$, while for $B \neq 0$

$$E_{ground} = \frac{\hbar^2}{2m_e}[k_{\gamma n}^2 + \pi^2/L^2]$$

where γ is not necessarily an integer. However if we require the ground state energy to be unchanged in the presence of B, then

$$\gamma^2 = m^2 - \beta^2 = 0, \quad m \text{ integer, and}$$

$$\pm m = eB\rho_a^2/2\hbar c \to \pi\rho_a^2 B = 2\pi N\hbar c/e,$$

where $N = \pm m = 0, \pm 1, \pm 2, \pm 3, \ldots\ldots$

26. $\psi \propto \exp[iS(x,t)/\hbar]$ and $H = i\hbar\partial\psi/\partial t$, where $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$. Thus $-(\hbar^2/2m)[\frac{\partial}{\partial x}(\frac{i\partial S}{\hbar\partial x}\psi)] + V(x)\psi = i\hbar[\frac{i\partial S}{\hbar\partial t}\psi]$ which simplifies to

$$-\frac{\hbar^2}{2m}[\frac{i\partial^2 S}{\hbar\partial x^2}\psi + (\frac{i\partial S}{\hbar\partial x})(\frac{i\partial S}{\hbar\partial x})\psi] + V(x)\psi = i\hbar[\frac{i\partial S}{\hbar\partial t}\psi]. \qquad (1)$$

If $\lim \hbar \to 0$ in some sense, (1) reduces to $\frac{1}{2m}(\partial S/\partial x)^2 + V(x) = -\partial S/\partial t$ and this is the Hamilton-Jacobi equation. For $V(x) = 0$ we have $\frac{1}{2m}(\partial S/\partial x)^2 = -\partial S/\partial t$ and seek a solution of separable form $S(x,t) = X(x) + T(t)$. Then $\frac{1}{2m}(\partial X/\partial x)^2 = -\partial T/\partial t = \alpha$(a constant), so $T(t) = -\alpha t$ + const and $X(x) = \sqrt{2\alpha m}\, x$ + const. Hence $\psi(x,t) = \exp[i(\sqrt{2\alpha m}\, x - \alpha t)/\hbar]$, a plane wave wave function. Our procedure works because S is linearly dependent on x (i.e. $\partial^2 S/\partial x^2 = 0$).

27. From (2.4.16), the flux $\vec{j}(\vec{x},t) = (-i\hbar/2m)[\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi]$, and the wave function

for a hydrogen atom is $\psi = R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)$ with $Y_{\ell m_\ell}(\theta,\phi) = C_{\ell m_\ell} P_\ell^{m_\ell}(\cos\theta)e^{im_\ell\phi}$.

In spherical coordinates:

$$\vec{\nabla} = \hat{e}_r\frac{\partial}{\partial r} + \hat{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} ,$$

hence $\vec{j} = (m_\ell/mr\sin\theta)|\psi|^2\hat{e}_\phi$, and thus $\vec{j}$ vanishes for $m_\ell = 0$. For $m_\ell \neq 0$, $j>0$ if $m_\ell>0$ and $\vec{j}<0$ if $m_\ell<0$, where $\vec{j}>0$ means that $\vec{j}$ has the same direction as $\hat{e}_\phi$ (i.e. in the direction of increasing ϕ) while $\vec{j}<0$ means that $\vec{j}$ has the opposite direction to $\hat{e}_\phi$ (i.e. in the direction of decreasing ϕ).

28. From (2.5.15) we have $K(x'',t;\, x',t_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp'\exp[\frac{ip'(x''-x')}{\hbar} - \frac{ip'^2(t-t_0)}{2m\hbar}]$.

The exponent can be written after completion of the square as the following

$$\frac{-i(t-t_0)}{2m\hbar}\{p'^2 - \frac{p'(x''-x')2m}{(t-t_0)}\} = \frac{-i(t-t_0)}{2m\hbar}[p' - \frac{m(x''-x')}{(t-t_0)}]^2 + \frac{im(x''-x')^2}{2\hbar(t-t_0)}.$$

Then with $\xi' = p'-m(x''-x')/(t-t_0)$, $d\xi' = dp'$, we have

$$K(x'',t;x',t_0) = \frac{1}{2\pi\hbar}\exp[\frac{im(x''-x')^2}{2\hbar(t-t_0)}]\int_{-\infty}^{\infty} d\xi\exp[-i(t-t_0)\xi^2/2m\hbar]$$

$$= \frac{1}{2\pi\hbar}\exp[\frac{im(x''-x')^2}{2\hbar(t-t_0)}][\frac{2\pi m\hbar}{i(t-t_0)}]^{\frac{1}{2}} = \{\frac{m}{2\pi\hbar i(t-t_0)}\}^{\frac{1}{2}}\exp[\frac{im(x''-x')^2}{2\hbar(t-t_0)}]$$

hence we have established (2.5.16). The three dimensional generalization is evidently

$$K(\vec{x}'',t;\vec{x}',t_0) = \{\frac{m}{2\pi\hbar i(t-t_0)}\}^{\frac{3}{2}}\exp[im(\vec{x}''-\vec{x}')^2/2\hbar(t-t_0)]$$

29. $Z = \int d^3x'\, K(\vec{x}',t;\,\vec{x}',0)|_{\beta = it/\hbar} = \sum_{a'}\exp[-\beta E_{a'}]$ from (2.5.22). The probability $P(E_{a'}) = \exp[-\beta E_{a'}]/Z$, hence the ground state energy (c.f. (1.4.6))

$$U = \sum_{a'} E_{a'}P(E_{a'}) = \sum_{a'} E_{a'}\exp[-\beta E_{a'}]/Z = -\frac{1}{Z}\frac{\partial Z}{\partial\beta} .$$

For a particle in a one dimensional box (with periodic boundary condition), $da' = \frac{L}{2\pi}dk = \frac{L}{2\pi\hbar}dp$, hence $Z = \sum_{a'}\exp[-\beta E_{a'}] \to (L/2\pi\hbar)\int_{-\infty}^{\infty}\exp[-\frac{p^2\beta}{2m}]dp = (\frac{2L}{2\pi\hbar})\int_0^{\infty} e^{-p^2\beta/2m}dp$, $= (L/\pi\hbar)\int_0^{\infty} e^{-p^2\beta/2m}dp$. Let $u^2 = p^2\beta/2m$, $p = \sqrt{2m/\beta}\,u$, $dp = \sqrt{2m/\beta}\,du$, then $Z =$

$(L/\pi\hbar)\sqrt{2m/\beta}\int_0^\infty \exp[-u^2]du = (L/\pi\hbar)\sqrt{2m/\beta}\,\sqrt{\pi}/2 = (L/\hbar)\sqrt{m/2\pi\beta}$. The ground state energy for a particle in a one dimensional "box" is

$$-\frac{1}{Z}\frac{dZ}{d\beta} = -\frac{1}{(L/\hbar)(m/2\pi\beta)^{\frac{1}{2}}}(L/\hbar)\sqrt{m/2\pi}\,(-\tfrac{1}{2})\beta^{-3/2} = 1/2\beta.$$

(Note in thermodynamics $\beta = 1/kT$, hence ground state energy $= kT/2$, an entirely reasonable result).

30. Analogous to (2.5.26) for $K(\vec{x}'',t;\vec{x}',t_0)$, we expect

$$K(\vec{p}'',t;\vec{p}',t_0) = \sum_{a'} \langle\vec{p}''|a'\rangle\langle a'|\vec{p}'\rangle\exp[-iE_{a'}(t-t_0)/\hbar]$$
$$= \sum_{a'} \langle\vec{p}''|\exp[-iHt/\hbar]|a'\rangle\langle a'|\exp[+iHt_0/\hbar]|\vec{p}'\rangle = \langle\vec{p}'',t|\vec{p}',t_0\rangle.$$

For a free particle, $H = p^2/2m$, hence

$$\langle\vec{p}'',t|\vec{p}',t_0\rangle = \sum_{a'} \langle\vec{p}''|\exp[-\frac{ip^2t}{2m\hbar}]|a'\rangle\langle a'|\exp[ip^2t_0/2m\hbar]|\vec{p}'\rangle.$$

31. (a) The classical Lagrangian for a SHO is $L = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2x^2$. The classical action is $S(t,t_0) = \int_{t_0}^{t}dt\,(\tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2x^2)$. For a finite time interval $\Delta t = t_n-t_{n-1}$ and $\Delta x = x_n-x_{n-1}$, we have $S(n,n-1) \cong \Delta t\cdot\frac{m}{2}\{(x_n-x_{n-1})^2/\Delta t^2 - \omega^2\left(\frac{x_n+x_{n-1}}{2}\right)^2\}$

$= \frac{m}{2}\{\frac{(x_n-x_{n-1})^2}{\Delta t} - \omega^2(x_n-\tfrac{1}{2}\Delta x)^2\Delta t\}$. Hence

$$S(n,n-1) \cong \frac{m}{2}\{\frac{(x_n-x_{n-1})^2}{\Delta t} - \omega^2x_n^2\Delta t\} \qquad (1)$$

where terms of order $\Delta x\Delta t$ and $(\Delta x)^2\Delta t$ have been neglected.

(b) The transition amplitude obtained from (1) is

$$\langle x_nt_n|x_{n-1}t_{n-1}\rangle \cong \sqrt{m/2\pi i\hbar\Delta t}\,\exp[iS(n,n-1)/\hbar]$$
$$= \sqrt{m/2\pi i\hbar\Delta t}\,\exp\{\frac{im}{2\hbar}[\frac{(x_n-x_{n-1})^2}{\Delta t} - \omega^2x_n^2\Delta t]\}\ . \qquad (2)$$

From (2.5.18) and (2.5.26)

$$\langle x_nt_n|x_{n-1}t_{n-1}\rangle = K(x_n,t_n;x_{n-1},t_{n-1}) \qquad (3)$$
$$= \sqrt{m\omega/2\pi i\hbar\sin(\omega\Delta t)}\exp[\{im\omega/2\hbar\sin(\omega\Delta t)\}\{(x_n^2+x_{n-1}^2)\cos(\omega\Delta t) - 2x_nx_{n-1}\}].$$

Up to order $(\Delta t)^2$, we have $\sin(\omega\Delta t) \cong \omega\Delta t$, $(x_n^2+x_{n-1}^2)\cos(\omega\Delta t) - 2x_nx_{n-1} \cong$

$(x_n-x_{n-1})^2-[(x_n^2+x_{n-1}^2)/2]\omega^2\Delta t^2 \cong (x_n-x_{n-1})^2 - \omega^2 x_n^2\Delta t^2$, where we have neglected also a term of order $\Delta x\Delta t^2$ because $(x_n^2+x_{n-1}^2)/2 = x_n^2 -[(x_n+x_{n-1})/2]\Delta x$ implies $(x_n^2+x_{n-1}^2)\Delta t^2/2 \cong x_n^2\Delta t^2$. Thus (3) becomes (up to order $(\Delta t)^2$)

$$<x_n t_n|x_{n-1}t_{n-1}> \cong \sqrt{m/2\pi i\hbar\Delta t}\, \exp(\frac{im}{2\hbar}[(x_n-x_{n-1})^2/\Delta t - \omega^2 x_n^2\Delta t]$$

in agreement with (2).

32. The Schwinger action principle states that the following condition determines the transformation function $<x_2t_2|x_1t_1>$ in terms of a given quantum mechanical Lagrangian L

$$\delta<x_2t_2|x_1t_1> = (i/\hbar)<x_2t_2|\delta\int_{t_1}^{t_2} Ldt|x_1t_1>.$$

To obtain $<x_2t_2|x_1t_1>$, let $\delta<x_2t_2|x_1t_1> = (i/\hbar)<x_2t_2|\delta W_{21}|x_1t_1>$ where W_{21} is action in going from initial state x_1t_1 to final state x_2t_2. Also, let $\delta W_{21} = \delta\omega_{21}$ where $\delta\omega_{21}$ is the well-ordered form (c.f. Finkelstein (1973), p.164) of δW_{21}. Then $\delta<x_2t_2|x_1t_1> = \frac{i}{\hbar}<x_2t_2|\ \delta\omega_{21}|x_1t_1> = \frac{i}{\hbar}\ \delta\omega'_{21}<x_2t_2|x_1t_1>$ and thus $\delta\ln<x_2t_2|x_1t_1> = \frac{i}{\hbar}\delta\omega'_{21}$ or

$$<x_2t_2|x_1t_1> = \exp[\frac{i}{\hbar}\omega'_{21}]. \quad (1)$$

The corresponding Feynman expression for $<x_2t_2|x_1t_1>$ [c.f. Finkelstein (1973), p.144] is

$$<x_2t_2|x_1t_1> = \frac{1}{N}\sum_{paths} \exp[(i/\hbar)S_{21}]. \quad (2)$$

The classical limit of (2) is such that as $\hbar/S \to$ small, the probability amplitude $<x_2t_2|x_1t_1>$ will be important only for those varied paths which lie in a narrow tube between x_1t_1 and x_2t_2 enclosing the classical path. On the other hand, to describe the classical limit for (1) (which has a well-ordered exponent instead of a sum over paths), is to consider first the operator Hamilton-Jacobi equation (c.f. Finkelstein (1973), p.166)

$$H(\frac{\partial\omega}{\partial x}\ldots\ldots x\ldots\ldots) + \partial\omega/\partial t = 0. \tag{3}$$

Since ω'_{21} satisfies (3), which arises from a variation of the final state (and is similar to the Schrödinger picture), it is seen that the correspondence limit of ω'_{21} is S, i.e. the probability amplitude (1) approaches the consideration of all possible paths as in the Feynman path integral case (2). Thus in the classical limit, (1) and (2) become equal provided they both are modulated by the factor 1/N (N = total number of individual steps in going from $x_1t_1 \to x_2t_2$).

33\. Take the plane wave $\psi(\vec{r},t) = e^{i(\vec{k}\cdot\vec{r}-\omega t)} = e^{i(\vec{p}\cdot\vec{r}/\hbar - \omega t)} = e^{i\phi(\vec{r},t)}$, where $E_k = p^2/2m = \hbar^2k^2/2m$. Also $\vec{r} = \vec{v}t$, hence $\phi(\vec{r},t) = \vec{p}\cdot\vec{r}/\hbar - \omega r/v$. Let us examine again Fig. 2.5 of text, like before the gravity-induced phase change associated with AB and also with CD are present, but the effects cancel as we compare the two alternative paths. Hence we are concerned with the phase changes $\Delta\phi_{BD}$ and $\Delta\phi_{AC}$, and their difference. Because we are concerned with a time-independent potential the sum of the kinetic energy and potential energy is constant, i.e. $\vec{p}^2/2m + mgz = E$, but the difference in height between level BD and level AC implies a slight difference in $\vec{p}$, or $\lambda\!\!\!^-$. As a result there is an accumulation of phase differences due to $\lambda\!\!\!^-$ difference. Along AC, $\Delta\phi_{AC} = p_{AC}\ell_1/\hbar - \omega\ell_1/v_{AC}$ while along BD $\Delta\phi_{BD} = p_{BD}\ell_1/\hbar - \omega\ell_1/v_{BD}$, where $p_{AC} = mv_{AC}$, $p_{BD} = mv_{BD}$, and [from $p^2/2m + mgz = \text{const}$] we have

$$v_{BD} = (2/m)^{\frac{1}{2}}[mv_{AC}^2/2 - mg\ell_2\sin\delta]^{\frac{1}{2}}.$$

The accumulation of phase difference is $\Delta\phi = |\Delta\phi_{BD} - \Delta\phi_{AC}| \cong |\frac{m}{\hbar}\ell_1(v_{BD}-v_{AC})| = \cdots$
$= (m^2g\ell_1\ell_2\lambda\!\!\!^-\sin\delta)/\hbar^2$ where $p_{AC} = mv_{AC} = \hbar/\lambda\!\!\!^-$.

34\. (a) To verify (2.6.25), i.e. $[\Pi_i,\Pi_j] = (i\hbar e/c)\varepsilon_{ijk}B_k$, we note that $\Pi_i = p_i - eA_i/c$

and $\Pi_j = p_j - eA_j/c$ while $p_{i,j} = \frac{\hbar}{i}\frac{\partial}{\partial x_{i,j}}$ and $\vec{B} = \vec{\nabla}\times\vec{A}$. Explicit calculation of $[\Pi_i,\Pi_j] = [p_i - eA_i/c,\ p_j - eA_j/c] = [p_i,p_j] + [p_i,-eA_j/c] + [-eA_i/c,p_j] + [-eA_i/c,$ $-eA_j/c] = -e[p_i,A_j/c] - e[A_i/c,p_j]$. From problem 29 of Chapter 1 we have $[p_i,$ $F(\vec{x})] = -i\hbar\partial F/\partial x_i$, hence setting $F \equiv A(\vec{x})$ we have $[\Pi_i,\Pi_j] = (i\hbar e/c)\epsilon_{ijk}B_k$.

To verify (2.6.27), with $H = (\vec{p}-e\vec{A}/c)^2 + e\phi$, let us note that from (2.6.22) we have $d\vec{x}/dt = (\vec{p}-e\vec{A}/c)/m$, hence $d^2\vec{x}/dt^2 = \frac{1}{m}(d\vec{p}/dt - \frac{e}{c}d\vec{A}/dt)$. Now $d\vec{p}/dt =$ $\frac{1}{i\hbar}[\vec{p},H]$, hence explicitly $d\vec{p}/dt = -e\vec{\nabla}\phi + \frac{e}{c}\vec{\nabla}(\frac{d\vec{x}}{dt}\cdot\vec{A})$ and $d\vec{A}/dt = \partial\vec{A}/\partial t + \frac{1}{i\hbar}[\vec{A},H]$ $= \vec{\nabla}\cdot\vec{A}\ d\vec{x}/dt + \partial\vec{A}/\partial t$. Thus $\frac{d}{dt}(\vec{p}-e\vec{A}/c) = -e\vec{\nabla}\phi + \frac{e}{c}\vec{\nabla}(\frac{d\vec{x}}{dt}\cdot\vec{A}) - \frac{e}{c}\vec{\nabla}\cdot\vec{A}\ d\vec{x}/dt - \frac{e}{c}\frac{\partial\vec{A}}{\partial t}$ or $\frac{d}{dt}(\vec{p}-e\vec{A}/c) = -e(\vec{\nabla}\phi + \frac{1}{c}\frac{\partial\vec{A}}{\partial t}) + \frac{e}{c}[d\vec{x}/dt \times (\vec{\nabla}\times\vec{A})]$. By symmetrization this can be written as $d\vec{\Pi}/dt = e[\vec{E} + \frac{1}{2c}\{d\vec{x}/dt \times \vec{B} - \vec{B}\times d\vec{x}/dt\}]$ and hence (2.6.27).

(b) To verify $\partial\rho/\partial t + \vec{\nabla}\cdot\vec{J} = 0$ (the continuity equation) with $\vec{J} = \frac{\hbar}{m}\,\mathrm{Im}(\psi^*\vec{\nabla}\psi) -$ $\frac{e}{mc}\vec{A}|\psi|^2$ which can be written as $\vec{J} = \frac{\hbar}{2im}[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*] - \frac{e}{mc}\vec{A}|\psi|^2$. Let us work in Coulomb gauge $\vec{\nabla}\cdot\vec{A} = 0$ (because of gauge invariance this is no loss of generality); we find

$$\vec{\nabla}\cdot\vec{J} = \frac{\hbar}{2mi}[\psi^*(\vec{\nabla}^2\psi)-\psi(\vec{\nabla}^2\psi^*)] - \frac{e}{mc}(\psi^*\vec{A}\cdot\vec{\nabla}\psi + \vec{\nabla}\psi^*\cdot\vec{A}\psi). \tag{1}$$

This can be simplified further by using the time-dependent Schrödinger equation

$$i\hbar\partial\psi/\partial t = \{\frac{-\hbar^2}{2m}\vec{\nabla}^2\psi + \frac{ie\hbar}{mc}(\vec{A}\cdot\vec{\nabla})\psi + \frac{e^2\vec{A}^2}{2m^2c^2}\psi + \phi\psi\} \tag{2}$$

$$-i\hbar\psi^*/\partial t = \{-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^* - \frac{ie\hbar}{mc}(\vec{A}\cdot\vec{\nabla})\psi^* + \frac{e^2\vec{A}^2}{2m^2c^2}\psi^* + \phi\psi^*\} \tag{3}$$

From (2) and (3) we may eliminate $\psi^*\vec{\nabla}^2\psi - \psi(\vec{\nabla}^2\psi^*)$ in (1), the result is

$$\vec{\nabla}\cdot\vec{J} = -(\psi^*\partial\psi/\partial t + \psi\partial\psi^*/\partial t) = -\frac{\partial}{\partial t}(\psi^*\psi) = -\partial\rho/\partial t.$$

35. Take $H_0 = p^2/2m + \phi(r)$, then $H = (\vec{p}-e\vec{A}/c)^2/2m + \phi(r)$. Now $(\vec{p}-e\vec{A}/c)^2 = \vec{p}^2 - [\frac{e}{c}\vec{A}\cdot\vec{p}$

$+\frac{e}{c}\vec{p}\cdot\vec{A}] + \frac{e^2}{c^2}\vec{A}^2$, and we note that $\vec{A}\cdot\vec{p}$ can be written as

$$\vec{A}\cdot\vec{p} = \tfrac{1}{2}(\vec{B}\times\vec{r})\cdot\vec{p} = \frac{\vec{B}}{2}\cdot(\vec{r}\times\vec{p}) = \tfrac{1}{2}\,\vec{B}\cdot\vec{L}$$

while $\vec{A}^2 = \tfrac{1}{4}(\vec{B}\times\vec{r})^2 = \tfrac{1}{4}\,B^2(x^2+y^2)$ when we choose B to be an uniform magnetic field along $\hat{z}$ - direction. Thus in Coulomb gauge $\vec{\nabla}\cdot\vec{A} = 0$, we have

$$H = H_o - \frac{eBL_z}{2mc} + \frac{e^2B^2}{8mc^2}(x^2+y^2).$$

Hence we are led to the correct expression for the interaction of the orbital magnetic moment $(e/2mc)\vec{L}$ with the magnetic field $\vec{B}$. There is also the quadratic Zeeman effect contribution proportional to $B^2(x^2+y^2)$ in H which contributes to the "diamagnetic susceptibility" χ appearing as an energy shift $= -\tfrac{1}{2}\,\chi B^2$.

36. (a) $[p_x-eA_x/c,\ p_y-eA_y/c] = -\frac{e}{c}[p_x,\ A_y] + \frac{e}{c}[p_y,\ A_x] = \frac{ie\hbar}{c}(\partial A_y/\partial x - \partial A_x/\partial y) = ie\hbar B/c$. Hence $[\Pi_x,\ \Pi_y] = ie\hbar B/c$.

(b) From the relation $[\Pi_x,\Pi_y] = ie\hbar B/c$, it is suggestive that we define $X = -c\Pi_y/eB$, then $[X,\Pi_x] = i\hbar$ (just like $[x,p] = i\hbar$). The Hamiltonian then reads

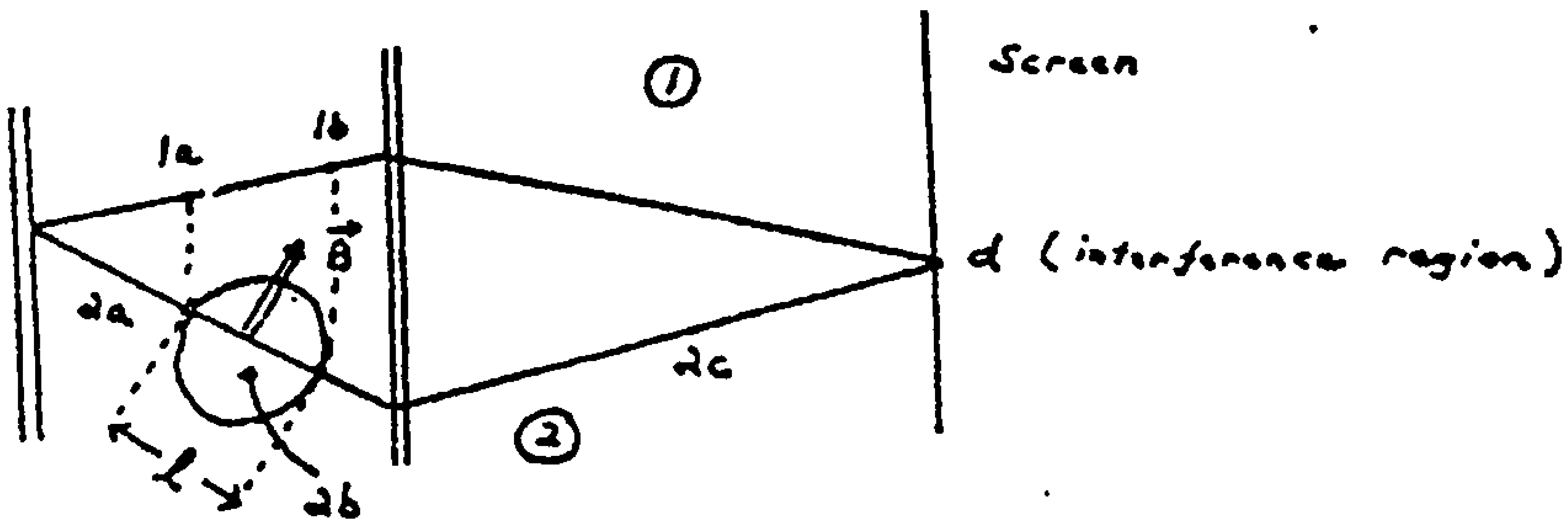
$$H = \Pi_x^2/2m + \Pi_y^2/2m + p_z^2/2m = \Pi_x^2/2m + e^2B^2X^2/2mc^2 + p_z^2/2m \qquad (1)$$

where p_z is same as Π_z because $A_z = 0$. Compare Eq.(1) with the one-dimensional simple harmonic oscillator

$$H_{SHO} = p^2/2m + m\omega^2x^2/2 \qquad (2)$$

for which we know $E_n = \hbar\omega(n+\tfrac{1}{2})$. So evidently the substitution $\omega \to |e\vec{B}|/mc$, we immediately get the energy eigenvalues of (1). (Note: Π_x and X satisfy the same commutation relations as p and x for the harmonic oscillator problem.) We must still add translational kinetic energy in the z-direction. The eigenvalues of p_z, $\hbar k$, are continuous. So the final answer is $E_{k,n} = \hbar^2k^2/2m + \hbar\frac{|eB|}{mc}(n+\tfrac{1}{2})$, where $n = 0,1,2,.......$

37.



Consider the paths ① and ② , and the two wave functions ψ_1 and ψ_2 where $\vec{B} = 0$. Then $\psi_2 = e^{i\delta}\psi_1$ since by symmetry $|\psi_2|^2 = |\psi_1|^2$ for $\vec{B} = 0$. If $\vec{B}$ is turned on in a region (drawn above) of length ℓ, the neutrons will cross the above length in a time T given by

$$v = \ell/T \text{ and } p \equiv m\ell/T \cong \hbar/\bar{\lambda}.$$

Therefore $T = m\ell\bar{\lambda}/\hbar$, and is the time in which the external B-field is acting on the particle. Now let us focus our attention on path ②; the Hamiltonian is

$$H = \begin{cases} H_o = p^2/2m \text{ for 2a, 2c regions} \\ H' = p^2/2m + g_n\mu\vec{\sigma}\cdot\vec{B} \text{ for 2b region} \end{cases}$$

where $\mu = -e\hbar/2mc$.

Now ψ_{2b} is related to ψ_{2a} via the time evolution operator viz: $\psi_{2b} = e^{-iHT/\hbar}\psi_{2a}$. Furthermore ψ_{2d} (wave function at screen via path ②) is given by

$$\psi_{2d} = \exp[-iH_o t/\hbar]\exp[-iH'T/\hbar]\psi_{2a},$$

where t is the time of transit along ② from 2b to 2d. Noting that $p^2/2m = \hbar^2/2m\bar{\lambda}^2$, we find $\exp[-iH'T/\hbar] = \exp[-(iT/\hbar)\{\hbar^2/2m\bar{\lambda}^2 + g_n\mu\vec{\sigma}\cdot\vec{B}\}]$. Choose next $\vec{B} = B\hat{e}_z$ (and remind that $T = m\ell\bar{\lambda}/\hbar$), we find

$$e^{-iH'T/\hbar} = e^{-i\phi}, \text{ where } \phi = \ell/2\bar{\lambda} + g_n\mu\sigma_z Bm\ell\bar{\lambda}/\hbar^2.$$

and

$$\psi_{2d} = e^{-iH_o t/\hbar}e^{-i\phi}\psi_{2a}. \quad (1)$$

A change in B, produces the following change in ϕ

$$\Delta\phi = g_n \mu \sigma_z m \ell \lambda \Delta B/\hbar^2 = \frac{g_n \mu m \ell \lambda}{\hbar^2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Delta B$$

For path 1 we see

$$\psi_{1d} = e^{-iH_o t/\hbar}\, e^{-iH_o T/\hbar} \psi_{1a} \tag{2}$$

where ψ_{1d} is wave function at screen via path 1 and t is the time of transit from 1b to 1d. From Eqs. (1) and (2) we see that maxima occur for $\Delta\phi = 2\pi$ (i.e. no "effect" on phase in region 2a to 2b), therefore

$$2\pi/\Delta B = g_n \mu m \ell \lambda/\hbar^2 \tag{3}$$

and with $|\mu| = |e|\hbar/2mc$, we have $|\Delta B| = 4\pi\hbar c/|e| g_n \lambda \ell$.

Chapter 3

1. The secular equation is $\det(\sigma_y-\lambda I) = 0$, where eigenfunction $\psi = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ satisfies equation $[\sigma_y-\lambda I]\psi = 0$. Roots of secular equation are ±1, hence $[\sigma_y-\lambda I]\psi = 0$ leads to $\alpha/\beta = -i(\lambda=+1)$, $\alpha/\beta = +i(\lambda=-1)$. Also from normalization we have $|\alpha|^2 + |\beta|^2 = 1$, hence $\psi_+ = \frac{1}{\sqrt{2}}\begin{pmatrix}-i\\ 1\end{pmatrix}$ (for $\lambda=+1$) and $\psi_- = \frac{1}{\sqrt{2}}\begin{pmatrix}i\\ 1\end{pmatrix}$(for $\lambda=-1$). Now $s_y = \frac{1}{2}\hbar\sigma_y$ and we know that $s_y\psi_+ = \hbar/2\ \psi_+$ (and $s_y\psi_- = -\hbar/2\ \psi_-$). The general situation is represented by an electron in spin-state $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$, hence the probability that electron will be found in ψ_+ with eigenvalue $+\hbar/2$ when s_y is measured is

$$|\langle\psi_+|s_y|\begin{pmatrix}\alpha\\ \beta\end{pmatrix}\rangle|^2 = \frac{\hbar^2}{4}\left(\frac{1}{\sqrt{2}}\right)^2|+i\alpha+\beta|^2 = \frac{\hbar^2}{8}[1-2\,\mathrm{Im}(\alpha\beta^*)]$$

if $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ is normalized.

2. (a) Write U as $U = (a_o + i\vec{\sigma}.\vec{a})(a_o - i\vec{\sigma}.\vec{a})^{-1} = A(A^\dagger)^{-1}$, than $UU^\dagger = A(A^\dagger)^{-1}A^{-1}A^\dagger = A(AA^\dagger)^{-1}A^\dagger = A\frac{1}{a_o^2+a_1^2+a_2^2+a_3^2}A^\dagger = 1$. Likewise $U^\dagger U = 1$, therefore U is unitary.

Now since $A = \begin{pmatrix}a_o+ia_3 & ia_1+a_2\\ ia_1-a_2 & a_o-ia_3\end{pmatrix}$ and $A^\dagger = \begin{pmatrix}a_o-ia_3 & -ia_1-a_2\\ -ia_1+a_2 & a_o+ia_3\end{pmatrix}$, we have

$\det A = \det A^\dagger = a_o^2+a_1^2+a_2^2+a_3^2$ while from $\det(A^\dagger(A^\dagger)^{-1}) = \det A^\dagger \det(A^{\dagger-1}) = 1$, it is evident that $\det(A^{\dagger-1}) = 1/\det(A^\dagger) = 1/(a_o^2+a_1^2+a_2^2+a_3^2)$. Thus $\det U = \det[A(A^\dagger)^{-1}] = \det A\ \det(A^\dagger)^{-1} = 1$, therefore U is unimodular..

(b) Since $AA^\dagger = (a_o^2+a_1^2+a_2^2+a_3^2)\underline{1} = \alpha\underline{1}$ say, we find

$$U = A(A^\dagger)^{-1} = A^2/\alpha = \frac{1}{\alpha}\cdot\begin{pmatrix}a_o^2-|\vec{a}|^2+2ia_oa_3 & 2a_oa_2+2ia_oa_1\\ -2a_oa_2+2ia_oa_1 & a_o^2-|\vec{a}|^2-2ia_oa_3\end{pmatrix}.$$

Compare with (3.3.7) and (3.3.10), we find angle and axis of rotation appropriate for U as $\cos\frac{\phi}{2} = (a_o^2 - \vec{a}^2)/\alpha$, $\sin\frac{\phi}{2} = 2a_o|\vec{a}|/\alpha$, $n_x = -a_1/|\vec{a}|$, $n_y = -a_2/|\vec{a}|$, and $n_z = -a_3/|\vec{a}|$.

3. The coupled representation has: $|11\rangle = |++\rangle$, $|10\rangle = \frac{1}{2^{1/2}}(|+-\rangle + |-+\rangle)$, $|1-1\rangle = |--\rangle$, and $|00\rangle = \frac{1}{2^{1/2}}(|+-\rangle - |-+\rangle)$ while $\vec{S}_1.\vec{S}_2 = (\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2)/2$. We are interested in the spin function of the system given by $\chi_+^{(e^-)}\chi_-^{(e^+)}$ hence in the $+-$ contribution arising from $|10\rangle$ and $|00\rangle$. So we are interested in the piece of Hamiltonian

$$(H) = \begin{pmatrix} \langle 10|H|10\rangle & \langle 10|H|00\rangle \\ \langle 00|H|10\rangle & \langle 00|H|00\rangle \end{pmatrix} = \begin{pmatrix} A\hbar^2/4 & eB\hbar/mc \\ eB\hbar/mc & -3A\hbar^2/4 \end{pmatrix}.$$

The eigenvalue equation is $(H)\psi = E\psi$, where E satisfies $\det[(H)-E\underline{1}] = 0$. We have $E_\pm = -\frac{1}{4}(A\hbar^2) \pm \frac{1}{2}[(A\hbar^2)^2 + 4(eB\hbar/mc)^2]^{1/2} = -\frac{1}{4}A\hbar^2(1 \mp 2/\cos\theta)$, where $\tan\theta = 2eB/mcA\hbar$.

For $\psi = \begin{pmatrix} x \\ y \end{pmatrix}$, the eigenvalue equation leads to normalized eigenvectors

$$\psi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \text{ for } E_+ \text{ and } \psi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} \text{ for } E_-$$

(a) In the case $A \to 0$, $eB/mc \neq 0$ we have $\theta = \pi/2$, hence $\psi_+ = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$ for $E_+ = +eB\hbar/mc$ and $\psi_- = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$ for $E_- = -eB\hbar/mc$. However the spin function of system is $\chi_+^{(e^-)}\chi_-^{(e^+)}$ and $|+-\rangle = \frac{1}{2^{1/2}}|10\rangle + \frac{1}{2^{1/2}}|00\rangle$ which corresponds to ψ_+ with $E_+ = +eB\hbar/mc$ as the respective eigenvector and eigenvalue.

(b) In the case $eB/mc \to 0$, $A \neq 0$, we have $\theta \to 0$. Hence $\psi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ for $E_+ = +A\hbar^2/4$ and $\psi_- = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$ for $E_- = -3A\hbar^2/4$. Our spin function $|+-\rangle = \frac{1}{2^{1/2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is not therefore an eigenvector corresponding to a definite energy eigenvalue. The expectation value can be computed by noting that $\langle +-|H|+-\rangle = \frac{1}{2}[\langle 10|H|10\rangle + \langle 00|H|10\rangle + \langle 10|H|00\rangle + \langle 00|H|00\rangle] = \frac{1}{2}[A\hbar^2/4 - 3A\hbar^2/4] = -\frac{1}{4}A\hbar^2$.

4. Choose a representation in which $\vec{S}^2$, and S_z are diagonal, so $\vec{S}^2|s,m\rangle = s(s+1)\hbar^2|s,m\rangle$ and $S_z|s,m\rangle = m\hbar|s,m\rangle$. Using ladder operations $S_+ = S_x + iS_y$, $S_- = S_x - iS_y$ where $S_\pm|s,m\rangle = [s(s+1)-m(m\pm 1)]^{1/2}\hbar|s,m\pm 1\rangle$, we have for $s = 1$ (spin 1 par-

ticle)

$$S_x = \frac{\hbar}{2^{1/2}}\begin{bmatrix}0&1&0\\1&0&1\\0&1&0\end{bmatrix},\quad S_y = \frac{\hbar}{2^{1/2}}\begin{bmatrix}0&-i&0\\i&0&-i\\0&i&0\end{bmatrix},\quad S_z = \hbar\begin{bmatrix}1&0&0\\0&0&0\\0&0&-1\end{bmatrix},\quad S^2 = 2\hbar^2\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}.$$

(a) $S_z(S_z + \hbar I)(S_z - \hbar I) = S_z(S_z^2 - \hbar^2 I) \equiv 0$. (b) $S_x(S_x + \hbar I)(S_x - \hbar I) = S_x(S_x^2 - \hbar^2 I) = (\hbar^3/2\sqrt{2})\times[0]$ where $[0]$ is the null matrix. This result is physically reasonable, since same quantity is considered with quantization axis S_x instead of S_z.

