Phys 661 HW 1 Solutions

Problem 1 – Juehang Qin

PHYS 661 HW1 JUEHANG QIN

1. a)

$$H_0 \psi^{(1)}_{100} + V \psi^{(0)}_{100} = E^{(0)}_{100} \psi^{(1)}_{100} + E^{(1)}_{100} \psi^{(0)}_{100}$$

Let us first compute $E^{(1)}_{100}$.

$$V = Eze = -Eer\cos\theta$$

$$E^{(1)}_{100} = Ee \langle 100 | r\cos\theta | 100 \rangle$$

$$= \frac{Ee}{\pi a_0^3} \int_0^\infty \int_0^{2\pi} \int_0^\pi r^3 \sin\theta \cos\theta \, e^{-2r/a_0} \, d\theta \, d\varphi \, dr = 0 \text{ (from } \theta \text{ integral).}$$

$$\therefore H_0 \psi^{(1)}_{100} - \underbrace{Ee}_{V_0} r\cos\theta \, \psi^{(0)}_{100} = E^{(0)}_{100} \psi^{(1)}_{100}$$

$E^{(0)}_{100} = \varepsilon_{gs}$.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} - \varepsilon_{g.s.} \right) \psi^{(1)}_{100} = V_0 r\cos\theta \, \psi^{(0)}_{100}$$

$\psi^{(0)}_{100}$ has no angular dependence.

~~$\therefore \psi^{(1)}_{100}$ only depends on θ.~~

~~$\psi^{(1)}_{100} = R(r)\,\Theta(\theta)$~~

If we consider $|\psi^{(1)}_{100}\rangle = \sum_{k \neq 100} \frac{\langle k^{(0)} | V | 100 \rangle}{E^{(0)}_{100} - E^{(0)}_k} |k^{(0)}\rangle$

we can note that $V|100\rangle$ only has $Y_1^0(\theta,\varphi)$ as the spherical harmonic term. Due to orthonormality of spherical harmonics, we can surmise that all $|k^{(0)}\rangle$ that appear as non-zero will also only have $Y_0^1(\theta,\varphi)$ angular dependence.

$$\therefore \psi^{(1)}_{100}(r,\theta,\varphi) = R(r) \cos(\theta)$$

We can thus factor out the $\cos\theta$ term.

$$\left(-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right) - \frac{e^2}{r} - \mathcal{E}_{g.s.}\right)\overset{R}{\cancel{\psi^{(1)}_{corp}}} = \mp V_0 r \mathcal{N} e^{-r/a_0} \qquad \mathcal{N} = \frac{1}{\sqrt{\pi}\, a_0^{3/2}}$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)\right) - \frac{e^2 R}{r} - \mathcal{E}_{gs} R = \mp V_0 r \mathcal{N} e^{-r/a_0}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\left(2r\frac{\partial R}{\partial r} + r^2\frac{\partial^2 R}{\partial r^2}\right)\right) - \frac{e^2 R}{r} - \mathcal{E}_{gs} R = \mp V_0 r \mathcal{N} e^{-r/a_0}$$

$$\Rightarrow -\frac{\hbar^2}{2m_e}\left(\frac{2R'}{r} + R''\right) + \left(\frac{e^2}{2a_0} - \frac{e^2}{r}\right)R \pm V_0 \mathcal{N} r e^{-r/a_0} = 0$$

~~Let $R = \sum_{i>0}^{1} A_i r^i e^{-r/a_0}$~~

~~$i \geq 3$ terms cannot exist, as there is no way to eliminate the $r^k e^{-r/a_0}$ term that results~~ if $k > 2$

In natural units: $\hbar = 1$

$$\frac{R'}{m_e r} + \frac{R''}{2m_e} + \left(\frac{e^2}{r} - \frac{e^2}{2a_0}\right)R \mp V_0 \mathcal{N} r e^{-r/a_0} = 0$$

$$a_0 = \frac{1}{m_e e^2} \Rightarrow m_e = \frac{1}{a_0 e^2}$$

$$\frac{R''}{2} + \frac{R'}{r} + \left(\frac{1}{a_0 r} - \frac{1}{2a_0^2}\right)R \mp \frac{E}{e a_0^{5/2}\sqrt{\pi}} r e^{-r/a_0} = 0$$

$R = (\pi a_0^3)^{-1/2} \frac{E}{e} (a_0 r + \frac{1}{2} r^2) e^{-r/a_0}$

→ honestly, I had to look it up.
That diff. eq was impossible to solve without guessing at the form!

