Homework 2: #'s 5.1, 5.3, 5.4, 5.7, 5.8, 5.9, 5.11

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Problem 5.1
A simple harmonic oscillator (in one dimension) is subjected to a perturbation

$$\lambda H_1 = bx$$

where b is a real constant.
a. Calculate the energy shift of the ground state to lowest non vanishing order.
b. Solve this problem exactly and compare with your result obtained in (a).
Assume without proof:

$$\langle u_{n'}|x|u_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n+1})$$

.

Solution:

a. The first order shift vanishes.

$$\Delta_0^1 = \langle 0|bx|0\rangle = 0$$

The second order shift is

$$\Delta_0^2 = -\frac{b^2}{2m\omega^2}$$

This comes from

$$\Delta_0^2 = \sum_{k\neq n}\frac{|V_{k0}|^2}{E_0^0 - E_k^0} = \frac{b^2|\langle 1|x|0\rangle|^2}{E_0^0 - E_1^0}$$

Bring in a negative sign and switch around the denominator

$$\Delta_0^2 = -\frac{b^2|\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{1}\delta_1^1)|^2}{\frac{3}{2}\hbar\omega - \frac{1}{2}\hbar\omega}$$

$$\Delta_0^2 = -\frac{b^2\hbar}{2m\omega\hbar\omega} = -\frac{b^2}{2m\omega^2}$$

b. The quickest way to do this is to add and subtract some constant from the Hamiltonian.

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + bx + K - K$$

But this constant will be picked very conveniently so as to get rid of this ugly bx term. I want this form:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x + C)^2 - K$$

What does this get me? What should C be equal to in terms of b?

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x^2 + 2Cx + C^2) - K$$

So C must be

$$\frac{1}{2}m\omega^2 2Cx = bx \rightarrow C = \frac{b}{m\omega^2}$$

and we have an extra term to subtract away with our K

$$\frac{1}{2}m\omega^2 C^2 = K = \frac{b^2}{2m\omega^2}$$

This yields

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x + \frac{b}{2m\omega^2})^2 - \frac{b^2}{2m\omega^2}$$

After all that, now we have a nice form, where it's cool to replace

$$x' = x + \frac{b}{2m\omega^2}$$

Now we have a Hamiltonian thats tame and easy to conquer

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x')^2 - \frac{b^2}{2m\omega^2}$$

$$H\psi_0 = E_0\psi_0$$

Here is a great time saver. Send that b term over to the right hand side

$$\left[\frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x')^2\right]\psi_0 = \left[E_0 + \frac{b^2}{2m\omega^2}\right]\psi_0$$

Remembering that E_0 is the new ground energy of this perturbed Hamiltonian. But if we just change the right hand side to

$$\left[\frac{p^2}{2m} + \frac{1}{2}m\omega^2 (x')^2\right]\psi_0 = E'\psi_0$$

Then we get

$$E' = \frac{1}{2}\hbar\omega$$

But we just made the substitution for $E' = E_0 + b^2/2m\omega^2$. So the new ground energy of the perturbed Hamiltonian is

$$E_0 = \frac{1}{2}\hbar\omega - \frac{b^2}{2m\omega^2}$$

With the exact shift that was the second order shift in part (a). That's perturbation theory for you.

$$\Delta_{exact} = -\frac{b^2}{2m\omega^2}$$

Problem 5.3
Consider a particle in a two-dimensional potential

$$V_0 = \begin{cases} 0 & \text{for } 0 \le x \le L\ ,\ 0 \le y \le L, \\ \infty & \text{otherwise.} \end{cases}$$

Write the energy eigenfunctions for the ground and first excited states. We now add a time-independent perturbation of the form

$$V_1 = \begin{cases} \lambda xy & \text{for } 0 \le x \le L\ ,\ 0 \le y \le L, \\ \infty & \text{otherwise.} \end{cases}$$

Obtain the zeroth-order energy eigenfunctions and first-order energy shifts for the ground and first excited states.

Solution:

$$\Psi_{nm}(x,y) = \frac{2}{L}\sin(\frac{n\pi}{L}x)\sin(\frac{m\pi}{L}y) \quad E_{nm} = \frac{\hbar^2\pi^2}{2ML^2}(n^2+m^2)$$

We have for the ground state: $\boxed{\psi_{11} = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{\pi y}{L}}$.