5. The Heisenberg equation of motion is $d\vec{K}/dt = \frac{i}{\hbar}[H, \vec{K}]$. Substitute $\vec{K}$ and H into this equation, we have $2d\vec{K}/dt = \frac{i}{\hbar}[K_1^2/I_1+K_2^2/I_2+K_3^2/I_3,\ K_1\vec{e}_1+K_2\vec{e}_2+K_3\vec{e}_3]$. Take the first component for definiteness, we have $2dK_1/dt = \frac{i}{\hbar}[K_2^2/I_2+K_3^2/I_3,\ K_1]$. Now $[K_2^2/I_2,\ K_1] = \frac{1}{I_2}\{K_2,[K_2,K_1]\}$, and since $[K_1,K_2] = -i\hbar K_3$ (true for a <u>rotating system of axis</u>), we have $[K_2^2/I_2,K_1] = i\hbar/I_2\ \{K_2,K_3\}$ and similarly $[K_3^2/I_3,\ K_1] = i\hbar/I_3\ \{K_1,K_3\}$. So $dK_1/dt = \frac{I_2 - I_3}{2I_2I_3}\{K_2,K_3\}$, and similarly $dK_2/dt = \frac{I_3-I_1}{2I_3I_1}\{K_3,K_1\}$ $dK_3/dt = \frac{I_1-I_2}{2I_1I_2}\{K_1,K_2\}$.

The correspondence limit gives $K_iK_j = K_jK_i$ and $K_i = I_i\omega_i$, hence $dK_i/dt = I_i\dot{\omega}_i$. Then the Heisenberg equation of motion for $\vec{K}$, reduces to $I_i\dot{\omega}_i = (I_j-I_k)\omega_j\omega_k$ (i,j,k cyclic permutation of 1,2,3) - that is the Euler's equation of motion.

6. If U represents the rotation with Euler angles α,β,γ, then U must satisfy for infinitesimal rotation angle ε(c.f. (3.1.7)) $U_x(\varepsilon)U_y(\varepsilon) - U_y(\varepsilon)U_x(\varepsilon) = U_z(\varepsilon^2) - 1$. Obviously $U_x(\varepsilon) = e^{iG_1\varepsilon}$, $U_y(\varepsilon) = e^{iG_2\varepsilon}$, and $U_z(\varepsilon) = e^{iG_3\varepsilon}$, and represent infinitesimal rotations around x,y,z axes respectively. In terms of Euler ang-

le rotation $U_x(\varepsilon) = e^{-iG_3\pi/2}e^{iG_2\varepsilon}e^{iG_3\pi/2}$, etc. where we have used (3.3.19). Expand $e^{iG_1\varepsilon}$, $e^{iG_2\varepsilon}$, and $e^{iG_3\varepsilon^2}$ in terms of Taylor series in $U_x(\varepsilon)U_y(\varepsilon)-U_y(\varepsilon)U_x(\varepsilon) = U_z(\varepsilon^2) - 1$, and compare coefficients of ε^2 on both sides. We have $[G_1,G_2] = iG_3$, and similarly $[G_2,G_3] = iG_1$ and $[G_3,G_1] = iG_2$, i.e. $[G_i,G_j] = i\varepsilon_{ijk}G_k$. Compare with commutation relations for $\vec{J}$, viz:- $[J_i,J_j] = i\hbar\varepsilon_{ijk}J_k$, we find $G_i = J_i/\hbar$.

7. A_ℓ are unrotated operators while $U^{-1}A_kU$ are operators under rotation. So $U^{-1}A_kU = \sum_\ell R_{k\ell}A_\ell$ is the connecting equation between unrotated operators and operators obtained after rotation. The operators after rotation are just combinations of unrotated operators. From $U^{-1}A_kU = A_k' = \sum_\ell R_{k\ell}A_\ell$, we obtain for matrix elements $\langle m|A_k'|n\rangle = \sum_\ell R_{k\ell}\langle m|A_\ell|n\rangle$. But this is the same as vector transformation $V_k' = \sum_\ell R_{k\ell}V_\ell$, hence $\langle m|A_k|n\rangle$ transforms like a vector.

8. We are given that $\mathcal{D}^{(\frac{1}{2})}(\alpha,\beta,\gamma)$ is such that (c.f. (3.3.21))

$$\mathcal{D}^{(\frac{1}{2})}(\alpha,\beta,\gamma) = \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos\frac{\beta}{2} & -e^{-i(\alpha-\gamma)/2}\sin\frac{\beta}{2} \\ e^{i(\alpha-\gamma)/2}\sin\frac{\beta}{2} & e^{i(\alpha+\gamma)/2}\cos\frac{\beta}{2} \end{pmatrix}, \tag{1}$$

but this is equivalent to (c.f. (3.2.45))

$$\mathcal{D}^{(\frac{1}{2})}(\hat{n};\theta) = e^{-\frac{i}{2}(\vec{\sigma}\cdot\hat{n})\theta} = \begin{pmatrix} \cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2} & (-in_x-n_y)\sin\frac{\theta}{2} \\ (-in_x+n_y)\sin\frac{\theta}{2} & \cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2} \end{pmatrix} \tag{2}$$

corresponding to rotation about some axis $\hat{n}$ through an angle θ. Since $\mathcal{D}^{(\frac{1}{2})}(\hat{n};\theta)$ is equivalent to $\mathcal{D}^{(\frac{1}{2})}(\alpha,\beta,\gamma)$, we have $\mathrm{Tr}\,\mathcal{D}^{(\frac{1}{2})}(\hat{n};\theta) = \mathrm{Tr}\,\mathcal{D}^{(\frac{1}{2})}(\alpha,\beta,\gamma)$, thence

$$2\cos\frac{\theta}{2} = 2\cos\frac{\beta}{2}\cos\frac{(\alpha+\gamma)}{2} \quad \text{or } \theta = 2\cos^{-1}[\cos\frac{\beta}{2}\cos\frac{(\alpha+\gamma)}{2}]$$

9. (a) A general state in spin ½ system can be written as (suitably normalized)

$$|\alpha\rangle = \cos\frac{\beta}{2}e^{i\alpha/2}|+\rangle + \sin\frac{\beta}{2}e^{-i\alpha/2}|-\rangle.$$

Then $\langle S_x\rangle = \langle\alpha|S_x|\alpha\rangle = \frac{\hbar}{2}\langle\alpha|(|+\rangle\langle-| + |-\rangle\langle+|)|\alpha\rangle = \frac{\hbar}{2}[\cos\frac{\beta}{2}e^{-i\alpha/2}\langle-|+\sin\frac{\beta}{2}e^{i\alpha/2}\langle+|]|\alpha\rangle$

$= \frac{\hbar}{2}[\cos\frac{\beta}{2}e^{-i\alpha/2}\sin\frac{\beta}{2}e^{-i\alpha/2} + \sin\frac{\beta}{2}e^{+i\alpha/2}\cos\frac{\beta}{2}e^{+i\alpha/2}] = \frac{\hbar}{2}\sin\beta\cos\alpha$. Similarly $\langle S_z\rangle = \frac{\hbar}{2}\cos\beta$ and $\langle S_y\rangle = -\frac{\hbar}{2}\sin\beta\sin\alpha$. If we know $\langle S_x\rangle$, $\langle S_z\rangle$ we can obtain β and $\cos\alpha$. However to know the sign of $\sin\alpha$ and hence specify α we need to know sign $(\langle S_y\rangle)$ but not the magnitude of $\langle S_y\rangle$.

(b) Let $\rho = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ be the density matrix in the S_z basis. The ensemble average of an operator O is $[O] = \mathrm{Tr}[\rho O]$. We have

$$[S_x] = \frac{\hbar}{2}\,\mathrm{Tr}[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}] = \frac{\hbar}{2}(b+c) \tag{1}$$

$$[S_y] = \frac{\hbar}{2}\,\mathrm{Tr}[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}] = \frac{i\hbar}{2}(b-c) \tag{2}$$

$$[S_z] = \frac{\hbar}{2}\,\mathrm{Tr}[\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}] = \frac{\hbar}{2}(a-d) \tag{3}$$

and the normalization condition is:

$$\mathrm{Tr}\,\rho = 1 \text{ or } (a+d) = 1. \tag{4}$$

Solving Eqs. (1)-(4), we obtain for elements of the density matrix

$$a=\tfrac{1}{2}[1+[S_z]/\hbar],\ b=\frac{1}{\hbar}[[S_x]-i[S_y]],\ c=\frac{1}{\hbar}[[S_x]+i[S_y]],\ d=\tfrac{1}{2}[1-2[S_z]/\hbar].$$

10. (a) Take (3.4.8) at time t, the density operator $\rho(t)$ reads

$$\rho(t) = \sum_i w_i|\alpha_i,t\rangle\langle\alpha_i,t|.$$

In the Schrödinger picture $|\alpha_i,t\rangle = U(t,t_o)|\alpha_i,t_o\rangle$, then

$$\rho(t) = \sum_i w_iU(t,t_o)|\alpha_i,t_o\rangle\langle\alpha_i,t_o|U^\dagger(t,t_o) = U(t,t_o)(\Sigma_i w_i|\alpha_i,t_o\rangle\langle\alpha_i,t_o|)\times$$
$$U^\dagger(t,t_o) = U(t,t_o)\rho(t_o)U^\dagger(t,t_o)$$

(b) $\rho^2(t) = U(t,t_o)\rho(t_o)U^\dagger(t,t_o)U(t,t_o)\rho(t_o)U^\dagger(t,t_o) = U(t,t_o)\rho^2(t_o)U^\dagger(t,t_o)$. At t=0 we have a pure ensemble (hence idempotent (3.4.13)) i.e. $\rho^2(t_o) = \rho(t_o)$. But $\rho^2(t) = U(t,t_o)\rho(t_o)U^\dagger(t,t_o) = \rho(t)$ and is also idempotent hence we have a pure ensemble at time t also.

11. From (3.4.9) we see that the density matrix of an ensemble of spin 1 systems has form

$$\rho = \begin{pmatrix} a & b & c \\ b^* & d & e \\ c^* & e^* & f \end{pmatrix}$$

where a,d,f are real, and b,c,e complex, i.e. 9 independent variables. However since Tr $\rho = 1$ (3.4.11), we have $a+d+f = 1$, and only 8 independent parameters are needed to characterize the density matrix. If we know $[S_x]$, $[S_y]$, $[S_z]$, we need five more independent quantities. They are: $[S_xS_y]$, $[S_yS_z]$, $[S_zS_x]$, $[S_x^2]$, $[S_y^2]$. Note $[S_xS_y]$, $[S_yS_z]$, and $[S_zS_x]$ may not be real, however the extra conditions (over 3) are not independent of $[S_x]$, $[S_y]$, $[S_z]$. Physically $[S_{x,y,z}]$ are related to measurement of dipole moments of the particles and to completely characterize a spin 1 system we need the five components of the quadrupole tensor.

12. Rotated state is given by

$$U_R|j,m=j\rangle = (1 - iJ_y\varepsilon/\hbar - (J_y^2)\varepsilon^2/2\hbar^2 \ldots\ldots)|j,m=j\rangle.$$

Probability amplitude for being found in the original state is

$$\langle j,m=j|U_R|j,m=j\rangle.$$

We must evaluate the expectation values of J_y, J_y^2, where from $J_y = (J_+ - J_-)/2i$ we have $J_y^2 = -\frac{1}{4}[J_+^2 + J_-^2 - J_+J_- - J_-J_+]$. Evidently $\langle J_y\rangle_{j,m=j} = 0$ and from (3.5.39) and (3.5.40) $\langle (J_y)^2\rangle_{j,m=j} = \frac{1}{4}\langle j,m=j|J_+J_-|j,m=j\rangle = 2j\hbar^2/4$. So

$$\langle j,m=j|U_R|j,m=j\rangle = 1 - (2j\hbar^2/2\hbar^2 4)\varepsilon^2 + \ldots\ldots\ldots$$

Hence probability to order $\varepsilon^2 = |\langle j,m=j|U_R|j,m=j\rangle|^2 = 1 - \frac{1}{2}j\varepsilon^2$.

Alternative solution:

Calculate the probability amplitude for being found in states other than $j=m$. To order ε(in the amplitude) only $m=j-1$ state gets populated. $U_R|j,m=j\rangle = |j,m=j\rangle - (i/\hbar)J_y\varepsilon|j,m=j\rangle = |j,m=j\rangle - \frac{\varepsilon}{2}\frac{1}{2}\sqrt{j}|j,m=j-1\rangle$. The probability for being found in the original state is reduced by $\varepsilon^2 j/2$. So the answer (for our problem) is $1 - \varepsilon^2 j/2$.

13. Looking at the matrix elements we have

$$[G_i,G_j]_{\ell n} = [G_iG_j-G_jG_i]_{\ell n} = (G_i)_{\ell m}(G_j)_{mn} - (G_j)_{\ell m}(G_i)_{mn}$$
$$= -\hbar^2[\varepsilon_{i\ell m}\varepsilon_{jmn} - \varepsilon_{j\ell m}\varepsilon_{imn}] = -\hbar^2[\varepsilon_{mi\ell}\varepsilon_{mnj} - \varepsilon_{mj\ell}\varepsilon_{mni}]$$
$$= -\hbar^2[(\delta_{in}\delta_{\ell j} - \delta_{ij}\delta_{\ell n}) - (\delta_{jn}\delta_{\ell i} - \delta_{ji}\delta_{\ell n})]$$
$$= \hbar^2(\delta_{i\ell}\delta_{jn} - \delta_{in}\delta_{j\ell}) = \hbar^2\varepsilon_{kij}\varepsilon_{k\ell n} = i\hbar\varepsilon_{ijk}(-i\hbar\varepsilon_{k\ell n})$$
$$= i\hbar\varepsilon_{ijk}(G_k)_{\ell n}.$$

Therefore $[G_i,G_j] = i\hbar\varepsilon_{ijk}G_k$. Let us find the unitary matrix which transforms G_i to J_i with J_3 diagonal, than $J_i = U^\dagger G_i U$ where U is made up of the eigenvectors of G_3. The explicit form of G_3 (from $(G_i)_{jk} = -i\hbar\varepsilon_{ijk}$ where j and k are the row and column indices) is

$$G_3 = i\hbar\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and the eigenvalues and eigenvectors are obtained from equation $(G_3-\lambda I)\vec{r}_\lambda = 0$ where λ is a root of $|G_3-\lambda I| = 0$. The eigenvalues and orthonormal eigenvectors can be readily seen to be

$$\lambda=0,\ \vec{r}_o = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix};\ \lambda = +\hbar,\ \vec{r}_+ = \frac{1}{2^{1/2}}\begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix};\ \lambda = -\hbar,\ \vec{r}_- = \frac{1}{2^{1/2}}\begin{pmatrix} -1 \\ i \\ 0 \end{pmatrix}.$$

Hence

$$U = \frac{1}{2^{1/2}}\begin{pmatrix} 1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ -1 & i & 0 \end{pmatrix},$$

and this unitary matrix transforms the Cartesian space representation of the angular momentum operator, i.e. $\vec{G}$, to its spherical basis representation, $\vec{J}$ (j=1). Since the G's and J's satisfy the same Lie algebra (and they both form a group), they are just different representations of the rotation group (irreducible). Therefore, the J's and G's are related via a rotation in the group space. This finite rotation can be obtained from compounding the infinitesimal rotation $\vec{V} \to \vec{V} + \hat{n}\delta\phi \times \vec{V}$ (or $\vec{G} \to \vec{G} + \hat{n}\delta\phi\times\vec{G}$).

14. (a) $J_+J_- = (J_x+iJ_y)(J_x-iJ_y) = J_x^2 + iJ_yJ_x - iJ_xJ_y + J_y^2 = J_x^2 + J_y^2 - i(J_xJ_y-J_yJ_x)$
$= \vec{J}^2-J_z^2-iJ_z(i\hbar) = \vec{J}^2 - J_z^2 + \hbar J_z$. So $\vec{J}^2 = J_z^2 + J_+J_- - \hbar J_z$.

(b) We have on the one hand $\langle jm|J_+J_-|jm\rangle = |c_-|^2$, while using $J_+J_- = \vec{J}^2-J_z^2+\hbar J_z$ we have on the other hand $\langle jm|J_+J_-|jm\rangle = (j(j+1)-m^2+m)\hbar^2$. So $|c_-|^2 = [j(j+1) - m^2 + m]\hbar^2 = (j+m)(j-m+1)\hbar^2$, and by convention we choose $c_- = \sqrt{(j+m)(j-m+1)}\,\hbar$. Thus $J_-|jm\rangle = c_-|j,m-1\rangle$ (or $J_-\psi_{jm} = c_-\psi_{j,m-1}$).

15. Rewrite the wave function in spherical coordinates, i.e. $\psi(\vec{x}) = rf(r)(\sin\theta\cos\phi + \sin\theta\sin\phi + 3\cos\theta)$.

(a) Since $Y_{11} \propto \sin\theta e^{i\phi}$, $Y_{1-1} \propto \sin\theta e^{-i\phi}$, $Y_{10} \propto \cos\theta$, while $e^{\pm i\phi} = \cos\phi \pm i\sin\phi$, it is evident that $\psi(\vec{x})$ is an eigenfunction of $\vec{L}^2$ with $\ell = 1$.

(b) Let us write

$$\sin\theta\cos\phi + \sin\theta\sin\phi + 3\cos\theta = \sin\theta\frac{(e^{i\phi}+e^{-i\phi})}{2} + \sin\theta\frac{(e^{i\phi}-e^{-i\phi})}{2i} + 3\cos\theta$$
$$= (4\pi/3)^{\frac{1}{2}}\{(1-i)Y_{11}/\sqrt{2} - (1+i)Y_{1-1}/\sqrt{2} + 3Y_{10}\}\ . \tag{1}$$

The probability for the particle to be found in the $m_\ell = 0$ state is $9/(9+1+1) = 9/11 = P_o$. Similarly the probabilities for particle to be found in the state $m_\ell = 1$ is $P_1 = 1/11$, and in state $m_\ell = -1$ is $P_{-1} = 1/11$.

(c) The procedure for finding the potential $V(r)$ is first to substitute the wave function into Schrödinger equation, and then use the fact that the wave function is the eigenfunction of $\vec{L}^2$. Now our $\psi(\vec{x}) = R(r)F(\theta,\phi)$, while the Schrödinger equation is $(-\hbar^2/2m)\nabla^2\psi + V(r)\psi = E\psi$. In spherical coordinates

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r}) + \frac{1}{r^2}[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}]$$
$$= [\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial R}{\partial r}) - \frac{\ell(\ell+1)R(r)}{r^2}]F(\theta,\phi) \tag{2}$$

where in (2) we have used (3.6.28) and the fact that $F(\theta,\phi)$ is a linear combination of spherical harmonics (c.f. (1)). Hence for $\ell = 1$, the Schrödinger equation leads to $\frac{-\hbar^2}{2m}[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial R}{\partial r}) - \frac{2}{r^2}R] + V(r)R(r) = ER(r)$, and therefore

$$V(r) = E - \hbar^2/mr^2 + \frac{\hbar^2}{2m}\frac{1}{rR}\frac{d^2}{dr^2}(rR) \tag{3}$$

16. From $L_\pm = L_x \pm iL_y$, we have $L_x = \frac{1}{2}(L_+ + L_-)$ and $L_y = \frac{-i}{2}(L_+ - L_-)$, and from (3.5.39) and (3.5.40) $L_\pm|\ell,m\rangle = c_\pm(\ell,m)|\ell,m\pm1\rangle = \hbar[\ell(\ell+1)-m(m\pm1)]^{\frac{1}{2}}|\ell,m\pm1\rangle$. Hence $\langle L_x\rangle = \langle\ell m|\frac{1}{2}(L_+ + L_-)|\ell m\rangle = 0$ since $\langle\ell m|\ell m'\rangle = \delta_{mm'}$. Similarly $\langle L_y\rangle = \langle\ell m|L_y|\ell m\rangle = 0$. Now $\langle L_x^2\rangle = \langle\ell m|\frac{1}{4}(L_+L_+ + L_+L_- + L_-L_+ + L_-L_-)|\ell m\rangle$. But $L_+L_-|\ell m\rangle = c_-(\ell,m) \times c_+(\ell,m-1)|\ell m\rangle$ and $L_-L_+|\ell m\rangle = c_+(\ell,m)c_-(\ell,m+1)|\ell m\rangle$ while $\langle\ell m|L_+L_+|\ell m\rangle = \langle\ell m|L_-L_-|\ell m\rangle = 0$ since states of different m values are orthogonal. Hence $\langle L_x^2\rangle = \frac{1}{4}\langle\ell m|L_+L_- + L_-L_+|\ell m\rangle = \frac{1}{4}\{c_-(\ell,m)c_+(\ell,m-1) + c_+(\ell,m)c_-(\ell,m+1)\} = \frac{1}{4}\{c_-^2(\ell,m) + c_+^2(\ell,m)\} = \frac{\hbar^2}{4}\{\ell(\ell+1)-m(m-1)+\ell(\ell+1)-m(m+1)\} = \frac{\hbar^2}{2}\{\ell(\ell+1)-m^2\}$. Similarly $\langle L_y^2\rangle = \langle\ell m|-\frac{1}{4}(L_+L_+ - L_+L_- - L_-L_+ + L_-L_-)|\ell m\rangle = \frac{1}{4}\langle\ell m|(L_+L_- + L_-L_+)|\ell m\rangle = \langle L_x^2\rangle$.

<u>Semiclassical interpretation</u>: We know that $\vec{L}^2|\ell m\rangle = \hbar^2\ell(\ell+1)|\ell m\rangle$, $L_z^2|\ell m\rangle = \hbar^2 m^2\ |\ell m\rangle$. Thus $\langle\vec{L}^2\rangle = \ell(\ell+1)\hbar^2$ and $\langle L_z^2\rangle = m^2\hbar^2$. In the classical correspondence $\vec{L}^2 = L_x^2 + L_y^2 + L_z^2$ expresses itself in terms of the corresponding expectation values, and indeed $\langle L_x^2\rangle + \langle L_y^2\rangle + \langle L_z^2\rangle = \frac{1}{2}\hbar^2(\ell(\ell+1)-m^2) + \frac{1}{2}\hbar^2(\ell(\ell+1)-m^2) + m^2\hbar^2 = \ell(\ell+1)\hbar^2 = \langle\vec{L}^2\rangle$.

17. Since (c.f. (3.6.13)) $L_\pm = -i\hbar e^{\pm i\phi}[\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}]$, and we may deduce as usual that $Y_{\frac{1}{2},\frac{1}{2}}(\theta,\phi) \propto e^{i\phi/2}\sqrt{\sin\theta}$ from $L_+Y_{\frac{1}{2},\frac{1}{2}}(\theta,\phi) = 0$.

(a) Apply L_- to $Y_{\frac{1}{2},\frac{1}{2}}$ gives

$$\begin{aligned}Y_{\frac{1}{2},-\frac{1}{2}}(\theta,\phi) &\propto e^{-i\phi}[-i\frac{\partial}{\partial\theta}(e^{i\phi/2}\sqrt{\sin\theta}) - \cot\theta(i/2)e^{i\phi/2}\sqrt{\sin\theta}] \\ &= e^{-i\phi/2}[\sin\theta]^{-\frac{1}{2}}\cos\theta \ .\end{aligned}$$

(b) From $0 = (-i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi})Y_{\frac{1}{2},-\frac{1}{2}}(\theta,\phi)$, we solve for $Y_{\frac{1}{2},-\frac{1}{2}}(\theta,\phi)$ in form $Y_{\frac{1}{2},-\frac{1}{2}} \sim e^{-i\phi/2}f(\theta)$ and obtain solution for $f(\theta)$ from defining differential equation. The answer is $Y_{\frac{1}{2},-\frac{1}{2}} \propto e^{-i\phi/2}(\sin\theta)^{-\frac{1}{2}}$.

Comparing (a) and (b) lead to contradictory results. So this is another argument against half integer ℓ for orbital angular momentum.

18. From (3.6.46) and (3.6.48), we have

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

where $m = 0$ initially. So the probability for finding $|\ell,m'\rangle$ is given by (c.f. (3.6.51))

$$|\mathcal{D}^{(\ell)}_{m'o}(\alpha=0,\beta,\gamma=0)|^2 = |(4\pi/2\ell+1)^{1/2}Y_\ell^{m'*}(\theta=\beta,\phi=0)|^2.$$

From table for $Y^m_{\ell=2}$ (c.f. Appendix A), the probabilities are

$$m'=0:\ \tfrac{1}{4}(3\cos^2\beta-1)^2;\ m'=\pm1:\ \tfrac{3}{2}\cos^2\beta\sin^2\beta;\ m'=\pm2:\ \tfrac{3}{8}\sin^4\beta.$$

It is easy to check that the total probability (summed over m') is unity as expected.

19. Here $K_+ \equiv a_+^\dagger a_-^\dagger$ and $K_- = a_+a_-$. Hence in the Schwinger scheme

$$K_+|n_+,n_-\rangle = \sqrt{(n_++1)(n_-+1)}|n_++1,n_-+1\rangle,\ K_-|n_+,n_-\rangle = \sqrt{n_+n_-}|n_+-1,n_--1\rangle. \quad (1)$$

Let $j = (n_++n_-)/2$ and $m = (n_+-n_-)/2$, and $|n_+,n_-\rangle \to |j,m\rangle$. Than (1) can be re-written as

$$K_+|j,m\rangle = \sqrt{(j+m+1)(j-m+1)}|j+1,m\rangle,\ K_-|j,m\rangle = \sqrt{(j+m)(j-m)}\ |j-1,m\rangle \quad (2)$$

i.e. K_+, K_- are the raising and lowering operators for $j = (n_++n_-)/2$ where n_++n_- corresponds to the total number of spin ½ "particles". The nonvanishing matrix elements of $K_\pm$ are from (2)

$$\begin{aligned}\langle j',m'|K_+|j,m\rangle &= \sqrt{(j+m+1)(j-m+1)}\delta_{j',j+1}\delta_{m',m}\,,\\ \langle j',m'|K_-|j,m\rangle &= \sqrt{(j+m)(j-m)}\delta_{j',j-1}\delta_{m',m}\,.\end{aligned} \quad (3)$$

20. We are to add angular momenta $j_1 = 1$ and $j_2 = 1$ to form $j = 2,1,0$ states. Express all nine $\{j,m\}$ eigenkets in terms of $|j_1j_2,m_1m_2\rangle$. The simplest states are $j_1=1,m_1=\pm1$; $j_2=1,m_2=\pm1$, i.e. $|j=2,m=2\rangle = |{++}\rangle$ and likewise $|j=2,m=-2\rangle = |{--}\rangle$. Using the ladder operator method we have $J_- = J_{1-} \oplus J_{2-}$ and (setting $\hbar = 1$ for convenience) from (3.5.40) $J_-|j,m\rangle = \sqrt{(j+m)(j-m+1)}|j,m-1\rangle$. So $J_-|j=2,m=2\rangle = \sqrt{4}|j=2,m=1\rangle = (J_{1-} \oplus J_{2-})|j_1=1,j_2=1;\ m_1=1,m_2=1\rangle = \sqrt{2}|0+\rangle + \sqrt{2}|{+0}\rangle$, i.e.

$|j=2,m=1\rangle = \frac{1}{2^{1/2}}(|0+\rangle + |+0\rangle)$. Now $J_-|j=2,m=1\rangle = \sqrt{6}|j=2,m=0\rangle = (J_{1-} \oplus J_{2-}) \times [\frac{1}{2^{1/2}}(|0+\rangle + |+0\rangle)] = |-+\rangle + 2|00\rangle + |+-\rangle$. Hence $|j=2,m=0\rangle = \frac{1}{6^{1/2}}(|-+\rangle+2|00\rangle+|+-\rangle)$. Also $J_-|j=2,m=0\rangle = \sqrt{6}|j=2,m=-1\rangle = \frac{1}{6^{1/2}}(\sqrt{2}|-0\rangle+2\sqrt{2}|0-\rangle+2\sqrt{2}|-0\rangle+\sqrt{2}|0-\rangle)$, therefore $|j=2,m=-1\rangle = \frac{1}{2^{1/2}}(|-0\rangle+|0-\rangle)$.

For the j=1 states, let us recognize that $|11\rangle = a|0+\rangle +b|+0\rangle$ with normalization $|a|^2+ |b|^2 = 1$. Since $\langle 21|11\rangle = 0$ by orthogonality, we have $a+b = 0$. Choosing our phase convention to be real, we can write $|11\rangle = \frac{1}{2^{1/2}}(|+0\rangle -|0+\rangle)$. Applying next $J_- = J_{1-} \oplus J_{2-}$ to the two sides respectively, we have $|10\rangle = \frac{1}{2^{1/2}}(|+-\rangle - |-+\rangle)$ and similarly $|1-1\rangle = \frac{1}{2^{1/2}}(|0-\rangle - |-0\rangle)$.

Finally we may write $|j=0,m=0\rangle = \alpha|+-\rangle + \beta|00\rangle + \gamma|-+\rangle$, determine α,β,γ by normalization $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$ and orthogonality to $|j=1,m=0\rangle$ and $|j=2,m=0\rangle$. Choosing α,β,γ to be real we have $|j=0,m=0\rangle = \frac{1}{3^{1/2}}(|+-\rangle - |00\rangle + |-+\rangle)$.

21. (a) Recall (3.5.50) and (3.5.51) that $d^{(j)}_{mm'}(\beta) = \langle jm|\mathcal{D}(\alpha=0,\beta,\gamma=0)|jm'\rangle = \langle jm|\mathcal{D}(R)|jm'\rangle$ where $\mathcal{D}^\dagger(R)J_z\mathcal{D}(R) = \sum_{q'} \mathcal{D}^{(1)*}_{oq'}(R)T^{(1)}_{q'}$ (from (3.10.22a)) and recognizing that J_z is a first rank tensor with q=0, i.e. $T^{(1)}_0$, we have

$$\frac{1}{\hbar}\langle jm'|\mathcal{D}^\dagger(R)J_z\mathcal{D}(R)|jm'\rangle = \frac{1}{\hbar}\sum_{m=-j}^{j}\langle jm'|\mathcal{D}^\dagger(R)J_z|jm\rangle\langle jm|\mathcal{D}(R)|jm'\rangle$$
$$= \sum_{m=-j}^{j}|\langle jm|\mathcal{D}(R)|jm'\rangle|^2 m. \qquad (1)$$

Similarly since only $q' = 0$ contributes, we have

$$\frac{1}{\hbar}\langle jm'|\sum_{q'}\mathcal{D}^{(1)*}_{oq'}T^{(1)}_{q'}|jm'\rangle = \frac{1}{\hbar}\langle jm'|\mathcal{D}^{(1)*}_{oo}(R)J_z|jm'\rangle$$
$$= (4\pi/2\ell+1)^{1/2}\,Y^o_o(\theta=\beta,\phi=0)m' = m'\cos\beta. \qquad (2)$$

So finally from (1) and (2), we have

$$\sum_{m=-j}^{j}|d^{(j)}_{mm'}(\beta)|^2 m = m'\cos\beta. \qquad (3)$$

Check for $j=\frac{1}{2}$, we have from (3.5.52) $d^{(1/2)} = \begin{pmatrix}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2}\end{pmatrix}$. For $m' = \frac{1}{2}$ case, l.h.s. of (3) = $\frac{1}{2}\cos^2\frac{\beta}{2} + (-\frac{1}{2})\sin^2\frac{\beta}{2} = \frac{1}{2}\cos\beta$ = r.h.s. of (3); for $m' = -\frac{1}{2}$ case, l.h.s. of (3) = $\frac{1}{2}(-\sin\frac{\beta}{2})^2 + (-\frac{1}{2})\cos^2\frac{\beta}{2} = -\frac{1}{2}\cos\beta$ = r.h.s. of (3).

(b) From (3.5.51), with $\hbar=1$, we note $d^{(j)}_{m'm}(\beta) = \langle jm'|e^{-i\beta J_y}|jm\rangle$. Now

$$\sum_{m=-j}^{j} m^2|d^{(j)}_{m'm}(\beta)|^2 = \sum_{m=-j}^{j} m^2\langle jm'|e^{-i\beta J_y}|jm\rangle\langle jm|e^{i\beta J_y}|jm'\rangle$$

$$\sum_{m=-j}^{j}\langle jm'|e^{-i\beta J_y}J_z^2|jm\rangle\langle jm|e^{i\beta J_y}|jm'\rangle = \langle jm'|e^{-i\beta J_y}J_z^2 e^{i\beta J_y}|jm'\rangle$$

$$= \langle jm'|\mathcal{D}(R)J_z^2\mathcal{D}^\dagger(R)|jm'\rangle \tag{4}$$

If we examine the rotational properties of J_z^2 using the spherical (irreducible) tensor language, we find $J_z^2 = \frac{1}{3}(\vec{J}^2 + Y_0^{(2)})$ where $\vec{J}^2$ is a scalar under rotation and $Y_0^{(2)}$ is a spherical tensor of rank 2. Hence $\mathcal{D}(R)J_z^2\mathcal{D}^\dagger(R) = \frac{1}{3}\vec{J}^2 + \frac{1}{3}\mathcal{D}(R)Y_0^{(2)}\mathcal{D}^\dagger(R)$ with $\mathcal{D}(R)Y_0^{(2)}\mathcal{D}^\dagger(R) = \sum_{k'=-2}^{2}\mathcal{D}^{(2)}_{k'0}Y^{(2)}_{k'}$. Therefore (4) can be recast as

$$\sum_{m=-j}^{j} m^2|d^{(j)}_{m'm}(\beta)|^2 = \frac{1}{3}j(j+1) + \frac{1}{3}\sum_{k'=-2}^{2}\langle jm'|\mathcal{D}^{(2)}_{k'0}Y^{(2)}_{k'}|jm'\rangle. \tag{5}$$

In the last term on r.h.s. of (5), only $k'=0$ contributes and $\mathcal{D}^{(2)}_{00} = \frac{(3\cos^2\theta-1)}{2}$ (from (3.6.53), (3.5.50), and (3.5.51)). Hence

$$\sum_{m=-j}^{j} m^2|d^{(j)}_{m'm}(\beta)|^2 = \frac{1}{3}j(j+1) + \frac{1}{3}\langle jm'|\mathcal{D}^{(2)}_{00}(3J_z^2-\vec{J}^2)|jm'\rangle$$

$$= \frac{j(j+1)}{2}\sin^2\beta + \frac{m'^2}{2}(3\cos^2\beta - 1)$$

22. (a) We have $J_y = \frac{1}{2i}(J_+ - J_-)$, then using (3.5.41) we derive easily

$$\langle jm'|J_y|jm\rangle = \frac{\hbar}{2i}[\sqrt{j(j+1)-m(m+1)}\langle jm'|j,m+1\rangle - \sqrt{j(j+1)-m(m-1)}\langle jm'|j,m-1\rangle]$$

and therefore for m and m' = +1,0,−1 and j=1 one finds the matrix form for $\langle j=1,m'|J_y|j=1,m\rangle$ as depicted in (3.5.54).

(b) Unlike the $j=\frac{1}{2}$ case, for j=1 only $[J_y^{(j=1)}]^2$ is <u>independent</u> of <u>1</u> and $J_y^{(j=1)}$, and in fact we have $(J_y/\hbar)^{2m+1} = (J_y/\hbar)$ and $(J_y/\hbar)^{2n} = (J_y/\hbar)^2$ where m and n are positive integers. By expansion of the exponential $e^{-iJ_y\beta/\hbar}$ in power series

$$e^{-iJ_y\beta/\hbar} = \sum_{n=0}^{\infty}\frac{(-iJ_y\beta/\hbar)^{2n}}{(2n)!} + \sum_{m=0}^{\infty}\frac{(-iJ_y\beta/\hbar)^{2m+1}}{(2m+1)!}$$

$$= \underline{1} + (J_y/\hbar)^2 \sum_{n=1}^{\infty} \frac{(+\beta)^{2n}(-1)^n}{(2n)!} - i(J_y/\hbar)\sum_{m=0}^{\infty} \frac{(+\beta)^{2m+1}(-1)^m}{(2m+1)!}$$

$$= \underline{1} - (J_y/\hbar)^2(1-\cos\beta) - i(J_y/\hbar)\sin\beta\ .$$

(c) Insert the 3×3 matrix form for J_y from (a), i.e. (3.5.54), into the exponential of part (b) above, we find

$$d^{(j=1)}(\beta) = e^{-iJ_y\beta/\hbar} = \begin{pmatrix} \frac{1+\cos\beta}{2} & -\sin\beta/\sqrt{2} & \frac{1-\cos\beta}{2} \\ \sin\beta/\sqrt{2} & \cos\beta & -\sin\beta/\sqrt{2} \\ \frac{1-\cos\beta}{2} & \sin\beta/\sqrt{2} & \frac{1+\cos\beta}{2} \end{pmatrix}$$

which is (3.5.57).

23.
$$\sum_{j,j'} \langle\alpha_2\beta_2\gamma_2|jmn\rangle\langle jmn|J_3^2|j'm'n'\rangle\langle j'm'n'|\alpha_1\beta_1\gamma_1\rangle = \langle\alpha_2\beta_2\gamma_2|J_3^2|\alpha_1\beta_1\gamma_1\rangle \quad (1)$$

where we note that $\langle jmn|J_3^2|j'm'n'\rangle = n^2\delta_{nn'}\delta_{jj'}\delta_{mm'}$. The l.h.s. of (1) is therefore $\sum_{j,m,n} n^2\mathcal{D}^j_{mn}(\alpha_2\beta_2\gamma_2)\mathcal{D}^{j*}_{mn}(\alpha_1\beta_1\gamma_1)$.

(Solution courtesy of Professor Thomas Fulton)

24. We will represent states as in (3.7.15). For $S_{tot.} = 0$: $\psi = \frac{1}{2^{1/2}}[|+-\rangle - |-+\rangle]$.

(a) Since B makes no measurement there are equal probabilities for measuring s_{1z} to be $\hbar/2$ and $-\hbar/2$. The same is true for s_{1x} because there is no preferred spatial direction.

(b) Now B measures $s_{2z} = \hbar/2$. (i) Since $s_{1z} + s_{2z} = 0$, A must obtain $-\hbar/2$. Now s_{2z} has picked the second piece of ψ which is $\sim\ -|-+\rangle$, therefore $s_{1z}(-|-+\rangle) = +\frac{\hbar}{2}|-+\rangle$. (ii) Since we know that $s_{1z}\psi = (-\hbar/2)\psi$ we cannot predict s_{1x} because $[s_{1x},s_{1z}] \neq 0$ and $|\hat{z}-\rangle = \frac{1}{2^{1/2}}[|\hat{x}+\rangle - |\hat{x}-\rangle]$ as in (3.9.3) yield equal probabilities for $s_{1x} = \hbar/2$ and $-\hbar/2$.

