PHY4370 ASSIGNMENT 4

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Problem 1. Problem 8.1

We know that

$$|\psi_n^{(1)}\rangle = \sum_{p\neq n} \frac{H'_{pn}}{(E_n^{(0)} - E_p^{(0)})} |\psi_p^{(0)}\rangle$$

Substitute into

$$\begin{aligned}
-\langle\psi_n^{(1)}|H_0 - E_n^{(0)}|\psi_n^{(1)}\rangle &= \langle\psi_n^{(1)}|E_n^{(0)} - H_0|\psi_n^{(1)}\rangle \\
&= \langle\psi_n^{(1)}|(E_n^{(0)} - H_0) \sum_{p\neq n} \frac{H'_{pn}}{(E_n^{(0)} - E_p^{(0)})} |\psi_p^{(0)}\rangle \\
&= \sum_{p\neq n} \frac{H'_{pn}}{(E_n^{(0)} - E_p^{(0)})} \langle\psi_n^{(1)}|E_n^{(0)} - H_0|\psi_p^{(0)}\rangle
\end{aligned}$$

Let's open up the sandwich

$$\begin{aligned}
\langle\psi_n^{(1)}|E_n^{(0)} - H_0|\psi_p^{(0)}\rangle &= \langle\psi_n^{(1)}|E_n^{(0)}|\psi_p^{(0)}\rangle - \langle\psi_n^{(1)}|H_0|\psi_p^{(0)}\rangle \\
&= E_n^{(0)}\langle\psi_n^{(1)}|\psi_p^{(0)}\rangle - E_p^{(0)}\langle\psi_n^{(1)}|\psi_p^{(0)}\rangle \\
&= (E_n^{(0)} - E_p^{(0)})\langle\psi_n^{(1)}|\psi_p^{(0)}\rangle \\
&= (E_n^{(0)} - E_p^{(0)})(a_{pn}^{(1)})^* \\
&= (E_n^{(0)} - E_p^{(0)})a_{np}^{(1)} \\
&= (E_n^{(0)} - E_p^{(0)})\frac{(H'_{pn})^*}{(E_n^{(0)} - E_p^{(0)})} \\
&= H'_{np}
\end{aligned}$$

Back into the original equation

$$\begin{aligned}
\sum_{p\neq n} \frac{H'_{pn}}{(E_n^{(0)} - E_p^{(0)})} \langle\psi_n^{(1)}|E_n^{(0)} - H_0|\psi_p^{(0)}\rangle &= \sum_{p\neq n} \frac{H'_{pn}}{(E_n^{(0)} - E_p^{(0)})} H'_{np} \\
&= \sum_{p\neq n} \frac{H'_{pn}H'_{np}}{(E_n^{(0)} - E_p^{(0)})} \\
&= \sum_{p\neq n} \frac{|H'_{pn}|^2}{(E_n^{(0)} - E_p^{(0)})} \\
&= E_n^{(2)}
\end{aligned}$$

Problem 2. Problem 8.4

Todo.

Problem 3. Problem 8.5

Expanding to third order in λ, the coefficients of λ^3 are (given by 8.12 on page 377)

$$\begin{aligned} H_0\psi_n^{(3)} + H'\psi_n^{(2)} &= E_n^{(0)}\psi_n^{(3)} + E_n^{(1)}\psi_n^{(2)} + E_n^{(2)}\psi_n^{(1)} + E_n^{(3)}\psi_n^{(0)} \\ 0 &= (H_0 - E_n^{(0)})\psi_n^{(3)} + (H' - E_n^{(1)})\psi_n^{(2)} - E_n^{(2)}\psi_n^{(1)} - E_n^{(3)}\psi_n^{(0)} \end{aligned}$$

Premultiply by $(\psi_n^{(0)})^*$ and integrate

$$0 = \langle\psi_n^{(0)}|H_0 - E_n^{(0)}|\psi_n^{(3)}\rangle + \langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_n^{(2)}\rangle - E_n^{(2)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle - E_n^{(3)}\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle$$

We want to solve for $E_n^{(3)}$. Note that $\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = a_{nn}^{(1)} = 0$.