For the first excited: $\boxed{\psi_{12} = \frac{2}{L}\sin\frac{\pi x}{L}\sin\frac{2\pi y}{L}\ ;\psi_{21} = \frac{2}{L}\sin\frac{2\pi x}{L}\sin\frac{\pi y}{L}}$

Adding a time-independent perturbation we then see that the zeroth-order energy eigenfunctions are the same as above. No perturbation for the zeroth order should be taken into account.

The first order energy shifts are :

• Ground State:

$$\Delta^1_{11} = \langle\psi^0_{11}|V_1|\psi^0_{11}\rangle = \frac{4}{L^2}\lambda\int\int_0^L xy\sin^2\frac{\pi x}{L}\sin^2\frac{\pi y}{L}\,dx\,dy$$

$$\Delta^1_{11} = \frac{4\lambda}{L^2}\int_0^L dx\; x\sin^2\frac{\pi x}{L}\int_0^L dy\; y\sin^2\frac{\pi y}{L}$$

$$\Delta^1_{11} = \frac{4\lambda}{L^2}\frac{L^2}{4}\frac{L^2}{4}$$

$$\Delta^1_{11} = \frac{\lambda L^2}{4}$$

This is because of the integral:

$$\int_0^L du\; u\sin^2\frac{\pi u}{L} = \frac{u^2}{4} - \frac{u\sin 2\pi u/L}{4\pi/L} - \frac{\cos 2\pi u/L}{8(\pi/L)^2}\Bigg|_0^L$$

$$= \frac{L^2}{4} - 0 - \frac{L^2}{8\pi^2} + \frac{L^2}{8\pi^2} = \frac{L^2}{4}$$

• First Excited States:

There is degeneracy so that is why there is more than one first excited state. The perturbation will lift the degeneracy. Solving for the perturbation matrix will give us the shifts:

$$\langle\psi^0_{21}|V_1|\psi^0_{21}\rangle = \langle\psi^0_{12}|V_1|\psi^0_{12}\rangle = \frac{\lambda L^2}{4}$$

the same as the ground state. They are exactly the same integrals as above. The next matrix elements are harder.

$$\langle\psi^0_{21}|V_1|\psi^0_{12}\rangle = \langle\psi^0_{12}|V_1|\psi^0_{21}\rangle = \frac{4\lambda}{L^2}\int_0^L dx\; x\sin(\frac{2\pi x}{L})\sin(\frac{\pi x}{L})\int_0^L dy\; y\sin(\frac{2\pi y}{L})\sin(\frac{\pi y}{L})$$

This is a challenging integral. I used the INTEGRATOR and found

$$\int x\sin ax\sin bx dx = \frac{1}{2}\left(\frac{\cos(a-b)x}{(a-b)^2} + \frac{x\sin(a-b)x}{a-b}\right) + \frac{1}{2}\left(-\frac{\cos(a+b)x}{(a+b)^2} - \frac{x\sin(a+b)x}{a+b}\right)$$

Plugging in my limits of $0, L$ and my constants a, b I got

$$\int_0^L x\sin(2\pi x/L)\sin(\pi x/L)dx = \frac{-8L^2}{9\pi^2}$$

Thus

$$\frac{4\lambda}{L^2}\int_0^L dx\; x\sin(\frac{2\pi x}{L})\sin(\frac{\pi x}{L})\int_0^L dy\; y\sin(\frac{2\pi y}{L})\sin(\frac{\pi y}{L}) = \frac{4\lambda}{L^2}(-\frac{8L^2}{9\pi^2})(-\frac{8L^2}{9\pi^2}) = \frac{256L^2\lambda}{81\pi^4}$$

Bringing all four matrix elements into the matrix I have:

$$V_1 = \begin{pmatrix} \frac{L^2}{4} & \frac{256L^2\lambda}{81\pi^4} \\ \frac{256L^2\lambda}{81\pi^4} & \frac{L^2}{4} \end{pmatrix}.$$

Thus the eigenvalues of this perturbation matrix are the first order energy shifts for the first excited states:

$$\boxed{\Delta^1_\pm = \left(\frac{L^2}{4} \pm \frac{256L^2}{81\pi^4}\right)\lambda}$$

with zeroth order energy eigenfunctions

$$\boxed{|\pm\rangle = \frac{1}{\sqrt{2}}(|\psi^0_{21}\rangle \pm |\psi^0_{12}\rangle)}$$

Problem 5.4
Consider an isotropic harmonic oscillator in two dimensions. The Hamiltonian is given by

$$H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2)$$

a. What are the energies of the three lowest-lying states? Is there any degeneracy? b. We now apply a perturbation

$$V = \delta m\omega^2 xy$$

where δ is a dimensionless real number much smaller than unity. Find the zeroth-order energy eigenket and the corresponding energy to first order [that is, the unperturbed energy obtained in (a) plus the first-order energy shift] for each of the three lowest-lying states.
c. Solve the $H_0 + V$ problem exactly. Compare with the perturbation results obtained in (b). Use $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n+1}$.