25.
$$\sum_{q'} d^{(1)}_{qq'}V^{(1)}_{q'} = \tfrac{1}{2}\begin{pmatrix} 1+\cos\beta & -\sqrt{2}\sin\beta & 1-\cos\beta \\ \sqrt{2}\sin\beta & 2\cos\beta & -\sqrt{2}\sin\beta \\ 1-\cos\beta & \sqrt{2}\sin\beta & 1+\cos\beta \end{pmatrix}\begin{pmatrix} V^{(1)}_+ \\ V^{(1)}_o \\ V^{(1)}_- \end{pmatrix} = \begin{pmatrix} V^{(1)'}_+ \\ V^{(1)'}_o \\ V^{(1)'}_- \end{pmatrix}. \quad (1)$$

Rewrite r.h.s. in terms of (V_x, V_y, V_z), we have

$$\sum_{q'} d^{(1)}_{qq'} V^{(1)}_{q'} = \begin{pmatrix} -\cos\beta\, V_x/\sqrt{2} - iV_y/\sqrt{2} - \sin\beta\, V_z/\sqrt{2} \\ -\sin\beta\, V_x + \cos\beta\, V_z \\ \cos\beta\, V_x/\sqrt{2} - iV_y/\sqrt{2} + \sin\beta\, V_z/\sqrt{2} \end{pmatrix}. \tag{2}$$

But a rotation through angle β about y-axis leads to $V_x \to V'_x = V_x\cos\beta + V_z\sin\beta$, $V'_y = V_y$, $V_z \to V'_z = V_z\cos\beta - V_x\sin\beta$. Therefore $V^{(1)\prime}_{+} = -(V'_x+iV'_y)/\sqrt{2} = \frac{-1}{2^{1/2}}\cos\beta\, V_x - iV_y/\sqrt{2} - \sin\beta\, V_z/\sqrt{2}$, $V^{(1)\prime}_{o} = V'_z = -\sin\beta\, V_x + V_z\cos\beta$, and $V^{(1)\prime}_{-} = (V'_x - iV'_y)/\sqrt{2} = \cos\beta\, V_x/\sqrt{2} - iV_y/\sqrt{2} + \sin\beta\, V_z/\sqrt{2}$. Thus the r.h.s. of (2) indeed gives r.h.s. of (1) which are just the expectations from the transformation properties of $V_{x,y,z}$ under rotations about the y-axis.

26. (a) Let us take (3.10.27) where $X^{(k_1)}_{q_1}$ and $Z^{(k_2)}_{q_2}$ are irreducible spherical tensors of rank k_1 and k_2 respectively. Then $T^{(k)}_q = \sum_{q_1}\sum_{q_2} \langle k_1k_2;q_1q_2|k_1k_2;kq\rangle X^{(k_1)}_{q_1} Z^{(k_2)}_{q_2}$ is a spherical (irreducible) tensor of rank k. For our problem $k_1 = k_2 = k = 1$, hence

$$T^{(1)}_q = \sum_{q_1}\sum_{q_2} \langle 11;q_1q_2|11;1q\rangle U^{(1)}_{q_1} V^{(1)}_{q_2} \tag{1}$$

From (1), we have $T^{(1)}_{-1} = \frac{1}{2^{1/2}}(-U^{(1)}_{-1}V^{(1)}_{o} + U^{(1)}_{o}V^{(1)}_{-1})$, $T^{(1)}_{o} = \frac{1}{2^{1/2}}(U^{(1)}_{1}V^{(1)}_{-1} - U^{(1)}_{-1}V^{(1)}_{1})$ and $T^{(1)}_{1} = \frac{1}{2^{1/2}}(-U^{(1)}_{o}V^{(1)}_{1} + U^{(1)}_{1}V^{(1)}_{o})$. In terms of $U_{x,y,z}$ and $V_{x,y,z}$, we have

$$\begin{aligned} T^{(1)}_{-1} &= \tfrac{1}{2}[-(U_x - iU_y)V_z + (V_x - iV_y)U_z] \\ T^{(1)}_{o} &= \tfrac{i}{2^{1/2}}[U_xV_y - U_yV_x] \\ T^{(1)}_{1} &= \tfrac{1}{2}[-(U_x + iU_y)V_z + (V_x + iV_y)U_z] \end{aligned} \tag{2}$$

(b) For $k_1 = k_2 = 1$, $k = 2$, we have

$$T^{(2)}_q = \sum_{q_1,q_2} \langle 11;q_1q_2|11;2q\rangle U^{(1)}_{q_1} V^{(1)}_{q_2} . \tag{3}$$

From (3), we find $T^{(2)}_{-2} = U^{(1)}_{-1}V^{(1)}_{-1}$, $T^{(2)}_{-1} = \frac{1}{2^{1/2}}(U^{(1)}_{-1}V^{(1)}_{o} + U^{(1)}_{o}V^{(1)}_{-1})$, $T^{(2)}_{o} = \frac{1}{6^{1/2}}(U^{(1)}_{-1}V^{(1)}_{+1} + 2U^{(1)}_{o}V^{(1)}_{o} + U^{(1)}_{+1}V^{(1)}_{-1})$, $T^{(2)}_{1} = \frac{1}{2^{1/2}}(U^{(1)}_{+1}V^{(1)}_{o} + U^{(1)}_{o}V^{(1)}_{+1})$, and $T^{(2)}_{2} = U^{(1)}_{+1}V^{(1)}_{+1}$. In terms of $U_{x,y,z}$ and $V_{x,y,z}$ we have

$$\begin{aligned}
&T^{(2)}_{-2} = \tfrac{1}{2}(U_x-iU_y)(V_x-iV_y),\; T^{(2)}_{-1} = \tfrac{1}{2}[(U_x-iU_y)V_z + U_z(V_x-iV_y)], \\
&T^{(2)}_{o} = \frac{1}{2\sqrt{6}}[-(U_x-iU_y)(V_x+iV_y) + 4U_zV_z - (U_x+iU_y)(V_x-iV_y)], \\
&T^{(2)}_{1} = -\tfrac{1}{2}[(U_x+iU_y)V_z + U_z(V_x+iV_y)],\; T^{(2)}_{2} = \tfrac{1}{2}(U_x+iU_y)(V_x+iV_y)
\end{aligned} \tag{4}$$

(Remark: (3) is similar to $Y^m_2 = \sum_{m_1m_2} \langle 11;m_1m_2|11;2m\rangle Y^{m_1}_1 Y^{m_2}_2$ for spherical harmonics)

27. (a) According to (3.10.31), the Wigner-Eckart theorem for our problem where $R^{(1)}_{\pm1} = \mp\frac{1}{2^{1/2}}(x\pm iy)$ and $R^{(1)}_{o} = z$ form three components of a spherical tensor of rank 1, reads

$$\langle n',\ell',m'|R^{(1)}_q|n,\ell,m\rangle = \frac{\langle \ell 1;mq|\ell 1;\ell' m'\rangle\langle n'\ell'||R^{(1)}||n\ell\rangle}{\sqrt{2\ell+1}} \tag{1}$$

where the "double bar" matrix element is independent of m and m'. Since $\langle \ell 1;mq|\ell 1;\ell' m'\rangle = 0$ unless $m' = m+q$ and $\ell' = |\ell\pm1|, \ell$, therefore $\langle n',\ell',m'|R^{(1)}_q|n,\ell,m\rangle = 0$ unless $m' = m+q$ and $\ell' = |\ell\pm1|, \ell$.

Furthermore, since we are dealing with a central force potential, the $|n,\ell,m\rangle$ are eigenstates of U_P (parity operator). Hence $U_P|n,\ell,m\rangle = (-1)^\ell|n,\ell,m\rangle$ and $U_P^{-1}R^{(1)}U_P = -R^{(1)}$ and we have $-\langle n',\ell',m'|R^{(1)}|n,\ell,m\rangle = (-1)^\ell(-1)^{\ell'}\langle n',\ell',m'|R^{(1)}|n,\ell,m\rangle$ or $\ell+\ell'$ = odd. Combine with Clebsch-Gordan selection rule from (1), we have

$$\langle n',\ell',m'|R^{(1)}_q|n,\ell,m\rangle = 0, \text{ unless } m'=m+q,\ \ell' = |\ell\pm1|. \tag{2}$$

Again from (1), we have

$$\frac{\langle n',\ell',m_1'|R^{(1)}_{\pm1}|n,\ell,m_1\rangle}{\langle n',\ell',m_2'|R^{(1)}_{o}|n,\ell,m_2\rangle} = \frac{\langle \ell 1;m_1,\pm1|\ell 1;\ell' m_1'\rangle}{\langle \ell 1;m_2,0|\ell 1;\ell' m_2'\rangle} \tag{3}$$

where ℓ', m' satisfy selection rule (2).

(b) Use now wave function $\psi(\vec{x}) = R_{n\ell}(r)Y_\ell^m(\theta,\phi)$. We have

$$<n',\ell',m'|R^{(1)}_{\pm,o}|n,\ell,m> = \int R^*_{n'\ell'}(r)Y_{\ell'}^{m'*}(\theta,\phi)[R^{(1)}_{\pm 1,o}]R_{n\ell}(r)Y_\ell^m(\theta,\phi)d^3\vec{x}$$

$$= \sqrt{4\pi/3}\int_0^\infty R^*_{n'\ell'}(r)r^3R_{n\ell}(r)dr\int d\Omega Y_{\ell'}^{m'*}(\theta,\phi)Y_1^{\pm,o}(\theta,\phi)Y_\ell^m(\theta,\phi). \quad (4)$$

Let $\overline{r^3_{n'n,\ell'\ell}} = \int_0^\infty r^3R^*_{n'\ell'}(r)R_{n\ell}(r)dr$, than (4) reads (using (3.7.73))

$$<n',\ell',m'|R^{(1)}_q|n,\ell,m> = (4\pi/3)^{\frac{1}{2}}\overline{r^3_{n'n,\ell'\ell}}\sqrt{(2\ell+1)3/4\pi(2\ell'+1)}<\ell 1;00|\ell 1;\ell' 0> \cdot$$

$$<\ell 1;mq|\ell' m'> = \overline{r^3_{n'n,\ell'\ell}}\frac{(2\ell+1)^{\frac{1}{2}}}{(2\ell'+1)^{\frac{1}{2}}}<\ell 1;00|\ell 1;\ell' 0><\ell 1;mq|\ell' m'>, \ \ell\neq\ell' \quad (5)$$

$$= 0, \text{ if } \ell = \ell'$$

where $q = \pm 1, 0$. We have thus the selection rule

$$<n',\ell',m'|R^{(1)}_q|n,\ell,m> = 0 \text{ unless } m' = m+q,\ \ell' = |\ell\pm 1| \quad (6)$$

which is identical to part (a). Also note from (5) we have at once the ratio equality (3) where $\ell' = |\ell\pm 1|$, $m_1' = m_1\pm 1$, $m_2' = m_2$.

28. (a) From (3.10.17), $Y_2^{\pm 2} = (\frac{15}{32\pi})^{\frac{1}{2}}\frac{(x^2-y^2\pm 2ixy)}{r^2}$, thence $xy = i(\frac{2\pi}{15})^{\frac{1}{2}}(Y_2^{-2}-Y_2^{+2})r^2$. Similarly, by $Y_2^{\pm 1} = \mp(\frac{15}{8\pi})^{\frac{1}{2}}\frac{(x\pm iy)z}{r^2}$, we have $xz = (\frac{2\pi}{15})^{\frac{1}{2}}(Y_2^{-1}-Y_2^{+1})r^2$, and again by $Y_2^{\pm 2}$ we have $x^2-y^2 = (8\pi/15)^{\frac{1}{2}}(Y_2^2+Y_2^{-2})r^2$. Note $Y_2^m(m=0,\pm 1,\pm 2)$ are components of a spherical (irreducible) tensor of rank 2.

(b) $Q \equiv e<\alpha,j,m=j|(3z^2-r^2)|\alpha,j,m=j>$. First note that $Y_2^o = (\frac{5}{16\pi})^{\frac{1}{2}}\frac{(3z^2-r^2)}{r^2}$, hence $Q = e<\alpha,j,j|\sqrt{16\pi/5}\ r^2Y_2^o|\alpha,j,j>$. Now apply the Wigner-Eckart theorem (3.10.31), we have

$$Q = e(\frac{16\pi}{5})^{\frac{1}{2}}\frac{<j2;j0|j2;jj><\alpha j||r^2Y_2||\alpha j>}{\sqrt{2j+1}} \quad (1)$$

By the same token use of W-E theorem on $e<\alpha,j,m'|(x^2-y^2)|\alpha,j,m=j> = e(\frac{8\pi}{15})^{\frac{1}{2}}\times$ $<\alpha,j,m'|r^2(Y_2^2+Y_2^{-2})|\alpha,j,m=j>$ leads to

$$e\left(\frac{8\pi}{15(2j+1)}\right)^{\frac{1}{2}}[\langle j2;j2|j2;jm'\rangle\langle\alpha j||r^2Y_2||\alpha j\rangle+\langle j2;j-2|j2;jm'\rangle\langle\alpha j||r^2Y_2||\alpha j\rangle] \tag{2}$$
$$= e\sqrt{8\pi/15(2j+1)}\langle j2;j-2|j2;jm'\rangle\langle\alpha j||r^2Y_2||\alpha j\rangle.$$

Substitute $\langle\alpha j||r^2Y_2||\alpha j\rangle$ of (1) into (2), we have

$$e\langle\alpha,j,m'|(x^2-y^2)|\alpha,j,m=j\rangle = (1/\sqrt{2})\left[\frac{\langle j2;j-2|j2;jm'\rangle}{\langle j2;j0|j2;jj\rangle}\right]Q. \tag{3}$$

29. In expression for $H_{int.}$, we recognize that $S_x^2 = \frac{1}{4}(S_+^2 + S_-^2 + \{S_+,S_-\})$ and $S_y^2 = -\frac{1}{4}(S_+^2 + S_-^2 - \{S_+,S_-\})$ with $S_\pm = S_x \pm iS_y$ and $\{S_+,S_-\} = 2(\vec{S}^2 - S_z^2)$. Thus

$$H_{int.} = \frac{eQ}{2s(s-1)\hbar^2}\left[\left(\frac{\partial^2\phi}{\partial x^2}\right)_o \tfrac{1}{4}\{S_+^2 + S_-^2 + 2(\vec{S}^2 - S_z^2)\} + \left(\frac{\partial^2\phi}{\partial y^2}\right)_o \frac{[2(\vec{S}^2-S_z^2)-S_+^2-S_-^2]}{4} + \left(\frac{\partial^2\phi}{\partial z^2}\right)_o S_z^2\right]$$

$$= \frac{eQ}{2s(s-1)\hbar^2}\left[\tfrac{1}{4}\left\{\left(\frac{\partial^2\phi}{\partial x^2}\right)_o - \left(\frac{\partial^2\phi}{\partial y^2}\right)_o\right\}(S_+^2+S_-^2) + \tfrac{1}{2}\left\{\left(\frac{\partial^2\phi}{\partial x^2}\right)_o + \left(\frac{\partial^2\phi}{\partial y^2}\right)_o\right\}(\vec{S}^2-S_z^2)+\left(\frac{\partial^2\phi}{\partial z^2}\right)_o S_z^2\right].$$

Using $\nabla^2\phi = 0$, we can write

$$H_{int.} = A(3S_z^2 - \vec{S}^2) + B(S_+^2 + S_-^2) \tag{1}$$

where $A = \frac{eQ}{4s(s-1)\hbar^2}(\partial^2\phi/\partial z^2)_o$ and $B = \frac{eQ}{8s(s-1)\hbar^2}\{(\partial^2\phi/\partial x^2)_o - (\partial^2\phi/\partial y^2)_o\}$.

From (1) we note that $H_{int.}$ acts on states of definite $|s,m\rangle$ where $s=3/2$ as follows:-

$$H_{int.}|sm\rangle = A(3S_z^2 - \vec{S}^2)|sm\rangle + B(S_+^2 + S_-^2)|sm\rangle$$
$$= 3Am^2\hbar^2|sm\rangle - \frac{15A\hbar^2}{4}|sm\rangle + B\sqrt{(s-m)(s+m+1)(s-m-1)(s+m+2)}\,\hbar^2|s,m+2\rangle$$
$$+ B\sqrt{(s+m)(s-(m-1))(s+m-1)(s-(m-2))}\,\hbar^2|s,m-2\rangle. \tag{2}$$

In the $m,m' = 3/2,-1/2$ and $m,m' = 1/2, -3/2$ basis, the matrix $H_{int.}$ using (2) can be written in block form as

$$H_{int.}^{mm'} = \begin{pmatrix} 3A & 2\sqrt{3}B & 0 & 0 \\ 2\sqrt{3}B & -3A & 0 & 0 \\ 0 & 0 & -3A & 2\sqrt{3}B \\ 0 & 0 & 2\sqrt{3}B & 3A \end{pmatrix}\hbar^2 \quad . \tag{3}$$

Diagonalizing each block of (3), we see that $\lambda_{\pm}\hbar^2 = \pm(12B^2 + 9A^2)^{\frac{1}{2}}\hbar^2$ are the energy eigenvalues for both m,m' = 3/2, -1/2 <u>and</u> m,m' = 1/2, -3/2 basis. The eigenstates $\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$ can be determined for each 2×2 matrix block as

$$\begin{pmatrix} 3A & 2\sqrt{3}B \\ 2\sqrt{3}B & -3A \end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \lambda_{\pm}\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}, \quad \begin{pmatrix} -3A & 2\sqrt{3}B \\ 2\sqrt{3}B & 3A \end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} = \lambda_{\pm}\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix} . \tag{4}$$

Hence for m,m' = 3/2, -1/2 we have $\alpha_2/\alpha_1 = (\lambda_{\pm}-3A)/2\sqrt{3}B$, while for m,m' = -3/2, 1/2 we have $\alpha_2/\alpha_1 = (\lambda_{\pm}+3A)/2\sqrt{3}B$. The energy eigenstates are

$$|\lambda_{\pm}\rangle = 2\sqrt{3}B|3/2,3/2\rangle + (\lambda_{\pm} - 3A)|3/2,-1/2\rangle \tag{5a}$$

$$|\lambda_{\pm}\rangle = 2\sqrt{3}B|3/2,-3/2\rangle + (\lambda_{\pm} + 3A)|3/2,+1/2\rangle . \tag{5b}$$

Note from (5a) and (5b), there exists a two-fold degeneracy, namely there exists two states corresponding to each value of $\lambda(\lambda_{+}$ and $\lambda_{-})$.

1. (a) Assume these particles can be distinguished, in other words they are non-identical particles. Since the three particles do not interact, so the Hamiltonian operator $H = -\frac{\hbar^2}{2m}\vec{\nabla}_1^2 - \frac{\hbar^2}{2m}\vec{\nabla}_2^2 - \frac{\hbar^2}{2m}\vec{\nabla}_3^2 + V(1,2,3)$ can be separated, thus the energy for particle i is $E^{(i)} = (\hbar^2\pi^2/2mL^2)\sum_{j=1}^{3} n_{ij}^2$ where n_{ij} are non-zero integers, and the total energy for the system is $E = E^{(1)}+E^{(2)}+E^{(3)} = \frac{\hbar^2\pi^2}{2mL^2}\sum_{i,j=1}^{3} n_{ij}^2$.

Obviously the lowest energy state is the state with all indices $n_{ij} = 1$, and $E_1 = \frac{9\hbar^2\pi^2}{2mL^2}$. The second lowest energy will be $E_2 = \frac{\hbar^2\pi^2}{2mL^2}(2^2+\underbrace{1+\ldots\ldots+1}_{8\text{ times}}) = \frac{12\hbar^2\pi^2}{2mL^2}$ $= 6\hbar^2\pi^2/mL^2$. The third lowest energy will be $E_3 = \frac{\hbar^2\pi^2}{2mL^2}(2^2+2^2+\underbrace{1+\ldots\ldots+1}_{7\text{ times}}) =$ $15\hbar^2\pi^2/2mL^2$.

Degeneracy. For energy E_1, we have only one spatial wave function, because all indices are 1. For energy E_2, we have 9 spatial wave functions. The reason is that the nine indices (n_{ij}) with $i,j = 1,2,3$ are such that each of them has an equal chance to be 2, while others equal to 1. So the number of distinct possibilities is $\frac{9!}{(9-1)!1!} = 9$. Evidently for E_3 we have $\frac{9!}{(9-2)!2!} = 36$ distinct spatial wave functions. In addition we have $2^3 = 8$ spin wave functions, they are $|{+}{+}{+}\rangle, |{+}{+}{-}\rangle, |{+}{-}{+}\rangle, |{+}{-}{-}\rangle, |{-}{+}{+}\rangle, |{-}{+}{-}\rangle, |{-}{-}{+}\rangle$, and $|{-}{-}{-}\rangle$. So in short E_1 has degeneracy 1x8 = 8, E_2 has degeneracy 9x8 = 72, while E_3 has degeneracy 36x8 = 288.

(b) For four non-identical spin-½ particles system, we have total energy $E = \frac{\hbar^2\pi^2}{2mL^2}\sum_{i=1}^{4}\sum_{j=1}^{3} n_{ij}^2$ where i refers to the i^{th} particle while j refers to the three dimensional space index. Therefore $E_1 = 12\hbar^2\pi^2/2mL^2 = 6\pi^2\hbar^2/mL^2$ and again the degeneracy for spatial wave function is 1. $E_2 = 15\hbar^2\pi^2/2mL^2$ and the number of distinct spatial wave function is $\frac{12!}{(12-1)!1!} = 12$. $E_3 = 9\hbar^2\pi^2/mL^2$, and the number of distinct spatial wave function is $\frac{12!}{(12-2)!2!} = 66$. At the same time we have $2^4 = 16$ spin wave functions $|{+}{+}{+}{+}\rangle, |{+}{+}{+}{-}\rangle, |{+}{+}{-}{+}\rangle, |{+}{+}{-}{-}\rangle$, etc. Hence the three lowest energy levels have degeneracies 16x1 = 16 for E_1, 16x12 = 192 for E_2, and 16x66 = 1056 for E_3.

2. (a) $T_{\vec{d}}\psi(\vec{x}) = \psi(\vec{x}+\vec{d})$, $T_{\vec{d}'}T_{\vec{d}}\psi(\vec{x}) = \psi(\vec{x}+\vec{d}'+\vec{d})$ and $T_{\vec{d}}T_{\vec{d}'}\psi(\vec{x}) = T_{\vec{d}}\psi(\vec{x}+\vec{d}') = \psi(\vec{x}+\vec{d}+\vec{d}')$, so $[T_{\vec{d}},T_{\vec{d}'}]\psi(\vec{x}) = 0$. Since $\psi(\vec{x})$ is arbitrary, we have $[T_{\vec{d}},T_{\vec{d}'}] = 0$. They commute.

(b) $\mathcal{D}(\hat{n},\phi)$ does not commute with $\mathcal{D}(\hat{n}',\phi')$. This is easily seen by taking the case $\hat{n} = \hat{x}$, $\hat{n}' = \hat{y}$ where we know the rotation around x-axis does not commute with the rotation around y-axis.

(c) $T_{\vec{d}}$ and Π do not commute. $\Pi\psi(\vec{x}) = \psi(-\vec{x})$ while $T_{\vec{d}}\Pi\psi(\vec{x}) = \psi(-\vec{x}+\vec{d})$. On the other hand, $T_{\vec{d}}\psi(\vec{x}) = \psi(\vec{x}+\vec{d})$ while $\Pi T_{\vec{d}}\psi(\vec{x}) = \psi(-\vec{x}-\vec{d}) \neq T_{\vec{d}}\,\Pi\psi(\vec{x})$. Hence $[\Pi,T_{\vec{d}}] \neq 0$.

(d) $\Pi\mathcal{D}(\hat{n},\phi)\psi(\vec{x}) = \Pi\psi(\vec{x}') = \psi(-\vec{x}')$ where $\vec{x}' = \mathcal{D}(\hat{n},\phi)\vec{x}$. On the other hand, $\mathcal{D}(\hat{n},\phi)\Pi\psi(\vec{x}) = \mathcal{D}(\hat{n},\phi)\psi(-\vec{x}) = \psi(-\vec{x}')$. So $\Pi\mathcal{D}(\hat{n},\phi)\psi(\vec{x}) = \mathcal{D}(\hat{n},\phi)\Pi\psi(\vec{x})$ and since $\psi(\vec{x})$ is arbitrary, we have $[\Pi,\mathcal{D}(\hat{n},\phi)] = 0$. They commute.

3. $\{A,B\} = AB+BA = 0$. Suppose it is possible, than there exists $|a',b'\rangle$ such that $AB|a',b'\rangle = -BA|a',b'\rangle$ or $a'b' = -b'a'$, thus $a' = 0$ or $b' = 0$. If $A = \vec{p}$ and $B = \Pi$, than $\{\vec{p},\Pi\} = 0$ [because $\Pi^{-1}\vec{p}\Pi = -\vec{p}$], hence momentum eigenstate is usually not parity eigenstate, except for $\vec{p}' = 0$ state.

4. From (3.7.64) we know that

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

(a) For $\ell=0$, only $j=\frac{1}{2}$ (upper sign) is possible, so from (1) we have

$$\mathcal{Y}_{\ell=0}^{j=\frac{1}{2},m=\frac{1}{2}} = \frac{1}{(4\pi)^{\frac{1}{2}}}\begin{pmatrix}1\\0\end{pmatrix} \tag{2}$$

(b)

$$\vec{\sigma}\cdot\vec{x}\,\frac{1}{(4\pi)^{1/2}}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{(4\pi)^{1/2}}\begin{pmatrix}z & x-iy\\ x+iy & -z\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{r}{(4\pi)^{1/2}}\begin{pmatrix}\cos\theta\\ \sin\theta e^{i\phi}\end{pmatrix}$$

$$= -r\begin{pmatrix}-Y_1^0(\theta,\phi)/\sqrt{3}\\ (2/3)^{1/2}Y_1^1(\theta,\phi)\end{pmatrix}, \tag{3}$$

where we recall $Y_1^0 = (3/4\pi)^{1/2}\cos\theta$ and $Y_1^1 = -(3/8\pi)^{1/2}\sin\theta e^{i\phi}$. Compare with $\mathcal{Y}_\ell^{j,m}$ in (1), we see that m must be ½, ℓ must be 1. Take lower sign in (1) hence $j = \ell-\frac{1}{2} = 1-\frac{1}{2} = \frac{1}{2}$. So (3) becomes

$$\vec{\sigma}\cdot\vec{x}\,\frac{1}{(4\pi)^{1/2}}\begin{pmatrix}1\\0\end{pmatrix} = (-r/\sqrt{3})\begin{pmatrix}-\sqrt{1-\frac{1}{2}+\frac{1}{2}}\;Y_1^0\\ \sqrt{1+\frac{1}{2}+\frac{1}{2}}\;Y_1^1\end{pmatrix} = -r\mathcal{Y}_{\ell=1}^{j=\frac{1}{2},m=\frac{1}{2}}\,.$$

Conclusion: Apart from $-r$, we get $\mathcal{Y}_\ell^{j,m}$ with ℓ changed ($\ell=0 \to \ell=1$) and j,m both unchanged from Eq.(2).

(c) The result obtained in (b) is not surprising: $\vec{S}\cdot\vec{x}$ is scalar (spherical tensor of rank 0) under rotation, hence by Wigner-Eckart theorem it cannot change j and m. But under space inversion $\vec{S}\cdot\vec{x}$ is odd. So $\vec{S}\cdot\vec{x}$ connects even parity with odd parity, and we note $\ell=0$ and $\ell=1$ have opposite parity.

5. $\vec{S}\cdot\vec{p}$ is invariant under rotations but changes sign under parity. So it is pseudoscalar. Now since $\delta^3(\vec{x})$ is scalar, so the entire V is pseudoscalar. This means V must connect ℓ odd with ℓ even but cannot change j,m. From elementary first order perturbation theory we have

$$C_{n'\ell'j'm'} = \frac{\langle n',\ell',j',m'|V|n,\ell,j,m\rangle}{E_{n\ell j} - E_{n'\ell'j'}} \tag{1}$$

where $\ell' = \ell\pm1$ (note however $|\Delta\ell| \geq 2$ is impossible because j must remain the same) and $m'=m$, $j'=j$. It is more difficult to evaluate $\langle n',\ell',j',m'|V|n,\ell,j,m\rangle$. The wave function for $|n,\ell,j,m\rangle$ can be written as $R_{n\ell j}\mathcal{Y}_\ell^{j=\ell\pm\frac{1}{2},m}$ where $\mathcal{Y}_\ell^{j,m}$ is the spin angular function and for low Z, $R_{n\ell j}$ has no dependence on j. So $\langle n',\ell',j',m'|V|n,\ell,j,m\rangle$ becomes

$$= \lambda \int d^3x\, R_{n'\ell'j'}(r) \mathcal{Y}_{\ell'}^{j'=\ell'\pm\frac{1}{2},m} \left[\delta^{(3)}(\vec{x})\vec{S}\cdot(-i\hbar\vec{\nabla})+(-i\hbar\vec{\nabla})\cdot\vec{S}\delta^{(3)}(\vec{x})\right]$$

$$\cdot\, R_{n\ell j}(r)\mathcal{Y}_{\ell}^{j=\ell\pm\frac{1}{2},m} \qquad (2)$$

where $(-i\hbar\vec{\nabla})$ in the second term of (2) operates on the wave function to the left. Because of $\delta^{(3)}(\vec{x})$ function, the matrix element vanishes unless $R_{n'\ell'j'}(r)$ or $R_{n\ell j}(r)$ is finite at the origin. This implies that we must have $S_{\frac{1}{2}}$ or $P_{\frac{1}{2}}$ for $|n,\ell,j,m\rangle$ to obtain non-vanishing contributions to $C_{n'\ell'j'm'}$.

6. (a) The plane wave is $\psi(\vec{x},t) = e^{i(\vec{p}.\vec{x}/\hbar-\omega t)}$, hence $\psi^*(\vec{x},-t) = e^{-i(\vec{p}.\vec{x}/\hbar+\omega t)} = e^{i(-\vec{p}.\vec{x}/\hbar-\omega t)}$ and is a plane wave with momentum direction reversed $(-\vec{p})$.

(b) From (3.2.52) with $\alpha=\gamma$, we have $\chi_+(\hat{n}) = \cos\beta/2\; e^{-i\gamma/2}\begin{pmatrix}1\\0\end{pmatrix} + \sin\beta/2\; e^{+i\gamma/2}\begin{pmatrix}0\\1\end{pmatrix}$. $\chi_+^*(\hat{n}) = \cos\beta/2\; e^{i\gamma/2}\begin{pmatrix}1\\0\end{pmatrix} + \sin\beta/2\; e^{-i\gamma/2}\begin{pmatrix}0\\1\end{pmatrix}$, thus $-i\sigma_2\chi_+^*(n)=\cos\frac{\beta}{2}\, e^{\frac{i\gamma}{2}}\begin{pmatrix}0&-1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} + \sin\frac{\beta}{2}e^{\frac{-i\gamma}{2}}\begin{pmatrix}0&-1\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \cos\frac{\beta}{2}e^{\frac{i\gamma}{2}}\begin{pmatrix}0\\1\end{pmatrix} + \sin\frac{\beta}{2}e^{\frac{-i\gamma}{2}}\begin{pmatrix}-1\\0\end{pmatrix}$. But by explicit calculation $(\vec{S}\cdot\hat{n})(-i\sigma_2\chi_+^*(\hat{n})) = (-\hbar/2)(-i\sigma_2\chi_+^*(\hat{n}))$ where $\vec{S} = (\hbar/2)\vec{\sigma}$. Hence $\chi_-(\hat{n}) = -i\sigma_2\chi_+^*(\hat{n})$ is the two component eigenspinor with the spin direction reversed.

7. (a) is proved in (4.4.59) and (4.4.60) of text. (b) The wave function of a plane wave $e^{i\vec{p}.\vec{x}/\hbar}$ can be complex without violating time reversal invariance, because it is degenerate with $e^{-i\vec{p}.\vec{x}/\hbar}$.

8. In momentum space $|\alpha\rangle = \int d^3p'|\vec{p}'\rangle\langle\vec{p}'|\alpha\rangle$ where $\langle\vec{p}'|\alpha\rangle = \phi(\vec{p}')$ is the momentum space wave function for $|\alpha\rangle$. Apply Θ to $|\alpha\rangle$ (using $\Theta|\vec{p}'\rangle = |-\vec{p}'\rangle$) we have

$$\Theta|\alpha\rangle = \int d^3p'|-\vec{p}'\rangle\langle\vec{p}'|\alpha\rangle^* = \int d^3p'|\vec{p}'\rangle\langle-\vec{p}'|\alpha\rangle^*$$

where $\langle-\vec{p}'|\alpha\rangle^*$ is the momentum space wave function for $\Theta|\alpha\rangle$. So $\phi^*(-\vec{p}')$ is the momentum space wave function for the time reversed state.

Alternative method: The momentum space wave function $\phi(\vec{p}')=[\frac{1}{(2\pi\hbar)}]^{\frac{3}{2}}\int d^3x' e^{\frac{-i\vec{p}'.\vec{x}'}{\hbar}}\psi$, when complex conjugated, becomes $\phi^*(\vec{p}')=[\frac{1}{(2\pi\hbar)}]^{\frac{3}{2}}\int d^3x' e^{i\vec{p}'.\vec{x}'/\hbar}\psi^*(\vec{x}')$. Thus momentum space wave function for time reversed state $\phi^*(-\vec{p}\,')$ is

$$\phi^*(-\vec{p}\,') = \frac{1}{(2\pi\hbar)^{3/2}}\left[\int d^3x'\; e^{-i\vec{p}\,'\cdot\vec{x}\,'/\hbar}\psi^*(\vec{x}\,')\right]$$

where $\psi^*(x')$ is the position space wave function for time reversed state.

9. (a) Let Θ be the time reversal operator than $|\alpha\rangle = \mathcal{D}(R)|j,m\rangle$ behaves under time reversal as follows: $\Theta|\alpha\rangle = \Theta\mathcal{D}(R)|j,m\rangle = \Theta e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}|j,m\rangle = \Theta e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}\Theta^{-1}\Theta|j,m\rangle$. But $\Theta\vec{J}\Theta^{-1} = -\vec{J}$ and Θ changes $i \to -i$, therefore $[\Theta,\mathcal{D}(R)] = 0$ and we have $\Theta|\alpha\rangle = \Theta\mathcal{D}(R)|j,m\rangle = \mathcal{D}(R)\Theta|j,m\rangle = (-1)^m\mathcal{D}(R)|j,-m\rangle$, where we have used (4.4.78).

(b) Consider the matrix element $\langle j,-m'|\Theta\mathcal{D}(R)|j,m\rangle = \langle j,-m'|(-1)^m\mathcal{D}(R)|j,-m\rangle = (-1)^m\mathcal{D}^{(j)}_{-m',-m}(R)$. But $\langle j,-m'|\,\Theta\mathcal{D}(R)|j,m\rangle = \sum_{m''}\langle j,-m'|\Theta|j,m''\rangle\langle j,m''|\mathcal{D}(R)|j,m\rangle^* = \sum_{m''}(-1)^{m''}\delta_{-m',-m''}\mathcal{D}^{*(j)}_{m'',m}(R) = (-1)^{m'}\mathcal{D}^{*(j)}_{m',m}(R)$ also (remember Θ contains complex conjugation). Comparing the two expressions for $\langle j,-m'|\Theta\mathcal{D}(R)|j,m\rangle$, we have

$$(-1)^m\mathcal{D}^{(j)}_{-m',-m}(R) = (-1)^{m'}\mathcal{D}^{*(j)}_{m',m}(R) \text{ or } (-1)^{m-m'}\mathcal{D}^{(j)}_{-m',-m}(R) = \mathcal{D}^{*(j)}_{m',m}(R).$$

(c) From part (a) we have $\Theta|\alpha\rangle = (-1)^m\mathcal{D}(R)|j,-m\rangle = \mathcal{D}(R)\Theta|j,m\rangle$, but $i^2 = (-1)$, hence $\mathcal{D}(R)\Theta|j,m\rangle = \mathcal{D}(R)(i^{2m})|j,-m\rangle$ or $\Theta|j,m\rangle = i^{2m}|j,-m\rangle$.

Remarks: The above discussion is for j integer. For $j=\frac{1}{2}$ integer we need to proceed with (4.4.73) with $\eta = +i$ to obtain consistency with (4.4.72a).

10. Under time reversal $\vec{p} \to -\vec{p}$, $\vec{r} \to \vec{r}$, then $[H,\Theta] = 0$ implies invariance under time reversal. Let $|\alpha\rangle$ be an energy eigenket, than $H\Theta|\alpha\rangle = \Theta H|\alpha\rangle = E\Theta|\alpha\rangle$. Hence $\Theta|\alpha\rangle$ is also an eigenket of H with same energy as $|\alpha\rangle$. By the non degenerate assumption we have $\Theta|\alpha\rangle = |\tilde{\alpha}\rangle = e^{i\delta}|\alpha\rangle$ where δ is real. Consider $\langle\alpha|\vec{L}|\alpha\rangle = \langle\tilde{\alpha}|\Theta\vec{L}\Theta^{-1}|\tilde{\alpha}\rangle = -\langle\tilde{\alpha}|\vec{L}|\tilde{\alpha}\rangle = -e^{-i\delta}\langle\alpha|\vec{L}|\alpha\rangle e^{i\delta} = -\langle\alpha|\vec{L}|\alpha\rangle$. Hence $\langle\alpha|\vec{L}|\alpha\rangle = 0$.

