SQ13

Consider an 1D harmonic oscillator with potential energy :

$$U(x) = \frac{1}{2} k (1+\epsilon) x^2$$

where $\epsilon << 1$,

Therefore , the term $\frac{1}{2} k \epsilon x^2$ can be treated as a perturbation.

The Hamiltonian is $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}k(1+\epsilon)x^2$.

Solve it exactly:

$$E_n = (n+\tfrac{1}{2})\hbar\sqrt{\frac{k(1+\epsilon)}{m}}$$

(Remember the angular fregency ω is equal $\sqrt{\frac{k}{m}}$ for unperturbed case , here we replace k by $k(1+\epsilon)$)

a. Expand the exact eigenvalues in power series of ϵ,

$$E_n = (n+\tfrac{1}{2})\hbar\omega \sqrt{1+\epsilon}$$

$$= (n+\tfrac{1}{2})\hbar\omega \left(1 + \tfrac{1}{2}\epsilon - \tfrac{1}{8}\epsilon^2 + \cdots\right)$$

See appendix for the Taylor series .

Since $(n+\frac{1}{2})\hbar\omega$ is the unperturbed eigenenergies , we denoted them as :

$$E_n^{(0)} = (n+\tfrac{1}{2})\hbar\omega$$

$$\therefore \quad E_n = E_n^{(0)}\left(1+\tfrac{1}{2}\epsilon - \tfrac{1}{8}\epsilon^2 + \cdots\right) //$$

Solve it by perturbation theory :

b. The perturbated hamiltonian can be reperated as :

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

where $\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$ is the unperturbed term.

$\hat{H}' = \frac{1}{2}k\epsilon x^2$ is the perturbation term.

$\therefore$ The first order perturbation in energy is :

$$E_n^{(1)} = \int \psi_n^{*(0)} \hat{H}' \psi_n^{(0)} \, d\tau$$

b. (cont.)

Recall those you have learned in PHYS 3021,

$$\psi_n^{(0)}(x) = A_n \, H_n(\sqrt{a}x)\, e^{-\frac{1}{2}ax^2},$$

where $A_n = \frac{1}{\sqrt{2^n n!}}\left(\frac{a}{\pi}\right)^{\frac{1}{4}}$ and $a = \frac{m\omega}{\hbar}$.

and $H_n(y)$ is called the Hermite polynomial.

So, $$E_n^{(1)} = \int_{-\infty}^{\infty}\left[A_n H_n(\sqrt{a}x)\, e^{-\frac{1}{2}ax^2}\right]\left[\frac{1}{2}k\epsilon x^2\right]\left[A_n H_n(\sqrt{a}x)\, e^{-\frac{1}{2}ax^2}\right]dx \quad \cdots (1)$$

Again, recall there is a recursive relation in the Hermite polynomial:
(at least you have proved it to be satisfied for the lowest three eigenstate in HW4 of PHYS3021 (Q4.4 c))

$$a^{\frac{1}{2}}x\, H_n(\sqrt{a}x) = n\, H_{n-1}(\sqrt{a}x) + \frac{1}{2}H_{n+1}(\sqrt{a}x) \quad \cdots (2)$$

In words, a "x" will bring H_n to H_{n+1} or H_{n-1}, i.e., step 1 up or step 1 down. So, "x^2" will bring H_n by 2 steps up, 2 steps down, or keep it as H_n.

Apply the relation (2) to formula (1),

$$E_n^{(1)} = \frac{1}{2}k\epsilon A_n^2\int_{-\infty}^{\infty}\left[x\, H_n(\sqrt{a}x)\right]\left[x\, H_n(\sqrt{a}x)\right] e^{-\frac{1}{2}ax^2} e^{-\frac{1}{2}ax^2}\, dx$$

$$= \frac{1}{2}k\epsilon A_n^2\int_{-\infty}^{\infty}\frac{1}{a}\underline{\left[n\, H_{n-1}(\sqrt{a}x) + \frac{1}{2}H_{n+1}(\sqrt{a}x)\right]^2}\, e^{-\frac{1}{2}ax^2} e^{-\frac{1}{2}ax^2}\, dx$$