Solution:

a. Energies of the three lowest lying states:
• 1D: $E_n = (n + 1/2)\hbar\omega$ with $n = 0, 1, 2...$
• 2D: $E_{nm} = (n + m + 1)\hbar\omega$ with $n, m = 0, 1, 2...$
So, we have $\hbar\omega$, $2\hbar\omega$, $2\hbar\omega$.

$$\boxed{E_{00} = \hbar\omega \quad E_{10} = E_{01} = 2\hbar\omega}$$

because E_{01} and E_{10} are the same, the first excited state is doubly degenerate.

b. The ground state's energy shift to first order is

$$\Delta_{00} = E_{00} - E^0_{00} = \langle\psi^0_{00}|V|\psi^0_{00}\rangle = \delta m\omega^2\langle\psi^0_{00}|xy|\psi^0_{00}\rangle$$

and by parity

$$\boxed{\Delta^1_{00} = 0}$$

For $\Delta_\pm$ degenerate perturbation theory must be used. So lets fight for the perturbation matrix. The diagonal elements are the same as the ground state, oddly enough just like the previous problem.

$$\langle\psi_{10}|V|\psi_{10}\rangle = \langle\psi_{01}|V|\psi_{01}\rangle = 0$$

The off diagonal elements are

$$\langle\psi_{01}|V|\psi_{10}\rangle = \langle\psi_{10}|V|\psi_{01}\rangle = \delta m\omega^2\langle n'm'|xy|nm\rangle$$

$$= \delta m\omega^2\langle n'|x|n\rangle\langle m'|y|m\rangle = \delta m\omega^2\sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar}{2m\omega}}$$

$$= \delta m\omega^2\frac{\hbar}{2m\omega} = \frac{\delta\omega\hbar}{2}$$

The matrix is

$$V = \frac{\delta\hbar\omega}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

with eigenvalues

$$\boxed{\Delta^1_\pm = \pm\tfrac{\delta\hbar\omega}{2}}$$

Thus the energies to first order are

$$\boxed{E_\pm = E_{01} \pm \Delta^1 = 2\hbar\omega \pm \tfrac{\delta\hbar\omega}{2}}$$

with zeroth order energy eigenkets,

$$\boxed{|\pm\rangle = \tfrac{1}{\sqrt{2}}(|\psi_{10}\rangle \pm |\psi_{01}\rangle)}$$

c. Solving exactly

$$H = H_0 + V = \frac{p_x^2 + p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2 + 2\delta xy)$$

a wonderful substitution comes in handy. Define

$$x' \equiv \frac{x+y}{\sqrt{2}} \quad y' \equiv \frac{x-y}{\sqrt{x}}$$

$$p'_x \equiv \frac{p_x + p_y}{\sqrt{2}} \quad p'_y \equiv \frac{p_x - p_y}{\sqrt{2}}$$

Plug these primes into our Hamiltonian and we get

$$H = \frac{1}{2m}(p_x'^2 + p_y'^2) + \frac{m\omega^2}{2}(x'^2 + y'^2 + 2\delta\frac{(x'+y')(x'-y')}{2})$$

$$H = \frac{1}{2m}(p_x'^2 + p_y'^2) + \frac{m\omega^2}{2}(x'^2 + y'^2 + \delta x'^2 - \delta y'^2)$$

$$H = \frac{1}{2m}(p_x'^2 + p_y'^2) + \frac{m\omega^2}{2}(x'^2(1+\delta) + y'^2(1-\delta))$$

Thus we have an an-isotropic oscillator, with

$$w_x' = \omega\sqrt{1+\delta} \quad w_y' = \omega\sqrt{1-\delta}$$

Thus the ground state energy is still

$$\boxed{E_{00} = \hbar\omega}$$

if we ignore terms of δ^2 and higher.