If $\psi_\alpha(\vec{x}) = \langle\vec{x}|\alpha\rangle = \sum_{\ell,m}\langle\vec{x}|\ell,m\rangle\langle\ell,m|\alpha\rangle = \sum_{\ell,m}\langle\hat{n}|\ell,m\rangle F_{\ell m}(r) = \sum_{\ell,m}F_{\ell m}(r)Y_\ell^m(\theta,\phi)$, where we have used (3.6.22) and (3.6.23), than $\langle\vec{x}|\Theta|\alpha\rangle = e^{i\delta}\langle\vec{x}|\alpha\rangle$ and thus $\psi_\alpha(\vec{x}) = e^{-i\delta}\langle\vec{x}|\tilde{\alpha}\rangle = e^{-i\delta}\psi_\alpha^*(\vec{x}) = e^{-i\delta}\sum_{\ell,m}F^*_{\ell m}(r)[Y_\ell^m(\theta,\phi)]^* = e^{-i\delta}[\sum_{\ell,m}F^*_{\ell m}(r)(-1)^mY_\ell^{-m}(\theta,\phi)]$

$= e^{-i\delta}\,[\sum_{\ell,m} F^*_{\ell,-m}(r)(-1)^m Y^m_\ell(\theta,\phi)]$, where we have used (3.6.38). Compare the coefficient of $Y^m_\ell(\theta,\phi)$ for the two forms of $\psi_\alpha(\vec{x})$ we have

$$F_{\ell,m}(r) = (-1)^m e^{-i\delta} F^*_{\ell,-m}(r)$$

11. Hamiltonian for a spin-one system is $H = AS_z^2 + B(S_x^2 - S_y^2)$. This problem is similar to problem 29 in Chapter 3. Here

$$S_x = (\hbar/\sqrt{2})\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix},\quad S_y = (\hbar/\sqrt{2})\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix},\quad S_z = \hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix},$$

$$H = \hbar^2\begin{pmatrix}A&0&B\\0&0&0\\B&0&A\end{pmatrix}$$

The 'block' matrix that needs to be diagonalized is of form $\begin{pmatrix}A&B\\B&A\end{pmatrix}$. Hence eigenvalues of H are $E = \hbar^2(A\pm B)$, 0 and the eigenvectors are (in terms of $|s,s_z\rangle$) $\frac{1}{2^{1/2}}(|1,1\rangle + |1,-1\rangle)$, $\frac{1}{2^{1/2}}(|1,1\rangle - |1,-1\rangle)$, and $|1,0\rangle$.

Assume that H is Hermitian than A,B are real, and $\Theta H\Theta^{-1} = A\Theta S_z\Theta^{-1}\Theta S_z\Theta^{-1} + B[\Theta S_x\Theta^{-1}\Theta S_x\Theta^{-1} - \Theta S_y\Theta^{-1}\Theta S_y\Theta^{-1}] = A(-S_z)^2 + B[(-S_x)^2 - (-S_y)^2] = H$. Hence Hamiltonian is invariant under time reversal. Since from (4.4.78) $\Theta|j,m\rangle = (-1)^m|j,-m\rangle$, we have $\Theta[\frac{1}{2^{1/2}}(|1,1\rangle + |1,-1\rangle)] = -\frac{1}{2^{1/2}}(|1,1\rangle + |1,-1\rangle)$, $\Theta[\frac{1}{2^{1/2}}(|1,1\rangle - |1,-1\rangle)] = +\frac{1}{2^{1/2}}(|1,1\rangle - |1,-1\rangle)$, $\Theta|1,0\rangle = |1,0\rangle$.

Chapter 5

1. (a) The first order correction is via (5.1.37) just $\langle 0|bx|0\rangle = 0$. The second order correction for the energy is (c.f. (5.1.42) and (5.1.43))

$$\Delta E = -\sum_n \frac{|\langle n|bx|0\rangle|^2}{E_n - E_o} = -b^2 \sum_n \frac{|\langle n|x|0\rangle|^2}{E_n - E_o},$$

where $E_n = (n+\frac{1}{2})\hbar\omega$. Now $\langle n|x|0\rangle = \sqrt{\hbar/2m\omega}\,\delta_{n1}$, so $\Delta E = -b^2(\sqrt{\hbar/2m\omega})^2/(E_1-E_o) = -b^2/2m\omega^2$ is the energy shift, and the energy of the ground state becomes $E^{(o)} = \frac{1}{2}\hbar\omega + \Delta E = \frac{1}{2}\hbar\omega - b^2/2m\omega^2$.

(b) The Schrödinger equation for this problem is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (\tfrac{1}{2}m\omega^2 x^2 + bx)\psi = E^{(o)}\psi.$$

Let $x' = x + b/m\omega^2$, than above equation can be reduced to

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx'^2} + \tfrac{1}{2}m\omega^2[x'^2 - (b/m\omega^2)^2]\psi = E^{(o)}\psi$$

that is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx'^2} + \tfrac{1}{2}m\omega^2 x'^2\psi = (E^{(o)} + b^2/2m\omega^2)\psi.$$

This is again a SHO equation with $E' = E^{(o)} + b^2/2m\omega^2$. For lowest energy value $E' = \frac{1}{2}\hbar\omega$, hence $E^{(o)} = \frac{1}{2}\hbar\omega - b^2/2m\omega^2$ which is exactly the same as the perturbation result in (a).

2. From (5.1.44) with $k \leftrightarrow n$ and $\lambda \to g$, we have

$$|k\rangle = |k^{(o)}\rangle + g \sum_{n\neq k} \frac{|n^{(o)}\rangle V_{nk}}{E_k^{(o)} - E_n^{(o)}} + \ldots\ldots\ldots$$

Using orthonormality of $|k^{(o)}\rangle$ and $|n^{(o)}\rangle$ we have

$$\langle k|k\rangle = 1 + g^2 \sum_{n\neq k} \frac{|V_{nk}|^2}{(E_k^{(o)} - E_n^{(o)})^2} + \ldots\ldots\ldots$$

and

$$\frac{|\langle k|k^{(o)}\rangle|^2}{|\langle k|k\rangle|^2} = 1 - g^2 \sum_{n\neq k} \frac{|V_{nk}|^2}{(E_k^{(o)} - E_n^{(o)})^2} + O(g^3)$$

3. Solving the Schrödinger equation for the unperturbed system, we can easily find the energy eigenfunctions. They are $\psi_G = \sqrt{2/L}\sqrt{2/L}\,\sin\pi x/L\,\sin\pi y/L = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi y}{L}$ for ground state, and $\psi_{el}^{(1)} = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{2\pi y}{L}$ or $\psi_{el}^{(2)} = \frac{2}{L}\sin\frac{2\pi x}{L}\,\sin\frac{\pi y}{L}$ for the first excited state. So obviously the <u>zeroth</u> order eigenfunction for the <u>ground</u> state is just $\psi_G = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi y}{L}$, with the first order energy shift of $<1|\lambda xy|1> = \int_0^L \int_0^L \frac{4}{L^2}\,\lambda xy\sin^2\pi x/L\,\sin^2\pi y/L\,dxdy = \frac{1}{4}\lambda L^2$, i.e. $\Delta E^{(o)} = \lambda L^2/4$. For the first excited state, there is degeneracy and the perturbation in general lift the degeneracy. We need to construct the perturbation matrix by evaluating

$$<\psi_{el}^{(1)}|V_1|\psi_{el}^{(1)}> = \frac{4\lambda}{L^2}\int_0^L\int_0^L xy\sin^2\pi x/L\,\sin^2 2\pi y/L\,dxdy = \frac{1}{4}\lambda L^2$$

$$<\psi_{el}^{(1)}|V_1|\psi_{el}^{(2)}> = \frac{4\lambda}{L^2}\int_0^L\int_0^L xy\sin\frac{\pi x}{L}\sin\frac{2\pi x}{L}\sin\frac{2\pi y}{L}\sin\frac{\pi y}{L}dxdy = \frac{4^4}{81}\lambda L^2/\pi^4$$

while by symmetry $<\psi_{el}^{(2)}|V_1|\psi_{el}^{(2)}> = <\psi_{el}^{(1)}|V_1|\psi_{el}^{(1)}>$ and $<\psi_{el}^{(2)}|V_1|\psi_{el}^{(1)}> = <\psi_{el}^{(1)}|V_1|\psi_{el}^{(2)}>$. So the perturbation matrix is

$$\Delta = \frac{\lambda L^2}{4\pi^4}\begin{pmatrix}\pi^4 & 4^5/81\\ 4^5/81 & \pi^4\end{pmatrix}.$$

Diagonalizing Δ with $\det(\Delta-\lambda' I) = 0$ and

$$(\Delta-\lambda' I)\begin{pmatrix}a\psi_{el}^{(1)}\\ b\psi_{el}^{(2)}\end{pmatrix} = 0$$

where $a^2 + b^2 = 1$ (normalization), we get $a = 1/\sqrt{2}$, $b = \pm 1/\sqrt{2}$ and

$$\Delta' = \frac{\lambda L^2}{4\pi^4}\begin{pmatrix}\pi^4+4^5/81 & 0\\ 0 & \pi^4-4^5/81\end{pmatrix}.$$

Hence energy shifts for the first excited state are

$$\frac{(\pi^4+4^5/81)\lambda L^2}{4\pi^4} \approx 0.28\lambda L^2 \text{ and } \frac{(\pi^4-4^5/81)\lambda L^2}{4\pi^4} \approx 0.22\lambda L^2$$

with corresponding zeroth order energy eigenfunctions

$$\frac{1}{\sqrt{2}}\,\frac{2}{L}\left[\sin\frac{\pi x}{L}\sin\frac{2\pi y}{L} + \sin\frac{2\pi x}{L}\sin\frac{\pi y}{L}\right] \quad\text{and}\quad \frac{1}{\sqrt{2}}\,\frac{2}{L}\left[\sin\frac{\pi x}{L}\sin\frac{2\pi y}{L} - \sin\frac{2\pi x}{L}\sin\frac{\pi y}{L}\right]$$

respectively.

4. (a) State vector for energy eigenstate is characterized by $|n_x,n_y\rangle$, and wave function is given by $\psi_{n_x}(x)\psi_{n_y}(y)$ where $\psi_{n_x}(x)$ and $\psi_{n_y}(y)$ are individually wave functions for one dimensional SHO. The energy for the isotropic two dimensional oscillator is just the sum of the energies for one dimensional oscillators, i.e. $E_{n_x n_y} = \hbar\omega(n_x + \frac{1}{2} + n_y + \frac{1}{2})$. The three lowest-lying states are $(n_x,n_y) = (0,0)$, $(1,0)$, $(0,1)$ with energies $\hbar\omega$, $2\hbar\omega$, $2\hbar\omega$, respectively. Evidently the first excited states are doubly degenerate.

(b) The first order energy shift is clearly zero for the ground state $(0,0)$, since $\langle 0,0|xy|0,0\rangle = 0$ because in $\langle 0|x|0\rangle$ (and $\langle 0|y|0\rangle$) $n_x(n_y)$ must change by one unit. For the first excited states we use the formalism of degenerate perturbation theory by diagonalizing $V = \delta m\omega^2 xy$. In the $(1,0)$ and $(0,1)$ basis

$$V = \delta m\omega^2\begin{pmatrix} 0 & x_{10}y_{01} \\ x_{01}y_{10} & 0 \end{pmatrix} = \tfrac{1}{2}\delta\hbar\omega\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and hence behaves like σ_x. By same method as problem 3 above, we get zeroth order energy eigenkets $\frac{1}{2^{1/2}}(|10\rangle+|01\rangle)$ with $\Delta^{(1)} = \frac{1}{2}\delta\hbar\omega$ and $\frac{1}{2^{1/2}}(|10\rangle-|01\rangle)$ with $\Delta^{(1)} = -\frac{1}{2}\delta\hbar\omega$. So to summarize we have ground state $|0,0\rangle$ with energy $E = \hbar\omega$ (no first order shift) and first excited states $\frac{1}{2^{1/2}}(|10\rangle+|01\rangle)$ with $E \simeq (2+\delta/2)\hbar\omega$ and $\frac{1}{2^{1/2}}(|10\rangle-|01\rangle)$ with $E \simeq (2-\delta/2)\hbar\omega$.

(c) Now $m\omega^2(x^2+y^2)/2 + \delta m\omega^2 xy = \frac{m\omega^2}{2}\{(1+\delta)(x+y)^2/2 + (1-\delta)(x-y)^2/2\}$. Let us rotate coordinates by 45°, than $X \equiv (x+y)/\sqrt{2}$, $Y \equiv (x-y)/\sqrt{2}$. So

$$H = p_X^2/2m + p_Y^2/2m + m[\omega^2(1+\delta)]X^2/2 + m[\omega^2(1-\delta)]Y^2/2$$

and is effectively again a two dimensional SHO with ω replaced by $\sqrt{1\pm\delta}\,\omega$ in the

(X,Y) system. The exact energy for the ground state is $\frac{1}{2}\hbar\omega\sqrt{1+\delta} + \frac{1}{2}\hbar\omega\sqrt{1-\delta} = \hbar\omega + O(\delta^2)$. There is therefore no change in energy if only terms linear in δ are kept. The exact energy for $(n_x,n_y) = (1,0)$ is $\hbar\omega\sqrt{1+\delta}(1+\frac{1}{2}) + \hbar\omega\sqrt{1-\delta}\,\frac{1}{2} = \hbar\omega(2+\delta/2) + O(\delta^2)$; similarly for $(n_x,n_y) = (0,1)$, by letting $\delta \to -\delta$, we have exact energy $\hbar\omega(2-\delta/2) + O(\delta^2)$. Ignoring $O(\delta^2)$ contributions, the results are the same as in (b).

5. The Hamiltonian for the system is $H = H_o + \frac{1}{2}\epsilon m\omega^2 x^2 = p_x^2/2m + \frac{1}{2}(1+\epsilon)m\omega^2 x^2$, hence $V_{ko} = \langle k|V|0\rangle = \langle k|\frac{1}{2}\epsilon m\omega^2 x^2|0\rangle \propto \langle k|x^2|0\rangle$. So our task is to evaluate $\langle k|x^2|0\rangle$ or x^2_{ko}. Since from (2.3.24) $x = \sqrt{\hbar/2m\omega}(a + a^\dagger)$ where a and $a^\dagger$ satisfy $a|n\rangle = c_-|n-1\rangle$ and $a^\dagger|n\rangle = c_+|n+1\rangle$, then $x|0\rangle = \sqrt{\hbar/2m\omega}(a|0\rangle + a^\dagger|0\rangle) = \sqrt{\hbar/2m\omega}|1\rangle$ while $x^2|0\rangle = (\sqrt{\hbar/2m\omega})^2(a + a^\dagger)|1\rangle = c_1|0\rangle + c_2|2\rangle$. So $V_{ko} \propto \langle k|x^2|0\rangle = c_1\delta_{ko} + c_2\delta_{k2}$, and only V_{oo} and V_{2o} are relevant to our discussion. Explicit evaluation of c_1 and c_2 (remembering that $(a^\dagger/\sqrt{2})|1\rangle = |2\rangle$ from (2.3.21)), we have $c_1 = \hbar/2m\omega$, $c_2 = \hbar\sqrt{2}/2m\omega$. Thus $V_{oo} = \frac{1}{2}\epsilon m\omega^2\langle 0|x^2|0\rangle = c_1\epsilon m\omega^2/2 = \frac{\hbar}{2m\omega}\frac{\epsilon m\omega^2}{2} = \epsilon\hbar\omega/4$, and $V_{2o} = \frac{1}{2}\epsilon m\omega^2\langle 2|x^2|0\rangle = c_2\epsilon m\omega^2/2 = \frac{\hbar\sqrt{2}}{2m\omega}\frac{\epsilon m\omega^2}{2} = \epsilon\hbar\omega/2\sqrt{2}$.

6. Consider our symmetric rectangular double-well potential, as divided into three regions: (I) $-a-b<x<-a$; (II) $-a\le x\le +a$; and (III) $a<x<a+b$. We have the symmetric states $u_I(x) = A\sin(k_s(x+a+b))$, $u_{II}(x) = B\cosh\kappa_s x$, $u_{III}(x) = -A\sin(k_s(x-a-b))$, and antisymmetric states $v_I(x) = C\sin(k_a(x+a+b))$, $v_{II}(x) = D\sinh\kappa_a x$, $v_{III}(x) = +C\sin(k_a(x-a-b))$. All of which satisfy Schrödinger's equations and the appropriate boundary conditions,

$$k_s = \sqrt{2mE_s/\hbar^2},\ k_a = \sqrt{2mE_a/\hbar^2},\ \kappa_s = \sqrt{2m(V_o-E_s)/\hbar^2},\ \kappa_a = \sqrt{2m(V_o-E_a)/\hbar^2}$$

where because we assume $V_o \gg E_a, E_s$, $\kappa = \kappa_s \cong \kappa_a$. Matching solutions and derivatives at each boundary we have $A\sin k_s b = B\cosh\kappa a$, $C\sin k_a b = -D\sinh\kappa a$ and

$Ak_s\cos k_s b = -B\kappa\sinh\kappa a$, $Ck_a\cos k_a b = +D\kappa\cosh\kappa a$. Therefore we have the eigenvalue conditions

$$\tan k_s b/k_s = -\coth\kappa a/\kappa \;,\; \tan k_a b/k_a = -\tanh\kappa a/\kappa. \qquad (1)$$

Since $V_o >> E_{a,s}$, we expect the energy levels to be approximately those of a particle in a box (one dimensional, with infinite walls) in regions (I) and (III). Hence $\tan k_{a,s}b = \tan(\pi+\varepsilon_{a,s}) = \tan\varepsilon_{a,s} \cong \varepsilon_{a,s} = k_{a,s}b - \pi$, and (1) can be rewritten as

$$(k_s b-\pi)/k_s = -\coth\kappa a/\kappa,\; (k_a b-\pi)/k_a = -\tanh\kappa a/\kappa. \qquad (2)$$

From (2) we have $k_s = \frac{\pi}{b+\coth\kappa a/\kappa}$, $k_a = \frac{\pi}{b+\tanh\kappa a/\kappa}$, and the lowest lying states are $E_s = \hbar^2k_s^2/2m = \frac{\hbar^2\pi^2}{2m}(b+\coth\kappa a/\kappa)^{-2}$ and $E_a = \hbar^2k_a^2/2m = \hbar^2\pi^2(b+\tanh\kappa a/\kappa)^{-2}/2m$. So $\Delta E = E_a - E_s = \frac{\hbar^2\pi^2}{2mb^2}\{(1+\tanh\kappa a/\kappa b)^{-2} - (1+\coth\kappa a/\kappa b)^{-2}\}$. (Note the method used here, actually illustrates the symmetric double well potential discussed in Chapter 4, section 2).

7. Here $V= -ez|\vec{E}|$, and the perturbed ground state ket $|1,0,0\rangle'$ and unperturbed ground state ket $|1,0,0\rangle$ in the $|n,\ell,m\rangle$ notation are related by

$$|1,0,0\rangle' = |1,0,0\rangle + \sum_{n\ell m}\frac{|\vec{E}|(-e)\langle n,\ell,m|z|1,0,0\rangle|n,\ell,m\rangle}{E_{100} - E_{n\ell m}}$$

where E_{100} and $E_{n\ell m}$ are unperturbed energies (actually independent of m). Take expectation value of ez

$$\left(\langle 1,0,0| + \sum_{n'\ell'm'}\frac{(-e)|\vec{E}|\langle 1,0,0|z|n',\ell',m'\rangle\langle n',\ell',m'|}{E_{100} - E_{n'\ell'm'}}\right)ez\left(|1,0,0\rangle + \sum_{n\ell m}\right.$$

$$\left.\frac{-e|\vec{E}|\langle n\ell m|z|100\rangle|n\ell m\rangle}{E_{100} - E_{n\ell m}}\right) = -2e^2\sum_{n\ell m}\frac{|\langle 100|z|n\ell m\rangle|^2}{E_{100}-E_{n\ell m}}|\vec{E}|, \quad (\ell=1, m=0 \text{ in our case}) \quad (1)$$

where we have used the fact that $\langle 100|z|100\rangle = 0$. Also from (5.1.63), (5.1.67), and (5.1.68) we have for the energy shift of the ground state computed to second order

$$\Delta = -\tfrac{1}{2}\alpha|\vec{E}|^2, \quad \alpha = -2e^2 \sum_{n\ell m} \frac{|\langle 100|z|n\ell m\rangle|^2}{E_{100} - E_{n\ell m}} . \tag{2}$$

Hence from (1), we have induced dipole moment $\alpha|\vec{E}|$, where α is the same α which appears in $\Delta = -\tfrac{1}{2}\alpha|\vec{E}|^2$ of (2).

8. (a) $\langle n=2,\ell=1,m=0|x|n=2,\ell=0,m=0\rangle = 0$, because x is rank 1 tensor $(k=1, q=\pm 1)$ and behaves like $Y_1^1 - Y_1^{-1}$, so m value must change.

(b) $\langle n=2,\ell=1,m=0|p_z|n=2,\ell=0,m=0\rangle = 0$, since $p_z = \frac{m}{i\hbar}[z,H]$ we get $\langle p_z\rangle = im/\hbar \times (E_{210}-E_{200})\langle n=2,\ell=1,m=0|z|n=2,\ell=0,m=0\rangle$, but $E_{210} - E_{200} = 0$ by "accidental degeneracy" (2s – 2p degeneracy).

(c) From (3.7.64), we note that $|j=9/2, m=7/2, \ell=4\rangle$ is represented by

$$y_{\ell=4}^{j=4+\frac{1}{2},7/2} = (1/\sqrt{9})\begin{pmatrix} \sqrt{4+7/2+1/2}\; Y_{\ell=4}^{7/2-1/2} \\ \sqrt{4-7/2+1/2}\; Y_{\ell=4}^{7/2+1/2} \end{pmatrix},$$

hence $\langle L_z\rangle = (\sqrt{8/9})^2 3\hbar + (\sqrt{1/9})^2 4\hbar = (28/9)\hbar$.

(Alternative method: Use $\langle L_z\rangle = m\hbar - \langle S_z\rangle$ with $S_z = \pm m\hbar/(2\ell+1)$ (c.f. (5.3.31)) for $j = \ell\pm\tfrac{1}{2}$.)

(d) To evaluate $\langle \text{singlet}, m=0|(S_z^{(e^-)} - S_z^{(e^+)})|\text{triplet}, m=0\rangle$, first note

$$(S_z^{(e^-)}-S_z^{(e^+)})|\text{triplet},m=0\rangle = (S_z^{(e^-)}-S_z^{(e^+)})\tfrac{1}{2^{1/2}}(|\uparrow\rangle_{e^-}|\downarrow\rangle_{e^+} + |\downarrow\rangle_{e^-}|\uparrow\rangle_{e^+})$$

$$= (\tfrac{1}{2}\hbar - (-\tfrac{1}{2})\hbar)\tfrac{1}{2^{1/2}}(|\uparrow\rangle_{e^-}|\downarrow\rangle_{e^+}) + ((-\tfrac{1}{2}\hbar) - (\tfrac{1}{2}\hbar))\tfrac{1}{2^{1/2}}(|\downarrow\rangle_{e^-}|\uparrow\rangle_{e^+})$$

$$= \tfrac{\hbar}{2^{1/2}}[|\uparrow\rangle_{e^-}|\downarrow\rangle_{e^+} - |\downarrow\rangle_{e^-}|\uparrow\rangle_{e^+}] = \hbar|\text{singlet},m=0\rangle.$$

So $\langle \text{singlet}, m=0|(S_z^{(e^-)} - S_z^{(e^+)})|\text{triplet}, m=0\rangle = \hbar$.

(e) Ground state of H_2 molecule: For "homopolar" binding, the space part is symmetric, hence spin part is in singlet state. Thus

$$\langle \vec{S}_1\cdot\vec{S}_2\rangle = \tfrac{1}{2}(\vec{S}^2_{tot.} - \vec{S}_1^2 - \vec{S}_2^2) = -\tfrac{1}{2}\cdot 2\cdot(3/4)\hbar^2 = -\tfrac{3}{4}\hbar^2$$

where expectation value of $\langle\vec{S}^2_{tot.}\rangle$ gives zero for a spin singlet state.

9. (a) $\langle n,\ell=1,m=\pm 1,0|V|n,\ell=1,m=\pm 1,0\rangle$, $\frac{V}{\lambda} = x^2-y^2 = r^2\sin^2\theta(\cos^2\phi - \sin^2\phi) =$ $r^2\sin^2\theta\cos 2\phi = r^2\sin^2\theta(e^{2i\phi}+ e^{-2i\phi})/2$. So the perturbation connects $m = \pm 1$ with $m = \mp 1$. The type of non vanishing V-matrix elements are of form

$$I = \lambda\int\frac{\sin^2\theta}{2}e^{\pm i\phi}e^{\mp 2i\phi}\sin^2\theta e^{\pm i\phi}d\Omega \int r^2 R_{nl}^2\, r^2 dr$$

between $m = +1$ to $m = -1$ and $m = -1$ to $m = +1$ respectively. Hence perturbation matrix

$$V = \begin{pmatrix} 0 & 0 & I \\ 0 & 0 & 0 \\ I & 0 & 0 \end{pmatrix}$$

and evidently the "correct" zeroth order energy eigenstates that diagonalize the perturbation is

$$\frac{1}{2^{1/2}}[\,|n,\ell=1,m=+1\rangle \pm |n,\ell=1,m=-1\rangle] \qquad (1)$$

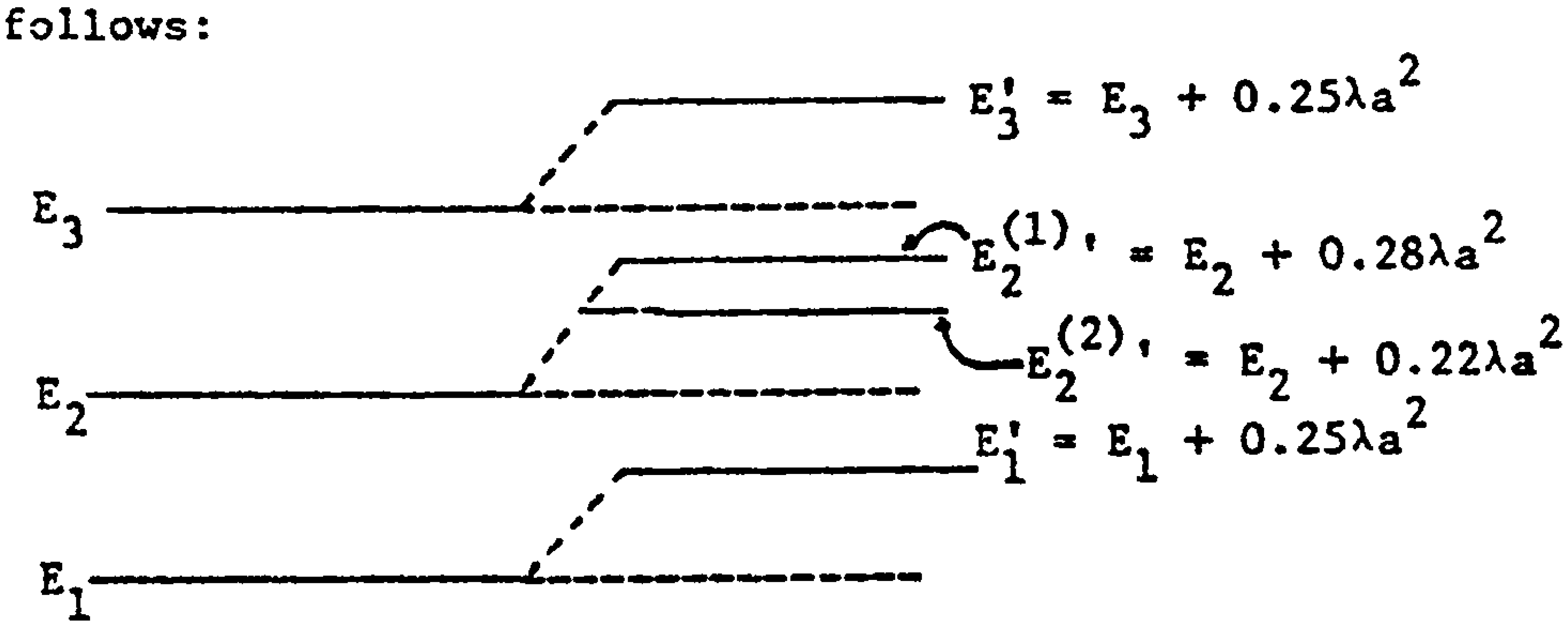
(b) We are dealing with states whose angular dependence are spherical harmonics. Under time reversal: $Y_\ell^m \to Y_\ell^{m*} = (-1)^m Y_\ell^{-m}$, hence $\Theta|n,\ell=1,m=\pm 1\rangle = -|n,\ell=1,m=\mp 1\rangle$. Therefore (1) evidently go into itself (up to a phase factor or sign) under time reversal.

0. This problem is rather similar to problem 3 above with L replaced by a. For (a) the Hamiltonian of the unperturbed system is H_o, where $H_o = -\frac{\hbar^2}{2m}\nabla^2 + V$, and by using the method of separation of variables, we can easily find the energy eigenvalues and eigenfunctions

$$E_n = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2),\quad \psi_n(x,y) = \sin(n_x\pi x/a)\sin(n_y\pi y/a) \qquad (1)$$

where n_x, n_y are non-zero integers. Thus the three lowest states correspond to $n_x=n_y=1$; $n_x=2$, $n_y=1$ and $n_x=1$, $n_y=2$; and $n_x=2$, $n_y=2$ respectively, and from (1) we have $E_1 = \hbar^2\pi^2/ma^2$ with $\psi_1(x,y) = (2/a)\sin(\frac{\pi x}{a})\sin(\frac{\pi y}{a})$ and nondegenerate, $E_2 =$ $5\hbar^2\pi^2/2ma^2$ with $\psi_2(x,y) = (2/a)\sin(\frac{2\pi x}{a})\sin(\frac{\pi y}{a})$ or $(2/a)\sin(\frac{\pi x}{a})\sin(\frac{2\pi y}{a})$ and hence two fold degenerate, $E_3 = 4\hbar^2\pi^2/ma^2$ with $\psi_3(x,y) = (2/a)\sin(\frac{2\pi x}{a})\sin(\frac{2\pi y}{a})$ and non-degenerate.

(b) For (i) the first order energy shift is $\Delta E_n = \langle n|V_1|n\rangle = \lambda\langle n|xy|n\rangle \propto \lambda$, hence the energy shift is <u>linear</u> in λ, in otherwords proportional to λ. For (ii) $\Delta E_3 = \langle 3|\lambda xy|3\rangle = (\frac{2}{a})^2\lambda \int_0^a\int_0^a x\sin^2(\frac{2\pi x}{a})y\sin^2(\frac{2\pi y}{a})dxdy = \frac{1}{4}\lambda a^2$. The energy shifts for degenerate state E_2 are given from problem 3 as $\Delta E_2^{(1)} = 0.28\lambda a^2$ and $\Delta E_2^{(2)} = 0.22\lambda a^2$, while that for nondegenerate E_1 is $\Delta E_1 = \frac{1}{4}\lambda a^2 = 0.25\lambda a^2$. (iii) The energy level diagrams for unperturbed levels (E_n) and perturbed levels $E_n + \Delta E_n = E_n'$ look as follows:



unperturbed levels perturbed levels

11. (a) The energy eigenvalues E_1 and E_2 are found from secular equation

$$\begin{vmatrix} E_1^o - E & \lambda\Delta \\ \lambda\Delta & E_2^o - E \end{vmatrix} = 0$$

therefore $E_{1,2} = (E_1^o + E_2^o)/2 \pm \sqrt{(E_1^o - E_2^o)^2/4 + \lambda^2\Delta^2}$. To find the eigenfunctions, we write $\psi_{1,2} = \begin{pmatrix} a_{1,2} \\ 1 \end{pmatrix}$, then $H\psi = E\psi$ gives $E_1^o a_{1,2} + \lambda\Delta = E_{1,2}a_{1,2}$ and thus up to normalization

$$\psi_{1,2} = \begin{pmatrix} \lambda\Delta/(E_{1,2} - E_1^o) \\ 1 \end{pmatrix}$$

with $E_{1,2}$ as given above. Note also that this problem is completely analogous to problem 11 of Chapter 1, if we make the substitution $E_1^o \leftrightarrow H_{11}$, $E_2^o \leftrightarrow H_{22}$, and $\lambda\Delta \leftrightarrow H_{12}$. Hence an alternative way to parametrize $\psi_{1,2}$ in normalized form is

$$\psi_1 = \begin{pmatrix} \cos\frac{\beta}{2} \\ \sin\frac{\beta}{2} \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} -\sin\frac{\beta}{2} \\ \cos\frac{\beta}{2} \end{pmatrix} \text{ where } \beta = \tan^{-1}\left[\frac{2\lambda\Delta}{E_1^o - E_2^o}\right]$$

(b) For H as given,

$$H_o = \begin{pmatrix} E_1^o & 0 \\ 0 & E_2^o \end{pmatrix}, \quad V = \begin{pmatrix} 0 & \lambda\Delta \\ \lambda\Delta & 0 \end{pmatrix},$$

hence $V_{11} = V_{22} = 0$, so first order energy shifts vanish in time-independent perturbation theory, and we must go to second-order. Here second order shifts are

$$\Delta_1^{(2)} = \frac{|V_{12}|^2}{E_1^o - E_2^o} = \frac{\lambda^2\Delta^2}{E_1^o - E_2^o}, \quad \Delta_2^{(2)} = \frac{|V_{21}|^2}{E_2^o - E_1^o} = \frac{\lambda^2\Delta^2}{E_2^o - E_1^o}.$$

But the exact energy solution for $\lambda|\Delta| << |E_1^o - E_2^o|$ is

$$E_{1,2} = \frac{(E_1^o + E_2^o)}{2} \pm \frac{(E_1^o - E_2^o)}{2}\left[1 + \frac{4\lambda^2\Delta^2}{(E_1^o - E_2^o)^2}\right]^{\frac{1}{2}} \cong \begin{cases} E_1^o + \lambda^2\Delta^2/(E_1^o - E_2^o) \\ E_2^o - \lambda^2\Delta^2/(E_1^o - E_2^o) \end{cases}$$

in agreement with perturbation results $E_1^o + \Delta_1^{(2)}$, and $E_2^o + \Delta_2^{(2)}$.

(c) Now suppose $E_1^o \sim E_2^o \equiv E^o$. Then $H = E^o\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \lambda\Delta\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Since the perturbation term is proportional to σ_x, we know right away that the eigenfunctions are those of σ_x,

$$\psi_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}; \text{ with } E_1 = E^o + \lambda\Delta, \; E_2 = E^o - \lambda\Delta.$$

Note $\psi_1 = \phi_1^o + \phi_2^o$, $\psi_2 = \phi_2^o - \phi_1^o$, i.e. linear combinations of degenerate states.

From (a), we have if $E_1^o = E_2^o = E^o$, than $E_{1,2} = E^o \pm \lambda\Delta$ and $\psi_{1,2} = \begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$ which agrees with (c).

12. Using the secular equation method, we diagonalize the perturbed Hamiltonian ma-

trix to obtain the exact energy eigenvalues. The secular equation reads

$$(E_1-\lambda)((E_1-\lambda)(E_2-\lambda) -|b|^2) + a((\lambda-E_1)a^*) = 0 .$$

Evidently $E_1 = \lambda$ is one solution, and the other two solutions are roots of $\lambda^2 - (E_1+E_2)\lambda + E_1E_2 -|a|^2 -|b|^2 = 0$, i.e. $\lambda_+ \cong E_1 + \frac{(|a|^2+|b|^2)}{(E_1 - E_2)}$ and $\lambda_- \cong E_2 - \frac{(|a|^2+|b|^2)}{(E_1 - E_2)}$, where we have assumed $|a|,|b| << |E_2-E_1|$.

Formally non-degenerate second order perturbation theory (5.1.42), translated into our notation, reads $\Delta_1 = |a|^2/(E_1-E_2)$, $\Delta_2 = |b|^2/(E_1-E_2)$ and $\Delta_3 = \frac{|a|^2+|b|^2}{E_2- E_1}$, hence energy levels are $E_1+\Delta_1$, $E_1+\Delta_2$, and $E_2+\Delta_3$ respectively. The non-degenerate second order perturbation results are unjustified because degeneracy is not removed to first order.

Use degenerate perturbation theory à la Gottfried (1966) (see p. 397, for details). We have here a degenerate two level subspace (E_1 twice and E_2), hence to second order in degenerate perturbation theory the energy shifts are given by

$$(\Delta - \frac{|a|^2}{E_1-E_2})(\Delta - \frac{|b|^2}{E_1-E_2}) = \left|\frac{ab}{E_1-E_2}\right|^2$$

i.e. $\Delta_1 = 0$, $\Delta_2 = \frac{|a|^2+|b|^2}{E_1-E_2}$, which agrees with the exact solution above where we had $E_1 = \lambda$(with $\Delta_1 = 0$), and $\lambda_+ \cong E_1 + (|a|^2+|b|^2)/(E_1-E_2) = E_1 + \Delta_2$, at least in the approximation $|a|,|b| << |E_2-E_1|$.

13. The Hamiltonian is $H = \vec{p}^2/2m - e^2/r + e\varepsilon z$, where $e\varepsilon z$ is the perturbation potential. In terms of the $2S_{1/2}$ and $2P_{1/2}$ levels of hydrogen, our Hamiltonian can be represented as

$$H \cong \begin{pmatrix} E_2^S + \langle s|e\varepsilon z|s\rangle+\delta & \langle s|e\varepsilon z|p\rangle \\ \langle p|e\varepsilon z|s\rangle & E_2^P + \langle p|e\varepsilon z|p\rangle \end{pmatrix} \qquad (1)$$

where δ is the Lamb shift, and E_2^S , E_2^P are the unperturbed energies for $2S_{1/2}$ and

$2P_{1/2}$ respectively. It is evident (from parity selection rule) that $\langle s|e\varepsilon z|s\rangle = \langle p|e\varepsilon z|p\rangle = 0$, while $\langle s|e\varepsilon z|p\rangle = \langle p|e\varepsilon z|s\rangle = e\varepsilon\langle s|r|p\rangle \int Y^{j=1/2,m\,*}_{\ell=0} Y^{j=1/2,m}_{\ell=1} \cos\theta d\Omega$. Using (3.7.64), we have $\langle s|e\varepsilon z|p\rangle = \langle p|e\varepsilon z|s\rangle = \mp\sqrt{3}e\varepsilon a_0$ for $m = \pm 1/2$. Hence (1) becomes

$$H = \begin{pmatrix} E_2^S + \delta & \mp\sqrt{3}e\varepsilon a_0 \\ \mp\sqrt{3}e\varepsilon a_0 & E_2^P \end{pmatrix}. \tag{2}$$

We diagonalize (2) to obtain eigenvalues Λ, where we recognize that $E_2^S = E_2^P = E_2$, this gives

$$\Lambda = E_2 + \delta/2 \pm [(\delta/2)^2 + 3e^2\varepsilon^2 a_0^2]^{1/2} \tag{3}$$

The energy shift from the mean $E_2+\delta/2$ is $\pm[(\delta/2)^2+3e^2\varepsilon^2a_0^2]^{1/2}$. Hence $\Delta E_S = -\Delta E_P = [(\delta/2)^2+3e^2\varepsilon^2a_0^2]^{1/2} \cong \frac{\delta}{2}[1 + 6e^2\varepsilon^2a_0^2/\delta^2]$ for $e\varepsilon a_0 \ll \delta$, and $[(\delta/2)^2+3e^2\varepsilon^2a_0^2]^{1/2} \cong \sqrt{3}e\varepsilon a_0(1 + \frac{\delta^2}{24e^2\varepsilon^2a_0^2})$ for $e\varepsilon a_0 \gg \delta$. Note for $e\varepsilon a_0 \ll \delta$ the shift from $E_2^S + \delta$ is quadratic in ε, while for $e\varepsilon a_0 \gg \delta$ the dominant shift is linear in ε.

