Advanced Quantum Mechanics: Assignment #4

Due on 8th November, 2018

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Let Hamiltonian $H = H_0 + \lambda V$, $H_0 \left|n^0\right\rangle = E_n^0 \left|n^0\right\rangle$, $H\left|n\right\rangle = E_n \left|n\right\rangle$. Let $\Delta_n = E_n - E_n^0$ and $\phi_n = 1 - \left|n^0\right\rangle\left\langle n^0\right|$ be the projector onto the orthogonal space of $\left|n^0\right\rangle$. $\left|n\right\rangle$ and Δ_n are given by,

$$\left|n\right\rangle = \left|n^0\right\rangle + \frac{\phi_n(\lambda V - \Delta_n)\left|n\right\rangle}{E_n^0 - H_0} = \left|n^0\right\rangle + \sum_{k\neq n} \frac{\lambda\left\langle k^0\middle|V\middle|n\right\rangle - \Delta_n\left\langle k^0\middle|n\right\rangle}{E_n^0 - E_k^0}\left|k^0\right\rangle \quad \text{and} \quad \Delta_n = \lambda\left\langle n^0\middle|V\middle|n\right\rangle$$

We work with normalization $\left\langle n\middle|n^0\right\rangle = 1 \implies \left\langle n^j\middle|n^0\right\rangle = 0 \quad ; \quad j \neq 0$. We assume the following,

$$\Delta_n = \lambda\Delta_n^1 + \lambda^2\Delta_n^2 + \dots \quad \text{and} \quad \left|n\right\rangle = \left|n^0\right\rangle + \lambda\left|n^1\right\rangle + \lambda^2\left|n^2\right\rangle + \dots$$

Putting these into the equations for $\left|n\right\rangle$ and Δ_n and equating order by order, we get,

$$\Delta_n^1 = \left\langle n^0\middle|V\middle|n^0\right\rangle \tag{1}$$

$$\left|n^1\right\rangle = \sum_{k\neq n}\frac{\left\langle k^0\middle|V\middle|n^0\right\rangle}{E_n^0 - E_k^0}\left|k^0\right\rangle \tag{2}$$

$$\Delta_n^2 = \sum_{k\neq n}\frac{\left|\left\langle k^0\middle|V\middle|n^0\right\rangle\right|^2}{E_n^0 - E_k^0}\left|k^0\right\rangle \tag{3}$$

$$\left|n^2\right\rangle = \sum_{k\neq n}\frac{\left\langle k^0\middle|V\middle|n^1\right\rangle - \Delta_n^1\left\langle k^0\middle|n^1\right\rangle}{E_n^0 - E_k^0}\left|k^0\right\rangle \tag{4}$$

Problem 1

We note that,

$$\begin{aligned}\left\langle E_n\middle|E_n\right\rangle &= \left\langle E_n\middle|E_n^0\right\rangle + \lambda\left(\left\langle E_n^1\middle|E_n^0\right\rangle + \left\langle E_n^0\middle|E_n^1\right\rangle\right) + \lambda^2\left(\left\langle E_n^2\middle|E_n^0\right\rangle + \left\langle E_n^0\middle|E_n^2\right\rangle + \left\langle E_n^1\middle|E_n^1\right\rangle\right)\\ &= 1 + \lambda^2\left(\left\langle E_n^1\middle|E_n^1\right\rangle\right)\end{aligned}$$

One needs to find the following,

$$\begin{aligned}\frac{\left\langle E_n^0\middle|E_n\right\rangle}{\sqrt{\left\langle E_n\middle|E_n\right\rangle\left\langle E_n^0\middle|E_n^0\right\rangle}} &= \frac{1}{\sqrt{1 + \lambda^2(\left\langle E_n^1\middle|E_n^1\right\rangle)}}\\ &= 1 - \frac{\lambda^2}{2}\sum_{k\neq n}\frac{\left|\left\langle E_k^0\middle|V\middle|E_n^0\right\rangle\right|^2}{(E_n^0 - E_k^0)^2}\end{aligned}$$

where we have used (2) in going to the last step. Hence, the required probability is $1 - \frac{\lambda^2}{2}\sum_{k\neq n}\frac{\left|\left\langle E_k^0\middle|V\middle|E_n^0\right\rangle\right|^2}{(E_n^0 - E_k^0)^2}$.