$$E_n^{(3)} = \langle\psi_n^{(0)}|H_0 - E_n^{(0)}|\psi_n^{(3)}\rangle + \langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_n^{(2)}\rangle$$

Dealing with the first term:

$$\begin{aligned} \langle\psi_n^{(0)}|H_0 - E_n^{(0)}|\psi_n^{(3)}\rangle &= \langle\psi_n^{(0)}|H_0|\psi_n^{(3)}\rangle - E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(3)}\rangle \\ &= \langle\psi_n^{(3)}|H_0|\psi_n^{(0)}\rangle^* - E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(3)}\rangle \\ &= E_n^{(0)}\langle\psi_n^{(3)}|\psi_n^{(0)}\rangle^* - E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(3)}\rangle \\ &= E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(3)}\rangle - E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(3)}\rangle \\ &= 0 \end{aligned}$$

So we see

$$E_n^{(3)} = \langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_n^{(2)}\rangle$$

An expression for $|\psi_n^{(2)}\rangle$ is obtained from the book on pg. 381 eq. 8.36b

$$|\psi_n^{(2)}\rangle = \sum_{l\neq n}\left[\sum_{k\neq n}\frac{H'_{lk}H'_{kn}}{(E_n^{(0)} - E_l^{(0)})(E_n^{(0)} - E_k^{(0)})} - \frac{H'_{nn}H'_{ln}}{(E_n^{(0)} - E_l^{(0)})^2}\right]|\psi_l^{(0)}\rangle - \frac{1}{2}\sum_{k\neq n}\frac{|H'_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})^2}|\psi_n^{(0)}\rangle$$

Substitute this into the expression for $E_n^{(3)}$:

$$\begin{aligned} E_n^{(3)} &= \sum_{l\neq n}\left[\sum_{k\neq n}\frac{H'_{lk}H'_{kn}}{(E_n^{(0)} - E_l^{(0)})(E_n^{(0)} - E_k^{(0)})} - \frac{H'_{nn}H'_{ln}}{(E_n^{(0)} - E_l^{(0)})^2}\right]\langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_l^{(0)}\rangle \\ &\quad -\frac{1}{2}\sum_{k\neq n}\frac{|H'_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})^2}\langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_n^{(0)}\rangle \end{aligned}$$

The second term is 0 because:

$$\langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_n^{(0)}\rangle = H'_{nn} - H'_{nn} = 0$$

Dealing with the sandwich in the first term:

$$\begin{aligned} \langle\psi_n^{(0)}|H' - E_n^{(1)}|\psi_l^{(0)}\rangle &= \langle\psi_n^{(0)}|H'|\psi_l^{(0)}\rangle - E_n^{(1)}\langle\psi_n^{(0)}|\psi_l^{(0)}\rangle \\ &= \langle\psi_n^{(0)}|H'|\psi_l^{(0)}\rangle \qquad (\text{since } \langle\psi_n^{(0)}|\psi_l^{(0)}\rangle = 0 \text{ for } l \neq n) \\ &= H'_{nl} \end{aligned}$$

Substituting this result back in

$$\begin{aligned} E_n^{(3)} &= \sum_{l\neq n}\left[\sum_{k\neq n}\frac{H'_{lk}H'_{kn}}{(E_n^{(0)} - E_l^{(0)})(E_n^{(0)} - E_k^{(0)})} - \frac{H'_{nn}H'_{ln}}{(E_n^{(0)} - E_l^{(0)})^2}\right]H'_{nl} \\ &= \sum_{l\neq n}\sum_{k\neq n}\frac{H'_{lk}H'_{kn}H'_{nl}}{(E_n^{(0)} - E_l^{(0)})(E_n^{(0)} - E_k^{(0)})} - H'_{nn}\sum_{l\neq n}\frac{H'_{ln}H'_{nl}}{(E_n^{(0)} - E_l^{(0)})^2} \end{aligned}$$

Note that $H'_{ln}H'_{nl} = |H'_{ln}|^2$. Rename the indices so that $l = k$ and $k = m$.