Whereas parity restricts $\langle s|e\varepsilon z|s\rangle = \langle p|e\varepsilon z|p\rangle = 0$, time reversal invariance of our Hamiltonian places no similar restriction. Nevertheless (c.f. (4.4.84)) it imposes the restriction that expectation value $\langle\vec{x}\rangle$ (hence $\langle z\rangle$ as a special case) vanishes when taken with respect to eigenstates of j,m. For example $|j,m\rangle$ of our problem need not be parity eigenkets, and could be $c_s|s_{1/2}\rangle + c_p|p_{1/2}\rangle$, yet it remains true that $\langle j,m|\vec{x}|j,m\rangle = 0$ under time reversal invariance - i.e. no electric dipole moment.

14.. Let the electric field be in z-direction, i.e. $\vec{\varepsilon} = \varepsilon\vec{k}$, so the potential is expressed as $V = +e\vec{\varepsilon}.\vec{r} = re\varepsilon\cos\theta$. Assuming ε is small, we can use perturbation theory. The wave functions for n=3 are $\psi_{n\ell m_\ell}$, $n = 3$, $\ell = 0,1,2$, obviously $\langle 3\ell m_\ell|V|3\ell' m_\ell'\rangle \propto \langle R_{3\ell}|r|R_{3\ell'}\rangle\langle Y_\ell^{m_\ell}|\cos\theta|Y_{\ell'}^{m_\ell'}\rangle$. Now $\langle Y_\ell^{m_\ell}|\cos\theta|Y_{\ell'}^{m_\ell'}\rangle \propto \delta_{m_\ell m_\ell'}\langle P_\ell^{m_\ell}|\cos\theta|P_{\ell'}^{m_\ell'}\rangle$, whi[illegible] $\cos\theta P_{\ell'}^{m_\ell'} \propto [(\ell'-|m_\ell'|+1)P_{\ell'+1}^{m_\ell'} + (\ell'+|m_\ell'|)P_{\ell'-1}^{m_\ell'}]$, thus $\langle Y_\ell^{m_\ell}|\cos\theta|Y_{\ell'}^{m_\ell'}\rangle$

$\propto \delta_{m_\ell m_\ell'}\{[\ell'-|m_\ell'|+1]\delta_{\ell,\ell'+1} + [\ell'+|m_\ell'|]\delta_{\ell,\ell'-1}\}$. So matrix elements vanish unless $m_\ell=m_\ell'$, $\ell=\ell'+1$ or $\ell=\ell'-1$, and we have non-vanishing matrix elements $\langle 321|V|311\rangle$, $\langle 32\text{-}1|V|31\text{-}1\rangle$, $\langle 320|V|310\rangle$, $\langle 310|V|320\rangle$, $\langle 311|V|321\rangle$, $\langle 31\text{-}1|V|32\text{-}1\rangle$, $\langle 310|V|300\rangle$, $\langle 300|V|310\rangle$. As a first step let us calculate these non-vanishing matrix elements, remembering that $\psi_{n\ell m}=R_{n\ell}Y_\ell^{m_\ell}$ where Y_ℓ^m is given by (A.5.6) and $R_{n\ell}(r)$ by (A.6.3). Straightforward evaluation leads to

$$\langle 321|V|311\rangle=\langle 311|V|321\rangle=\langle 32\text{-}1|V|31\text{-}1\rangle=\langle 31\text{-}1|V|32\text{-}1\rangle= - 27\varepsilon a_o e/2$$

$$\langle 320|V|310\rangle =\langle 310|V|320\rangle= -9\sqrt{3}\varepsilon a_o e$$

$$\langle 310|V|300\rangle =\langle 300|V|310\rangle= -9\sqrt{6}\varepsilon a_o e.$$

Diagonalizing the (9×9) V-matrix ($\sum_{m_\ell=o}^{2} (2m_\ell+1) = 9$), we have the matrix equation (with eigenvalues $\lambda= e\varepsilon a_o r$)

$$\begin{pmatrix} r & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 & 0 & b & 0 & 0 \\ 0 & 0 & 0 & r & 0 & 0 & 0 & a & 0 \\ 0 & 0 & 0 & 0 & r & 0 & 0 & 0 & 0 \\ 0 & a & 0 & 0 & 0 & r & 0 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & 0 & r & 0 & c \\ 0 & 0 & 0 & a & 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & c & 0 & r \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \\ A_7 \\ A_8 \\ A_9 \end{pmatrix} = 0 \qquad (1)$$

where $a = 27/2$, $b = 9\sqrt{3}$, $c = 9\sqrt{6}$. and secular equation is $r^3[r^2-a^2]^2[r^2-b^2-c^2] = 0$ i.e. $r=0$. $r=\pm a$, $r=\pm(b^2+c^2)^{\frac{1}{2}}$. Substitute $r=0$ into Eq. (1) gives $A_2=A_4=A_6=A_7=A_8=0$, $A_3b+cA_9 = 0$, no information on A_1 and A_5. So for $r=0$, we can choose three combinations for A_1, A_3, A_5, A_9. They are $A_1=1$, $A_i=0$ ($i\neq 1$), i.e. ψ_{322}; $A_5=1$, $A_i = 0$ ($i\neq 5$), i.e. ψ_{32-2}; $A_i = 0$ ($i\neq 3,9$), $A_3 = \sqrt{2/3}$, $A_9 = -\sqrt{1/3}$, i.e. $(\sqrt{2/3}\psi_{320} - \sqrt{1/3}\psi_{300})$. Here our notation is $A_1\ldots\ldots A_5$ correspond to $\ell=2$, $m_\ell=2,1,0,-1,-2$; A_6, A_7, A_8 correspond to $\ell=1$, $m_\ell=1,0,-1$; A_9 corresponds to $\ell=0$, $m_\ell=0$. To summarize:

For $r=0$, $\Delta E=0$, wave functions are $\psi_{322}, \psi_{32-2}, \sqrt{2/3}\psi_{320} - \sqrt{1/3}\psi_{300}$. (2)

For $r=a=27/2$, i.e. $\lambda= 27e\varepsilon a_o/2$, we have from Eq.(1), $A_1=0$, $A_5=0$, $A_3=A_7=A_9=0$ and either $A_2 = -A_6 = 1/\sqrt{2}$, $A_4=A_8=0$ or $A_2=A_6=0$, $A_4= -A_8 = 1/\sqrt{2}$ i.e.

$$r=a,\ \Delta E = 27e\varepsilon a_o/2;\ \text{wave functions}\ \begin{cases}\frac{1}{2^{1/2}}(\psi_{321}-\psi_{311}) \\ \frac{1}{2^{1/2}}(\psi_{32-1}-\psi_{31-1})\end{cases} . \tag{3}$$

For $r= -a = -27/2$, i.e. $\lambda = -27e\varepsilon a_o/2$, we find from Eq.(1) $A_1=A_5=0$, $A_3=A_7=A_9 = 0$ and either $A_2=A_6=1/\sqrt{2}$, $A_4=A_8=0$ or $A_2=A_6=0$, $A_4=A_8=1/\sqrt{2}$, i.e.

$$r=-a,\ \Delta E = -27e\varepsilon a_o/2;\ \text{wave functions}\ \begin{cases}\frac{1}{2^{1/2}}(\psi_{321}+\psi_{311}) \\ \frac{1}{2^{1/2}}(\psi_{32-1}+\psi_{31-1})\end{cases} . \tag{4}$$

Finally, for $r=\pm(b^2+c^2)^{1/2} = \pm 9\sqrt{9}$, i.e. $\lambda = \pm 9\sqrt{9}e\varepsilon a_o$, we find $A_1=A_5=A_2=A_4=A_6=A_8=0$. For $r=+9\sqrt{9}$, $A_3=1/\sqrt{6}$, $A_7= -1/\sqrt{2}$, $A_9=1/\sqrt{3}$, i.e.

$$r=+(b^2+c^2)^{1/2},\ \Delta E=+9\sqrt{9}e\varepsilon a_o:\ \text{wave function is}\ [\tfrac{1}{6^{1/2}}\psi_{320}-\tfrac{1}{2^{1/2}}\psi_{310}+\tfrac{1}{3^{1/2}}\psi_{300}] \tag{5}$$

and for $r=-9\sqrt{9}$, $A_3=1/\sqrt{6}$, $A_7=1/\sqrt{2}$, $A_9=1/\sqrt{3}$, i.e.

$$r=-(b^2+c^2)^{1/2},\ \Delta E=-9\sqrt{9}e\varepsilon a_o;\ \text{wave function is}\ [\tfrac{1}{6^{1/2}}\psi_{320}+\tfrac{1}{2^{1/2}}\psi_{310}+\tfrac{1}{3^{1/2}}\psi_{300}] \tag{6}$$

15. For electric dipole $V = -\vec{\mu}_e\cdot\vec{E}$ where $\vec{\mu}_e = \mu_e\vec{\sigma}$. The Coulomb field of the nucleus may be written as: $\vec{E} = -\frac{1}{e}\hat{r}dV_c/dr$ (V_c = Coulomb potential). Now $\vec{\sigma}\cdot\hat{r}$ may be written as: $\vec{\sigma}\cdot\hat{r} = [\sigma_+(x-iy)+\sigma_-(x+iy)+\sigma_z z]/r = (4\pi/3)^{1/2}[\sqrt{2}(\sigma_+Y_1^{-1}-\sigma_-Y_1^1)+\sigma_z Y_1^0]$. Hence there are selection rules governing which matrix elements of V are non-zero. For $\Delta m_\ell=0$ the matrix elements of Y_1^0 are needed. These vanish unless $\Delta\ell=\pm1$. For $\Delta m_\ell=\pm1$, $\Delta\ell$ is also ±1. This is expected since $\hat{r}$ is a vector operator and connects states of different parity. The radial contribution is proportional to: $\int_0^\infty R_{n\ell}\frac{dV}{dr}cR_{n'\ell'}r^2dr = -\int_0^\infty R_{n\ell}R_{n'\ell'}dr$. One may verify that for $\ell-\ell' =\pm1$, this integral vanishes for $n=n'$.

The ground state of Na has n=3 (degeneracy $n^2=9$). But from the above, we know that $\Delta n \neq 0$ therefore the effects of this perturbation V on the energy levels are seen in second order. Mixings will occur between 3s and 4p states and similarly between 4s and 3p, 3d and 4p etc. Using eigenstates of L^2, L_z, S^2, S_z, the following expression for $\langle 3s|V|4p\rangle$ is true for $\Delta \ell_z = 0$.

$$\langle 3s|V|4p\rangle_{\Delta\ell_z=0} = \frac{Z}{(-e)}\int_0^\infty R_{30}(r)R_{41}(r)dr\left(\frac{4\pi}{3}\right)^{1/2}\langle 00\tfrac{1}{2}\tfrac{1}{2}|Y_1^0\sigma_z|10\tfrac{1}{2}\tfrac{1}{2}\rangle$$

$$= \frac{Z}{-e}\int_0^\infty R_{30}R_{41}dr\left(\frac{4\pi}{3}\right)^{1/2}\int_{-1}^{+1}\int_0^{2\pi}\left(\frac{1}{4\pi}\right)^{1/2}\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta\times\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta d(\cos\theta)d\phi$$

$$= \left(\frac{Z}{-e}\right)\left(\frac{1}{3}\right)^{1/2}\int_0^\infty R_{30}R_{41}dr = \left(\frac{Z}{-e}\right)\left(\frac{1}{3}\right)^{1/2}I_R .$$

So the second (lowest) order shift in the 3s state of Na would be (using (5.2.18))

$$\Delta_{3s} = \left(\frac{-\mu_e Z I_R}{e\sqrt{3}}\right)^2 \Big/ (E_{n=3} - E_{n=4})$$

where $E_n = -Z^2me^4/2\hbar^2n^2$.

16. (a) This is the central force problem with spherically symmetric potential V(r). As usual let $\psi(r) = cu(r)/r$ where $\psi(r)$ satisfies the usual radial Schrödinger equation and u(r) satisfies (c.f. (A.5.8))

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V(r)u = Eu \text{ (for } \ell=0 \text{ S-states).} \qquad (1)$$

Multiply (1) by $u' \equiv du/dr$, we have

$$-\frac{\hbar^2}{2m}\frac{1}{2}\frac{d(u')^2}{dr} + \frac{1}{2}\frac{d(uVu)}{dr} - \frac{1}{2}\frac{dV}{dr}u^2 = \frac{E}{2}\frac{d(u^2)}{dr}. \qquad (2)$$

Integrate (2) from 0 to ∞ on both sides, we have

$$-\frac{\hbar^2}{4m}(u')^2\Big|_0^\infty + \tfrac{1}{2}(uVu)\Big|_0^\infty - \tfrac{1}{2}\int_0^\infty\frac{dV}{dr}u^2dr = \frac{E}{2}u^2\Big|_0^\infty . \qquad (3)$$

But $\lim_{r\to 0} u(r) = 0$, and $\lim_{r\to\infty} u(r) = 0$, therefore (3) gives

$$-\frac{\hbar^2}{4m}(u')^2\Big|_0^\infty - \tfrac{1}{2}\int_0^\infty \frac{dV}{dr}u^2dr = 0. \qquad (4)$$

From $u(r) = r\psi(r)/c$, we get $u'(r) = \psi(r)/c + r\psi'(r)/c$, where at ∞ the right hand side functions are well behaved and must vanish as $r\to\infty$. Thus (4) gives

$$\frac{\hbar^2}{4mc^2}|\psi(0)|^2 = \frac{1}{2c^2}\int_0^\infty r^2(dV/dr)\psi^2(r)dr = \frac{1}{4\pi(2c^2)}\langle\frac{dV}{dr}\rangle ,$$

and therefore

$$|\psi(0)|^2 = (\frac{m}{2\pi\hbar^2})\langle dV/dr\rangle \tag{5}$$

(b) For the hydrogen atom $V(r) = -e^2/r$ and for the ground state (from (A.6.7)) we have $R_{10}(\rho) = (2/a_o^{3/2})e^{-\rho/2}$, where $\rho = 2r/a_o$ and $a_o = \hbar^2/m_e e^2$ is the Bohr radius (c.f. (A.6.3)). $R_{10}(0) = 2/a_o^{3/2} = 2/(\hbar^2/me^2)^{3/2} = 2e^3m^{3/2}/\hbar^3$, and

$$\langle dV/dr\rangle = e^2 4\pi\int_0^\infty \frac{1}{r^2}\, r^2R_{10}^2(r)dr = \frac{4\pi e^2.4}{a_o^3}\int_0^\infty e^{-\rho}dr$$

and since $dr = a_o d\rho/2$, we have $\langle dV/dr\rangle = 8\pi e^2/a_o^2$. Therefore $\frac{m}{2\pi\hbar^2}\langle dV/dr\rangle =$ $\frac{m}{2\pi\hbar^2}\cdot\frac{8\pi e^2}{a_o^2} = 4me^2/\hbar^2a_o^2 = 4/a_o^3 = |R_{10}(0)|^2$. Hence relation (5) is verified.

For the three dimensional harmonic oscillator $V(r) = \frac{1}{2}kr^2$, the ground state is $n_x=n_y=n_z=0$, and wave function $\psi = X_o(x)Y_o(y)Z_o(z)$ is such that

$$X_o(x)=N_oH_o(\alpha x)e^{-\frac{1}{2}\alpha^2x^2},\ Y_o(y)=N_oH_o(\alpha y)e^{-\frac{1}{2}\alpha^2y^2},\ Z_o(z)=N_oH_o(\alpha z)e^{-\frac{1}{2}\alpha^2z^2}$$

where $N_o=(\alpha/\pi^{\frac{1}{2}})^{\frac{1}{2}}$ and $\alpha = (mk/\hbar^2)^{\frac{1}{4}}$. So $|\psi(0)|^2 = N_o^6H_o^6(0)$, while

$$\langle dV/dr\rangle = N_o^6\int_{-\infty}^{+\infty}H_o^2(\alpha x)H_o^2(\alpha y)H_o^2(\alpha z)[kr]e^{-\alpha^2r^2}dxdydz.$$

From (A.4.5) we see that $H_o(\xi) = 1$, hence $|\psi(0)|^2 = N_o^6$, while $\langle dV/dr\rangle = N_o^6\int_0^\infty kr\times$ $e^{-\alpha^2r^2}r^2dr(4\pi) = N_o^6(4\pi)k\int_0^\infty r^3e^{-\alpha^2r^2}dr = N_o^6(4\pi)k\frac{1}{2\alpha^4} = N_o^6(2\pi)\hbar^2/m$. Thus $(\frac{m}{2\pi\hbar^2})\times$ $\langle dV/dr\rangle = N_o^6 = |\psi(0)|^2$ for the three dimensional isotropic harmonic oscillator also.

(a) Rotate the system in such a way that the z'-axis is along the magnetic field

$\vec{B}$, we then have $H = A\vec{L}^2+(B^2+C^2)^{1/2}L'_z$ where in the y-z plane the angle θ between Oz and Oz' is given by $\tan\theta = C/B$. We then have eigenkets $|\ell,m'\rangle$ with eigenvalues

$$E = A\ell(\ell+1)\hbar^2 + (B^2+C^2)^{1/2}m'\hbar \tag{1}$$

where $|\ell,m'\rangle = \mathcal{D}(\pi/2,\beta,0)|\ell,m\rangle = \sum_{m=-\ell}^{\ell}|\ell,m\rangle\mathcal{D}^{(\ell)}_{mm'}(\pi/2,\beta,0)$. When $B \gg C$, we treat $H_o = A\vec{L}^2 + BL_z$ as the unperturbed Hamiltonian, and CL_y as the perturbation, than unperturbed eigenvalues $E^{(o)}_{\ell,m}$ and eigenkets are $A\hbar^2\ell(\ell+1)+Bm\hbar$ and $|\ell,m\rangle$ respectively. Hence to second order in perturbation

$$E^{(2)}=A\hbar^2\ell(\ell+1)+Bm\hbar + \langle\ell,m|CL_y|\ell,m\rangle + C^2\sum_{\substack{\ell',m'\\ \neq\ell,m}}\frac{|\langle\ell',m'|L_y|\ell,m\rangle|^2}{E^{(o)}_{\ell,m} - E^{(o)}_{\ell',m'}}. \tag{2}$$

Use next $L_y = \frac{1}{2i}(L_+-L_-)$ and (3.5.41), (2) becomes

$$E^{(2)} = A\hbar^2\ell(\ell+1) + Bm\hbar + C^2\hbar m/2B. \tag{3}$$

From the exact solution (1), we may expand for $B \gg C$ to get

$$E = A\ell(\ell+1)\hbar^2 + Bm'\hbar + \frac{C^2}{2B}\hbar m' + \ldots\ldots\ldots \tag{4}$$

Hence in this approximation ($B \gg C$), the second-order perturbed energy (3) reproduces the exact solution for $m'\to m$.

(b) We consider $\langle n'\ell'm'_\ell m'_s|O|n\ell m_\ell m_s\rangle$ where $O = 3z^2-r^2$, xy. Note that the operator O is <u>spin-independent</u>, hence $\Delta m_s = m'_s-m_s=0$. Now $3z^2-r^2 \sim (3\cos^2\theta-1) \sim Y_2^0$, hence $\langle\ell';m'_\ell|Y_2^0|\ell,m_\ell\rangle$ must satisfy $\Delta m_\ell = m_{\ell'}-m_\ell = 0$, and $-2\leq\Delta\ell=\ell'-\ell\leq +2$. However $|\Delta\ell| \neq 1$ because of parity conservation. <u>Summary</u>: $\Delta m_s = m'_s - m_s = 0$, $\Delta m_\ell = m_{\ell'}-m_\ell=0$, $\Delta\ell= 0,\pm2$.(Actually we have also the constraint $\ell+\ell'\geq 2$.)

Consider next O =xy, now $Y_2^2 \propto (x+iy)^2$, $Y_2^{-2} \propto (x-iy)^2$, hence $Y_2^2 - Y_2^{-2} \propto xy$. So $\langle\ell'm'_\ell|(Y_2^2-Y_2^{-2})|\ell m_\ell\rangle$ satisfies $\Delta m_\ell=2,-2$;$\Delta\ell= \pm1$ remains forbidden by parity conservation, hence $\Delta\ell=0,\pm2$. <u>Summary</u>: $\Delta m_s = m'_s-m_s=0$,$\Delta m_\ell = \pm2$,$\Delta\ell=0,\pm2$ ($\ell+\ell'\geq2$).

<u>Remarks</u>: The above selection rules are different from those for dipole radia-

tions which require $\Delta m_s = 0, \Delta m_\ell = 0, \pm 1$, $\Delta\ell = 0, \pm 1$, which is not surprising since for instance $3z^2 - r^2$ relates to quadrupole radiation.

18. The perturbation Hamiltonian (see (5.3.25)) is $e^2A^2/2m_ec^2 = e^2B^2(x^2+y^2)/8m_ec^2$, where we have used $A_x = -\frac{1}{2}By$, $A_y = \frac{1}{2}Bx$, $A_z = 0$ and noted that the perturbation is spin independent (hence okay to ignore spin). So we must evaluate $\langle x^2+y^2\rangle$ for the ground state. Now by symmetry $\langle x^2+y^2\rangle = \frac{2}{3}\langle r^2\rangle$ because $\langle x^2\rangle = \langle y^2\rangle = \langle z^2\rangle$ and $\langle x^2+y^2+z^2\rangle = \langle r^2\rangle$. So the integral to be evaluated relative to the ground-state of hydrogen atom is $4\pi\int(1/\pi a_o^3)e^{-2r/a_o}\, r^2r^2dr = \frac{4}{a_o^3}(a_o/2)^5 4!$. Hence

$$\Delta = \frac{e^2B^2a_o^2}{m_ec^2}\,\frac{4.4.3.2}{8.2.2.2.2.2}(2/3) = \frac{e^2B^2a_o^2}{4m_ec^2}$$

and $\chi = -\,e^2a_o^2/2m_ec^2$, the negative sign is because the induced dipole moment has opposite sign for diamagnetism.

19. In this problem, we work out the quadratic Zeeman effect with the help of vector potential $\vec{A} = \frac{1}{2}\vec{B}\times\vec{r}$ for uniform magnetic field $\vec{B} = B_o\hat{e}_z$ (we notice $\vec{B} = \vec{\nabla}\times\vec{A}$). Using the Lorentz gauge $\vec{\nabla}.\vec{A} = 0$, then $[\vec{p},\vec{A}] = -i\hbar\vec{\nabla}.\vec{A} = 0$ or $\vec{A}.\vec{p} = \vec{p}.\vec{A}$ for particle momentum $\vec{p}$. Then $\vec{A}.\vec{p} = \frac{1}{2}(\vec{B}\times\vec{r}).\vec{p} = \frac{1}{2}\vec{B}.\vec{r}\times\vec{p} = \frac{1}{2}\vec{B}.\vec{L} = \frac{1}{2}B_oL_z$, $\vec{A}^2 = \frac{1}{4}(\vec{B}\times\vec{r}).(\vec{B}\times\vec{r}) = \frac{1}{4}[\vec{B}^2\vec{r}^2 - (\vec{B}.\vec{r})^2] = \frac{1}{4}B_o^2(x^2+y^2)$, and the total Hamiltonian will be

$$E = \frac{1}{2m_e}(\vec{p} - \frac{e}{c}\vec{A})^2 = \frac{\vec{p}^2}{2m_e} - \frac{eB_o}{2m_ec}L_z + e^2B_o^2(x^2+y^2)/8m_ec^2 - \frac{Ze^2}{r}$$

with the perturbation term $V = \frac{-eB_o}{2m_ec}L_z + \frac{e^2B_o^2}{8m_ec^2}(r^2\sin^2\theta)$. For zero angular momentum $\ell=0$ (S-state), we have $\vec{L} = 0$, $L_z = 0$, and in this simple case, for an atomic electron in the n=1 ground state of an atom with atomic number Z, the energy change will be

$$\Delta E^{(1)}_{Z,m_\ell=0} = \int_0^{2\pi}d\phi\int_{-1}^{+1}d(\cos\theta)\int_0^\infty r^2dr\frac{Z^3}{\pi a_o^3}\, e^{-2Zr/a_o}(e^2B_o^2r^2\sin^2\theta/8m_ec^2)$$

$$= [1/(2Z)^2].\frac{e^2B_o^2a_o^2}{m_ec^2} = [1/(2Z)]^2.\lambda_e^3B_o^2/\alpha \qquad (1)$$

in which $\lambda\!\!\!^{-}_e = \hbar/m_e c$ is the electron Compton wavelength and $a_o = \hbar^2/m_e e^2$ is the Bohr atomic radius and $\alpha = e^2/\hbar c \simeq 1/137$ is the fine structure constant. The above integral was carried out by using $\int_0^\infty d\xi\,\xi^N e^{-\rho\xi} = N!/\rho^{N+1}$.

Now for the helium atom the result would be twice that we obtained for an atomic electron in (1) with effective atomic number $Z = 2-5/16 \simeq 1.7$:

$$\Delta E^{(1)}_{He,m_\ell=0} = 2\times \frac{1}{(2Z)^2\alpha}\lambda\!\!\!^{-3}_e B_o^2\Big|_{Z\simeq 1.7} \simeq 23.7\lambda\!\!\!^{-3}_e B_o^2\,. \tag{2}$$

For one mole of helium the energy change is $N_o\Delta E^{(1)}_{He,m_\ell=0}$ where $N_o \simeq 6.022\times 10^{23}$/mole (the Avogadro's number). Thus the magnetic susceptibility per mole of helium, χ_{He}, is going to be

$$N_o\Delta E^{(1)}_{He,m_\ell=0} = -\tfrac{1}{2}\chi_{He}B_o^2 \;\rightarrow\; \chi_{He} = -2N_o\times 23.7\lambda\!\!\!^{-3}_e. \tag{3}$$

Expressed in terms of a_o(atomic unit), we have $\lambda\!\!\!^{-}_e = 7.2973\times 10^{-3}a_o$, then

$$\chi_{He} = -1.109\times 10^{19}a_o^3\,/\text{mole} \equiv -1.643\times 10^{-6}\text{cm}^3/\text{mole}. \tag{4}$$

The experimental result is $-1.88\times 10^{-6}\text{cm}^3$/mole which is in fairly good agreement with our perturbation calculation.

20.
$$\overline{H} = \frac{(-\hbar^2/2m)\int_{-\infty}^{+\infty}e^{-\beta|x|}\frac{d^2}{dx^2}e^{-\beta|x|}dx + \int_{-\infty}^{+\infty}e^{-2\beta|x|}(m\omega^2x^2/2)dx}{\int_{-\infty}^{+\infty}e^{-2\beta|x|}dx}$$

$$= \frac{-\frac{2\hbar^2}{2m}\int_0^\infty \beta^2 e^{-2\beta x}dx - \frac{\hbar^2}{2m}(-2\beta) + \frac{m\omega^2}{2}(2)\int_0^\infty e^{-2\beta x}x^2dx}{2\int_0^\infty e^{-2\beta x}dx}$$

where the term $-\frac{\hbar^2}{2m}(-2\beta)$ in numerator is the contribution from the first derivative at $x=0$. So $\overline{H} = \hbar^2\beta^2/2m + m\omega^2/4\beta^2$, and $\partial\overline{H}/\partial\beta = 0$ implies $2\hbar^2\beta/2m - m\omega^2/2\beta^3 = 0$ or $\beta^2 = m\omega/\sqrt{2}\hbar$. Hence $(\overline{H})_{min} = \frac{\hbar^2}{2\sqrt{2}}\frac{m\omega}{m\hbar} + \frac{m\omega^2\sqrt{2}\hbar}{4m\omega} = \hbar\omega(\frac{1}{2\sqrt{2}} + \frac{\sqrt{2}}{4}) = \frac{\hbar\omega\sqrt{2}}{2}$,

where $(\hbar\omega/2)$ is the true energy.

21. The equation $d^2\psi/dx^2 + (\lambda-|x|)\psi = 0$ can be written as $-d^2\psi/dx^2 + |x|\psi = \lambda\psi$ and hence is like Schrödinger equation $H\psi = \lambda\psi$ with $\hbar^2/2m = 1$. Let us set c=1 and worry about normalization later, than

$$d\psi/dx = \begin{cases} -1 \text{ for } 0<x<\alpha \\ +1 \text{ for } -\alpha<x<0 \end{cases}, \quad \int_{-\varepsilon}^{\varepsilon} d^2\psi/dx^2\, dx = (d\psi/dx)_{x=\varepsilon} - (d\psi/dx)_{x=-\varepsilon},$$

hence $d^2\psi/dx^2 = -2\delta(x)$, and $\langle\psi|H|\psi\rangle = 2\psi(0) + 2\int_0^\alpha x(\alpha-x)^2 dx = 2\alpha + \alpha^4/12$. Also $\langle\psi|\psi\rangle = 2\int_0^\alpha(\alpha-x)^2 dx = 2\alpha^3/3$. Therefore from (5.4.2), we have

$$\lambda \leqslant \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{2\alpha+2\alpha^4/12}{2\alpha^3/3} = \frac{3}{\alpha^2} + \frac{\alpha}{4}\,. \tag{1}$$

Hence $d\lambda/d\alpha = 0$ implies $(3/\alpha^3)(-2) + \frac{1}{4} = 0$ or $\alpha = 24^{1/3} = 2\times3^{1/3}$, and $\lambda <$ $3/4\times3^{2/3} + 2\times3^{1/3}/4 = 1.081$. So the true λ must be lower than 1.081 which is not bad compared to exact value 1.019 for such a crude trial function. Note normalization of ψ is taken care of via $\langle\psi|\psi\rangle$ in denominator of (1).

22. Here $V(t) = F_o x\cos\omega t$, and we set $\omega_{1o} \equiv (E_1-E_0)/\hbar = \omega_0$. From (5.6.17) we see that $c_o(t) \cong 1$ up to first order, while

$$\begin{aligned} c_1(t) &\cong (-i/\hbar)\frac{F_o}{2}\int_0^t \langle 1|x|0\rangle e^{i\omega_{1o}t'}[e^{i\omega t'} + e^{-i\omega t'}]dt' \\ &= -(F_o/2\hbar)\langle 1|x|0\rangle\left[\frac{e^{i(\omega_o+\omega)t}-1}{(\omega_o+\omega)} + \frac{e^{i(\omega_o-\omega)t}-1}{(\omega_o-\omega)}\right]. \end{aligned} \tag{1}$$

Let us compute x in the Schrödinger picture, than

$$\begin{aligned} \langle x\rangle_S &= (\langle 0|e^{i\omega_o t/2} + c_1^*\langle 1|e^{3i\omega_o t/2})x(|0\rangle e^{-i\omega_o t/2} + c_1|1\rangle e^{-3i\omega_o t/2}) \\ &= c_1^*(t)\langle 1|x|0\rangle e^{i\omega_o t} + c_1(t)\langle 0|x|1\rangle e^{-i\omega_o t} \\ &= -\left(\frac{F_o}{2\hbar}\right)|\langle 1|x|0\rangle|^2\left[\frac{e^{-i(\omega_o+\omega)t}e^{i\omega_o t} - e^{i\omega_o t}}{(\omega_o+\omega)} + \frac{e^{i(\omega_o-\omega)t}e^{-i\omega_o t} - e^{-i\omega_o t}}{(\omega_o-\omega)}\right] \\ &\quad + \text{c.c. (complex conjugate)} \end{aligned} \tag{2}$$

where we have used (1) and the constancy of F_o in arriving at (2). Since $\langle 1|x|0\rangle = (\hbar/2m\omega_o)^{\frac{1}{2}}$, (2) becomes

$$\langle x\rangle_S = -\frac{F_o}{m}\left(\frac{\cos\omega t - \cos\omega_o t}{\omega_o^2 - \omega^2}\right) . \tag{3}$$

This is more or less what you expect classically. As $\omega \approx \omega_o$, $\cos\omega t - \cos\omega_o t \approx -\frac{1}{2}\omega^2 t^2 + \frac{1}{2}\omega_o^2 t^2 = \frac{1}{2}t^2(\omega_o^2-\omega^2)$, thus $\langle x\rangle_S \approx \frac{-F_o}{m}\frac{1}{2}t^2$. Treating $-F_o/m$ as a classical uniform acceleration a, $\langle x\rangle_S = \frac{1}{2}at^2$ is the classical rectilinear motion starting from rest, however procedure breaks down for $\omega \approx \omega_o$.

23. (a) For a force $F(t) = F_o e^{-t/\tau}$, we have $-dV/dx = F_o e^{-t/\tau}$, hence $V = -F_o x e^{-t/\tau}$. Again from (5.6.17), $c_o^{(o)}(t) = 1$, and $\omega_{1o} \equiv (E_1-E_0)/\hbar = \omega$, while

$$c_1^{(1)}(t) = (-i/\hbar)\int_0^t e^{i\omega t'}e^{-t'/\tau}dt'\langle 1|x|0\rangle F_o$$

$$= (-i/\hbar)\left[\frac{e^{i\omega t-t/\tau}-1}{(i\omega -1/\tau)}\right]\langle 1|x|0\rangle F_o . \tag{1}$$

Hence

$$|c_1^{(1)}(t)|^2 = \frac{1}{\hbar^2}\left[\frac{1+e^{-2t/\tau}-(2\cos\omega t)e^{-t/\tau}}{\omega^2 + (1/\tau)^2}\right]|F_o|^2(\hbar/2m\omega) . \tag{2}$$

Note that as $t \to \infty$, $|c_1^{(1)}(t)|^2$ is independent of t. This is reasonable since for sufficiently large t, the perturbation is no longer on.

(b) Take (5.6.17) again, we see to first order the nth excited state is

$$c_n^{(1)}(t) = (-i/\hbar)\int_0^t e^{i\omega_{no}t'}V_{no}(t')dt' \tag{3}$$

where $\omega_{no} \equiv (E_n-E_o)/\hbar$, and $n\geq 2$. However $V_{no}(t')$ would contain multiplicative factor $\langle n|x|0\rangle$ which vanishes for $n\geq 2$.. Nevertheless for $\langle n'|x|n\rangle=\sqrt{\hbar/2m\omega}(\sqrt{n}\delta_{n',n-1} +\sqrt{n+1}\delta_{n',n+1})$, we know that $\langle 2|x|1\rangle =\sqrt{2}(\hbar/2m\omega)^{1/2}$ while $\langle 1|x|0\rangle =\sqrt{\hbar/2m\omega}$. Thus to <u>second order</u>

$$c_2^{(2)}(t) = (-i/\hbar)^2\int_0^t dt'\int_0^{t'} dt'' e^{i\omega_{21}t'}V_{21}(t')e^{i\omega_{1o}t''}V_{10}(t'') \tag{4}$$

gives a non-vanishing contribution, since V_{21} and V_{10} are non-vanishing ($\omega_{21} = (E_2-E_1)/\hbar$). Thus there is a finite probability to find the oscillator in its <u>second</u> excited state E_2, and the argument can be pursued to even higher order terms and corresponding higher order excited states.

24. The initial state is $|0\rangle$, so from (5.6.17), we have

$$c_n^{(0)}(t) = \delta_{n0},\ c_n^{(1)}(t) = (-i/\hbar)\int_0^t e^{-i(E_0-E_n)t'/\hbar}\langle n|H'(x,t')|0\rangle dt'. \quad (1)$$

Next we note that

$$\langle n|H'(x,t)|0\rangle = Ae^{-t/\tau}\langle n|x^2|0\rangle \quad (2)$$

and from (2.3.24), we have $x^2|0\rangle = \frac{1}{2}(\hbar/m\omega)(a+a^\dagger)(a+a^\dagger)|0\rangle$. Since $a|0\rangle = 0$, $a^\dagger|0\rangle = |1\rangle$, $a|1\rangle = |0\rangle$, $a^\dagger|1\rangle = \sqrt{2}|2\rangle$, thus $x^2|0\rangle = (\hbar/2m\omega)[|0\rangle + \sqrt{2}|2\rangle]$, and therefore $\langle n|x^2|0\rangle = (\hbar/2m\omega)[\delta_{n0} + \sqrt{2}\delta_{n2}]$. We see that if $n \neq 0$ or $n \neq 2$, $c_n^{(1)}(t)$ of (1) vanishes because $\langle n|x^2|0\rangle$ vanishes in (2). Only the following coefficients are relevant to our discussion: $c_0^{(0)}=1$, $c_2^{(0)}=0$, $c_0^{(1)} = (-i/\hbar)\int_0^t(\hbar/2m\omega) \times Ae^{-t'/\tau}dt' = \frac{iA}{2m\omega}(e^{-t/\tau} - 1)\tau$ (which for $t/\tau \gg 1$, gives $c_0^{(1)} \approx -iA\tau/2m\omega$), $c_2^{(1)} = (-i/\hbar)\frac{\hbar}{2m\omega}\sqrt{2}\int_0^t \exp[-i(E_0-E_2)t'/\hbar]Ae^{-t'/\tau}dt' = -i\sqrt{2}A/2m\omega(1/\tau - 2\omega i)$.

After a long time duration of perturbation, the state becomes [see (5.5.4) and (5.6.1)]

$$|\psi\rangle = [1 - iA\tau/2m\omega]e^{-i\omega t/2}|0\rangle - \frac{i\sqrt{2}A}{2m\omega(1/\tau-2i\omega)}e^{-i5\omega t/2}|2\rangle \quad (3)$$

(Remark: higher order terms like A^2, A^3,...... are ignored.) So the probability for the system to be transmitted to the second excited state is

$$P_2 = \frac{|A|^2}{2m^2\omega^2(1/\tau^2+4\omega^2)} \Big/ [1+\frac{|A|^2\tau^2}{4m^2\omega^2} + \frac{1}{2}\frac{|A|^2}{m^2\omega^2(4\omega^2+1/\tau^2)}]. \quad (4)$$

There is no probability for transition to other states such as $|1\rangle, |3\rangle$,.......