Problem 2

Part (a)
From the form of the Hamiltonian, we can see that the energy will have the form,

$$E_{n_x,n_y} = (n_x + 0.5 + n_y + 0.5)\omega = (n_x + n_y + 1)\omega$$

The three lowest lying states are,

$$\begin{aligned} n_x = 0 \quad &, \quad n_y = 0 \implies E_{00}^{(0)} = \omega \\ n_x = 1 \quad &, \quad n_y = 0 \implies E_{10}^{(0)} = 2\omega \\ n_x = 0 \quad &, \quad n_y = 1 \implies E_{01}^{(0)} = 2\omega \end{aligned}$$

We see that there is a double-degeneracy with energy 2ω.

Part (b)
Let's denote states by $|n_x n_y\rangle$. x and y can be written in terms of corresponding creation and annhilation operators as follows,

$$x = \frac{1}{\sqrt{2m\omega}}(a_x + a_x^\dagger) \quad \text{and} \quad y = \frac{1}{\sqrt{2m\omega}}(a_y + a_y^\dagger)$$

The perturbation is $V = \lambda m\omega^2 xy$. Let's denote the m-th order energy shift by $\Delta^m_{n_x n_y}$. Let's first consider $|00\rangle$. The zeroth order energy eigenstate is given by,

$$\psi_{00}^0 = \psi_0(x)\psi_0(y) = \sqrt{\frac{m\omega}{\pi}} e^{-\frac{m\omega}{2}(x^2+y^2)}$$

Consider Δ^1_{00},

$$\begin{aligned} \Delta^1_{00} &= \langle 00|V|00\rangle \\ &= \frac{m\omega^2}{2m\omega}\big(\langle 00|a_x a_y|00\rangle + \langle 00|a_x a_y^\dagger|00\rangle + \langle 00|a_x^\dagger a_y^\dagger|00\rangle + \langle 00|a_x^\dagger a_y|00\rangle\big) \\ \Delta^1_{00} &= 0 \end{aligned}$$

The states $|10\rangle$ and $|01\rangle$ are degenerate, and hence we need to apply degenerate perturbation formalism. For this, we construct the matrix elements of V between the degenerate states. As we have seen in the $|00\rangle$ case, the operator xy changes a given state to one which has at least one of the quantum numbers different (by 1). Hence $\langle 01|V|01\rangle = \langle 10|V|10\rangle = 0$. We proceed to calculate $\langle 01|V|10\rangle$,

$$\begin{aligned} \langle 01|V|10\rangle &= \frac{\lambda m\omega^2}{2m\omega}\big(\langle 01|a_x a_y|10\rangle + \langle 01|a_x a_y^\dagger|10\rangle + \langle 01|a_x^\dagger a_y^\dagger|10\rangle + \langle 01|a_x^\dagger a_y|10\rangle\big) \\ &= \frac{\lambda\omega}{2}(0 + 1 + 0 + 0) \\ \langle 01|V|10\rangle &= \frac{\lambda\omega}{2} \\ \implies \langle 10|V|01\rangle &= \frac{\lambda\omega}{2} \\ \therefore V &= \frac{\lambda\omega}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

The eigenvalues of the above matrix are $\pm\frac{\lambda\omega}{2} \implies E = 2\omega \pm \lambda\frac{\omega}{2}$ with eigenstates $\frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle)$

Part (c)

The aim is to now solve for the Hamiltonian exactly.

$$
\begin{aligned}
H &= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2 + 2\lambda xy) \\
&= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{4}((x+y)^2 + (x-y)^2 + \lambda[(x+y)^2 - (x-y)^2]) \\
&= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}\left[\left(\frac{x+y}{\sqrt{2}}\right)^2(1+\lambda) + \left(\frac{x-y}{\sqrt{2}}\right)^2(1-\lambda)\right]
\end{aligned}
$$

Let $\alpha = \dfrac{x+y}{\sqrt{2}}$ and $\beta = \dfrac{x-y}{\sqrt{2}}$. We can see that $\dot{\alpha}^2 + \dot{\beta}^2 = \dot{x}^2 + \dot{y}^2 \implies p_\alpha^2 + p_\beta^2 = p_x^2 + p_y^2$. In the new coordinates, the Hamiltonian is,

$$
H = \frac{p_\alpha^2}{2m} + \frac{m(\omega\sqrt{1+\lambda})^2}{2}\alpha^2 + \frac{p_\beta^2}{2m} + \frac{m(\omega\sqrt{1-\lambda})^2}{2}\beta^2
$$

We have essentially decoupled the Hamiltonian into two harmonic oscillators of frequencies $\omega_1 = \omega\sqrt{1+\lambda}$ and $\omega_2 = \omega\sqrt{1-\lambda}$. The three lowest energies are,

$$
\begin{aligned}
\frac{\omega(\sqrt{1+\lambda} + \sqrt{1-\lambda})}{2} &= \omega + \mathcal{O}(\lambda^2) \\
\frac{\omega(3\sqrt{1+\lambda} + \sqrt{1-\lambda})}{2} &= 2\omega + \lambda\frac{\omega}{2} + \mathcal{O}(\lambda^2) \\
\frac{\omega(\sqrt{1+\lambda} + 3\sqrt{1-\lambda})}{2} &= 2\omega - \lambda\frac{\omega}{2} + \mathcal{O}(\lambda^2)
\end{aligned}
$$

We see that the above values match with those calculated from perturbation theory.