$$E_n^{(3)} = \sum_{k\neq n}\sum_{m\neq n} \frac{H'_{km}H'_{mn}H'_{nk}}{(E_n^{(0)} - E_k^{(0)})(E_n^{(0)} - E_m^{(0)})} - H'_{nn}\sum_{k\neq n} \frac{|H'_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})^2}$$

Problem 4. Problem 8.6

We want to find the first order energy correction to the ground state energy ($n = 0$) and the first excited state ($n = 1$) of the linear harmonic oscillator perturbed by $H' = \lambda e^{-ax^2}$. The ground state and first excited state are given by

$$\begin{aligned}\psi_0(x) &= \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\alpha^2x^2/2} \\ \psi_1(x) &= \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x e^{-\alpha^2x^2/2}\end{aligned}$$

Where $\alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$ and $\omega = \left(\frac{k}{m}\right)^{1/2}$. We need to calculate $E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle$.

Using the ground state:

$$\begin{aligned}E_0^{(1)} &= \langle\psi_0^{(0)}|H'|\psi_0^{(0)}\rangle \\ &= \langle\psi_0^{(0)}|\lambda e^{-ax^2}|\psi_0^{(0)}\rangle \\ &= \lambda\langle\psi_0^{(0)}|e^{-ax^2}|\psi_0^{(0)}\rangle \\ &= \lambda\int_{-\infty}^{\infty} \psi_0^* e^{-ax^2}\psi_0 dx \\ &= \lambda\Big(\frac{\alpha}{\sqrt{\pi}}\Big)\int_{-\infty}^{\infty} e^{-\alpha^2x^2 - a^2x^2} dx = \lambda\Big(\frac{\alpha}{\sqrt{\pi}}\Big)\int_{-\infty}^{\infty} e^{-(\alpha^2+a)x^2} dx \\ &= \lambda\Big(\frac{\alpha}{\sqrt{\pi}}\Big)\sqrt{\frac{\pi}{\alpha^2+a}} \qquad \Big(\int_{-\infty}^{\infty} e^{-ax^2} = \sqrt{\frac{\pi}{a}}\Big) \\ E_0^{(1)} &= \lambda\frac{\alpha}{\sqrt{\alpha^2+a}}\end{aligned}$$

Now the same for the first excited state

$$\begin{aligned}E_1^{(1)} &= \lambda\langle\psi_1^{(0)}|e^{-ax^2}|\psi_1^{(0)}\rangle \\ &= \lambda\int_{-\infty}^{\infty}\Big(\frac{\alpha}{2\sqrt{\pi}}\Big)(2\alpha x e^{-\alpha^2x^2/2})^2 e^{-ax^2} dx \\ &= \lambda\Big(\frac{\alpha}{2\sqrt{\pi}}\Big)(4\alpha^2)\int_{-\infty}^{\infty} x^2 e^{-(\alpha^2+a)x^2} dx \\ &= \lambda\frac{2\alpha^3}{\sqrt{\pi}}\frac{1}{2(\alpha^2+a)}\sqrt{\frac{\pi}{\alpha^2+a}} \qquad \Big(\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}\Big) \\ E_1^{(1)} &= \lambda\frac{\alpha^3}{(\alpha^2+a)^{3/2}}\end{aligned}$$

Problem 5. Problem 8.13

The trial function is

$$\phi_0(x) = \begin{cases}(c^2 - x^2)^2 & |x| < c \\ 0 & |x| \geq c\end{cases}$$

The Hamiltonian of the linear harmonic oscillator is

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2$$

First we compute the energy functional as a function of the parameter c and then minimize it. $E[\phi] = E(c)$:

$$E(c) = \frac{\int \phi^* H \phi dx}{\int \phi^* \phi dx}$$

Doing the denominator:

$$\begin{aligned}
\int_{-\infty}^{\infty} \phi^* \phi dx &= \int_{-c}^{c} (c^2 - x^2)^4 dx \\
&= \int_{-c}^{c} c^8 + 4c^6x^2 + 6c^4x^4 + 4c^2x^6 + x^8 dx \\
&= c^8 x + \frac{4}{3}c^6x^3 + \frac{6}{5}c^4x^5 + \frac{4}{7}c^2x^7 + \frac{1}{9}x^9 \Big|_{-c}^{c} \\
&= c^8(2c) + \frac{4}{3}c^6(2c^3) + \frac{6}{5}c^4(2c^5) + \frac{4}{7}c^2(2c^7) + \frac{1}{9}(2c^9) \\
&= \Big(2 + \frac{8}{3} + \frac{12}{5} + \frac{8}{7} + \frac{2}{9}\Big)c^9 \\
&= \frac{2656}{315}c^9
\end{aligned}$$