25.

$$H = \begin{pmatrix} E_1^{(0)} & \lambda\cos\omega t \\ \lambda\cos\omega t & E_2^{(0)} \end{pmatrix} = H_0 + V(t)$$

(a) Let us write $|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. A general state is

$$|\alpha,t\rangle = c_1(t)\exp[-iE_1^{(0)}t/\hbar]\ |1\rangle + c_2(t)\exp[-iE_2^{(0)}t/\hbar]\ |2\rangle$$

with $c_1(0) = 1$, and $c_2(0) = 0$. Now this problem can be solved exactly, but we are told to proceed via time-dependent perturbation theory. Take (5.6.17) - (5.6.19) of text, we have (for n=2)

$$c_2^{(1)}(t) = -\frac{i}{\hbar}\lambda\int_0^t \exp[i\omega_{21}t']\cos\omega t'\,dt'$$

$$= (-i/\hbar)\lambda\int_0^t \tfrac{1}{2}[\exp(i[\omega_{21}+\omega]t' + \exp(i[\omega_{21}-\omega]t')]dt'$$

$$= (\frac{-\lambda i}{\hbar})[\frac{e^{i(\omega_{21}+\omega)t/2}\sin(\omega_{21}+\omega)t/2}{(\omega_{21}+\omega)} + \frac{e^{i(\omega_{21}-\omega)t/2}\sin(\omega_{21}-\omega)t/2}{(\omega_{21}-\omega)}].$$

Now $|c_2^{(1)}(t)|^2$ is the transition probability which becomes

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

(b) Since $\omega_{21} = (E_2^{(o)} - E_1^{(o)})/\hbar$, we see that $\omega_{21}\pm\omega = 0$ would correspond to vanishing denominators in our perturbation expression for $|c_2^{(1)}(t)|^2$ above, and hence a breakdown of the approximation scheme.

26. Perturbation potential added is $-F(t)x$. The ground state energy $E_o = \tfrac{1}{2}\hbar\omega$ and the first excited state has energy $E_1 = \hbar\omega(1+\tfrac{1}{2})$ where $\omega_{1o} = \frac{1}{\hbar}(E_1-E_0) = \omega$. From (5.6.17), we have

$$c_1^{(1)}(\infty) = +(i/\hbar)\frac{F_o\tau}{\omega}\langle 1|x|0\rangle \int_{-\infty}^{+\infty}\frac{e^{i\omega t}}{\tau^2+t^2}dt = (i/\hbar)\frac{F_o\tau}{\omega}\langle 1|x|0\rangle I\ . \qquad (1)$$

The integral I may be evaluated using complex variable theory. Since $\omega>0$, we close contour in upper half t-plane ($\mathrm{Im}(t)>0$) with no contribution from semi-circle as $|t| \to \infty$. The pole at $t=+i\tau$ gives through the method of residues, contribution $I = (\pi/\tau)e^{-\omega\tau}$. Since $\langle 1|x|0\rangle = \sqrt{\hbar/2m\omega}\,(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}) = \sqrt{\hbar/2m\omega}$ for $n=0, n'=1$, we have putting everything together

$$c_1^{(1)}(\infty) = \frac{i}{\hbar}\frac{F_o\tau}{\omega}\sqrt{\hbar/2m\omega}(\frac{\pi}{\tau})e^{-\omega\tau}\ . \qquad (2)$$

Probability for being found in the first excited state is $|c_1^{(1)}(\infty)|^2 = \frac{\pi^2F_o^2}{2m\hbar\omega^3}e^{-2\omega\tau}$.

"Challenge for experts". Yes, it is reasonable. If the perturbation is turned on very slowly, and then turned off very slowly (as in the $\tau >> \frac{1}{\omega}$ case), the oscillator can be visualized to be in the ground state all the time. This is because the only effect of the applied force (uniform in space) is just a very slow change in the equilibrium point of the oscillator; at each instant of time, you can solve the time-independent Schrödinger equation for the ground state.

This problem can also be attacked semiclassically. The action integral $\oint p\,dq$ (related to $(n+\frac{1}{2})\hbar$) is "adiabatically invariant". This means that there is no sudden quantum jump as long as the external parameters change very slowly. –

27. (a) Again from (5.6.17), $c^{(1)}(t) = (-i/\hbar)\int_{t_o}^{t} \langle f|V(t')|i\rangle e^{i\omega_{fi}(t'-t_o)}dt'$, and using fact that $\delta(x-ct') = \frac{1}{c}\delta(x/c-t')$, we have

$$c^{(1)}(t) = (-i/\hbar)\int_{t_o}^{t} dt'\int dx \langle f|x\rangle \frac{A}{c}\delta(x/c-t')\langle x|i\rangle e^{i\omega_{fi}(t'-t_o)}$$

$$= (-iA/\hbar c)\int_{-\infty}^{+\infty} dx \langle f|x\rangle\langle x|i\rangle e^{i\omega_{fi}x/c} \underbrace{e^{-i\omega_{fi}t_o}}_{\text{uninteresting phase factor}}$$

as $t_o \to -\infty$, and $t \to \infty$. So probability for finding system in state $|f\rangle$ is given by $|c^{(1)}(t)|^2 = \frac{|A|^2}{\hbar^2 c^2}|\int_{-\infty}^{\infty} u_f^*(x)u_i(x)e^{i\omega_{fi}x/c}dx|^2$ with $\omega_{fi} \equiv (E_f-E_i)/\hbar$.

(b) $\delta(x-ct)$ pulse can be regarded as superposition of harmonic perturbation of form $e^{i\omega x/c}e^{-i\omega t}$ with $\omega>0$ (absorption) as well as $\omega<0$ (emission). Our result in (a) shows that the travelling pulse can give up energy $\hbar\omega = E_f-E_i$ so that the particle gets excited to state $|f\rangle$. The form of $|c^{(1)}|^2$ shows that only that part of the harmonic perturbation with the "right" frequency is relevant, just as expected from energy conservation. Note that the space integral $\int u_f^* u_i dx \times e^{i\omega_{fi}}$ is identical to the case where only one frequency component ("monochromatic wave") is present.

28. To first order 1s →2s transition is forbidden since the matrix element of perturbation is $\langle 200|z|100\rangle = 0$ by parity. Likewise, since z is proportional to a spherical tensor of rank 1, the only 1s → 2p transition which is allowed, to this (first) order, is when $\Delta m = 0$.

With potential energy $V = -eE_o z e^{-t/\tau}$ for t>0, we have for the only non vanishing transition amplitude is (see (5.6.17))

$$c^{(1)}(t) = -(-i/\hbar)eE_o \int_0^t dt' \langle 210|z|100\rangle e^{(i\omega-1/\tau)t'} \quad . \tag{1}$$

Therefore to this first order we have selection rule $\Delta\ell = 1$, $\Delta m = 0$. By simple integration, (1) can be rewritten as

$$c^{(1)}(t) = \frac{-(-ieE_o/\hbar)\langle 210|z|100\rangle(e^{[i\omega-1/\tau]t} - 1)(-i\omega - 1/\tau)}{(\omega^2 + 1/\tau^2)} \quad . \tag{2}$$

From (2) we have probability

$$|c^{(1)}(t)|^2 = \frac{e^2E_o^2}{\hbar^2}\frac{|\langle 210|z|100\rangle|^2}{(\omega^2+1/\tau^2)}[1+e^{-2t/\tau} - 2e^{-t/\tau}(\cos\omega t)] . \tag{3}$$

After a long time $t >> \tau$ (essentially set $t \to \infty$), we have

$$|c^{(1)}(\infty)|^2 = \frac{e^2E_o^2}{\hbar^2}\frac{|\langle 210|z|100\rangle|^2}{(\omega^2 + 1/\tau^2)} \tag{4}$$

where $\langle 210|z|100\rangle = 2\pi\int_{-1}^{+1} d(\cos\theta) \int_0^\infty r^2 dr R_{21}Y_1^o r\cos\theta R_{10}Y_o^o = \frac{2^{15/2}}{3^5} a_o$, and $\omega = (E_{2p}-E_{1s})/\hbar = 3e^2/8a_o\hbar$ (with $a_o = \hbar^2/me^2$).

29. First we observe that

$$\frac{1}{\hbar^2}\vec{S}_1\cdot\vec{S}_2 = \frac{-(\vec{S}_1^2 + \vec{S}_2^2) + (\vec{S}_1 + \vec{S}_2)^2}{2\hbar^2} = \begin{cases} 1/4 \text{ for triplet} \\ -3/4 \text{ for singlet} \end{cases} .$$

Therefore eigenkets of H are triplet and singlet, and eigenvalues are

$$E = \begin{cases} \Delta \text{ for triplet} \\ -3\Delta \text{ for singlet} \end{cases}$$

(a) At $t=0$, $|+-\rangle = \frac{1}{2^{1/2}}(|1,0\rangle + |0,0\rangle)$ where $|1,0\rangle$ is a triplet $m=0$ state and $|0,0\rangle$ is a singlet state. For a later time

$$|\alpha;t\rangle = \frac{1}{2^{1/2}}(|1,0\rangle e^{-i\Delta t/\hbar} + |0,0\rangle e^{+3i\Delta t/\hbar})$$

where $|1,0\rangle = \frac{1}{2^{1/2}}(|+-\rangle+|-+\rangle)$ and $|0,0\rangle = \frac{1}{2^{1/2}}(|+-\rangle-|-+\rangle)$. So

$$|\langle +-|\alpha;t\rangle|^2 = \tfrac{1}{4}|e^{-i\Delta t/\hbar} + e^{3i\Delta t/\hbar}|^2 = \tfrac{1}{2} + \tfrac{1}{2}\cos(4\Delta t/\hbar)$$
$$|\langle -+|\alpha;t\rangle|^2 = \tfrac{1}{4}|e^{-i\Delta t/\hbar} - e^{3i\Delta t/\hbar}|^2 = \tfrac{1}{2} - \tfrac{1}{2}\cos(4\Delta t/\hbar) \qquad (1)$$

and obviously $|\langle ++|\alpha;t\rangle|^2 = |\langle --|\alpha;t\rangle|^2 = 0$.

(b) Use first order perturbation theory

$$c_{+-}^{(1)}(t) = (-i/\hbar)\int_0^t \langle +-|\frac{4\Delta}{\hbar^2}\vec{S}_1\cdot\vec{S}_2|+-\rangle dt', \quad c_{-+}^{(1)}(t) = \left(\frac{-i}{\hbar}\right)\int_0^t \langle -+|\frac{4\Delta}{\hbar^2}\vec{S}_1\cdot\vec{S}_2|+-\rangle dt'$$

where we note that $\langle +-| = \frac{1}{2^{1/2}}\langle 1,0| + \frac{1}{2^{1/2}}\langle 0,0|$, $\langle -+| = \frac{1}{2^{1/2}}\langle 1,0| - \frac{1}{2^{1/2}}\langle 0,0|$ and similarly for the dual corresponding (DC) kets. Hence $c_{+-}^{(1)}(t) = -\frac{i\Delta t}{\hbar}(1-3)/2 = \frac{i\Delta t}{\hbar}$; $c_{-+}^{(1)}(t) = -\frac{i\Delta t}{\hbar}(1+3)/2 = -i2\Delta t/\hbar$. Note that $c_{--}^{(1)}(t) = c_{++}^{(1)}(t) = 0$ because $\vec{S}_1\cdot\vec{S}_2$ connects only states of the same $m_{tot.}$ values.

Probability for $|+-\rangle$ is $|1+i\Delta t/\hbar|^2 = 1 + \Delta^2t^2/\hbar^2$, this does <u>not</u> quite agree with exact treatment because $c_{+-}^{(2)}$ interfering with $c_{+-}^{(0)}$ also gives Δ^2t^2 term. Probability for $|-+\rangle$ is $4\Delta^2t^2/\hbar^2$ which agrees with exact treatment up to $O(\frac{\Delta^2t^2}{\hbar^2})$. Note expansion of exact results from (1) gives

$$|\langle +-|\alpha;t\rangle|^2 \cong 1 - \frac{1}{2}\frac{16\Delta^2t^2}{\hbar^2}, |\langle -+|\alpha;t\rangle|^2 \cong \tfrac{1}{2} - \tfrac{1}{2}(1 - \frac{16\Delta^2t^2}{2\hbar^2}). \qquad (2)$$

Hence validity of first order perturbation theory for $|+-\rangle$ is never satisfied, for $|-+\rangle$ validity is questionable when $t \gg \hbar/\Delta$ since lowest order expansion in (2) gives a poor approximation to the exact answer.

30. (a) From (5.5.17) for a two channel problem we have

$$i\hbar\begin{pmatrix}\dot{c}_1\\ \dot{c}_2\end{pmatrix} = \begin{pmatrix}0 & \gamma e^{i\omega t}e^{i\omega_{12}t}\\ \gamma e^{-i\omega t}e^{i\omega_{21}t} & 0\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} \qquad (1)$$

where $\omega_{21} = -\omega_{12} = (E_2-E_1)/\hbar$. Try for a solution of form

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} e^{i(\omega-\omega_{21})t/2}\, a_1 \\ e^{-i(\omega-\omega_{21})t/2}\, a_2 \end{pmatrix} \tag{2}$$

into (1), we have upon simplification

$$\frac{i(\omega-\omega_{21})}{2}\, a_1 + \dot{a}_1 = \frac{\gamma}{i\hbar}\, a_2; \quad \frac{-i(\omega-\omega_{21})}{2}\, a_2 + \dot{a}_2 = \frac{\gamma}{i\hbar}\, a_1 \tag{3}$$

It is straightforward to see from (3) that

$$\ddot{a}_1 = -[\gamma^2/\hbar^2 + \frac{(\omega-\omega_{21})^2}{4}]a_1; \quad \ddot{a}_2 = -[\gamma^2/\hbar^2 + \frac{(\omega-\omega_{21})^2}{4}]a_2. \tag{4}$$

Hence for instance

$$a_2 \sim \{{}^{\sin}_{\cos}\}\ [(\gamma^2/\hbar^2 + (\omega-\omega_{21})^2/4)^{1/2}t]\ . \tag{5}$$

Since $c_2(0) = 0$, we must have from (2)

$$c_2(t) \propto e^{-i(\omega-\omega_{21})t/2}\sin\{[\gamma^2/\hbar^2 + (\omega-\omega_{21})^2/4]^{1/2}t\} \tag{6}$$

Again from (1), we have since $c_1(0) = 1$, that $i\hbar\dot{c}_2|_{t=0} = \gamma$. Hence

$$c_2(t) = \frac{\gamma}{i\hbar[\gamma^2/\hbar^2+(\omega-\omega_{21})^2/4]^{1/2}}e^{-i(\omega-\omega_{21})t/2}\sin\{[\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4}]^{1/2}t\} \tag{7}$$

and

$$|c_2(t)|^2 = \frac{(\gamma^2/\hbar^2)}{(\gamma^2/\hbar^2)+(\omega-\omega_{21})^2/4}\sin^2\{[\gamma^2/\hbar^2+(\omega-\omega_{21})^2/4]^{1/2}t\}. \tag{8}$$

Now from (1), we have $i\hbar\dot{c}_2 = \gamma e^{-i\omega t}e^{i\omega_{21}t}\, c_1$, hence

$$c_1 = (i\hbar/\gamma)e^{i(\omega-\omega_{21})t/2}\, \dot{c}_2 \tag{9}$$

and using (7) it is easy to verify that

$$|c_1(t)|^2 = 1 - |c_2(t)|^2 \tag{10}$$

with $|c_2(t)|^2$ given by (8).

(b) Perturbation approach, let us use (5.6.17), than

$$c_2^{(1)}(t) = \left(\frac{-i}{\hbar}\right)\gamma\int_0^t e^{-i(\omega-\omega_{21})t'}dt' = \frac{(\gamma/\hbar)[e^{-i(\omega-\omega_{21})t}-1]}{(\omega-\omega_{21})} \tag{11}$$

and

$$|c_2^{(1)}(t)|^2 = \frac{4(\gamma/\hbar)^2}{(\omega-\omega_{21})^2}\sin^2\left[\frac{(\omega-\omega_{21})t}{2}\right]. \tag{12}$$

Compare (12) with exact result (8), we see that γ^2 in denominator (as well as the γ^2 in the radical sign) is missing in the perturbation expression. However, as long as $|\omega-\omega_{21}| >> 2|\gamma|/\hbar$, the perturbation result is justifiable. When $\omega \cong \omega_{21}$, $|c_2^{(1)}|^2$ can exceed unity even with small γ. As for c_1, we have $c_1^{(1)} = 0$ (since $i\hbar\dot{c}_1^{(1)} = 0$), so $|c_1|^2 \cong |c_1^{(o)}|^2 = 1$.

31. If the perturbation potential V is constant in time, then the second term in Eq. (5.6.36) will be rapidly oscillating and gives no contribution to the transition probability.

However, if the perturbation is assumed to be slowly time-dependent, i.e. $V \to Ve^{\eta t}$, where η is small, the rapid oscillating term does give some non-vanishing contribution, which grows linearly in time: With $V\to Ve^{\eta t}$, (5.6.36) becomes

$$\begin{aligned}
c_n^{(2)}(t) &= \left(\frac{-i}{\hbar}\right)^2\sum_m V_{nm}V_{mi}\int_{-\infty}^t dt' e^{i\omega_{nm}t'+\eta t'}\int_{-\infty}^{t'} dt'' e^{i\omega_{mi}t''+\eta t''} \\
&= (i/\hbar)\sum_m \frac{V_{nm}V_{mi}}{E_m-E_i-i\eta\hbar}\int_{-\infty}^t dt' e^{i\omega_{ni}t'+2\eta t'} = \frac{e^{i\omega_{ni}t+2\eta t}}{E_n-E_i-2i\eta\hbar}\cdot\sum_m\frac{V_{nm}V_{mi}}{E_m-E_i-i\eta\hbar} \\
&= \sum_m \frac{V_{nm}V_{mi}}{(E_m-E_i-i\eta\hbar)(E_n-E_i-2i\eta\hbar)} + \frac{e^{i\omega_{ni}t+2\eta t}-1}{E_n-E_i-2i\eta\hbar}\sum_m\frac{V_{nm}V_{mi}}{E_m-E_i-i\eta\hbar}.
\end{aligned} \tag{1}$$

When $\eta\to 0$, the first term above (in (1)) is exactly the first term in (5.6.36). On the other hand, the second term has a coefficient

$$\lim_{\omega_{ni}\to 0}\frac{e^{i\omega_{ni}t}-1}{E_n-E_i} \to (i/\hbar)t \tag{2}$$

which is linear in time when $\omega_{ni}\to 0$. That $|c_n^{(2)}(t)|^2$ has a quadratic dependence on time is not disturbing (c.f. (5.6.26) and subsequent discussion). Hence a non vanishing contribution to the transition probability from the second term in (5.6.36) is realizable since the total transition rate $\Gamma_{i\to n}(t)$ is defined to be

$$\Gamma_{i\to n}(t) = \frac{d}{dt}\left(\sum_{\alpha}|c_n^{(\alpha)}|^2\right). \tag{3}$$

32. Our Hamiltonian is

$$H = H_o + V = A\vec{S}_1\cdot\vec{S}_2 + (eB/m_ec)(S_{1z} - S_{2z}). \tag{1}$$

The four unperturbed states of positronium are

$$\begin{aligned} &\psi_1^{+1} = |{++}\rangle,\ \psi_1^o = \tfrac{1}{2^{1/2}}[|{+-}\rangle+|{-+}\rangle],\ \psi_1^{-1} = |{--}\rangle \qquad \text{(triplet)} \\ &\psi_o^o = \tfrac{1}{2^{1/2}}[|{+-}\rangle-|{-+}\rangle] \qquad \text{(singlet)}. \end{aligned} \tag{2}$$

The unperturbed energy levels must be determined, with $H_o = A\vec{S}_1\cdot\vec{S}_2 = \frac{A}{2}[(\vec{S}_1+\vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2]$, hence $H_o\psi_1^{\pm1,0} = \frac{A\hbar^2}{2}[2-3/4-3/4]\psi_1^{\pm1,0} = \frac{A\hbar^2}{4}\psi_1^{\pm1,0}$, while $H_o\psi_o^o = (A\hbar^2/2)\times[0-3/4-3/4]\psi_o^o = \frac{-3A\hbar^2}{4}\psi_o^o$. So unperturbed energy levels are

$$E_1^{(o)} = A\hbar^2/4 \text{ (triplet state)},\ E_o^{(o)} = -3A\hbar^2/4 \text{ (singlet state)}. \tag{3}$$

Now it is evident from (2) that $(S_{1z} - S_{2z})\psi_1^{\pm1} = 0$ and $(S_{1z}-S_{2z})\psi_{0,1}^0 = \hbar\psi_{1,0}^0$, therefore the first order energy level shifts are zero. Because the matrix elements of V between degenerate states are all vanishing, there is no problem about using non-degenerate perturbation theory in this case. We next compute the first order corrections to the unperturbed states. From $\langle\psi_1^{\pm1}|S_{1z}-S_{2z}|\psi_{0,1}^0\rangle$, we see that there is no mixing of the $S_z = \pm1$ states with the $S_z = 0$ states. Using (5.1.53a), the mixing between the two $S_z = 0$ states are given by

$$\delta\psi_o^o = \frac{\psi_1^o\langle\psi_1^o|V|\psi_o^o\rangle}{E_o^{(o)} - E_1^{(o)}},\quad \delta\psi_1^o = \frac{\psi_o^o\langle\psi_o^o|V|\psi_1^o\rangle}{E_1^{(o)} - E_o^{(o)}} \tag{4}$$

where $\langle\psi_1^o|V|\psi_o^o\rangle = \frac{eB}{m_ec}\langle\psi_1^o|S_{1z} - S_{2z}|\psi_o^o\rangle = \frac{eB}{m_ec}\hbar$. Hence using (3), we have

$$\delta\psi_0^0 = \psi_1^0 \frac{eB\hbar}{m_e c}(-1/A\hbar^2) \text{ and } \delta\psi_1^0 = \psi_0^0 \frac{eB\hbar}{m_e c}(1/A\hbar^2). \tag{5}$$

Also from (5.1.53b), we have

$$\Delta E_0 = (\frac{eB\hbar}{m_e c})^2(-1/A\hbar^2),\ \Delta E_1 = (\frac{eB\hbar}{m_e c})^2(1/A\hbar^2). \tag{6}$$

Therefore to second order in perturbation theory

$$E_1(m=\pm 1) = A\hbar^2/4,\ E_1(m=0) = \frac{A\hbar^2}{4}[1+4(eB/m_e cA\hbar)^2],$$
$$E_0 = -\frac{A\hbar^2}{4}[3+4(eB/m_e cA\hbar)^2]. \tag{7}$$

Assuming the field B to be weak, the term $[1+4(eB/m_e cA\hbar)^2]^{\frac{1}{2}}$ may be approximated by $1+2(eB/m_e cA\hbar)^2$ in the exact expression for energy, than we see that exact expression for the m = 0 energy levels yields the second order results found above.

(b) We may write this new time dependent perturbation as

$$V'(t) = \frac{eB'e^{i\omega t}}{m_e c}(S_{1\hat{B}'} - S_{2\hat{B}'}) \tag{8}$$

where ω is the angular frequency of the energy difference. To determine which direction to orient $\hat{B}'$ the matrix elements of $(S_{1j} - S_{2j})$ with j=x,y,z between χ_1 and χ_0 will be examined, where $\chi_1 = Z_1^{\frac{1}{2}}(\psi_1^0 + a_1\psi_0^0)$ and $\chi_0 = Z_0^{\frac{1}{2}}(\psi_0^0 + a_0\psi_1^0)$ are the general forms of mixture between the two m=0 states. Let us use $S_x = \frac{\hbar}{2} \times [|+\rangle\langle-| + |-\rangle\langle+|]$ representation, than from (2)

$$S_{1x}\psi_0^0 = \frac{\hbar}{2}\times\frac{1}{2^{\frac{1}{2}}}[|--\rangle-|++\rangle],\ S_{2x}\psi_0^0 = \frac{\hbar}{2}\times\frac{1}{2^{\frac{1}{2}}}[|++\rangle-|--\rangle], \tag{9}$$

hence

$$(S_{1x} - S_{2x})\psi_0^0 = \frac{\hbar}{2^{\frac{1}{2}}}(\psi_1^{-1} - \psi_1^{+1}), \tag{10}$$

also

$$S_{1x}\psi_1^0 = \frac{\hbar}{2}\times\frac{1}{2^{\frac{1}{2}}}[|--\rangle+|++\rangle],\quad S_{2x}\psi_1^0 = \frac{\hbar}{2}\times\frac{1}{2^{\frac{1}{2}}}[|++\rangle+|--\rangle]. \tag{11}$$

and thus

$$(S_{1x} - S_{2x})\psi_1^0 = 0. \tag{12}$$

From (10) and (12), we see that by orthonormality of ψ_ℓ^m states, $\langle\chi_0|(S_{1x}-S_{2x})\times$

$|\chi_1\rangle = 0$; similarly it can be shown that $\langle\chi_o|(S_{1y}-S_{2y})|\chi_1\rangle = 0$. However we have $(S_{1z}-S_{2z})\psi^o_{o,1} = \hbar\psi^o_{1,o}$, thence $(S_{1z}-S_{2z})|\chi_1\rangle = Z_1^{\frac{1}{2}}\hbar(\psi^o_o + a_1\psi^o_1)$ and $\langle\chi_o|(S_{1z}-S_{2z})\times|\chi_1\rangle = Z_1^{\frac{1}{2}}Z_o^{\frac{1}{2}}\hbar(1+a_o^*a_1)$. From orthogonality of χ_1 and χ_o we know that $a_o^* = -a_1$, hence in general $\langle\chi_o|(S_{1z}-S_{2z})|\chi_1\rangle$ does not vanish. Therefore the $\hat{B}'$ field should be in the z-direction.

33. From (5.7.1) the photon-electron interaction is written as

$$V = \frac{-e}{m_e c}\vec{A}.\vec{p} \tag{1}$$

and for emission (see (5.7.6)), we have $\vec{A} = A_o\vec{\varepsilon}e^{-i\omega\hat{n}.\vec{x}/c+i\omega t}$ where $\vec{\varepsilon}$ is the polarization. Matrix element

$$V_{ni} = \frac{-eA_o}{m_e c}\langle n|e^{-i\omega\hat{n}.\vec{x}/c}\vec{\varepsilon}.\vec{p}|i\rangle \tag{2}$$

and the transition rate from $i\to n$ is (c.f. analogous case for absorption in (5.7.8))

$$w_{i\to n} = (2\pi/\hbar)\frac{e^2}{m_e^2c^2}|A_o|^2|\langle n|e^{-i\omega\hat{n}.\vec{x}/c}\ \vec{\varepsilon}.\vec{p}|i\rangle|^2\delta(E_n-E_i+\hbar\omega). \tag{3}$$

In the dipole approximation $e^{-i(\omega/c)\hat{n}.\vec{x}} \to 1$, so

$$w_{i\to n} = (2\pi/\hbar)\frac{e^2|A_o|^2}{m_e^2c^2}|\vec{\varepsilon}.\langle n|\vec{p}|i\rangle|^2\delta(E_n-E_i+\hbar\omega). \tag{4}$$

From $[x,H_o] = i\hbar p/m_e$ we write as in (5.7.21) $\langle n|p_x|i\rangle = im_e\omega_{ni}\langle n|x|i\rangle$, etc. Hence

$$w_{i\to n} = (2\pi/\hbar)\frac{e^2|A_o|^2}{m_e^2c^2}m_e^2\omega_{ni}^2|\vec{\varepsilon}.\langle n|\vec{x}|i\rangle|^2\delta(E_n-E_i+\hbar\omega). \tag{5}$$

Now $m_n - m_i = -1$, and remember that $\vec{x}$ is a spherical tensor of rank 1, we have from Sakurai (1967) [see equations (2.127) and (2.128)] that $\vec{d}_{ni} = \langle n|\vec{x}|i\rangle \sim \hat{x}-i\hat{y}$ and

$$|\vec{\varepsilon}.\vec{d}_{ni}|^2 \sim |\varepsilon_x-i\varepsilon_y|^2 = \varepsilon_x^2 + \varepsilon_y^2 . \tag{6}$$

Since $\hat{n}$ is perpendicular to $\vec{\varepsilon}$, if we have a rotating polarization vector $\vec{\varepsilon}$, its projection on to the x-y plane will be $(\varepsilon_x^2+\varepsilon_y^2)^{1/2} = |\vec{\varepsilon}|\cos\theta$ where θ is the angle between $\hat{n}$ and the z-axis. Therefore the angular distribution is proportional to $\cos^2\theta$.

Since the atom loses one unit of angular momentum in the z-direction, this must be carried off by the photon. Therefore if the photon is emitted in the positive z direction it must be right polarized (i.e. spin parallel to momentum) and if the photon is emitted in the negative z direction then its spin point in the +z direction and its polarization must be left-handed.

Since the electron's wave function does not change discontinuously, it remains in the ground state of ^{3}H for a short while, before it leaks into a definite eigenstate of ^{3}He. Thus all we need is the overlap of the initial wave function with the ground state of ^{3}He.

$$^3\text{H}: \psi_{o,o}(r) = \frac{1}{\pi^{1/2}}\frac{1}{a_o^{3/2}}e^{-r/a_o}\ , \quad a_o = \hbar/m_e c\alpha = 0.53\text{Å}$$

$$^3\text{He}: \psi_{o,o}(r) = \frac{1}{\pi^{1/2}}(2/a_o)^{3/2}e^{-2r/a_o}\ .$$

The probability amplitude $C_o = \int d^3x\psi^{*\,^3\text{He}}_{oo}\psi^{\,^3\text{H}}_{oo}$ (where $\int d\Omega = 4\pi$) $= \int_0^\infty drr^2 4(\frac{2}{a_o^2})^{3/2} \times e^{-3r/a_o} = 4(2/a_o^2)^{3/2}(a_o/3)^3\int_0^\infty dxx^2e^{-x} = 16\sqrt{2}/27 = 0.838$. Hence probability $= |C_o|^2 = 0.702$ (or a 70% chance).

Write $V(\vec{x},t) = \frac{1}{2}[V_o\exp(i\omega z/c - i\omega t) + V_o\exp(-i\omega z/c + i\omega t)]$ where $V_o e^{i\omega z/c - i\omega t}$ is responsible for absorption of energy $\hbar\omega$ while $V_o e^{-i\omega z/c+i\omega t}$ is responsible for emission of energy $\hbar\omega$. Since $E_i<E_f$, only absorption part contributes and absorption rate is

$$|c^{(1)}|^2/t = (2\pi/\hbar)|V_o/2|^2|\langle\vec{k}_f|e^{i\omega z/c}|S\rangle|^2\delta(E_{\vec{k}_f}-E_S-\hbar\omega) \quad (1)$$

where $\langle\vec{k}_f|$ is a plane wave bra state and $|S\rangle$ is atomic ket state.

The basic differences with photoelectric case are (i) $|V_o/2|^2$ in place of $e^2|A_o|^2/m_e^2c^2$ (c.f. (5.7.1) and (5.7.3)) and (ii) $|\langle\vec{k}_f|e^{i\omega z/c}|S\rangle|^2$ in place of $|\langle\vec{k}_f|\vec{\varepsilon}.\vec{p}e^{i\omega z/c}|S\rangle|^2$, where note $\vec{\varepsilon}.\vec{p}$ is absent in our case.

The integral to be evaluated is

$$\int \frac{e^{-i\vec{k}_f.\vec{x}}\,e^{i\omega z/c}}{L^{3/2}}\psi_S(\vec{x})d^3x \tag{2}$$

where $\psi_S(x)$ is the atomic wave function. Compare (2) with the space integral in the photoelectric case (see (5.7.33))

$$\int \frac{e^{-i\vec{k}_f.\vec{x}}}{L^{3/2}}\,\vec{\varepsilon}.(-i\hbar\vec{\nabla})e^{i\omega z/c}\psi_S(\vec{x})d^3x \tag{3}$$

where we let $-i\hbar\vec{\nabla}$ operate on plane wave (i.e. integrate by part, or use Hermiticity of $-i\hbar\vec{\nabla}$). This picks up $\vec{k}_f.\vec{\varepsilon}$ which can be taken <u>outside</u> integral in (3). Thus

$$|\langle\vec{k}_f|e^{i\omega z/c}|S\rangle|^2 = \frac{1}{\hbar^2(\vec{k}_f.\vec{\varepsilon})^2}|\langle\vec{k}_f|\vec{\varepsilon}.\vec{p}e^{i\omega z/c}|S\rangle|^2 \tag{4}$$

and in terms of angles shown in Fig.5.10, we have

$$(\vec{k}_f.\vec{\varepsilon})^2 = k_f^2\sin^2\theta\cos^2\phi. \tag{5}$$

So the angular distribution differs by the absence (our case) or presence (photoelectric) of $\sin^2\theta\cos^2\phi$.

The energy dependence is such that energy conservation $E_{\vec{k}_f} - E_S = \hbar\omega$ must be be satisfied in both cases. This means that k_f is determined by $\hbar^2k_f^2/2m - E_S = \hbar\omega$. But suppose we now vary ω . Then the transition rate integrated with the density of final states (linear in k_f) goes as k_f (our case) but k_f^3 (in photoelectric case).

36. Use periodic boundary conditions in two dimensions. Than $k_x = \frac{2\pi n_x}{L}$, $k_y = \frac{2\pi n_y}{L}$

and $n^2 = n_x^2 + n_y^2 = k^2(L/2\pi)^2$. The number of states in differential area in polar coordinates (n,ϕ) is $nd\phi dn = (L/2\pi)^2 k d\phi dk$. To convert dk into dE, use $E = \hbar^2k^2/2m$ and thus $\hbar^2 kdk/m = dE$ or $dk = mdE/\hbar^2 k$. Hence $\rho(E)dEd\phi = (L/2\pi)^2(\frac{m}{\hbar}2)dEd\phi$ where factor $(L/2\pi)^2(\frac{m}{\hbar}2)$ is independent of k (or E)!!

37. A particle of mass m, constrained by an infinite-wall potential within the interval $0\leq x\leq L$, satisfies the boundary condition $\sin kL = \sin(n\pi)$, or

$$k = n\pi/L,\ n=0,\pm1,\pm2,\ldots\ldots \tag{1}$$

The (one dimensional) energy is $E = \hbar^2k^2/2m = \hbar^2n^2\pi^2/2mL^2$. What we need to calculate is ndn expressed as the density of states (i.e. number of states per unit energy interval) viz: $\rho(E)dE$. Here $dE = \hbar^2\pi^2 ndn/mL^2$, so $ndn = (mL^2/\hbar^2\pi^2)dE$. The assumption of high energy is needed in order to work in a n-continuum space rather than the discrete set given by (1). Dimension is consistent with that found in problem 36 above for two dimensions, namely <u>dimensionless</u> as required.

38. Use (5.7.32) and (5.7.33) where in (5.7.33) we replace the hydrogen atom wave function by ψ_S, the ground state wave function of a three-dimensional isotropic harmonic oscillator of angular frequency ω_o. The differential cross section reads therefore as

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2\alpha\hbar}{m^2\omega}\left|\int\frac{e^{-i\vec{k}_f\cdot\vec{x}}}{L^{3/2}}e^{i\omega\hat{n}\cdot\vec{x}/c}(-i\hbar\vec{\nabla})\cdot\hat{\varepsilon}\psi_S d^3x\right|^2\frac{mL^3k_f}{\hbar^2(2\pi)^3} \tag{1}$$

where $(-i\hbar\vec{\nabla})$ operates on the final state wave function using Hermiticity. Equation (1) simplifies to

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2\alpha m}{m^2\omega}\frac{}{\hbar}\frac{k_f\hbar^2}{(2\pi)^3}(\vec{k}_f\cdot\hat{\varepsilon})^2\left|\int e^{-i\vec{q}\cdot\vec{x}}\psi_S d^3x\right|^2 \tag{2}$$

where $\vec{q} \equiv \vec{k}_f - \frac{\omega}{c}\hat{n}$, and $\psi_S = (m\omega_o/\pi\hbar)^{3/4}\, e^{-m\omega_o r^2/2\hbar}$ (note: $\omega \neq \omega_o$, the oscillator frequency). Energy conservation requires that

$$\hbar\omega + \tfrac{1}{2}\hbar\omega_o = \hbar^2k_f^2/2m. \tag{3}$$

Let us evaluate the integral in Eq.(2), i.e.

$$I = \int e^{-i\vec{q}.\vec{x}}\psi_S d^3x = (\frac{m\omega_o}{\pi\hbar})^{3/4} I_x I_y I_z \tag{4}$$

where $I_x \equiv \int_{-\infty}^{+\infty} e^{-iq_x x} e^{-m\omega_o x^2/2\hbar} dx$, I_y, I_z are similar expressions with $x \to y,z$ and $q_x \to q_y, q_z$. By method of quadrature, we have $I_x = \int_{-\infty}^{+\infty} e^{-m\omega_o(x+iq_x\hbar/m\omega_o)^2/2\hbar}\cdot$ $e^{-\frac{1}{2}(\hbar q_x^2/m\omega_o)}dx = \sqrt{2\pi\hbar/m\omega_o}\; e^{-\hbar q_x^2/2m\omega_o}$. So

$$I^2 = (\frac{m\omega_o}{\pi\hbar})^{3/2}(\frac{2\pi\hbar}{m\omega_o})^3 e^{-\hbar(q_x^2+q_y^2+q_z^2)/m\omega_o} \tag{5}$$

and in terms of the angles (θ,ϕ) shown in Fig. 5.10, we have $(\vec{k}_f.\hat{\varepsilon})^2 = k_f^2\sin^2\theta \times \cos^2\phi$, and

$$I^2 = (\frac{4\pi\hbar}{m\omega_o})^{3/2} e^{-\frac{\hbar}{m\omega_o}[k_f^2-2k_f(\omega/c)\cos\theta+(\omega/c)^2]}. \tag{6}$$

Thus from (2) we have putting everything together

$$\frac{d\sigma}{d\Omega} = \frac{4\alpha\hbar^2 k_f^3}{m^2\omega\omega_o}(\frac{\pi\hbar}{m\omega_o})^{\frac{1}{2}} e^{\frac{-\hbar}{m\omega_o}[k_f^2+(\omega/c)^2]}\sin^2\theta\cos^2\phi\, e^{(\frac{2\hbar k_f}{m\omega_o}\frac{\omega}{c})\cos\theta} \tag{7}$$

Let's check the dimension of (7), α: dimensionless, $\hbar$: ML^2/T, k_f: $1/L$, ω,ω_o: $1/T$, hence dimension of (7) is

$$\frac{M^2L^4}{T^2}\;\frac{1}{L^3}\;\frac{T^2}{M^2}\;[ML^2/T/M/T]^{\frac{1}{2}} = L^2 \text{ (dimension of area)} \tag{8}$$

39. Via Fourier transform, we know

$$\phi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3\vec{x}\; e^{-i\vec{p}.\vec{x}/\hbar}\psi_{100}(\vec{r}). \tag{1}$$

Now $d^3\vec{x} = r^2 dr\sin\theta d\theta d\phi$, and for ground-state of hydrogen atom we have $\psi_{100}(\vec{r}) = \psi_{100}(r) = (1/\pi a_o^3)^{\frac{1}{2}}e^{-r/a_o} = \gamma e^{-r/a_o}$. Then

$$\phi(\vec{p}) = \frac{-\gamma}{(2\pi\hbar)^{3/2}}\int_0^\infty\int_0^\pi\int_0^{2\pi} r^2 dr d(\cos\theta)d\phi e^{-(r/a_o+i\vec{p}.\vec{r}/\hbar)}. \tag{2}$$

We choose the z-axis in the direction of $\vec{p}$, therefore $\vec{p}.\vec{r} = p_z z = pz = pr\cos\theta$, and we integrate out θ,ϕ variables to get

$$\phi(\vec{p}) = \frac{4\pi\gamma\hbar}{p(2\pi\hbar)^{3/2}} \int_0^\infty r dr e^{-r/a_o} \sin(pr/\hbar). \tag{3}$$

The r-integration is also straightforward, we have

$$\phi(\vec{p}) = \frac{4\pi\gamma\hbar}{p(2\pi\hbar)^{3/2}} \left\{ \frac{re^{-r/a_o}[-\frac{1}{a_o}\sin(pr/\hbar) - \frac{p}{\hbar}\cos(pr/\hbar)]}{(\frac{1}{a_o^2} + p^2/\hbar^2)} \right.$$
$$\left. - e^{-r/a_o} \frac{\{[\frac{1}{a_o^2} - \frac{p^2}{\hbar^2}]\sin(pr/\hbar) + \frac{2p}{a_o\hbar}\cos(pr/\hbar)\}}{(\frac{1}{a_o^2} + p^2/\hbar^2)^2} \right\} \Bigg|_0^\infty , \tag{4}$$

at $r\to\infty$ contribution vanishes because of dominance of e^{-r/a_o}, the $r=0$ contribution gives

$$\phi(\vec{p}) = \frac{4\pi\gamma\hbar}{p(2\pi\hbar)^{3/2}} \frac{(2p/a_o\hbar)}{[\frac{1}{a_o^2} + p^2/\hbar^2]^2} . \tag{5}$$

Since $\gamma = (1/\pi a_o^3)^{\frac{1}{2}}$, $|\phi(\vec{p})|^2$ assumes form

$$|\phi(\vec{p})|^2 = (\frac{2^3}{\pi^2}) \frac{a_o^3 \hbar^5}{[\hbar^2 + a_o^2 p^2]^4} . \tag{6}$$

10. This problem is spontaneous emission in the dipole approximation (E1) for a hydrogen atom (or a hydrogen-like atom with only one valence electron). The complete treatment leading to $\tau(2p\to 1s) = 1.6\times 10^{-9}$ sec. is well described on p.41 - 44 of J. J. Sakurai, Advanced Quantum Mechanics (1967).