Problem 3

We first note that $x^2 - y^2 = r^2\sin^2\theta\cos 2\phi = r^2\sin^2\theta\dfrac{e^{2i\phi} + e^{-2i\phi}}{2}$ when expressed in polar coordinates. As we are dealing with states that differ only in their m values, we label the states as $|m\rangle$. We note the following eigenstates $\psi_{n,l,m}$ of the hydrogen atom,

$$
\psi_{2,1,\pm1}(r,\theta,\phi) = |\pm1\rangle = \frac{1}{8\sqrt{\pi}a_0^{5/2}} r e^{-\frac{2r}{a_0}} \sin\theta e^{\pm i\phi} \quad \text{and} \quad \psi_{2,1,0}(r,\theta,\phi) = |0\rangle = \frac{\sqrt{2}}{8\sqrt{\pi}a_0^{5/2}} r e^{-\frac{2r}{a_0}} \cos\theta
$$

The above eigenstates are degenerate. The perturbing Hamiltonian is $V = \lambda(x^2 - y^2) = \lambda r^2\sin^2\theta\cos 2\phi = \lambda V'$. As we are dealing with states that differ only in their m values, we label the states as $|m\rangle$. As in the previous problem, we proceed to construct the matrix elements of V'. In each element $\langle p|V|q\rangle$, the ϕ integral will be $\sim \int_0^{2\pi} e^{i(q-p)\phi}(e^{2i\phi} + e^{-2i\phi})d\phi$. We can see that this integral will be zero unless $q - p = \pm 2$. Hence, only terms where $p - q = \pm 2$ will contribute, ie $p = 1, q = -1$ and $p = -1, q = 1$. Let's evaluate $\langle -1|V'|1\rangle$,

$$
\begin{aligned}
\langle -1|V'|1\rangle &= -\frac{1}{64\pi a_0^5}\int_0^{2\pi}\frac{e^{4i\phi}+1}{2}d\phi\int_0^{\pi}\sin^4\theta d(\cos\theta)\int_0^{\infty} r^6 e^{-\frac{4r}{a_0}}dr \\
&= -\frac{1}{64\pi a_0^5}(\pi)\int_0^{\pi}(1-\cos^2\theta)^2 d(\cos\theta)\int_{-\infty}^{0}\left(\frac{a_0}{4}\right)^7 t^6 e^t dr \qquad \left(\Longleftarrow\ t = -\frac{4r}{a_0}\right) \\
&= -\frac{1}{64\pi a_0^5}(\pi)\int_0^{\pi}(\cos^4\theta - 2\cos^2\theta + 1)d(\cos\theta)\left[\left(\frac{a_0}{4}\right)^7 6!\right] \\
&= -\frac{a_0^2}{64}\left(\frac{-2}{5} + \frac{4}{3} - 2\right)\left[\left(\frac{45}{2^{10}}\right)\right] = \frac{a_0^2}{64}\left(\frac{16}{15}\right)\left[\left(\frac{45}{2^{10}}\right)\right] = \frac{3}{2^{12}}a_0^2 = \alpha
\end{aligned}
$$

$$\therefore \langle -1|V'|1\rangle = \langle -1|V'|1\rangle = \alpha = \frac{3}{2^{12}} a_0^2$$

$$V' = \begin{pmatrix} 0 & 0 & \alpha \\ 0 & 0 & 0 \\ \alpha & 0 & 0 \end{pmatrix}$$

The eigenvalues of V' are 0, $\pm\alpha$ and the corresponding eigenstates are $|0\rangle$, $\dfrac{|1\rangle \pm |{-1}\rangle}{\sqrt{2}}$ respectively. So the first order energy shifts are 0, $\pm\alpha$.