Expanding the underlined square will give 4 terms, but the cross-terms depending on $H_{n-1}(\sqrt{a}x)\,H_{n+1}(\sqrt{a}x)$ will vanish (orthogonality).

$$\therefore\ E_n^{(1)} = \frac{1}{2}k\epsilon A_n^2\,\frac{1}{a}\int_{-\infty}^{\infty}\left[n^2 H_{n-1}^2(\sqrt{a}x) + \frac{1}{4}H_{n+1}^2(\sqrt{a}x)\right] e^{-\frac{1}{2}ax^2} e^{-\frac{1}{2}ax^2}\, dx$$

$$= \frac{1}{2}k\epsilon A_n^2\,\frac{1}{a}\int_{-\infty}^{\infty}\left(n^2\frac{1}{A_{n-1}^2}(\psi_{n-1}(x))^2 + \frac{1}{4}\frac{1}{A_{n+1}^2}(\psi_{n+1}(x))^2\right)dx$$

b. (cont.)

By orthonormal properties,

$$E_n^{(1)} = \frac{1}{2}k\epsilon A_n^2 \frac{1}{a} \left(n^2 \frac{1}{A_{n-1}^2} + \frac{1}{4}\frac{1}{A_{n+1}^2} \right)$$

$$= \frac{1}{2}k\epsilon \frac{1}{a} \left(n^2 \frac{A_n^2}{A_{n-1}^2} + \frac{1}{4}\frac{A_n^2}{A_{n+1}^2} \right)$$

put $A_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{a}{\pi}\right)^{\frac{1}{4}}$,

$$E_n^{(1)} = \frac{1}{2}k\epsilon \frac{1}{a} \left(n^2 \frac{2^{n-1}(n-1)!}{2^n n!} + \frac{1}{4} \frac{2^{n+1}(n+1)!}{2^n n!} \right)$$

$$= \frac{1}{2}k\epsilon \frac{1}{a} \left(\frac{n}{2} + \frac{n+1}{2} \right)$$

$$= \frac{1}{2}\left(n+\frac{1}{2}\right) k\epsilon \frac{1}{a}$$

$$= \frac{1}{2}\left(n+\frac{1}{2}\right) \hbar\omega \epsilon \qquad \left(a = \frac{m\omega}{\hbar}, \quad k = m\omega^2 \right)$$

$$= \frac{1}{2} E_n^{(0)} \epsilon,$$

$\therefore$ This matches with the 1st order expansion of the exact solution in a).

c. 2nd order perturbation of Ground State:

$$E_n^{(2)} = \sum_{i \neq n} \frac{|\langle \psi_i^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_i^{(0)}}$$

put $n=0$,

$$\langle \psi_i^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle = \int_{-\infty}^{\infty} \psi_i^{(0)}(x)^* \frac{1}{2}k\epsilon x^2 \psi_0^{(0)}(x)\, dx$$

$$= \int_{-\infty}^{\infty} \frac{1}{2}k\epsilon \left(A_i H_i(\sqrt{a}x) e^{-\frac{1}{2}ax^2} \right) x^2 \left(A_0 H_0(\sqrt{a}x) e^{-\frac{1}{2}ax^2} \right) dx$$

By the recursive relation (2) in b),

$$H_i(\sqrt{a}x)\, x = a^{-\frac{1}{2}} \left(i H_{i-1}(\sqrt{a}x) + \frac{1}{2} H_{i+1}(\sqrt{a}x) \right),$$

and $x H_0(\sqrt{a}x) = \frac{1}{2} a^{-\frac{1}{2}} H_1(\sqrt{a}x)$,

c) cont.