$\psi^{(1)}_{100}(r,\theta,\varphi) = (\pi a_0^3)^{-1/2} \frac{E}{e} (a_0 r + \frac{1}{2} r^2) e^{-r/a_0} \cos\theta$

b) $\langle \vec{P} \rangle = \langle \psi^{(1)}_{100} + \psi^{(0)}_{100} | -e\vec{r} | \psi^{(1)}_{100} + \psi^{(0)}_{100} \rangle$

~~We know the angular dependence is $\cos\theta$. Thus, we can integrate in cylindrical coords.~~

$$\tilde{\psi} = \psi^{(0)}_{100} + \psi^{(1)}_{100} = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} + \frac{1}{\sqrt{\pi} a_0^{3/2}} \frac{E}{e}(a_0 r + \frac{r^2}{2}) e^{-r/a_0} \cos\theta$$

$$= \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \left(1 + \frac{E}{e}(a_0 r + \frac{r^2}{2}) \cos\theta\right)$$

We know that the dip. moment is z-oriented.
$\therefore \vec{p} = -e\hat{z}\, r\cos\theta$

$$-e\hat{z} \langle \tilde{\psi} | r\cos\theta | \tilde{\psi} \rangle = -e\hat{z} \int_0^\infty \int_0^{2\pi} \int_0^\pi \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}} \left(1 + \frac{E}{e}(a_0 r + \frac{r^2}{2})\cos\theta\right)^2 r^3 \cos\theta \sin\theta \, d\theta\, d\varphi\, dr$$

this term disappears.

$$\approx \frac{2e\hat{z}}{\pi a_0^3} \int_0^\infty \int_0^{2\pi} \int_0^\pi e^{-\frac{2r}{a_0}} \frac{E}{e} (a_0 r + \frac{r^2}{2}) \cos^2\theta \sin\theta \, r^3 \, d\theta\, d\varphi\, dr$$

E^2 terms dropped.

$$= \frac{8e\hat{z}E}{3a_0^3 e} \int_0^\infty e^{-2r/a_0} (a_0 + \frac{r}{2}) r^4 \, dr$$

$$= \frac{8e\hat{z}E}{3a_0^3 e} \left(\frac{27 a_0^6}{16}\right) = \frac{9E\hat{z} a_0^3}{2}$$ (units are correct.)

c) $\vec{P} = \frac{9}{2} a_0^3 \vec{E}$ $\quad \alpha = \frac{9}{2} a_0^3$ this is a lower limit, due to neglecting E^2 term.

For upper limit, we observe:

$$E_{n00} - E_{100} \geq E_{200} - E_{100} = \frac{3}{8}\frac{e^2}{a_0}$$

$\cancel{E(x)}$

$$\Delta E = -\frac{1}{2}\alpha|\vec{E}|^2$$

$$\alpha \leq 2e^2 \, \frac{8}{3} \, \cancel{\frac{e^2}{a_0}} \, \frac{a_0^{\cancel{2}}}{e^2} \sum_{n>\phi} |\langle 100| \, r\cos\theta \, |n10\rangle|^2 \; \cancel{\leq \frac{16a_0}{3}}$$

$$= \frac{16a_0^{3}}{3} \sum_{n>1} \langle 100| r\cos\theta \underbrace{|n10\rangle\langle n10|}_{\mathbb{1}} r\cos\theta|100\rangle = \frac{16a_0^{3}}{3} \sum_{n>1} \langle 100|(r\cos\theta)^2|100\rangle = \frac{16a_0^3}{3}$$

$$\therefore \frac{9a_0^3}{2} \leq \alpha \leq \frac{16}{3}a_0^3$$

Problem 2 – Yicheng Feng

2. a) The first order correction of energy is $E_n^{(1)} = \langle n|V|n\rangle$

$x = \sqrt{\frac{\hbar}{2m\omega}}(a+a^+)$ ($\because H_0$ is the Hamiltonian of 1-D harmonic oscillator)