Problem 4

$$H = \begin{pmatrix} E_1 & 0 & \lambda a \\ 0 & E_1 & \lambda b \\ \lambda a^* & \lambda b^* & E_2 \end{pmatrix} = \underbrace{\begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_2 \end{pmatrix}}_{H_0} + \lambda \underbrace{\begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix}}_{V}$$

H has the following three eigenvalues.

$$\frac{E_1 + E_2}{2} \pm \sqrt{\lambda^2 \left(a^2 + b^2\right) + \left(\frac{E_1 - E_2}{2}\right)^2} \quad \text{and} \quad E_1$$

Problem 5

Let $L^2 = L_x^2 + L_y^2 + L_z^2$. We work in the basis of states $|l, m\rangle$ such that $L^2 |l, m\rangle = l(l+1)|l, m\rangle$ and $L_z |l, m\rangle = m |l, m\rangle$. The Hamiltonian then is,

$$H = H_0 + \lambda V = AL^2 + BL_z + \lambda C L_y$$

The eigenstates of H_0 are,

$$H_0 |l, m\rangle = (Al(l+1) + Bm)|l, m\rangle = E_{lm} |l, m\rangle$$

For future use, let's evaluate $\langle l', m'|V|l, m\rangle$,

$$\begin{aligned}
\langle l', m'|V|l, m\rangle &= C \langle l', m'|L_y|l, m\rangle \\
&= \frac{C}{2i} \langle l', m'|L_+ - L_-|l, m\rangle \\
&= \frac{C}{2i}\left(\sqrt{l(l+1) - m(m+1)}\delta_{l',l}\delta_{m',m+1} - \sqrt{l(l+1) - m(m-1)}\delta_{l',l}\delta_{m',m-1}\right) \\
|\langle l', m'|V|l, m\rangle|^2 &= \frac{C^2}{4}\left([l(l+1) - m(m+1)]\delta_{l',l}\delta_{m',m+1} + [l(l+1) - m(m-1)]\delta_{l',l}\delta_{m',m-1}\right)
\end{aligned}$$

The first order energy shift is given by,

$$\begin{aligned}
\Delta_{lm}^{(1)} &= \langle l, m|V|l, m\rangle \\
&= \frac{C}{2i}\left(\sqrt{l(l+1) - m(m+1)}\delta_{l,l}\delta_{m,m+1} - \sqrt{l(l+1) - m(m-1)}\delta_{l,l}\delta_{m,m-1}\right) \\
\Delta_{lm}^{(1)} &= 0
\end{aligned}$$

Problem 5 continued on next page. . .

Then one needs to find higher order energy shifts. Considering Δ^2_{lm} and using (3),

$$\begin{aligned}
\Delta^2_{lm} &= \sum_{l\neq l', m\neq m'} \frac{|\langle l', m'|V|l, m\rangle|^2}{E_{lm} - E_{l'm'}} \\
&= \frac{C^2}{4} \sum_{l\neq l', m\neq m'} \frac{([l(l+1) - m(m+1)]\delta_{l',l}\delta_{m',m+1} + [l(l+1) - m(m-1)]\delta_{l',l}\delta_{m',m-1})}{Al(l+1) + Bm - Al'(l'+1) - Bm'} \\
&= \frac{C^2}{4}\left(\frac{-[l(l+1) - m(m+1)]}{B} + \frac{[l(l+1) - m(m-1)]}{B}\right) \\
&= \frac{mc^2}{2B}
\end{aligned}$$

Problem 6

The Hamiltonian to deal with is,

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2$$

and the given trial wavefunction is,

$$\psi_\beta(x) = Ne^{-\beta|x|}$$

where N is some normalization. Let's calculate $\langle\psi_\beta|H|\psi_\beta\rangle$,

$$\begin{aligned}
\langle\psi_\beta|H|\psi_\beta\rangle &= N^2 \int_{-\infty}^{\infty} e^{-2\beta|x|}\left(-\frac{1}{2m}\beta^2 + \frac{m\omega^2}{2}x^2\right)dx \\
&= \lim_{\epsilon\to 0} N^2\left[2\int_{\epsilon}^{\infty} e^{-2\beta x}\left(-\frac{1}{2m}\beta^2 + \frac{m\omega^2}{2}x^2\right)dx + \int_{-\epsilon}^{\epsilon} e^{-2\beta|x|}\left(-\frac{1}{2m}\beta^2 + \frac{m\omega^2}{2}x^2\right)dx\right] \\
&= N^2\left[\left(-\frac{\beta}{2m} + \frac{m\omega^2}{4\beta^3}\right) + \lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} e^{-2\beta|x|}\left(-\frac{1}{2m}\beta^2 + \frac{m\omega^2}{2}x^2\right)dx\right]
\end{aligned}$$

$$\begin{aligned}
N^2 \int_{-\infty}^{\infty} e^{-2\beta|x|} &= 1 \\
N^2 &= \beta
\end{aligned}$$

$$\langle\psi_\beta|H|\psi_\beta\rangle = -\frac{\beta^2}{2m} + \frac{m\omega^2}{4\beta^2}$$