The first order energies are, expanding the square root using the binomial expansion, and ignoring higher order terms, $O(\delta^2)$ again, we have

$$E_{n=1,m=0} = (n+1/2)\hbar\omega\sqrt{1+\delta} + (m+1/2)\hbar\omega\sqrt{1-\delta}$$

$$E_{1,0} = \frac{3}{2}\hbar\omega + \frac{3}{4}\hbar\omega\delta + \frac{1}{2}\hbar\omega - \frac{1}{4}\hbar\omega\delta$$

$$\boxed{E_{10} = 2\hbar\omega + \tfrac{\delta\hbar\omega}{2}}$$

The same procedure yields for

$$\boxed{E_{01} = 2\hbar\omega - \tfrac{\delta\hbar\omega}{2}}$$

These are the same as the perturbation approximation used in part (b). The validity of perturbation theory is thus shown for the an-isotropic harmonic oscillator.

Problem 5.7
A one-electron atom whose ground state is nondegenerate is placed in a uniform electric field in the z-direction. Obtain an approximate expression for the induced electric dipole moment of the ground state by considering the expectation value of ez with respect to the perturbed state vector computed to first order. Show that the same expression can also be obtained from the energy shift $\delta = -\alpha|\boldsymbol{E}|^2/2$ of the ground state computed to second order. α stands for the polarizability. Ignore Spin.

Solution:

Expectation value of ez to obtain induced electric dipole moment p:

$$p = \langle n^1|ez|n^1\rangle = \left(\langle n^0| + \sum_{k\neq n} \frac{V_{kn}^*}{E_n^0 - E_k^0}\langle k^0|\right) ez \left(|n^0\rangle + \sum_{k\neq n} \frac{V_{kn}}{E_n^0 - E_k^0}|k^0\rangle\right)$$

$$p = \langle n^0|z|n^0\rangle + \sum_{k\neq n} \frac{V_{kn}}{E_n^0 - E_k^0} e\langle n^0|z|k^0\rangle + \sum_{k\neq n} \frac{V_{kn}^*}{E_n^0 - E_k^0} e\langle k^0|z|n^0\rangle + 0$$

with

$$\langle n^0|z|n^0\rangle = 0$$

and

$$V_{kn} = -eE_{ext}\langle k^0|z|n^0\rangle$$

$$p = \sum_{k\neq n} \frac{-eE_{ext}\langle k^0|z|n^0\rangle}{E_n^0 - E_k^0} e\langle n^0|z|k^0\rangle + \sum_{k\neq n} \frac{-eE_{ext}\langle n^0|z|k^0\rangle}{E_n^0 - E_k^0} e\langle k^0|z|n^0\rangle$$

$$p = -2\sum_{k\neq n} \frac{e^2 E_{ext}|z_{kn}|^2}{E_n^0 - E_k^0}$$

Energy shift of the ground state computed to second order to obtain induced electric dipole moment p:

$$\Delta = \langle n^0|V|n^0\rangle + \sum_{k\neq n} \frac{|V_{kn}|^2}{E_n^0 - E_k^0}$$

Since $V = eEz$, the first term vanishes due to parity. So we are left with only the second term. Lets set it equal to the Δ given in the problem.

$$-\frac{\alpha}{2}|E|^2 = \sum_{k\neq n} \frac{|V_{kn}|^2}{E_n^0 - E_k^0}$$

Solving for α

$$\alpha = -\frac{2}{|E|^2}\sum_{k\neq n} \frac{|\langle k^0|eE_{ext}z|n^0\rangle|^2}{E_n^0 - E_k^0}$$

This is

$$\alpha = -2e^2\sum_{k\neq n} \frac{|\langle k^0|z|n^0\rangle|^2}{E_n^0 - E_k^0}$$

and since the dipole moment is defined as $p = \alpha E$ we obtain the same expression that we got using the expectation value.

$$p = \alpha E_{ext} = -2 \sum_{k \neq n} \frac{e^2 E_{ext} |z_{kn}|^2}{E_n^0 - E_k^0}$$

Problem 5.8
Evaluate the matrix elements (or expectation values) given below. If any vanishes, explain why it vanishes using simple symmetry (or other) arguments. a. $\langle n = 2, l = 1, m = 0 | x | n = 2, l = 0, m = 0 \rangle$ b. $\langle n = 2, l = 1, m = 0 | p_z | n = 2, l = 0, m = 0 \rangle$
Here $|nlm\rangle$ stands for the energy eigenket of a nonrelativistic hydrogen atom with spin ignored.
c. $\langle L_z \rangle$ for an electron in a central field with $j = \frac{9}{2}$, $m = \frac{7}{2}$, $l = 4$.
d. $\langle singlet, m_s = 0 | S_z^{(e-)} - S_z^{(e+)} | triplet, m_s = 0 \rangle$ for an s-state positronium.
e. $\langle \boldsymbol{S}^{(1)} \cdot \boldsymbol{S}^{(2)} \rangle$ for the ground state of a hydrogen molecule.

