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,

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

One needs to find the following,

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

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

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,

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

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 $V = \lambda m\omega^2 xy$. Consider $\langle q_x q_y|V|n_x n_y\rangle$

$$\begin{aligned} \langle q_x q_y|V|n_x n_y\rangle &= \lambda m\omega^2\big(\langle q_x q_y|a_x a_y|n_x n_y\rangle + \langle q_x q_y|a_x a_y^\dagger|n_x n_y\rangle + \langle q_x q_y|a_x^\dagger a_y^\dagger|n_x n_y\rangle + \langle q_x q_y|a_x^\dagger a_y|n_x n_y\rangle\big) \\ &= \lambda m\omega^2(\sqrt{n_x n_y}\delta_{q_x,n_x-1}\delta_{q_y,n_y-1} + \sqrt{n_x(n_y+1)}\delta_{q_x,n_x-1}\delta_{q_y,n_y+1} \\ &\quad + \sqrt{(n_x+1)(n_y+1)}\delta_{q_x,n_x+1}\delta_{q_y,n_y+1} + \sqrt{(n_x+1)(n_y)}\delta_{q_x,n_x+1}\delta_{q_y,n_y-1}) \\ \implies \langle n_x n_y|V|n_x n_y\rangle = 0 \implies E^{(1)}_{n_x n_y} = 0 \end{aligned}$$

This means that there will be no energy shift at the first order in λ for any state under consideration. We now proceed to calculate $\left|n_x n_y^{(1)}\right\rangle$,

$$\begin{aligned} \left|00^{(1)}\right\rangle &= \sum_{(q_x,q_y)\neq(0,0)} \frac{\langle q_x q_y|V|00\rangle}{E^{(0)}_{00} - E^{(0)}_{q_x q_y}} |q_x q_y\rangle \\ &= \lambda m\omega^2 \sum_{(q_x,q_y)\neq(0,0)} \frac{\delta_{q_x,1}\delta_{q_y,1}}{E^{(0)}_{00} - E^{(0)}_{q_x q_y}} |q_x q_y\rangle \\ \left|00^{(1)}\right\rangle &= -\frac{\lambda m\omega}{2} |11\rangle \end{aligned}$$

$$\begin{aligned} \left|10^{(1)}\right\rangle &= \sum_{(q_x,q_y)\neq(1,0)} \frac{\langle q_x q_y|V|10\rangle}{E^{(0)}_{10} - E^{(0)}_{q_x q_y}} |q_x q_y\rangle \\ &= \lambda m\omega^2 \sum_{(q_x,q_y)\neq(0,0)} \frac{\delta_{q_x,1}\delta_{q_y,1}}{E^{(0)}_{00} - E^{(0)}_{q_x q_y}} |q_x q_y\rangle \\ \left|10^{(1)}\right\rangle &= -\frac{\lambda m\omega}{2} |11\rangle \end{aligned}$$

Problem 3

We first note that $x^2 - y^2 = r^2 \sin^2\theta \cos 2\phi$ when expressed in polar coordinates, and also the following eigenstates $\psi_{n,l,m}$ of the hydrogen atom,

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

The perturbing Hamiltonian is $V = \lambda(x^2 - y^2) = \lambda r^2 \sin^2\theta \cos 2\phi = \lambda V'$
The first order correction for $m = \pm 1$ is given by,

$$\begin{aligned}
\Delta_{\pm 1} &= -\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi^*_{2,1,\pm 1}\psi_{2,1,\pm 1} V' r^2 d(\cos\theta) dr d\theta d\phi \\
&= -\frac{1}{64\pi a_0^5}\int_0^{2\pi} \cos 2\phi d\phi \int_0^{\pi} \sin^4\theta d(cos\theta) \int_0^{\infty} r^6 e^{-\frac{4r}{a_0}} dr \qquad = 0
\end{aligned}$$

Problem 4

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

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

The first order energy shift is given by,

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

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 $\langle\psi_\beta|H|\psi_\beta\rangle$,

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

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

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