$\therefore \quad \langle \psi_i^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle = \int_{-\infty}^{\infty} \frac{1}{2} k\epsilon \left(A_i a^{-\frac{1}{2}}\right) \left(i\, H_{i-1}(\sqrt{a}x) + \frac{1}{2} H_{i+1}(\sqrt{a}x)\right) e^{-\frac{1}{2}ax^2}$
$\frac{1}{2}\left(A_0 a^{-\frac{1}{2}}\right)\left(H_1(\sqrt{a}x)\right) e^{-\frac{1}{2}ax^2}\, dx$

The integral will be non-zero only if :

$i = 2$ or $i = 0$ (this is rejected since $i \neq 0$)

For $i = 2$,

$$\langle \psi_2^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle = \int_{-\infty}^{\infty} \frac{1}{2} k\epsilon \frac{1}{a} (A_2)\left(2 H_1(\sqrt{a}x)\, e^{-\frac{1}{2}ax^2}\right) \frac{1}{2}(A_0)\left(H_1(\sqrt{a}x)\, e^{-\frac{1}{2}ax^2}\right) dx$$

$$= \frac{1}{2} k\epsilon \frac{1}{a} \frac{A_0 A_2}{A_1^2} \int_{-\infty}^{\infty} (\psi_1(x))^2\, dx$$

$$= k\epsilon \frac{1}{a} \frac{A_0 A_2}{A_1^2}$$

$$= \frac{1}{2\sqrt{2}} \frac{k\epsilon}{a}$$

For $i = 0$, (no need to compute for this problem)

$$\langle \psi_0^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle = \int_{-\infty}^{\infty} \frac{1}{2} k\epsilon \frac{1}{a} \left(A_0 \frac{1}{2} H_1(\sqrt{a}x)\right)\left(\frac{1}{2} A_0 H_1(\sqrt{a}x)\right) e^{-\frac{1}{2}ax^2} e^{-\frac{1}{2}ax^2}\, dx$$

$$= \frac{1}{2} k\epsilon \frac{1}{a} \frac{A_0^2}{A_1^2} \frac{1}{4} \int_{-\infty}^{\infty} |\psi_1(x)|^2\, dx$$

$$= \frac{1}{4a} k\epsilon$$

Put the values of the inner products to $E_0^{(2)}$,

$$E_0^{(2)} = \frac{|\langle \psi_2^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle|^2}{E_0^{(0)} - E_2^{(0)}}$$

$$= \left(\frac{1}{2\sqrt{2}} \frac{k\epsilon}{a}\right)^2 \frac{1}{\frac{1}{2}\hbar\omega - \frac{5}{2}\hbar\omega}$$

$$= -\frac{1}{16} \hbar\omega \epsilon^2$$

$$= E_0^{(0)} \left(-\frac{1}{8}\epsilon^2\right)$$

$\therefore$ The ground state energy up to 2nd order is

$$E_0 \approx E_0^{(0)} + E_0^{(1)} + E_0^{(2)} = E_0^{(0)} \left(1 + \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2\right)$$

d) The result matches with that we obtained in part a).

e) 1st order correction to the Ground state wavefunction :

$$\psi_0^{(1)}(x) = \sum_{i \neq 0} \frac{\langle \psi_i^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle}{E_0^{(0)} - E_i^{(0)}} \psi_i^{(0)}(x)$$

From c), only $i=2$ is left,

$$\psi_0^{(1)}(x) = \frac{\langle \psi_2^{(0)} | \hat{H}' | \psi_0^{(0)} \rangle}{E_0^{(0)} - E_2^{(0)}} \psi_2^{(0)}(x)$$

$$= \frac{\left(\frac{1}{2\sqrt{2}} \frac{k\epsilon}{a} \right)}{-2\hbar\omega} \psi_2^{(0)}(x)$$

$$= -\frac{\epsilon}{4\sqrt{2}} \psi_2^{(0)}(x)$$

$\therefore$ Up to 1st order in ϵ,

$$\psi_0(x) \simeq \psi_0^{(0)}(x) + \psi_0^{(1)}(x)$$

$$\simeq \psi_0^{(0)}(x) - \frac{\epsilon}{4\sqrt{2}} \psi_2^{(0)}(x) \,//$$

Some remarks :

① The wavefunction $\psi_0(x)$ is not normalised.

② The coeff. of $\psi_2^{(0)}(x)$, $-\frac{\epsilon}{4\sqrt{2}}$, is much less than the coeff. of $\psi_0^{(0)}(x)$, 1.

