HW2: solutions. Sakurai



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

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 <u>doubly degenerate</u>.

(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 <u>degenerate</u> 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 $\sigma_x$. By same method as problem 3 above, we get zeroth order energy eigenkets $\frac{1}{2^{\frac{1}{2}}}(|10\rangle+|01\rangle)$ with $\Delta^{(1)} = \frac{1}{2}\delta\hbar\omega$ and $\frac{1}{2^{\frac{1}{2}}}(|10\rangle-|01\rangle)$ 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 $\frac{1}{2^{\frac{1}{2}}}(|10\rangle+|01\rangle)$ with $E = (2+\delta/2)\hbar\omega$ and $\frac{1}{2^{\frac{1}{2}}}(|10\rangle-|01\rangle)$ with $E = (2-\delta/2)\hbar\omega$.

(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 $\omega$ 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 $\delta$ 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. Let $\omega = \omega_x = \omega_y$, $\omega_z = (1+\epsilon)\omega$ where $\epsilon \ll 1$. Full Hamiltonian is

$$H = \frac{1}{2\mu}(\vec{p} - q\vec{A}/c)^2 + \frac{1}{2}\mu\omega^2(x^2+y^2) + \frac{1}{2}\mu(1+\epsilon)^2\omega^2 z^2. \tag{1}$$

Choosing $\vec{A} = \frac{1}{2}\vec{B}_o\times\vec{r}$ with $\vec{B}_o$ along x-axis, $\vec{r} = x\vec{i}+y\vec{j}+z\vec{k}$, we have

$$H = \frac{1}{2\mu}p^2 + \frac{1}{2}\mu\omega^2 r^2 - \frac{qB_o}{2\mu c}L_x + \epsilon\mu\omega^2 z^2 + \frac{1}{2}\epsilon^2\mu\omega^2 z^2 + \frac{q^2B_o^2}{8\mu c^2}(y^2+z^2). \tag{2}$$

We are told third and fourth terms on r.h.s. of (2) are comparably small, hence to <u>lowest (first) order</u> in perturbation theory we can drop fifth and sixth terms on r.h.s. of (2) [of order $\epsilon^2$ and $B_o^2$]. In this approximation

$$H = \frac{1}{2\mu}p^2 + \frac{1}{2}\mu\omega^2 r^2 - \frac{qB_o}{2\mu c}L_x + \epsilon\mu\omega^2 z^2. \tag{3}$$

To simplify, rotate through 90° in x - z plane s.t. $x \to z'$, $-z \to x'$, $y \to y'$ and then drop primes, Eq. (3) becomes

$$\begin{vmatrix} \frac{5}{2}\hbar\omega - E + \frac{\varepsilon\hbar\omega}{2} & 0 & 0 \\ 0 & \frac{5}{2}\hbar\omega - E + \varepsilon\hbar\omega - \frac{qB_o\hbar}{2\mu c} & \frac{1}{2}\varepsilon\hbar\omega \\ 0 & \frac{1}{2}\varepsilon\hbar\omega & \frac{5}{2}\hbar\omega - E + \varepsilon\hbar\omega + \frac{qB_o\hbar}{2\mu c} \end{vmatrix} = 0 \qquad (8)$$

So one solution is $E_1 = (5/2)\hbar\omega + (\varepsilon/2)\hbar\omega$, and the other two solutions are $E_2 = (5/2 + \varepsilon)\hbar\omega - \frac{1}{2}[(\varepsilon\hbar\omega)^2 + (qB_o\hbar/\mu c)^2]^{\frac{1}{2}}$, $E_3 = (5/2 + \varepsilon)\hbar\omega + \frac{1}{2}[(\varepsilon\hbar\omega)^2 + (qB_o\hbar/\mu c)^2]^{\frac{1}{2}}$.

<u>Various limiting cases</u>. In limit that $\varepsilon \to 0$, we just get the Zeeman splittings

$$E_1 = \varepsilon_1 = \frac{5}{2}\hbar\omega,\ E_2 = \frac{5}{2}\hbar\omega - \frac{qB_o\hbar}{2\mu c},\ E_3 = \frac{5}{2}\hbar\omega + \frac{qB_o\hbar}{2\mu c}. \qquad (9)$$

In the limit that $B_o \to 0$,

$$E_1 \to \frac{1}{2}(5 + \varepsilon)\hbar\omega,\ E_2 \to \frac{5}{2}\hbar\omega + \hbar\omega/2 = E_1,\ E_3 \to (5/2 + 3\varepsilon/2)\hbar\omega. \qquad (10)$$

Thus we have degeneracy between $E_1$ and $E_2$.

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

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

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 $\alpha$ is the same $\alpha$ 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 $(k=1, q=\pm1)$ 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

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

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) $\langle n,\ell=1,m=\pm1,0|V|n,\ell=1,m=\pm1,0\rangle$, $\frac{V}{\lambda} = x^2-y^2 = r^2\sin^2\theta(\cos^2\phi - \sin^2\phi) = r^2\sin^2\theta\cos2\phi = r^2\sin^2\theta(e^{2i\phi}+ e^{-2i\phi})/2$. So the perturbation connects $m = \pm1$ with $m = \mp1$. The type of non vanishing V-matrix elements are of form

$$I = \lambda\int\frac{\sin^2\theta}{2}e^{\pm i\phi}e^{\mp2i\phi}\sin^2\theta e^{\pm i\phi}d\Omega \int r^2R_{nl}^2\; r^2dr$$

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

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

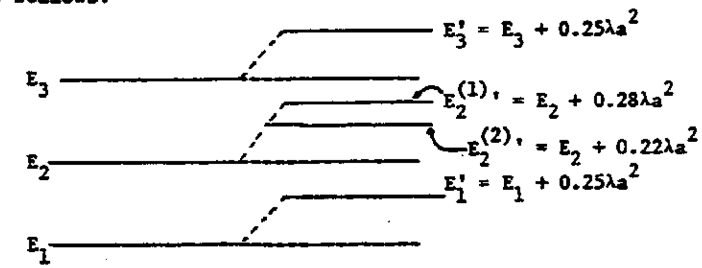
(b) We are dealing with states whose angular dependence are spherical harmonics. Under time reversal: $Y_\ell^m \to Y_\ell^{m*} = (-1)^mY_\ell^{-m}$, hence $\Theta|n,\ell=1,m=\pm1\rangle = -|n,\ell=1,m=\mp1\rangle$. Therefore (1) evidently go into itself (up to a phase factor or sign) under time reversal.

10. 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 $H_o = -\frac{\hbar^2\nabla^2}{2m} + V$, and by using the method of separation of variables, we can easily find the energy eigenvalues and eigenfunctions

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

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 $\lambda$, in otherwords proportional to $\lambda$. 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 $\lambda|\Delta| \ll |E_1^o - E_2^o|$ is

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

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 $\sigma_x$, we know right away that the eigenfunctions are those of $\sigma_x$,

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

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-