(a) Assume each particle's motion is only due to the SHO potential, than the energy states for any one particle are $\frac{1}{2}\hbar\omega$, $3\hbar\omega/2, \ldots\ldots (n+\frac{1}{2})\hbar\omega, \ldots$. From Fermi -Dirac statistical distribution, we have the probability for state with energy E being occupied is $p = 2/(1 + e^{(E-E_F)/kT})$ where E_F is the Fermi energy and the constant 2 is due to spin multiplicity (2s+1). So

$$N = \Sigma p_i = \sum_{E_i} \frac{2}{1 + \exp[(E_i-E_F)/kT]} \; ; \; E_i=(n_i+\tfrac{1}{2})\hbar\omega. \qquad (1)$$

In principle, if we know ω and temperature T, solving (1) for E_F would yield the Fermi energy E_F. In practice this is far from being elementary. The ground state $E^{(0)}$ is

$$E^{(0)} = 2\{\tfrac{1}{2}\hbar\omega+3\hbar\omega/2+\ldots+([N/2]-\tfrac{1}{2})\hbar\omega\}+([N/2]+\tfrac{1}{2})\hbar\omega\delta \qquad (2)$$

where $\delta = 0$ if N is even, $\delta = 1$ for N odd, and [N/2] is the integer part of $\frac{N}{2}$. $E^{(0)}$ can be rewritten as

$$E^{(0)} = [N/2]\hbar\omega+[N/2]([N/2]-1)\hbar\omega+([N/2]+\tfrac{1}{2})\hbar\omega\delta. \qquad (3)$$

Thence for N even and N odd, we have

$$E^{(0)} = \frac{N^2}{4}\hbar\omega \text{ (N even)}, \; E^{(0)} = [(N-1)^2/4 + N/2]\hbar\omega \text{ (N odd)}. \qquad (4)$$

Note for N even, we have N/2 energy states while for N odd we have [N/2]+1 states. Also for the ground state, we have from the definition of Fermi energy that

$$E_F = \begin{cases} (N-1)\hbar\omega/2 \text{ for N even} \\ (N/2)\hbar\omega \text{ for N odd} \end{cases} \qquad (5)$$

(b) If we assume N >> 1, and no mutual interaction as in part (a), than from (4) and (5) ground state energy $E^{(0)} \cong \frac{N^2}{4}\hbar\omega$ while Fermi energy $E_F \cong (N/2)\hbar\omega$.

2. From the Clebsch-Gordan Coefficients table, the combination of two spin-1 particles lead to 9 states. These are in the $|m_1,m_2\rangle$ basis representation,

$$j=2 \ : |11\rangle, |-1-1\rangle, \frac{1}{6^{1/2}}[|1-1\rangle+2|00\rangle+|-11\rangle], \frac{1}{2^{1/2}}[|10\rangle+|01\rangle], \frac{1}{2^{1/2}}[|0-1\rangle+|-10\rangle] \quad (1a)$$

$$j=1: \quad \frac{1}{2^{1/2}}[|10\rangle-|01\rangle], \frac{1}{2^{1/2}}[|1-1\rangle-|-11\rangle], \frac{1}{2^{1/2}}[|0-1\rangle-|-10\rangle] \quad (1b)$$

$$j=0: \quad \frac{1}{3^{1/2}}[|1-1\rangle-|00\rangle+|-11\rangle]. \quad (1c)$$

For two identical particles which are bosons (with no orbital angular momentum) and both of spin 1, Bose statistics require symmetry for the states. Evidently from (1b) the j=1 states are anti-symmetric under $m_1 \leftrightarrow m_2$ while (1a) and (1c) are acceptable, forming six symmetric states with j=2 and j=0 respectively.

If the electron were a spinless boson, then the total wave function (with now no spin part) must be symmetric, viz:-

$$\psi(x_1,x_2) = \frac{1}{2^{1/2}}(\psi_\alpha(x_1)\psi_\beta(x_2) + \psi_\beta(x_1)\psi_\alpha(x_2)) \quad \text{if } \alpha \neq \beta$$

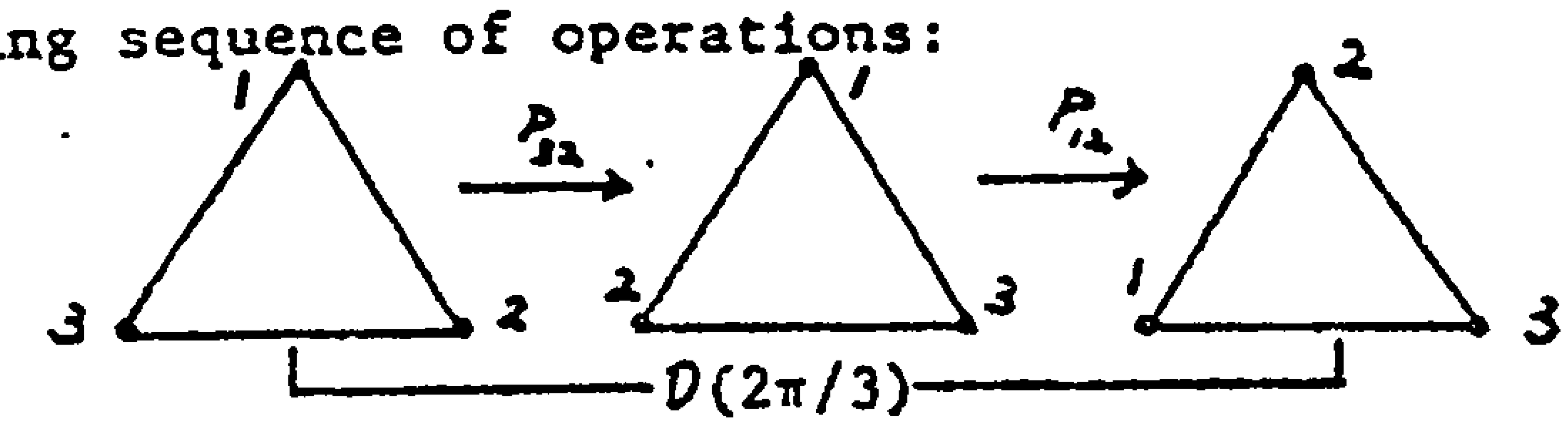
$$= \psi_\alpha(x_1)\psi_\alpha(x_2). \quad \text{if } \alpha = \beta$$

We have only "singlet" parahelium. If we assume that the interaction due to spin is small, then there is no "triplet" orthohelium and the levels of parahelium remains the same.

Consider rotation operator around z-axis:

$$\mathcal{D}(\phi) = e^{-iJ_z\phi/\hbar}. \quad (1)$$

Let $\phi = 2\pi/3$, $(4\pi/3,\ldots\ldots)$. Note however that rotation by $2\pi/3$, is equivalent to the following sequence of operations:



The system must return to its original configuration, and from (1) we have

$$\mathcal{D}(2\pi/3)|\alpha\rangle = \text{const.}|\alpha\rangle \quad (2)$$

where const. in (2) must be +1 because $P_{12}P_{32}$ gives +1. Therefore $e^{-im\phi}|_{\phi=2\pi/3} = 1$, which in turn implies

$$m = 0, \pm 3, \pm 6, \pm 9, \ldots\ldots\ldots\ldots\ldots \quad (3)$$

5. (a) The spin states must be totally symmetric. (i) $|+\rangle|+\rangle|+\rangle$ is obviously of $S=3$ where S is total spin. (ii) $\frac{1}{3^{1/2}}(|+\rangle|+\rangle|0\rangle + |+\rangle|0\rangle|+\rangle + |0\rangle|+\rangle|+\rangle)$. This construction can be obtained by applying $S_- = S_{1-} + S_{2-} + S_{3-}$ to $|+\rangle|+\rangle|+\rangle$. Since $S^2_{tot.}$ commutes with S_-, we have $S = 3$ in this case also. (iii) Simply write down all possible states with +,-,0 and of equal amplitude, we have $\frac{1}{6^{1/2}}[|+\rangle|0\rangle|-\rangle + |+\rangle|-\rangle|0\rangle + |0\rangle|-\rangle|+\rangle + |0\rangle|+\rangle|-\rangle + |-\rangle|+\rangle|0\rangle + |-\rangle|0\rangle|+\rangle]$. This <u>cannot</u> be a pure $S=3$ state since $S=3$, $m_s=0$ would contain $|0\rangle|0\rangle|0\rangle$. Proof: Imagine applying $(S_-)^3$ to $|+\rangle|+\rangle|+\rangle$, there would be a contribution from $S_{3-}S_{2-}S_{1-}|+\rangle|+\rangle|+\rangle \propto |0\rangle|0\rangle|0\rangle$. It cannot be a pure $S=1$ state either. Proof: The symmetric $S=1$ state would look like $\vec{a}(\vec{b}.\vec{c}) + \vec{b}(\vec{c}.\vec{a}) + \vec{c}(\vec{a}.\vec{b})$ which necessarily contains $|0\rangle|0\rangle|0\rangle$. Now $S=2$ states cannot be totally symmetric. Proof: $S=2$ states with $m_s=1$ must be orthogonal to the symmetric $S=3$ state. We can construct only one totally symmetric state out of ++0, +0+, and 0++. Answer for part (iii) is some linear combination of $S=3$ and $S=1$.

(b) This time the spin part must be totally antisymmetric by Bose statistics. Cases (i) and (ii) above are clearly impossible for total antisymmetry, e.g. for ++0, +0+, 0++ no matter how we distribute the signs we cannot arrange for an antisymmetric state of spin. For case (iii) it is possible, we have:- $\frac{1}{6^{1/2}}[|+\rangle|0\rangle|-\rangle - |+\rangle|-\rangle|0\rangle + |0\rangle|-\rangle|+\rangle - |0\rangle|+\rangle|-\rangle + |-\rangle|+\rangle|0\rangle - |-\rangle|0\rangle|+\rangle]$. There is in fact only one totally antisymmetric spin state possible. It goes like $\vec{a}.(\vec{b}\times\vec{c})$ and is necessarily a singlet $S=0$.

6. Possible spin states for spin 3/2 particles are $2\cdot\frac{3}{2} + 1 = 4$. So the configuration is $(1s)^4(2s)^4(2p)^{12}$. High degeneracy is because the 2p orbitals can accomodate up to $4(2\ell+1) = 12$ electrons, typically $\binom{12}{2} = \frac{12!}{2!10!} = \frac{12\times 11}{2} = 66$, i.e. 66-fold degeneracy and hence a very large number.

The ground state (lowest term) should have spin states as symmetric as possible, and space states as antisymmetric as possible [c.f. discussion of C-atom]. The only antisymmetric space states are P-wave, i.e. $\ell_1=\ell_2=1$, $\ell_{tot.}=1$. With $S_{tot.}= 3/2 + 3/2 = 3$, we have a spin 7-plet. For the total angular momentum, $\vec{L}$ and $\vec{S}$ should be as "antiparallel" as possible, this implies that $J_{tot.}= 2$. Hence ground state is $^7P_2$.

7. (a) The wave function for a single particle is $\psi_n^{(1)}(x_i) = \sqrt{2/L}\,\sin(n\pi x_i/L)$ with energy $E_n^{(1)} = n^2\pi^2\hbar^2/2mL^2$. For a two particle system the wave function is

$$\psi^{(2)}(x_1,x_2) = \sum_{i,j} c_{ij}\psi_i^{(1)}(x_1)\psi_j^{(1)}(x_2) \qquad (1)$$

where c_{ij} is determined by symmetry and the filling of energy levels according to Pauli principle. For ground state of two spin ½ fermions, the total wave function must be antisymmetric and the spin part is triplet (hence symmetric), therefore the space wave function (1) must be antisymmetric. Thus $\psi^{(2)} = \frac{1}{2^{1/2}}(\psi_1^{(1)}(x_1)\psi_2^{(1)}(x_2) - \psi_2^{(1)}(x_1)\psi_1^{(1)}(x_2))$ and to obtain a non-vanishing ground state space wave function, we must choose

$$\psi^{(2)}(x_1,x_2) = (2/\sqrt{2}L)[\sin\pi x_1/L\ \sin 2\pi x_2/L - \sin 2\pi x_1/L\ \sin\pi x_2/L] \qquad (2)$$

and $E_{tot.} = \frac{\pi^2\hbar^2}{2mL^2}(1^2+2^2) = 5\pi^2\hbar^2/2mL^2$.

(b) If spin part is a singlet state (which is antisymmetric), than space wave function must be symmetric. Hence (1) must assume for the ground state the form

$$\psi^{(2)}(x_1,x_2) = (2/L)\sin\pi x_1/L\ \sin\pi x_2/L \qquad (3)$$

and $E_{tot.}= \frac{\pi^2\hbar^2}{2mL^2}(1^2+1^2) = \pi^2\hbar^2/mL^2$.

(c) First for triplet and singlet state the first order energy shift is

$$\Delta E = -\lambda\int dx_1dx_2\psi^{(2)*}(x_1,x_2)\delta(x_1-x_2)\psi^{(2)}(x_1,x_2). \qquad (4)$$

Use the explicit form (2) and integrate over δ-function, we find for triplet state $\Delta E = (2/L)^2(-\lambda/2)\int dx_1(\sin\pi x_1/L \sin 2\pi x_1/L - \sin 2\pi x_1/L \sin\pi x_1/L)^2 = 0$ and for singlet state $\Delta E = -\lambda(2/L)^2\int_0^L \sin^4(\pi x_1/L)dx_1 = -3\lambda/2L$.

Chapter 7

1. (a) From (7.1.6) and (7.1.7), the Lippmann-Schwinger equation reads (in one dimension) $|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_o \pm i\varepsilon} V|\psi^{(\pm)}\rangle$ or $\langle x|\psi^{(\pm)}\rangle = \langle x|\phi\rangle + \int dx'\langle x|$ $\frac{1}{E - H_o \pm i\varepsilon}|x'\rangle\langle x'|V|\psi^{(\pm)}\rangle$ in position basis. The singular operator $\frac{1}{E-H_o}$ is handled by the $E \to E+i\varepsilon$ prescription if we are to have a transmitted wave for $x>a$; for reflected wave in $x<-a$ we need prescription $E \to E-i\varepsilon$. Hence for transmitted-reflected Green's function we have $G_\pm(x,x') = \frac{\hbar^2}{2m}\langle x|\frac{1}{E-H_o\pm i\varepsilon}|x'\rangle$. So

$$
\begin{aligned}
G_\pm(x,x') &= (\tfrac{\hbar^2}{2m})\int\int_{-\infty}^{+\infty} dp''\langle x|p'\rangle\langle p'|\frac{1}{E-H_o\pm i\varepsilon}|p''\rangle\langle p''|x'\rangle dp' \\
&= (\tfrac{\hbar^2}{2m}) \int_{-\infty}^{+\infty} dp'(e^{ip'x/\hbar}/\sqrt{2\pi})\frac{1}{E-p'^2/2m\pm i\varepsilon}(e^{-ip'x'/\hbar}/\sqrt{2\pi}) \qquad (1) \\
&= (1/2\pi)\int_{-\infty}^{+\infty} dq[e^{iq(x-x')}/(k^2-q^2\pm i\varepsilon)]
\end{aligned}
$$

where we have used the one dimensional version of (7.1.14) and (7.1.15). The poles of (1) are at $q = \pm(k^2\pm i\varepsilon)^{\frac{1}{2}} \equiv \pm k\pm i\varepsilon'$. By straightforward method of residue contour integration in q-plane, we have

$$G_+(x,x') = -\frac{i}{2k}\, e^{ik|x-x'|}, G_-(x,x') = -\frac{i}{2k}\, e^{-ik|x-x'|}. \qquad (2)$$

Hence integral equation for $\langle x|\psi^{(+)}\rangle$ is

$$\langle x|\psi^{(+)}\rangle = \langle x|\phi\rangle - (i/2k)(2m/\hbar^2)\int_{-a}^{+a} dx' e^{ik|x-x'|}V(x')\langle x'|\psi^{(+)}\rangle \qquad (3)$$

For transmitted wave $x>a$ (hence $|x-x'| = x-x'$), we have

$$\langle x|\psi^{(+)}\rangle = e^{ikx}/\sqrt{2\pi} - \frac{im}{k\hbar^2} \int_{-a}^{+a} e^{ik(x-x')}V(x')\langle x'|\psi^{(+)}\rangle dx'. \qquad (3')$$

Similarly for a reflected wave $x<-a$, we have from (2)

$$\langle x|\psi^{(-)}\rangle = e^{ikx}/\sqrt{2\pi} - \frac{im}{k\hbar^2} \int_{-a}^{+a} e^{-ik(x-x')}V(x')\langle x'|\psi^{(-)}\rangle dx', \qquad (4)$$

where the first term on r.h.s. of (4) is really the original wave for $x<-a$.

(b) Take now $V = -(\gamma\hbar^2/2m)\delta(x)$ where $\gamma>0$, and substitute into (3) we have

$$\langle x|\psi^{(+)}\rangle = \langle x|\phi\rangle + \frac{i\gamma}{2k}\, e^{ik|x|}\langle 0|\psi^{(+)}\rangle. \qquad (5)$$

Set x=0 (center of range $-a<x<a$ where $V(x) \neq 0$), (5) becomes

$$\langle 0|\psi^{(+)}\rangle = \frac{1}{(2\pi)^{1/2}}\frac{1}{[1 - i\gamma/2k]} . \tag{6}$$

Substitute (6) into (5), we have

$$\langle x|\psi^{(+)}\rangle = e^{ikx}/\sqrt{2\pi} + \frac{1}{(2\pi)^{1/2}} e^{ik|x|}[i\gamma/(2k-i\gamma)]. \tag{7}$$

Hence for $x>a$, transmission coefficient is $T = 1 + i\gamma/(2k-i\gamma)$. Similarly from (4) for $x<-a$, we have for reflection coefficient $R = i\gamma/(2k-i\gamma)$. This checks with Gottfried (1966), p.52.

(c) It is seen explicitly from our expressions for T and R, that they have poles at $k = i\gamma/2$, and $\langle x|\psi\rangle \sim e^{-\gamma|x|/2}$. From problem 22 (Chapter 2), we see that the Schrödinger equation

$$-\frac{\hbar^2}{2m} d^2\psi/dx^2 - \frac{\gamma\hbar^2}{2m}\delta(x)\psi = -|E|\psi \tag{8}$$

has solutions of form $\psi = Ae^{-\kappa x}$ $(x>0)$ and $\psi = Ae^{+\kappa x}$ $(x<0)$ with $k = i\kappa = i(\frac{2m|E|}{\hbar^2})^{1/2}$, and satisfy

$$d\psi/dx|_{0^+} - d\psi/dx|_{0^-} = -\gamma\psi(0). \tag{9}$$

Eq.(9) implies that $\kappa = \gamma/2$ (or $k = i\gamma/2$) thus $\psi \propto e^{-\gamma|x|/2}$ in agreement with the discussion of T and R and bound state poles when k is treated as a complex variable.

2. (a) From (7.1.33) - (7.1.36), we have $\langle\vec{x}|\psi^{(+)}\rangle = (1/2\pi)^{3/2}[e^{i\vec{k}.\vec{x}}+f(\vec{k}',\vec{k})e^{ikr}/r]$ and the differential cross-section $d\sigma/d\Omega = |f(\vec{k},\vec{k}')|^2$ where $f(\vec{k},\vec{k}')$ in the first Born approximation is given by (7.2.2)

$$f^{(1)}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}(2m/\hbar^2)\int d^3x' e^{i(\vec{k}-\vec{k}').\vec{x}'}V(\vec{x}'). \tag{1}$$

Hence

$$d\sigma/d\Omega = (m^2/4\pi^2\hbar^4)\int d\vec{x}'d\vec{x}''\, e^{i(\vec{k}-\vec{k}').\vec{x}'}V(\vec{x}')e^{-i(\vec{k}-\vec{k}').\vec{x}''}V(\vec{x}'') \tag{2}$$

and

$$\sigma = \int(m^2/4\pi^2\hbar^4)\int d\Omega_{k'}e^{-i\vec{k}'.(\vec{x}'-\vec{x}'')}\, d\vec{x}'d\vec{x}''e^{i\vec{k}.(\vec{x}'-\vec{x}'')}V(\vec{x}')V(\vec{x}''). \tag{3}$$

Now $\int d\Omega_{k'} e^{-i\vec{k}'\cdot(\vec{x}'-\vec{x}'')} = 2\pi\int_{-1}^{+1} e^{ik|\vec{x}'-\vec{x}''|\cos\theta} d(\cos\theta) = 4\pi \sin k|\vec{x}'-\vec{x}''|/k|\vec{x}'-\vec{x}''|$,

where θ is angle between $\vec{k}'$ and $\vec{x}''-\vec{x}'$, and $|\vec{k}| = |\vec{k}'| = k$.

We now average over all incident beam direction $\vec{k}$ (assuming that V is spherically symmetric), than

$$\bar{\sigma} = \frac{m^2}{\pi\hbar^4}\int d\vec{x}'d\vec{x}''\ \frac{\sin k|\vec{x}'-\vec{x}''|}{k|\vec{x}'-\vec{x}''|}V(|\vec{x}'|)V(|\vec{x}''|)\frac{1}{4\pi}\int d\Omega_k e^{i\vec{k}\cdot(\vec{x}'-\vec{x}'')}$$

$$= \frac{m^2}{\pi\hbar^4}\int d\vec{x}'d\vec{x}''\ V(r')V(r'')\sin^2 k|\vec{x}'-\vec{x}''|/k^2|\vec{x}'-\vec{x}''|^2 \qquad (4)$$

(b) Let us now apply the optical theorem for $\vec{k} = \vec{k}'$ (forward scattering) given by (7.3.9) in the second-order Born approximation (7.2.23)

$$\sigma_{tot.} = \frac{4\pi}{k}\ \mathrm{Im}\{f_B^{(2)}(\vec{k}=\vec{k}')\}$$
$$= \mathrm{Im}\{\frac{4\pi}{k}(-\frac{1}{4\pi}\frac{2m}{\hbar^2})^2\int d^3x'\int d^3x'' e^{-i\vec{k}\cdot(\vec{x}'-\vec{x}'')}e^{ik|\vec{x}'-\vec{x}''|}V(\vec{x}')V(\vec{x}'')/|\vec{x}'-\vec{x}''|\}. \qquad (5)$$

Since (5) is dependent on the angle between $\vec{k}$ and $(\vec{x}'-\vec{x}'')$, we need to take an average over all $\hat{k}$ direction, i.e. $\frac{1}{4\pi}\int d\Omega_k e^{-i\vec{k}\cdot(\vec{x}'-\vec{x}'')}$ must be computed. Hence

$$\bar{\sigma}_{tot.} = \mathrm{Im}\ \{\frac{m^2}{\pi k\hbar^4}\int d^3x'\int d^3x''\ \frac{\sin k|\vec{x}'-\vec{x}''|}{k|\vec{x}'-\vec{x}''|}\ \frac{e^{ik|\vec{x}'-\vec{x}''|}}{|\vec{x}'-\vec{x}''|}V(r')V(r'')\}$$

$$= \frac{m^2}{\pi\hbar^4}\int d^3x'\int d^3x''\ V(r')V(r'')\sin^2 k|\vec{x}'-\vec{x}''|/k^2|\vec{x}'-\vec{x}''|^2. \qquad (6)$$

This is the same as (4) and again V is assumed to be spherically symmetric.

From (7.6.35) and (7.6.34), and the method of partial waves (7.6.50), we have $\beta_\ell = (\frac{r dA_\ell}{A_\ell dr})_{r=R}$, $\tan\delta_\ell = (kRj_\ell'(kR) - \beta_\ell j_\ell(kR))/(kRn_\ell'(kR)-\beta_\ell n_\ell(kR))$ and $\sigma_{tot.} = \frac{4\pi}{k^2}\sum_{\ell=0}^{\ell\approx kR}(2\ell+1)\sin^2\delta_\ell$.

Again from (7.6.36) - (7.6.38), we have for the radial wave function $A_\ell = u_\ell/r$, $u_\ell'' + [k'^2-\ell(\ell+1)/r^2]u_\ell = 0$ where $k'^2 = 2m(E-V_0)/\hbar^2$, and $u_\ell = 0$ at $r=0$. So our solution is $u_\ell(k'r) = rj_\ell(k'r)$ or $A_\ell(k'r) = j_\ell(k'r)$, hence $\beta_\ell = k'Rj_\ell'(k'R)/j_\ell(k'R)$. Since $kR \ll 1$, and $|V_0| \ll E = \hbar^2k^2/2m$, therefore $k'R \ll 1$. But from the general recursion for $j_\ell(kR)$, we have $j_\ell'(k'R) = \ell j_\ell(k'R)/k'R$ -

$j_{\ell+1}(k'R)$. Hence

$$\beta_\ell = \ell - (k'R)j_{\ell+1}(k'R)/j_\ell(k'R) \simeq \ell - (k'R)^2/(2\ell+3). \quad (1)$$

Our expression for $\tan\delta_\ell$ becomes

$$\tan\delta_\ell = \frac{(k'R)^2 j_\ell(kR) - (2\ell+3)(kR)j_{\ell+1}(kR)}{(k'R)^2 n_\ell(kR) - (2\ell+3)(kR)n_{\ell+1}(kR)}$$

$$\simeq \frac{(k'^2-k^2)R^2 2^\ell \ell!(kR)^\ell 2^{\ell+1}(\ell+1)!}{(2\ell+1)!(2\ell+3)!\ (kR)^{-(\ell+1)}}$$

$$\simeq \frac{-2mV_oR^2}{\hbar^2(2\ell+3)}[2^\ell \ell!/(2\ell+1)!]^2(kR)^{2\ell+1} \simeq \sin\delta_\ell \simeq \delta_\ell. \quad (2)$$

Clearly only S-wave ($\ell=0$) will have significant contribution to total scattering, hence

$$\sigma_{tot.} \simeq \frac{4\pi}{k^2}\sin^2\delta_o = \frac{16\pi}{9\hbar^4}m^2V_o^2R^6. \quad (3)$$

If the energy is raised slightly, we must take into account δ_1 contribution. From (2) above we have $\delta_1 \simeq -2mV_oR^2(kR)^3/45\hbar^2$. Now from (7.6.17) we have

$$f(\theta) = \frac{1}{k}(e^{i\delta_o}\sin\delta_o + 3e^{i\delta_1}\sin\delta_1 P_1(\cos\theta) + \ldots\ldots), \quad (4)$$

hence $|f(\theta)|^2 = (1/k^2)\sin^2\delta_o + \frac{3}{k}2(e^{i(\delta_1-\delta_o)} + e^{+i(\delta_o-\delta_1)})\sin\delta_1\sin\delta_o\cos\theta + \ldots\ldots$ or

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = A+B\cos\theta \simeq \sin^2\delta_o/k^2 + 6\cos(\delta_1-\delta_o)\sin\delta_1\sin\delta_o\cos\theta/k^2.$$

We see therefore that $B/A = 6\sin\delta_1\sin\delta_o\cos(\delta_1-\delta_o)/\sin^2\delta_o \simeq 6\sin\delta_1/\sin\delta_o$ and using (2) $B/A \simeq \frac{2}{5}(kR)^2$ where we have set $\cos(\delta_1-\delta_o) = 1$.

(a) Let's take

$$f_k^{(1)}(\theta) = \sum_{\ell=o}^{\infty}\frac{(2\ell+1)}{k}e^{i\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta) = -\frac{2mV_o}{\hbar^2\mu}\frac{1}{2k^2[(1+\mu^2/2k^2)-\cos\theta]}$$

and denote $\xi = \cos\theta$, $\zeta = 1+\mu^2/2k^2 > 1$ (for $\mu>0$). Then we know how to expand $1/(\zeta-\xi) = \sum_{\ell=o}^{\infty} a_\ell P_\ell(\xi)$ in the domain $-1\leq\xi\leq+1$ where $a_\ell = \frac{(2\ell+1)}{2}\int_{-1}^{+1}\frac{P_\ell(\xi)d\xi}{\zeta-\xi} =$

$(2\ell+1)Q_\ell(\zeta)$ (and we have in mind the orthogonality of the Legendre Polynomials $\int_{-1}^{+1}d\xi P_\ell(\xi)P_{\ell'}(\xi) = \frac{2}{(2\ell+1)}\delta_{\ell\ell'}$).

Again let us rewrite $f_k^{(1)}(\theta)$ as

$$f_k^{(1)}(\theta) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2ik}(e^{2i\delta_\ell}-1)P_\ell(\xi) \cong \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{k}\left[\frac{-mV_oQ_\ell(\zeta)}{\hbar^2\mu k}\right]P_\ell(\xi).$$

Hence compare coefficient of $P_\ell(\xi)$ on both sides, we have

$$(e^{2i\delta_\ell}-1)/2i = \frac{-mV_o}{\hbar^2\mu k}Q_\ell(\zeta).$$

Assume $|\delta_\ell| \ll 1$ than $e^{2i\delta_\ell}-1 \cong 2i\delta_\ell$, and we find

$$\delta_\ell \cong -\frac{mV_o}{\hbar^2\mu k}Q_\ell(\zeta) = -\frac{mV_o}{\hbar^2\mu^2}\sqrt{2(\zeta-1)}\,Q_\ell(\zeta).$$

(b) (i) Obviously from above we can write $\delta_\ell \cong -V_oK_\ell(\zeta)$ with

$$K_\ell(\zeta) = \frac{m}{\hbar^2\mu^2}\sqrt{2(\zeta-1)}\,Q_\ell(\zeta) > 0, \quad (\zeta>1).$$

This is evident from the explicit expansion form for $Q_\ell(\zeta)$ (or at least $K_\ell(\zeta) \to 0$ for $k \to 0$). Hence we see for repulsive potential $V_o>0$: $\delta_\ell = -V_oK_\ell(\zeta)<0$, and for attractive potential $V_o<0$: $\delta_\ell = -V_oK_\ell(\zeta)>0$.

(ii) Now the deBroglie wave length $\lambda = h/p = 2\pi\hbar/p = 2\pi/k$ (or $\lambdabar = 1/k$), while the range of the potential $R = 1/\mu$. Hence $\lambdabar/R \gg 1$ implies $\eta = \mu/k \gg 1$. Hence $1/\zeta = 1/[1+\frac{1}{2}(\mu/k)^2] \cong 2(k/\mu)^2 = 2\eta^{-2}$ and therefore the polynomial $K_\ell(\zeta)$ will be reduced to $K_\ell(\eta)$ as follows

$$K_\ell(\zeta) \cong \frac{m}{\hbar^2\mu^2}\eta\frac{\ell!}{(2\ell+1)!!}\left[(2\eta^{-2})^{\ell+1} + \ldots\ldots\right].$$

This gives the approximate form for δ_ℓ in terms of η as follows:

$$\delta_\ell \cong -\frac{mV_o}{\hbar^2\mu^2}\cdot\frac{2^{\ell+1}\ell!}{(2\ell+1)!!}\eta^{-2\ell-1} = -\frac{2mV_o}{\hbar^2\mu^{2\ell+3}}\cdot\frac{(2\ell)!!}{(2\ell+1)!!}k^{2\ell+1}. \tag{1}$$

According to Gottfried (1966) [p.124, Eq. (17)] for small δ_ℓ

$$\delta_\ell(k)_{\ell\gg\ell_{max}} \cong \tan\delta_\ell = -\frac{k^{2\ell+1}}{[(2\ell+1)!!]^2}\int_0^\infty r^{2\ell+2}U(r)dr \tag{2}$$

where $U(r) = (2m/\hbar^2)V(r) = (2mV_o/\hbar^2)e^{-\mu r}/\mu r$. Since $\int_0^\infty \rho^{2\ell+1}e^{-\rho}d\rho = (2\ell+1)!$ (remember $\int_0^\infty x^n e^{-x}dx = n!$), we have

$$\delta_\ell \cong -\frac{k^{2\ell+1}.2^{2\ell}.(\ell!)^2}{[(2\ell+1)!]^2}\left(\frac{2mV_o}{\hbar^2\mu^{2\ell+3}}\int_0^\infty e^{-\rho}\rho^{2\ell+1}d\rho\right)_{\rho=\mu r} .$$

We notice that $1/(2\ell+1)!! = 2^\ell\ell!/(2\ell+1)!$, hence

$$\delta_\ell \cong -\frac{2mV_o}{\hbar^2\mu^{2\ell+3}}\cdot\frac{(2^\ell\ell!)^2}{(2\ell+1)!}k^{2\ell+1} = -\frac{2mV_o}{\hbar^2\mu^{2\ell+3}}\cdot\frac{(2\ell)!!}{(2\ell+1)!!}k^{2\ell+1}, \qquad (3)$$

and (3) is the same as (1) above obtained using the $Q_\ell(\zeta)$ expansion formula.

. The ground state wave function for the hard sphere can be written as $\psi(r,\theta,\phi) = Y_{oo}(\theta,\phi)R(r) \equiv (1/4\pi)^{1/2}\chi(r)/r$, where $\chi(r)$ obeys the equation $(-\hbar^2/2m)d^2\chi/dr^2 = E_o\chi$ $(r<a)$ and $\chi(r) = 0$ for $r>a$. Thus $\chi(r) = A\sin\alpha r + B\cos\alpha r$ for $r<a$, with $\alpha = [2mE_o/\hbar^2]^{1/2}$. The requirement that $R(r)$ be finite at $r=0$ demands that $B = 0$. At the boundary $r=a$, $\chi(a)=0$. Thus we impose $\alpha a = \pi$ or $E_o = \frac{\hbar^2}{2m}(\pi/a)^2$. The normalization constant A is fixed by $\int\psi^*\psi r^2 d\phi d\cos\theta dr = \frac{1}{4\pi}\int_0^\infty 4\pi\chi^2(r)dr = 1$, or $A^2\int_0^a \sin^2\alpha r dr = 1$. This in turn implies $A = \sqrt{2\alpha/\pi} = [8mE_o/\pi^2\hbar^2]^{1/4} = \sqrt{2/a}$.