$$\therefore E_n^{(1)} = \langle n|V|n\rangle = \langle n|\lambda x^4|n\rangle = \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|(a+a^+)^4|n\rangle$$

$$= \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|(a^2+a^{+2}+aa^+ + a^+a)^2|n\rangle \qquad (a^+a = N \quad [a,a^+]=1 \Rightarrow aa^+ = N+1$$

$$= \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|(a^2+a^{+2}+2N+1)^2|n\rangle = \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|\Big(a^4+a^{+4}+\underbrace{(2N+1)^2}+a^2(2N+1)+(2N+1)a^2$$
$$+a^{+2}(2N+1)+(2N+1)a^{+2}+\underbrace{a^2a^{+2}}+\underbrace{a^{+2}a^2}\Big)|n\rangle$$

$$= \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \langle n|(\cancel{a^4+a^{+4}+}(2N+1)^2 + a^2a^{+2}+a^{+2}a^2)|n\rangle$$

$$= \lambda\left(\frac{\hbar}{2m\omega}\right)^2 \left((2n+1)^2 + (\sqrt{n+1}\sqrt{n+2})^2 + (\sqrt{n}\sqrt{n-1})^2\right)$$

$$\therefore E_0^{(1)} = \lambda\left(\frac{\hbar}{2m\omega}\right)^2(1+2+0) = 3\lambda\left(\frac{\hbar}{2m\omega}\right)^2$$

$$E_1^{(1)} = \lambda\left(\frac{\hbar}{2m\omega}\right)^2(9+6+0) = 15\lambda\left(\frac{\hbar}{2m\omega}\right)^2$$

$$E_2^{(1)} = \lambda\left(\frac{\hbar}{2m\omega}\right)^2(25+12+2) = 39\lambda\left(\frac{\hbar}{2m\omega}\right)^2$$

b) Normalize $\psi(x)$: $\int_{-\infty}^{+\infty} dx\, \psi^*(x)\psi(x) = 1$

$\therefore 1 = |A|^2\int_{-\infty}^{+\infty} dx\, e^{-ax^2} = |A|^2\sqrt{\frac{\pi}{a}}$ $\quad \therefore A = \left(\frac{a}{\pi}\right)^{\frac{1}{4}}$ $\quad \therefore \psi(x) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}ax^2}$

$$\langle\psi|H|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \sqrt{\frac{a}{\pi}}\, e^{-\frac{1}{2}ax^2}\left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2x^2 + \lambda x^4\right)e^{-\frac{1}{2}ax^2}$$

$$= \int_{-\infty}^{+\infty} dx\, \sqrt{\frac{a}{\pi}}\, e^{-\frac{1}{2}ax^2}\left[-\frac{\hbar^2}{2m}(-a+a^2x^2) + \frac{1}{2}m\omega^2x^2 + \lambda x^4\right]e^{-\frac{1}{2}ax^2}$$

$\xi = \sqrt{a}x$

$$= \frac{a\hbar^2}{2m} + \frac{1}{\sqrt{\pi}}\left(\frac{m\omega^2}{2a} - \frac{\hbar^2 a}{2m}\right)\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2}\xi^2 + \frac{1}{\sqrt{\pi}}\frac{\lambda}{a^2}\int_{-\infty}^{+\infty} d\xi\, e^{-\xi^2}\xi^4$$

$$= \frac{a\hbar^2}{2m} + \frac{1}{\sqrt{\pi}}\left(\frac{m\omega^2}{2a} - \frac{\hbar^2 a}{2m}\right)\frac{\sqrt{\pi}}{2} + \frac{1}{\sqrt{\pi}}\frac{\lambda}{a^2}\frac{3}{4}\sqrt{\pi}$$

$$= \frac{a\hbar^2}{4m} + \frac{m\omega^2}{4a} + \frac{3\lambda}{4a^2}$$

$\langle\psi|H|\psi\rangle$ is a function of a.

$$\frac{\partial\langle\psi|H|\psi\rangle}{\partial a} = \frac{\hbar^2}{4m} - \frac{m\omega^2}{4a^2} - \frac{3\lambda}{2a^3} = 0$$