Now the numerator:

$$\int_{-\infty}^{\infty} \phi^* H \phi dx = \int_{-c}^{c} (c^2 - x^2)^2 \Big(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(c^2 - x^2)^2 + \frac{1}{2}m\omega^2 x^2 (c^2 - x^2)^2 \Big) dx$$

$$\begin{aligned}
\frac{d}{dx}(c^2 - x^2)^2 &= -4x(c^2 - x^2) \\
\frac{d^2}{dx^2}(c^2 - x^2)^2 &= -4(c^2 - 3x^2)
\end{aligned}$$

$$\begin{aligned}
\int_{-\infty}^{\infty} \phi^* H \phi dx &= \int_{-c}^{c} (c^2 - x^2)^2 \Big(-\frac{\hbar^2}{2m}(-4(c^2 - 3x^2)) + \frac{1}{2}m\omega^2 x^2 (c^2 - x^2)^4 \Big) dx \\
&= \int_{-c}^{c} \frac{4\hbar^2}{2m}(c^2 - x^2)^2(c^2 - 3x^2) dx + \frac{1}{2}m\omega^2 \int_{-c}^{c} x^2 (c^2 - x^2)^4 dx \\
&= \frac{4\hbar^2}{2m}\Big(c^6 x - \frac{5c^4x^3}{3} + \frac{7c^2x^5}{5} - \frac{3x^7}{7}\Big)_{-c}^{c} + \frac{1}{2}m\omega^2 \Big(\frac{c^8x^3}{3} - \frac{4c^6x^5}{5} + \frac{6c^4x^7}{7} - \frac{4c^2x^9}{9} + \frac{x^{11}}{11}\Big)_{-c}^{c} \\
&= \frac{4\hbar^2 c^7}{2m}\Big(2 - \frac{10}{3} + \frac{14}{5} - \frac{6}{7}\Big) + \frac{1}{2}m\omega^2 c^{11}\Big(\frac{2}{3} - \frac{8}{3} + \frac{12}{7} - \frac{8}{9} + \frac{2}{11}\Big) \\
&= \frac{128\hbar^2}{105m}c^7 + \frac{128}{3465}m\omega^2 c^{11}
\end{aligned}$$

Back into the functional:

$$\begin{aligned}
E(c) &= \Big(\frac{2656}{315}c^9\Big)^{-1}\Big(\frac{128\hbar^2}{105m}c^7 + \frac{128}{3465}m\omega^2 c^{11}\Big) \\
&= \frac{315}{2656}\Big(\frac{128\hbar^2}{105mc^2} + \frac{128}{3465}m\omega^2 c^2\Big) \\
&= \frac{40320}{2656}\Big(\frac{\hbar^2}{105mc^2} + \frac{m\omega^2c^2}{3465}\Big) \\
&= \frac{40320}{2656}\Big(\frac{3465\hbar^2 + 105m^2\omega^2c^4}{363825mc^2}\Big)
\end{aligned}$$

Now to minimize it

$$\begin{aligned}
0 = \frac{dE}{dc} &= -\frac{40320}{2656(363825mc^2)^2}(3465\hbar^2 + 105m^2\omega^2c^4) + \frac{40320}{2656(363825mc^2)}(4c^3(105m^2\omega^2)) \\
&= -\frac{(1.1\times 10^{-10})(3465\hbar^2 + 105m^2\omega^2c^4)}{m^2c^4} + (4.2\times 10^{-5})(4c(105m\omega^2)) \\
&=
\end{aligned}$$

Out of time.

Problem 6. Problem 8.12

Todo.