Therefore, it is just a <u>perturbation</u> on the unperturbed ground state $\psi_0^{(0)}(x)$.

SQ14

We use the perturbation theory to treat the hydrogen atom, and the Hamiltonian is divided into two parts: a solvable part H_0 and a perturbation part H', i.e.

$$H = H_0 + H',$$

where

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r},$$

$$H' = -\frac{p^4}{8m^3c^2} = -\frac{\hbar^4}{8m^3c^2}\nabla^4.$$

(a) Applying the 1st order perturbation theory, the correction to the hydrogen atom energy is:

$$E_n^{(1)} = \int \psi_{nlm_l}^{*(0)}(r,\theta,\phi)H'\psi_{nlm_l}^{(0)}(r,\theta,\phi)d\tau$$

$$= \int \psi_{nlm_l}^{*(0)}(r,\theta,\phi)(-\frac{\hbar^4}{8m^3c^2}\nabla^4)\psi_{nlm_l}^{(0)}(r,\theta,\phi)d\tau.$$

(b) Firstly we would like to find a relation between $E_n^{(1)}$ and $\langle\left(H_0 - U(r)\right)^2\rangle$, where $U(r) = -e^2/(4\pi\epsilon_0 r)$.

$$H_0 - U(r) = -\frac{\hbar^2}{2m}\nabla^2,$$

$$H' = -\frac{\hbar^4}{8m^3c^2}\nabla^4 = -\frac{1}{2mc^2}\left(-\frac{\hbar^2}{2m}\nabla^2\right)^2 = -\frac{1}{2mc^2}\left(H_0 - U(r)\right)^2.$$

Therefore their expectation values should also satisfy

$$E_n^{(1)} = \langle H'\rangle = -\frac{1}{2mc^2}\langle\left(H_0 - U(r)\right)^2\rangle.$$

We further write $E_n^{(1)}$ as

$$E_n^{(1)} = -\frac{1}{2mc^2}\langle\left(E_n^{(0)} - U(r)\right)^2\rangle$$

$$= -\frac{1}{2mc^2}\left[\left(E_n^{(0)}\right)^2 - 2E_n^{(0)}\langle U(r)\rangle + \langle U^2(r)\rangle\right]$$

$$= -\frac{1}{2mc^2}\left[\left(E_n^{(0)}\right)^2 - 2E_n^{(0)}\left(\frac{e^2}{4\pi\epsilon_0}\right)\langle\frac{1}{r}\rangle + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\langle\frac{1}{r^2}\rangle\right].$$

The involved integrals are given by

$$\langle\frac{1}{r}\rangle_{nlm_l} = \int \psi_{nlm_l}^{*(0)}(r,\theta,\phi)\frac{1}{r}\,\psi_{nlm_l}^{(0)}(r,\theta,\phi)d\tau = \frac{1}{n^2 a_0},$$

$$\langle\frac{1}{r^2}\rangle_{nlm_l} = \int \psi_{nlm_l}^{*(0)}(r,\theta,\phi)\frac{1}{r^2}\psi_{nlm_l}^{(0)}(r,\theta,\phi)d\tau = \frac{1}{(l+1/2)n^3 a_0^2},$$

where $a_0 = 4\pi\epsilon_0\hbar^2/(me^2)$ is the Bohr radius. And the original Hydrogen atom energy is given by

$$E_n^{(0)} = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2 n^2} = -\frac{e^2}{8\pi\epsilon_0 a_0 n^2}.$$

Then we have

$$E_n^{(1)} = -\frac{1}{2mc^2}\left[\left(E_n^{(0)}\right)^2 - 2E_n^{(0)}\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{n^2 a_0} + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{1}{(l+1/2)n^3 a_0^2}\right]$$

$$= E_n^{(0)}\frac{\alpha^2}{n^2}\left[\frac{n}{l+1/2} - \frac{3}{4}\right],$$

where $\alpha = e^2/(4\pi\epsilon_0\hbar c) \simeq 1/137$ is the fine structure constant. We see that the magnitude of the correction term is governed by α^2, which is about $(1/137)^2$ of the unperturbed energy $E_n^{(0)}$.