Now we check explicitly the uncertainty relation in $x - p_x$, $(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$ but $\langle x^2\rangle = \int r^2\sin^2\theta\cos^2\phi|\psi|^2 r^2 d\phi d\cos\theta dr = \frac{1}{2a\pi}\cdot\frac{4\pi}{3}\int_0^a r^2\sin^2\alpha r dr = \frac{1}{3\alpha^2}[\pi^2/3 - \tfrac{1}{2}]$ and $\langle x\rangle = 0$. On the other hand $\langle p_x^2\rangle = -\hbar^2\int\psi^*\frac{d^2}{dx^2}\psi d^3x$, now

$$\frac{d^2\psi}{dx^2} = \frac{1}{(4\pi)^{1/2}}\sqrt{2/a}\,\frac{d^2}{dx^2}(\sin\alpha r/r) = \sqrt{1/2a\pi}\left\{\frac{d}{dx}\left[-\frac{\sin\alpha r}{r^2} + \frac{\alpha\cos\alpha r}{r}\right]\frac{\partial r}{\partial x}\right\}$$
$$= \left(\frac{1}{2a\pi}\right)^{1/2}\left[\frac{2\sin\alpha r}{r^3} - \frac{2\alpha\cos\alpha r}{r^2} - \frac{\alpha^2\sin\alpha r}{r}\right]\left(\frac{\partial r}{\partial x}\right)^2 + \left(\frac{1}{2a\pi}\right)^{1/2}\left[-\frac{\sin\alpha r}{r^2} + \frac{\alpha\cos\alpha r}{r}\right]\frac{\partial^2 r}{\partial x^2}$$

therefore

$$\langle p_x^2\rangle = -\frac{\hbar^2}{2a\pi}\int\left[\frac{\sin^2\alpha r}{r^4}(2-\alpha^2r^2) - \frac{2\alpha\sin\alpha r\cos\alpha r}{r^3}\right](\sin^2\theta\cos^2\phi)r^2 d\phi d\cos\theta dr$$
$$-\frac{\hbar^2}{2a\pi}\int\left[-\frac{\sin^2\alpha r}{r^3} + \frac{\alpha\sin\alpha r\cos\alpha r}{r^2}\right]\frac{1}{r}(1-\sin^2\theta\cos^2\phi)r^2 d\phi d\cos\theta dr$$

$$= -\frac{\hbar^2}{2a\pi}\cdot\frac{4\pi}{3}\int_0^a\left[\frac{\sin^2\alpha r}{r^2}(2-\alpha^2r^2) - \frac{2\alpha\sin\alpha r\cos\alpha r}{r}\right]dr$$

$$-\frac{\hbar^2}{2a\pi}\cdot\frac{8\pi}{3}\int_0^a\left[-\frac{\sin^2\alpha r}{r^2} + \frac{\alpha\sin\alpha r\cos\alpha r}{r}\right]dr = +\frac{2\hbar^2\alpha^2}{3a}\int_0^a \sin^2\alpha r dr = \frac{\alpha^2}{3}\hbar^2.$$

It can be readily seen that $\langle p_x\rangle = 0$, thus we have

$$(\Delta x)^2(\Delta p_x)^2 = \frac{1}{9}[\pi^2/3 - \tfrac{1}{2}]\hbar^2 \simeq \hbar^2/4,$$

which is consistent with the Heisenberg uncertainty relation.

6. (a) The full wave function for $r>a$ can be written in partial wave analysis as

$$\langle\vec{x}|\psi^{(+)}\rangle = \frac{1}{(2\pi)^{3/2}}\sum_\ell i^\ell(2\ell+1)A_\ell(r)P_\ell(\cos\theta)$$

with $A_\ell = c_\ell^{(1)}h_\ell^{(1)}(kr) + c_\ell^{(2)}h_\ell^{(2)}(kr)$ where $h_\ell^{(1)}$ and $h_\ell^{(2)}$ are the Hankel functions of the first and second kind, respectively. When we consider large r behavior, we have (c.f. (7.6.33)):

$$A_\ell(r) = e^{i\delta_\ell}[j_\ell(kr)\cos\delta_\ell - n_\ell(kr)\sin\delta_\ell].$$

Asymptotically $h_\ell^{(1)} \to e^{i(kr-\ell\pi/2)}/ikr$, $h_\ell^{(2)} \to e^{-i(kr-\ell\pi/2)}/ikr$, while the large r behavior of $\langle\vec{x}|\psi^{(+)}\rangle$ is (from (7.6.8) and (7.6.16))

$$\langle\vec{x}|\psi^{(+)}\rangle \to \frac{1}{(2\pi)^{3/2}}\sum_\ell(2\ell+1)[e^{2i\delta_\ell}e^{ikr}/2ikr - e^{-i(kr-\ell\pi)}/2ikr]P_\ell(\cos\theta).$$

So clearly $c_\ell^{(1)} = \frac{1}{2}e^{2i\delta_\ell}$ and $c^{(2)} = \frac{1}{2}$. Thus

$$A_\ell(r) = e^{i\delta_\ell}[\cos\delta_\ell j_\ell(kr) - \sin\delta_\ell n_\ell(kr)].$$

For hard sphere, the boundary condition at $r=a$ is $A_\ell(r)|_{r=a} = 0$ because the sphere is impenetrable. This means $j_\ell(ka)\cos\delta_\ell - n_\ell(ka)\sin\delta_\ell = 0$ or $\tan\delta_\ell = j_\ell(ka)/n_\ell(ka)$. For $\ell=0$ $\tan\delta_0 = \dfrac{\sin(ka)/ka}{-\cos(ka)/ka} = -\tan(ka)$ or $\delta_0 = -ka$.

(b) We have $f(\theta) = \frac{1}{k}\sum_{\ell=0}^\infty(2\ell+1)e^{i\delta_\ell}\sin\delta_\ell\, P_\ell(\cos\theta)$ and in the limit when $k \to 0$, the $\ell=0$ partial wave dominates the scattering. Thus $f(\theta) \simeq \frac{1}{k}e^{-ika}\sin(ka)$, and knowing that $d\sigma/d\Omega = |f(\theta)|^2$ we have for the total cross section $\sigma = \int(\frac{d\sigma}{d\Omega}).d\Omega = \int|f(\theta)|^2d\Omega = \int\frac{1}{k^2}\sin^2(ka)d\Omega = 4\pi\sin^2(ka)/k^2 \simeq 4\pi a^2$.

Classically, the "geometric cross section" is πa^2. By "geometric cross section" we mean the area of the disc of radius a that blocks the propagation of the plane wave (and has the same cross section area as that of a hard sphere). Low energy scattering of course means a very large wave length scattering and we do not necessarily expect a classically reasonable result.

7. (a) For the Gaussian potential (c.f. (7.4.14)), we have $\Delta_G(b) \equiv \frac{-m}{2k\hbar^2}\int_{-\infty}^{\infty} V(\sqrt{b^2+z^2})dz$ where $V(r) = V_o e^{-r^2/a^2}$. This implies that

$$\Delta_G(b) = \frac{-mV_o}{2k\hbar^2}\int_{-\infty}^{\infty} e^{-(b^2+z^2)/a^2}dz$$

$$= \frac{-mV_o}{2k\hbar^2} e^{-(b/a)^2}\int_{-\infty}^{\infty} e^{-(z/a)^2}dz = -\frac{\sqrt{\pi}}{2}\frac{mV_o a}{k\hbar^2} e^{-(b/a)^2}.$$

Since we are given that $\delta_\ell^G = \Delta(b)|_{b=\ell/k}$, hence

$$\delta_\ell^G = -\frac{\sqrt{\pi}}{2}\frac{mV_o a}{k\hbar^2} e^{-(\ell/ka)^2}$$

(b) For the Yukawa potential $V(r) = V_o e^{-\mu r}/\mu r$, we have

$$\Delta_Y(b) = -\frac{mV_o}{2k\hbar^2}\int_{-\infty}^{\infty}\frac{1}{\mu r}e^{-\mu r}\Big|_{r=\sqrt{b^2+z^2}}dz = -\frac{mV_o}{2k\hbar^2}\int_{-\infty}^{\infty}\frac{e^{-\mu\sqrt{b^2+z^2}}}{\mu(b^2+z^2)^{\frac{1}{2}}}dz.$$

The integral (remembering $r^2 = b^2+z^2$)

$$I = \int_{-\infty}^{\infty}\frac{e^{-\mu(b^2+z^2)^{\frac{1}{2}}}}{(b^2+z^2)^{\frac{1}{2}}}dz = 2\int_0^{\infty}\frac{e^{-\mu(b^2+z^2)^{\frac{1}{2}}}}{(b^2+z^2)^{\frac{1}{2}}}dz = 2\int_0^{\infty}\frac{e^{-\mu r}}{r}\frac{rdr}{(r^2-b^2)^{\frac{1}{2}}}$$

$$= 2\int_0^{\infty}\frac{e^{-\mu r}dr}{(r^2-b^2)^{\frac{1}{2}}} = 2K_o(\mu b)$$

where K_o is the modified Bessel function. Thus

$$\Delta_Y(b) = -\frac{mV_o}{2k\hbar^2}\frac{2K_o(\mu b)}{\mu} = -\frac{mV_o}{\mu k\hbar^2}K_o(\mu b)$$

hence $\delta_\ell^Y = \Delta_Y(b)|_{b=\ell/k}$ assumes value

$$\delta_\ell^Y = -\frac{mV_o}{\mu k\hbar^2}K_o(\mu\ell/k).$$

In case of Gaussian potential $\delta_\ell^G \propto e^{-(\ell/ka)^2}$, and as ℓ increases $\delta_\ell^G \to 0$ very rapidly as $e^{-\ell^2/k^2a^2}$. In the case of the Yukawa potential $\delta_\ell^Y \propto K_0(\mu\ell/k)$, for $\ell >> k/\mu$ $(R\sim 1/\mu)$ we have $K_0(\mu\ell/k) \sim \sqrt{\pi/2}(k/\mu\ell)^{\frac{1}{2}}e^{-\mu\ell/k}$ thus δ_ℓ^Y also goes to zero very rapidly as ℓ increases.

8. (a) From (7.1.11) and (7.1.12), we have

$$\frac{\hbar^2}{2m}\langle\vec{x}|\frac{1}{E-H_0+i\varepsilon}|\vec{x}'\rangle = G_+(\vec{x},\vec{x}') = -\frac{1}{4\pi}\frac{e^{+ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}. \tag{1}$$

This Green's function turns out to be the out-going wave solution to the Helmholtz equation:

$$(\vec{\nabla}^2 + k^2)G_+(\vec{x},\vec{x}') = \delta^{(3)}(\vec{x}-\vec{x}'). \tag{2}$$

To solve this equation, first notice that the δ-function in spherical coordinates can be represented as

$$\delta(\vec{x}-\vec{x}') = \frac{1}{r^2}\delta(r-r')\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}Y_{\ell m}^*(\theta',\phi')Y_{\ell m}(\theta,\phi). \tag{3}$$

Expanding the Green's function in spherical harmonics, we have

$$G_+(\vec{x},\vec{x}') = -\sum_{\ell,m} g_\ell(r,r')Y_{\ell m}^*(\theta',\phi')Y_{\ell m}(\theta,\phi). \tag{4}$$

Substitute (3) and (4) into (2), we are led to an equation for $g_\ell(r,r')$

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2 - \frac{\ell(\ell+1)}{r^2}\right]g_\ell = -\frac{1}{r^2}\delta(r-r'). \tag{5}$$

The boundary conditions are that g_ℓ be finite at the origin and infinity. This in turn requires that

$$g_\ell(r,r') = Aj_\ell(kr_<)h_\ell^{(1)}(kr_>). \tag{6}$$

When we match the discontinuity in slope (at $r=r'$), we find

$$A = +ik. \tag{7}$$

Thus the expansion of the Green's function is

$$\frac{\hbar^2}{2m}\langle\vec{x}|\frac{1}{E-H_0+i\varepsilon}|\vec{x}'\rangle = -ik\sum_{\ell=0}^{\infty}j_\ell(kr_<)h_\ell^{(1)}(kr_>)\sum_{m=-\ell}^{\ell}Y_{\ell m}^*(\theta',\phi')Y_{\ell m}(\theta,\phi) \tag{8}$$

(b) In $\vec{x}$ - representation

$$\langle\vec{x}|E\ell m(+)\rangle = \langle\vec{x}|E\ell m\rangle + \int d^3x' d^3x'' \langle\vec{x}|\frac{1}{E-H_0+i\varepsilon}|\vec{x}'\rangle\langle\vec{x}'|V|\vec{x}''\rangle\langle\vec{x}''|E\ell m(+)\rangle \quad (9)$$

where $\langle\vec{x}|\frac{1}{E-H_0+i\varepsilon}|\vec{x}'\rangle$ can be evaluated from (8), and (c.f. (7.5.21b)) $\langle\vec{x}|E\ell m\rangle = \frac{i^\ell}{\hbar}\sqrt{2mk/\pi}\ j_\ell(kr)Y_\ell^m(\hat{r})$ while we write $\langle\vec{x}|E\ell m(+)\rangle \equiv \frac{i^\ell}{\hbar}\sqrt{2mk/\pi}A_\ell(k;r)Y_\ell^m(\hat{r})$. Assume that the potential is local, i.e. $\langle\vec{x}'|V|\vec{x}''\rangle = V(\vec{x}')\delta^{(3)}(\vec{x}'-\vec{x}'')$, then (9) can be rewritten as

$$A_\ell(k;r)Y_\ell^m(\hat{r}) = j_\ell(kr)Y_\ell^m(\hat{r}) - \frac{2mik}{\hbar^2}\int d^3x' d^3x'' \sum_{\ell'}\sum_{m'} Y_{\ell'}^{m'}(\hat{r})Y_{\ell'}^{m'*}(\hat{r})Y_\ell^m(\hat{r}')$$
$$\times j_{\ell'}(kr_<)h_{\ell'}^{(1)}(kr_>)V(\vec{x}')\delta^{(3)}(\vec{x}'-\vec{x}'')A_\ell(k;r'). \quad (10)$$

The second term on r.h.s. of (10) becomes

$$\frac{2mik}{\hbar^2}\int d^3x' \sum_{\ell'}\sum_{m'} Y_{\ell'}^{m'}(\hat{r})Y_{\ell'}^{m'*}(\hat{r}')Y_\ell^m(\hat{r}')j_{\ell'}(kr_<)h_{\ell'}^{(1)}(kr_>)V(\vec{x}')A_\ell(k;r')$$
$$= \frac{2mik}{\hbar^2}\int_0^\infty r'^2dr' \sum_{\ell'}\sum_{m'} Y_{\ell'}^{m'}(\hat{r})\delta_{\ell\ell'}\delta_{mm'}j_{\ell'}(kr_<)h_{\ell'}^{(1)}(kr_>)V(\vec{x}')A_\ell(k;r')$$
$$= \frac{2mik}{\hbar^2}Y_\ell^m(\hat{r})\int_0^\infty r'^2dr' j_\ell(kr_<)h_\ell^{(1)}(kr_>)V(r')A_\ell(k;r'). \quad (11)$$

Thus

$$A_\ell(k;r) = j_\ell(kr) - \frac{2mik}{\hbar^2}\int_0^\infty j_\ell(kr_<)h_\ell^{(1)}(kr_>)V(r')A_\ell(k;r')r'^2dr'. \quad (12)$$

As $r \to \infty$, it is clear that we should identify $r_>$ as r, and $r_< = r'$. But from (7.6.7) and (A.5.19), we have

$$j_\ell(kr) \xrightarrow[r\to\infty]{} \frac{e^{i(kr-\ell\pi/2)} - e^{-i(kr-\ell\pi/2)}}{2ikr},\quad h_\ell^{(1)}(kr) \xrightarrow[r\to\infty]{} \frac{e^{i(kr-(\ell+1)\pi/2)}}{kr}. \quad (13)$$

So from (12)

$$A_\ell(k;r) \xrightarrow[r\to\infty]{} \frac{i^{-\ell}}{2ik}\left\{\left[1-\frac{4mik}{\hbar^2}\int_0^\infty j_\ell(kr')A_\ell(k;r')V(r')r'^2dr'\right]\frac{e^{ikr}}{r} - \frac{e^{-i(kr-\ell\pi)}}{r}\right\}. \quad (14)$$

On the other hand, for sufficiently large r, there are only the plane incoming wave and the spherical outgoing wave, with scattering amplitude $f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\theta)$. The ℓ^{th} partial wave $f_\ell(k)$ contributes to $A_\ell(k;r)$

[c.f. (7.6.8)] as

$$A_\ell(k;r) \xrightarrow[r\to\infty]{} \frac{i^{-\ell}}{2ik}\{[1+2ikf_\ell(k)]\frac{e^{ikr}}{r} - \frac{e^{-i(kr-\ell\pi)}}{r}\}. \tag{15}$$

Comparing (14) and (15) and noting (c.f. (7.6.14) and (7.6.15)) that $S_\ell \equiv e^{2i\delta_\ell}$ $= 1 + 2ikf_\ell(k)$, we have

$$f_\ell(k) = \frac{e^{i\delta_\ell}\sin\delta_\ell}{k} = -(2m/\hbar^2)\int_0^\infty j_\ell(kr)A_\ell(k;r)V(r)r^2dr. \tag{16}$$

9. (a) From (7.6.29), the scattering wave is $\langle\vec{x}|\psi^{(+)}\rangle = \frac{1}{(2\pi)^{3/2}}\sum_\ell i^\ell(2\ell+1)A_\ell(r)\times$ $P_\ell(\cos\theta)$ and $A_\ell(r)$ satisfies (c.f. (7.6.36)) $u_\ell'' + (k^2 - \frac{2mV(r)}{\hbar^2} - \frac{\ell(\ell+1)}{r^2})u_\ell(r) =$ 0 with $u_\ell(r) = rA_\ell$. For S-wave and $(2m/\hbar^2)V(r) = \gamma\delta(r-R)$, we consider $\ell=0$ only. Hence $u_o'' + (k^2-\gamma\delta(r-R))u_o = 0$ and for $r<R$ the solution can be written as $u_o(r)$ $= B_o r\sin kr/kr$ while for $r>R$ (using (7.6.33) and (7.6.45)) we have $u_o(r) =$ $re^{i\delta_o}\sin(kr+\delta_o)/kr$. These two solutions must match at $r=R$, i.e. $u_o|_{r=R+} =$ $u_o|_{r=R-} = u_o(R)$ while $u_o'|_{r=R+} - u_o'|_{r=R-} = \gamma u_o(R)$. Therefore

$$\begin{aligned}\frac{Re^{i\delta_o}\sin(kr+\delta_o)}{kR} &= \frac{B_oR\sin(kR)}{kR}\\ e^{i\delta_o}\cos(kR+\delta_o) - B_o\cos(kR) &= \frac{\gamma B_o}{k}\sin(kR).\end{aligned} \tag{1}$$

Solving (1) for $\tan\delta_o$, we have

$$\tan\delta_o = \frac{(-\gamma/k)\sin^2(kR)}{1+(\gamma/k)\sin(kR)\cos(kR)}. \tag{2}$$

(b) Assume $\gamma \gg 1/R,\ k$, from (1) we obtain

$$\tan(kR+\delta_o) = \frac{\sin(kR)}{\cos(kR)+(\gamma/k)\sin(kR)} \cong \frac{\tan(kR)}{(\gamma/k)\tan(kR)} = \frac{k}{\gamma} \ll 1, \tag{3}$$

thus $-kR\cong\delta_o$, and this resembles the hard sphere scattering (7.6.44). Again from (2) above we have

$$\cot\delta_o = 0 \text{ when } 1+(\gamma/k)\sin(kR)\cos(kR) = 0 \tag{4}$$

i.e. $\sin(2kR) = -2k/\gamma \cong 0$. Ostensibly we have solutions $(kR)_r \cong n\pi$, $(n+\frac{1}{2})\pi$, but $(n+\frac{1}{2})\pi$ is eliminated since $\cot\delta_o$ then goes through zero from below (negative side). So we write $k_rR \cong n\pi$ (where $d\cot\delta_o/dk < 0$ as k increases) and $k_rR = n\pi - \varepsilon$, $\varepsilon \ll 1$. Hence $\sin(2k_rR) = -\sin(2\varepsilon) = -2k/\gamma$, and $\varepsilon \cong k/\gamma$ to first order, and $k_rR = n\pi - k/\gamma$ as the resonance condition. The resonance energy is

$$E_r = \hbar^2k_r^2/2m \cong \frac{\hbar^2}{2m}\frac{n^2\pi^2}{R^2}(1 - 2/R\gamma). \tag{5}$$

For a particle confined inside potential $V = 0$, $r<R$, and $V = \infty$ for $r>R$ and in S-wave, we have $u'' + k^2u = 0$ where $u(0) = 0$ and $u(R) = 0$. Solution is $u(r) = A\sin(kr)$ $(0\leq r\leq R)$ and from boundary condition $kR = n\pi$, bound state energies are $E_b = \hbar^2k^2/2m = \hbar^2n^2\pi^2/2mR^2$. Hence from (5), we have

$$E_r \cong E_b(1-2/R\gamma). \tag{6}$$

Finally from (2), we have

$$\begin{aligned} d(\cot\delta_o)/dE &= (d(\cot\delta_o)/dk)(dk/dE) \\ &= \frac{1}{\gamma\sin^4(kR)}[R\cos(kR)(k+\gamma\sin(2kR)/2)\sin(kR) - (1+\gamma R\cos(kR))\sin^2(kR)]\frac{m}{\hbar^2k}. \end{aligned} \tag{7}$$

At $E=E_r$, since $k_rR \cong n\pi(1-\frac{1}{\gamma R})$, $\sin^2(k_rR) \cong (n\pi/\gamma R)^2$ and $\cos(2k_rR) \cong 1$, we have from (7)

$$\Gamma = -2/[d(\cot\delta_o)/dE]\big|_{E=E_r} \cong \frac{2\hbar^2}{m}\frac{(n\pi)^3}{\gamma^2R^4}. \tag{8}$$

Notice that because of the $1/\gamma^2$ dependence in (8), $\Gamma \to 0$ as γ becomes large, thus the resonances become extremely sharp.

Assume that initially (t=0) the particle is in an eigenstate $|i\rangle$. The potential $V(\vec{r},t) = V(\vec{r})\cos\omega t$ is turned on at t=0. Take the perturbation expansion of the state amplitudes $c_n(t)$ up to first order $c_n(t) = c_n^{(o)}(t) + c_n^{(1)}(t) + \ldots\ldots$ Then obviously $c_n^{(o)}(t) = \delta_{ni}$. Let the final state be $|f\rangle$, then

$$c_f^{(1)}(t) = (-i/\hbar)\int_0^t V_{fi}(\vec{r})\cos\omega t' e^{i\omega_{fi}t'}dt', \tag{1}$$

where $V_{fi}(\vec{r}) \equiv \langle f|V(\vec{r})|i\rangle$ and $\omega_{fi} = (E_f-E_i)/\hbar$. Integrate (1) gives

$$c_f^{(1)}(t) = \frac{V_{fi}}{2\hbar}\left[\frac{1-e^{i(\omega+\omega_{fi})t}}{(\omega+\omega_{fi})} + \frac{1-e^{i(\omega_{fi}-\omega)t}}{(-\omega+\omega_{fi})}\right]. \tag{2}$$

Obviously, as $t\to\infty$, $|c_f^{(1)}|^2$ is appreciable only if

$$\begin{aligned}&\text{(i) } \omega_{fi}+\omega \cong 0 \text{ or } E_f \cong E_i - \hbar\omega \\ &\text{(ii) } \omega_{fi}-\omega \cong 0 \text{ or } E_f \cong E_i + \hbar\omega .\end{aligned} \tag{3}$$

The transition rate is then

$$w_{i\to f} = \frac{2\pi}{\hbar}|V_{fi}|^2\{\rho(E_f)|_{E_f=E_i-\hbar\omega} + \rho(E_f)|_{E_f=E_i+\hbar\omega}\}. \tag{4}$$

Using box normalization (c.f. (7.11.23)), we have

$$\rho(E_f) = n^2dn/dE_f = (L/2\pi)^3k_fm/\hbar^2, \tag{5}$$

where k_f is the momentum of the final state. On the other hand, the incident flux $\vec{j}$ (c.f. (7.11.26)) is $|\vec{j}| = \hbar k_i/mL^3$. From (7.11.25) we know that the transition rate $w_{i\to f}$ = (incident flux)×$(d\sigma/d\Omega)d\Omega$, we obtain

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \left(\frac{mL^3}{\hbar k_i}\right)\left(\frac{2\pi}{\hbar}\right)\left(\frac{L}{2\pi}\right)^3\frac{m}{\hbar^2}|\langle f|V(\vec{r})|i\rangle|^2\{k_f|_{E_f=E_i-\hbar\omega} + k_f|_{E_f=E_i+\hbar\omega}\} \\ &= \frac{m^2}{4\pi^2\hbar^4}\left|\int d^3\vec{r}\,V(\vec{r})e^{i(\vec{k}_f-\vec{k}_i)\cdot\vec{r}}\right|^2\times\frac{1}{k_i}\{(k_i^2-2m\omega/\hbar)^{\frac{1}{2}} + (k_i^2+2m\omega/\hbar)^{\frac{1}{2}}\}\end{aligned} \tag{6}$$

where initial and final states are assumed to be plane waves and momentum of the two final states are related by $E_f = \hbar^2k_f^2/2m = E_i\pm\hbar\omega = \hbar^2k_i^2/2m \pm \hbar\omega$.

Since

$$c_f^{(2)} = (-i/\hbar)^2\sum_m\int_0^t dt' e^{i\omega_{fm}t'}V_{fm}(t')\int_0^{t'}dt'' e^{i\omega_{mi}t''}V_{mi}(t''), \tag{7}$$

similar to (2) we have

$$\begin{aligned}c_f^{(2)}(t) &= \frac{i}{2}\left(\frac{-i}{\hbar}\right)^2\sum_m\int_0^t dt\, e^{i\omega_{fm}t'}V_{fm}\cos\omega t'.V_{mi}\left[\frac{1-e^{i(\omega+\omega_{mi})t'}}{\omega+\omega_{mi}} + \frac{1-e^{i(\omega_{mi}-\omega)t'}}{-\omega+\omega_{mi}}\right] \\ &= \left(\frac{i}{2}\right)^2\left(\frac{-i}{\hbar}\right)^2\sum_m V_{fm}V_{mi}\left\{\left(\frac{1}{\omega+\omega_{mi}} + \frac{1}{-\omega+\omega_{mi}}\right).\left[\frac{1-e^{i(\omega+\omega_{fm})t}}{\omega+\omega_{fm}}\right.\right.\end{aligned}$$

$$+ \frac{1-e^{i(\omega_{fm}-\omega)t}}{-\omega + \omega_{fm}}] + \frac{(-1)}{\omega+\omega_{mi}}\cdot[\frac{1-e^{i(2\omega+\omega_{mi}+\omega_{fm})t}}{2\omega + \omega_{mi} + \omega_{fm}} + \frac{1-e^{i(\omega_{mi}+\omega_{fm})t}}{\omega_{mi} + \omega_{fm}}]$$

$$+ \frac{-i}{-\omega+\omega_{mi}}\cdot[\frac{1-e^{i(\omega_{fm}+\omega_{mi}+\omega)t}}{\omega + \omega_{fm} + \omega_{mi}} + \frac{1-e^{i(\omega_{fm}+\omega_{mi}-\omega)t}}{-\omega + \omega_{fm} + \omega_{mi}}]\} . \tag{8}$$

Looking at the square brackets of (8) we see that these terms contribute only if the denominators are close to zero, which means

$$\omega_f \cong \omega_m \pm \omega,\ \omega_f \cong \omega_i - 2\omega,\ \omega_f \cong \omega_i,\ \omega_f \cong \omega_i \pm \omega . \tag{9}$$

The $\omega_f \cong \omega_i \pm \omega$ last condition of (9) is the same as in the first order transition (3) whereas the other three conditions are new. In particular, there can be a "second harmonic" generation where $\omega_i - \omega_f \cong 2\omega$.

Furthermore, the first condition ($\omega_f \cong \omega_m \pm \omega$) of (9) implies that the intermediate states that are $\pm\omega\hbar$ away from the final state $|f\rangle$ will contribute most among all intermediate states.

These observations can be generalized to even higher order perturbations. For example, in 3rd order perturbation we expect to see a "third harmonic" transition with $\omega_f \cong \omega_i \pm 3\omega$.

11. The potential for the elastic scattering of a fast electron by the ground state of the hydrogen atom is

$$V = -e^2/r + e^2/|\vec{x} - \vec{x}'| \ , \ r = |\vec{x}|. \tag{1}$$

So the matrix element for elastic scattering is

$$\langle\vec{k}'0|V|\vec{k}0\rangle = \frac{1}{L^3}\int d^3x e^{i\vec{q}\cdot\vec{x}}\langle 0|\frac{-e^2}{r} + \frac{e^2}{|\vec{x}-\vec{x}'|}|0\rangle$$

$$= \frac{1}{L^3}\int d^3x e^{i\vec{q}\cdot\vec{x}}\int d^3x'\psi_o^*(\vec{x}')[\frac{-e^2}{r} + \frac{e^2}{|\vec{x}-\vec{x}'|}]\psi_o(\vec{x}') \tag{2}$$

where $\vec{q} = \vec{k}'-\vec{k}$.

As explained in section 7.12, the first term in V does not contribute to the $\int d^3x'$ integration, and from Eq. (7.12.10)

$$\int d^3\vec{x}\; e^{i\vec{q}\cdot\vec{x}}/r = 4\pi/q^2. \tag{3}$$

Furthermore, after shifting the coordinate variable $\vec{x} \to \vec{x} + \vec{x}'$ we have

$$\int d^3\vec{x}\; e^{i\vec{q}\cdot\vec{x}}/|\vec{x}-\vec{x}'| = \frac{4\pi}{q^2}\, e^{i\vec{q}\cdot\vec{x}'} \tag{4}$$

so

$$\langle\vec{k}'0|V|\vec{k}0\rangle = \frac{4\pi e^2}{q^2}[-\langle 0|0\rangle + \langle 0|e^{i\vec{q}\cdot\vec{x}}|0\rangle]L^{-3}. \tag{5}$$

Notice that $\langle 0|0\rangle = 1$, and $\langle\vec{x}|0\rangle = (1/a_o)^{3/2} 2e^{-r/a_o}\, Y_{oo} = \frac{2}{(4\pi)^{1/2}}\left(\frac{1}{a_o}\right)^{3/2} e^{-r/a_o}$, so

$$\langle 0|e^{i\vec{q}\cdot\vec{x}'}|0\rangle = \left(\frac{1}{a_o}\right)^3 \int_{-1}^{+1}\int_0^\infty 2r'^2 d\cos\theta\, dr' e^{-2r'/a_o}\, e^{iqr'\cos\theta}$$

$$= \left(\frac{1}{a_o}\right)^3 \frac{4}{q}\int_0^\infty r' e^{-2r'/a_o} \sin qr' dr' ,$$

therefore

$$\langle 0|e^{i\vec{q}\cdot\vec{x}}|0\rangle = \left(\frac{1}{a_o}\right)^3 \frac{4}{q}\cdot \frac{4q/a_o}{(4/a_o^2+q^2)^2} = \frac{16}{[4+(qa_o)^2]^2}. \tag{6}$$

Thus

$$\langle\vec{k}'0|V|\vec{k}0\rangle = -\frac{4\pi e^2}{q^2}\{1 - \frac{16}{[4 + (qa_o)^2]^2}\}L^{-3} . \tag{7}$$

For the differential cross section (c.f. (7.12.6)) with $k' = k$

$$\frac{d\sigma}{d\Omega} = L^6\left|\frac{1}{4\pi}\frac{2m}{\hbar^2}\langle\vec{k}'0|V|\vec{k}0\rangle\right|^2 = \frac{4m^2e^4}{\hbar^4 q^4}\{1 - \frac{16}{[4+(qa_o)^2]^2}\}^2 \tag{8}$$

12. (See Finkelstein: <u>Non Relativistic Mechanics</u> (1973), p.292 for background material). Energy E is

$$E = E(J_1, J_2, J_3) \tag{1}$$

In the case of a central potential, it turns out that

$$E = E(J_r, J_\phi + J_\theta), \tag{2}$$

where

$$J_\phi = \oint p_\phi d\phi = \oint \frac{\partial W}{\partial \phi}\, d\phi = 2\pi\alpha_\phi$$

$$J_\theta = \oint p_\theta d\theta = \oint \frac{\partial W}{\partial \theta}\, d\theta \;\; {}^2 - \alpha_\theta^2 /\sin^2\theta]^{1/2} d\theta = 2\pi(\alpha_\theta - \alpha_\phi)$$

$$J_r = \oint p_r dr = \oint \frac{\partial W}{\partial r} dr = \oint [2\mu\alpha_1 - 2\mu V + \alpha_\theta^2/r^2]^{1/2} dr \tag{3}$$

and the function W and constants α_ϕ, α_θ, and α_1 are defined by the Hamilton-Jacobi equation:

$$H(\partial W/\partial q_i, q_i) = \alpha_1 = E. \tag{4}$$

Equation (2) arises because (3) gives

$$J_r = \oint [2\mu E - 2\mu V(r) - (J_\theta + J_\phi)^2/4\pi^2 r^2]^{1/2} dr. \tag{5}$$

When V(r) is the Coulomb potential, $V(r) = -e^2/r$, we have

$$J_r = \oint [2\mu E + 2\mu e^2/r - (J_\theta + J_\phi)^2/4\pi^2 r^2]^{1/2} dr$$

and with some algebra, this integration gives (c.f. Goldstein, Classical Mechanics (1980), p.475)

$$E = -\frac{2\pi^2 \mu e^4}{(J_r + J_\theta + J_\phi)^2} = E(J_r + J_\theta + J_\phi). \tag{6}$$

Compare (2) and (3), we see that for a central potential in general, J_ϕ and J_θ always appear in the combination $(J_\theta + J_\phi)$, hence there is at least 'singly' degeneracy. On the otherhand, in the Coulomb case J_r, J_ϕ, J_θ appear always in combination $(J_r + J_\theta + J_\phi)$, hence there is at least a double degeneracy.

In the case of Coulomb potential, there is, in addition to the angular momentum $\vec{L}$, yet another invariance of the action $\vec{A}$:

$$\vec{A} = \vec{L} \times \vec{p} + e^2 \mu \hat{r} \tag{7}$$

which determines the direction of the major axis and the eccentricity of the conic.

If one writes for the general central potential

$$V(r) = -e^2/r + \phi(r) \tag{8}$$

then

$$d\vec{A}/dt = \left(\frac{-d\phi}{r\,dr}\right)(\vec{L} \times \vec{r}). \tag{9}$$

Therefore, $\vec{A}$ precesses in general according to this equation. Consequently, the general case of motion in a central potential may be pictured in terms of a precessing conic, that also has a changing eccentricity. In terms of action and angle variables, this means that the Coulombian motion is distinguished by a single period whereas the motion of a central field problem is generally characterized by two periods which are not commensurable.

The explicit expression of $\vec{A}^2$ from (7) (for our classical system) is

$$\vec{A}^2 = \ell^2\vec{p}^2 - \frac{2e^2\mu\ell^2}{r} + \mu^2e^4 = 2\mu\ell^2(\vec{p}^2/2\mu - \frac{e^2}{r}) + \mu^2e^4. \tag{10}$$

Other than the last term μ^2e^4 in $\vec{A}^2$ of (10), the first two terms are proportional to the kinetic and potential energies of the Coulomb problem. It is thus clear that the Hamiltonian $H = \vec{p}^2/2\mu + V(r) + F(\vec{A}^2)$ is a polynomial in $(\frac{\vec{p}^2}{2\mu} - \frac{e^2}{r})$ plus the extra term $\phi(r)$ in (8). It follows that all the algebra of the Poisson brackets remain the same (as that without $F(\vec{A}^2)$), and the previous statements are still valid.

To describe quantum systems, we modify the Poisson brackets into commutators:

$$\begin{aligned} [L_i,L_j] &= i\hbar\varepsilon_{ijk}\, L_k \\ [L_i,M_j] &= i\hbar\varepsilon_{ijk}\, M_k \\ [M_i,M_j] &= i\hbar\varepsilon_{ijk}\, L_k \end{aligned} \tag{11}$$

where $M_i \equiv \sqrt{1/2\mu H}\, A_i$ and $L_i \equiv \frac{1}{2}\varepsilon_{ijk}(L_jp_k+p_kL_j)$ such that L_i is Hermitian. It follows that (for Hamiltonian H)

$$\vec{A}^2 = (\mu e^2)^2+(2\mu H)(\vec{L}^2+\hbar^2),\ \vec{M}^2 = \frac{\mu^2e^4}{-2\mu H} - \vec{L}^2 - \hbar^2. \tag{12}$$

These lead to

$$H = -\frac{1}{2}\left(\frac{\mu e^2}{\vec{L}^2 + \vec{M}^2 + \hbar^2}\right). \tag{13}$$

Let

$$\vec{J} = \tfrac{1}{2}(\vec{M} + \vec{L}),\ \vec{K} = \tfrac{1}{2}(\vec{M} - \vec{L}) \tag{14}$$

then one has

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k,\ [K_i, K_j] = -i\hbar\epsilon_{ijk}K_k,\ [K_i, J_j] = 0 \tag{15}$$

with the constraint $\vec{J}^2 = \vec{K}^2$ (c.f. also discussion in Schiff, Quantum Mechanics (1968), p.236-239). Thus $H = -\tfrac{1}{2}\dfrac{\mu e^4}{(4\vec{J}^2+\hbar^2)}$ and the possible values of $\vec{J}^2$ are $j(j+1)\hbar^2$. The complete set of commuting observables can thus be chosen as $\vec{J}^2$, J_z and K_z, with

$$\begin{aligned}
\vec{J}^2\mathcal{D}^k_{mn}(\alpha\beta\gamma) &= k(k+1)\hbar^2\mathcal{D}^k_{mn}(\alpha\beta\gamma)\\
J_z\mathcal{D}^k_{mn}(\alpha\beta\gamma) &= m\hbar\mathcal{D}^k_{mn}(\alpha\beta\gamma)\\
K_z\mathcal{D}^k_{mn}(\alpha\beta\gamma) &= n\hbar\mathcal{D}^k_{mn}(\alpha\beta\gamma)\\
H\ \mathcal{D}^k_{mn}(\alpha\beta\gamma) &= E(k)\mathcal{D}^k_{mn}(\alpha\beta\gamma)
\end{aligned} \tag{16}$$

where $E(k) = -\dfrac{\mu e^4}{2\hbar^2}\cdot\dfrac{1}{(2k+1)^2}$.

In terms of the usual quantum numbers (n,ℓ,m) we have

$$H = -\frac{\mu e^4}{2\hbar^2}\cdot\frac{1}{(2\ell+1)^2} \equiv -\frac{\mu e^4}{2\hbar^2}\cdot\frac{1}{n^2}\,. \tag{17}$$

Thus the eigenvalues depend only on the principal quantum number n, and the number of degeneracy is

$$n^2 = (2\ell+1)^2 \tag{18}$$

for the Coulomb problem. The degeneracy for the central potential problem, on the other hand, is most easily seen by the (k,m,n) representation defined by Eqs. (14) - (16). While in the Coulomb problem the two commuting conserved vectors $\vec{J}$ and $\vec{K}$ are derived from the conserved vectors $\vec{A}$ and $\vec{L}$, in the central potential problem $\vec{A}$ is no longer a conserved vector (in general). Thus the two commuting sets of observables reduce to one, and the degeneracy reduces to

$$k = (2m+1) \tag{19}$$

Since the Schrödinger equation in x-space governing the wave function D^k_{mn} separates the same way as the Hamilton-Jacobi equation, namely, in spherical (and parabolic) coordinates, we get Laguerre functions for the spherical case.