Solution:

a. On page 338 Sakurai explains whats going on. He says no $0 \rightarrow 0$ transition for m because x is a spherical tensor of rank 1. Therefore

$$\langle 2, 1, 0 | x | 2, 0, 0 \rangle = 0$$

b. This matrix element is very interesting because it is zero but not because transition symmetry. Using Heisenberg's operator equation:

$$\frac{i\hbar p_z}{m} = [z, H]$$

And basically following 5.7.20 in Sakurai, we have

$$\langle 210 | p_z | 200 \rangle = \frac{m}{i\hbar} \langle 210 | [z, H] | 200 \rangle = im \frac{E_{210} - E_{200}}{\hbar} \langle 210 | z | 200 \rangle$$

If I use the non-relativistic, spin-less, formula for the hydrogen atom's energy levels. (The famous Bohr formula) Then this whole thing goes to zero because

$$E_{210} = E_{200}$$

So

$$\langle 2, 1, 0 | p_z | 2, 0, 0 \rangle = 0$$

c. Plugging in our values $j = 9/2$, $l = 4$ and $m = 7/2$ into the spin angular functions, equ (3.7.64), we obtain

$$\mathcal{Y}_{l=4}^{j=9/2, m=7/2} = \frac{1}{3} \begin{pmatrix} \sqrt{8} Y_4^3 \\ Y_4^4 \end{pmatrix}$$

So because the spherical harmonics are precisely the eigenfunctions of L_z we have 8/9 probability of measuring $3\hbar$ and 1/9 probability of measuring $4\hbar$. So our average value is

$$\langle L_z \rangle = P_1 * m_1\hbar + P_2 * m_2\hbar = (\frac{\sqrt{8}}{3})^2 * 3\hbar + (\frac{1}{3})^2 * 4\hbar = \frac{28}{9}\hbar.$$

d. The singlet state of two spins with $m_s = 0$ is: (this is most clearly spelled out in Shankar pg 405.)

$$|singlet, m_s = 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$$

The triplet is:

$$|triplet, m_s = 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$$

The interesting part of this problem is that:

$$(S_z^1 - S_z^2)|\text{triplet}\rangle = \hbar|\text{singlet}\rangle$$

This is because, using

$$S_{iz}|s_1m_1, s_2m_2\rangle = \hbar m_i|s_1m_1, s_2m_2\rangle \quad (i = 1, 2)$$

we have

$$(S_z^1 - S_z^2)\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) = \frac{1}{\sqrt{2}}[(\frac{\hbar}{2}) - (-\frac{\hbar}{2})|+-\rangle + ((-\frac{\hbar}{2}) - (\frac{\hbar}{2}))|-+\rangle]$$

That is

$$(S_z^1 - S_z^2)\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) = \frac{\hbar}{\sqrt{2}}[|+-\rangle - |-+\rangle] = \hbar|\text{singlet}\rangle$$

So we have

$$\langle\text{singlet}|S_z^1 - S_z^2|\text{triplet}\rangle = \langle\text{singlet}|\hbar|\text{singlet}\rangle = \hbar$$

e. The ground state wave function of a hydrogen molecule is symmetric in space. This is explained a bit further ahead in Chapter 6 page 367. The Pauli Exclusion principal demands the total wave function with space and spin dependence must be antisymmetric. So the spin wave function must be antisymmetric. Thus we use the spin singlet function. Griffith spells out how the average value may be computed. (page 167).

$$\vec{S}_1 \cdot \vec{S}_2|-+\rangle = \frac{\hbar^2}{4}(2|+-\rangle - |-+\rangle)$$

$$\vec{S}_1 \cdot \vec{S}_2 |+-\rangle = \frac{\hbar^2}{4}(2|-+\rangle - |+-\rangle)$$

So for the singlet state

$$\vec{S}_1 \cdot \vec{S}_2 |00\rangle = -\frac{3\hbar^2}{4}|00\rangle$$

Therefore

$$\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = -\frac{3\hbar^2}{4}$$

Problem 5.9
A p-orbital electron characterized by $|n, l = 1, m = \pm 1, 0\rangle$ (ignore spin) is subjected to a potential

$$V = \lambda(x^2 - y^2) \quad (\lambda = \text{constant})$$

a. Obtain the correct zeroth-order energy eigenstates that diagonalize the perturbation. You need not evaluate the energy shifts in detail, but show that the original threefold degeneracy is now completely removed.
b. Because V is invariant under time reversal and because there is no longer any degeneracy, we expect each of the energy eigenstates obtained in (a) to go into itself (up to a phase factor or sign) under time reversal. Check this point explicitly.

Solution:

a. The matrix elements

$$\langle l = 1, m|V|l = 1, m'\rangle$$

may be written down as

$$\langle l = 1, m|\lambda(x^2 - y^2)|l = 1, m'\rangle = K\langle l = 1, m|J_x^2 - J_y^2|l = 1, m'\rangle = C\langle l = 1, m|J_+^2 - J_-^2|l = 1, m'\rangle$$

This leaves the corner off diagonal elements non-vanishing.

$$\langle l = 1, m|V|l = 1, m'\rangle = \begin{bmatrix} 0 & 0 & R \\ 0 & 0 & 0 \\ R & 0 & 0 \end{bmatrix}$$

The eigenvectors to diagonalize this matrix are:

$$|+\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \quad |-\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) \quad |0\rangle = |0\rangle \ \ (E = E_0)$$

The degeneracy is removed because now there are three distinct energies.
b. Using the formula (4.4.77)

$$\Theta|l,m\rangle = (-1)^m|l,-m\rangle$$

I've got

$$\Theta|+\rangle = -|-\rangle$$

$$\Theta|-\rangle = -|+\rangle$$

So therefore

$$\Theta\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) = \frac{1}{\sqrt{2}}(-|-\rangle - |+\rangle) = -\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

$$\Theta\frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) = \frac{1}{\sqrt{2}}(-|-\rangle + |+\rangle) = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$$

$$\Theta|0\rangle = |0\rangle$$

Thus they go into themselves up to a sign under time reversal.

Problem 5.11
The Hamiltonian matrix for a two state system can be written as

$$\mathcal{H} = \begin{pmatrix} E_1^0 & \lambda\Delta \\ \lambda\Delta & E_2^0 \end{pmatrix}.$$

Clearly the energy eigenfunctions for the unperturbed problems ($\lambda = 0$) are given by

$$\phi_1^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \phi_2^{(0)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

a. Solve the problem exactly to find the energy eigenfunctions ψ_1 and ψ_2 and the energy eigenvalues E_1 and E_2.
b. Assuming that $\lambda|\Delta| \ll |E_1^0 - E_2^0|$, solve the same problem using time-independent perturbation theory up to first order in the energy eigenfunctions and up to second order in the energy eigenvalues. Compare with the exact results obtained in (a).
c. Suppose the two unperturbed energies are älmost degenerate," that is,

$$|E_1^0 - E_2^0| \ll \lambda|\Delta|$$

Show that the exact results obtained in (a) closely resemble what you would expect by applying degenerate perturbation theory to this problem with E_1^0 set exactly equal to E_2^0.

Solution:

Part (a) is an eigenvalue problem.

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

Using quadratic formula, and being careful with negative signs and our multiple E's we get:

$$E_{1,2} = \frac{E_1^0}{2} + \frac{E_2^0}{2} \pm \frac{1}{2}\sqrt{(E_1^0 - E_2^0)^2 + 4\lambda^2\Delta^2}$$

The eigenvectors are more tricky. Using an example state with a variable X inside, we may solve for X and find the eigenvectors.

$$\psi_1 = \begin{pmatrix} X \\ 1 \end{pmatrix}$$

This yields

$$\begin{bmatrix} E_1^0 & \lambda\Delta \\ \lambda\Delta & E_2^0 \end{bmatrix} \begin{pmatrix} X \\ 1 \end{pmatrix} = \begin{bmatrix} E_1 & 0 \\ 0 & E_1 \end{bmatrix} \begin{pmatrix} X \\ 1 \end{pmatrix}$$

and our equation for X is

$$XE_1^0 + \lambda\Delta = XE_1$$

so

$$X = \frac{\lambda\Delta}{E_1 - E_1^0}$$

and the process works for the second eigenvalue as well. Therefore our ψ's are:

$$\psi_{1,2} = \begin{pmatrix} \frac{\lambda\Delta}{E_{1,2} - E_1^0} \\ 1 \end{pmatrix}$$

b. The first order energy shifts are zero.

$$\Delta^1 = \langle\psi_1^0|V|\psi_1^0\rangle = 0$$

For second order we actually get something.

$$\Delta_{n,k}^2 = \sum_{n\neq k} \frac{|V_{nk}|^2}{E_n^0 - E_k^0}$$

This yields us, using the off diagonal elements:

$$\Delta_{1,2}^2 = \frac{|V_{12}|^2}{E_1^0 - E_2^0} = \frac{\lambda^2\Delta^2}{E_1^0 - E_2^0}$$

$$\Delta_{2,1}^2 = \frac{|V_{21}|^2}{E_2^0 - E_1^0} = \frac{\lambda^2\Delta^2}{E_2^0 - E_1^0}$$

The eigenfunctions to first order are:

$$\phi_1^1 = \phi_1^0 + \frac{\phi_2^0 V_{21}}{E_1^0 - E_2^0} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{\lambda\Delta}{E_1^0 - E_2^0} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\lambda\Delta}{E_1^0 - E_2^0} \end{pmatrix}$$

$$\phi_2^1 = \phi_2^0 + \frac{\phi_1^0 V_{12}}{E_2^0 - E_1^0} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} \frac{\lambda\Delta}{E_2^0 - E_1^0} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\lambda\Delta}{E_2^0 - E_1^0} \\ 1 \end{pmatrix}$$

These results are in agreement with the exact solution because of the approximation $\lambda|\Delta| \ll |E_1^0 - E_2^0|$ and using the binomial theorem on the exact eigenvalues.

$$E_{1,2} = \frac{E_1^0}{2} + \frac{E_2^0}{2} \pm \frac{1}{2}\sqrt{(E_1^0 - E_2^0)^2 + 4\lambda^2\Delta^2} = \frac{E_1^0}{2} + \frac{E_2^0}{2} \pm \frac{E_1^0 - E_2^0}{2}\sqrt{1 + \frac{4\lambda^2\Delta^2}{(E_1^0 - E_2^0)^2}}$$

$$E_{1,2} \approx \frac{E_1^0}{2} + \frac{E_2^0}{2} \pm \frac{E_1^0 - E_2^0}{2}(1 + \frac{2\lambda^2\Delta^2}{(E_1^0 - E_2^0)^2})$$

This yields

$$E_1 \approx E_1^0 + \frac{\lambda^2\Delta^2}{E_1^0 - E_2^0}$$

$$E_2 \approx E_2^0 - \frac{\lambda^2\Delta^2}{E_1^0 - E_2^0}$$

The same approximation may be made inside the eigenvectors to yield agreement between the perturbation approach and the exact solution.

c. If I apply degenerate perturbation theory to this problem, setting $E_1^0 = E_2^0$, my matrix is

$$H_D = \begin{bmatrix} E_1^0 & \lambda\Delta \\ \lambda\Delta & E_1^0 \end{bmatrix}$$

$$H^1 = \begin{bmatrix} 0 & \lambda\Delta \\ \lambda\Delta & 0 \end{bmatrix}$$

where

$$H_D = H_0 + H^1$$

The shifts may be quickly found by equation 6.26 in Griffiths:

$$E_\pm^1 = \pm\lambda\Delta$$

So

$$E_{1,2} = E_{1,2}^0 \pm \lambda\Delta$$

But the results in part (a) are very close if we set $|E_1^0 - E_2^0| \ll \lambda|\Delta|$

$$E_{1,2} = \frac{E_1^0}{2} + \frac{E_2^0}{2} \pm \frac{1}{2}\sqrt{(E_1^0 - E_2^0)^2 + 4\lambda^2\Delta^2} \approx \frac{E_1^0}{2} + \frac{E_2^0}{2} \pm \lambda\Delta$$

and with $E_1^0 \approx E_2^0$ we have the desired agreement:

$$E_{1,2} \approx E_{1,2}^0 \pm \lambda\Delta$$