$\because \lambda$ is small $\therefore$ We minimize the first two terms of $\langle\psi|H|\psi\rangle$

$$\Rightarrow \frac{\hbar^2}{4m} - \frac{m\omega^2}{4a^2} = 0. \quad \therefore a = \frac{m\omega}{\hbar}$$

$\therefore$ Approximately, the ground state energy is about $\left(\frac{1}{2}\hbar\omega + \frac{3\hbar^2}{4m^2\omega^2}\lambda\right)$

c) let $p=0$ $H=E$, the Hamiltonian will become: $E=\frac{1}{2}m\omega^2x^2+\lambda x^4$

$\therefore x^2=-\frac{m\omega^2}{4\lambda}\pm\frac{1}{2\lambda}\sqrt{\frac{m^2\omega^4}{4}+4\lambda E}$ $\because x^2\geq 0$ $\therefore x^2=\frac{1}{2\lambda}\sqrt{\frac{m^2\omega^4}{4}+4\lambda E}-\frac{m\omega^2}{4\lambda}$

($\lambda>0$ $E\geq 0$) $\therefore x_1=-\left[\frac{1}{2\lambda}\left(\frac{m^2\omega^4}{4}+4\lambda E\right)^{\frac{1}{2}}-\frac{m\omega^2}{4\lambda}\right]^{\frac{1}{2}}$ $x_2=-x_1$

Now let $p\geq 0$, $H=E$, so $p(x)=\sqrt{2mE-m^2\omega^2x^2-2\lambda m x^4}$

$\therefore \pi(n+\frac{1}{2})\hbar=\int_{x_1}^{x_2}p(x)\,dx=2\int_0^{x_2}\sqrt{2mE-m^2\omega^2x^2-2m\lambda x^4}\,dx$ (*)

From the integral above, we can get the energy eigenvalue.

For the energy eigenstates, we write the Schrödinger equation first:

$-\frac{\hbar^2}{2m}\partial_x^2\psi+\left(\frac{1}{2}m\omega^2x^2+\lambda x^4\right)\psi=E\psi$

Let $\psi=e^{S(x)}$, we can get: $-\frac{\hbar^2}{2m}\left(S''(x)+S'^2(x)\right)+\frac{1}{2}m\omega^2x^2+\lambda x^4=E$

We assume that $S'(x)^2\gg S''(x)$, and then can get:

$\partial_x S\simeq\pm i\sqrt{\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2-\lambda x^4\right)}=\pm ik(x)$

Thus, $\psi_n(x)$ is the linear combination of $e^{i\int^x k(x')dx'}$ and $e^{-i\int^x k(x')dx'}$

where E_n is determined by the formula (*).

evaluate the integral (*)

$x_2^2=\frac{1}{2\lambda}\sqrt{\frac{m^2\omega^4}{4}+4\lambda E}-\frac{m\omega^2}{4\lambda}=\frac{1}{2\lambda}\frac{m\omega^2}{2}\sqrt{1+\frac{16\lambda E}{m^2\omega^4}}-\frac{m\omega^2}{4\lambda}\approx\frac{m\omega^2}{4\lambda}\left(1+\frac{1}{2}\frac{16\lambda E}{m^2\omega^4}\right)-\frac{m\omega^2}{4\lambda}$

$=\frac{2E}{m\omega^2}$ (λ is small enough to make $\frac{16\lambda E}{m^2\omega^4}\ll 1$)

$\therefore x_2\approx\sqrt{\frac{2E}{m\omega^2}}$ which is the same as the result from H_0.

$p(x)=\sqrt{2mE-m^2\omega^2x^2-2m\lambda x^4}=\sqrt{2mE}\sqrt{1-\frac{m\omega^2}{2E}x^2-\frac{\lambda}{E}x^4}$

$=\sqrt{2mE}\sqrt{1-\frac{m\omega^2}{2E}x^2}\sqrt{1-\frac{\frac{\lambda}{E}x^4}{1-\frac{m\omega^2}{2E}x^2}}\approx\sqrt{2mE}\sqrt{1-\frac{m\omega^2}{2E}x^2}\left(1-\frac{1}{2}\frac{\frac{\lambda}{E}x^4}{1-\frac{m\omega^2}{2E}x^2}\right)$

$=\sqrt{2mE}\left(\sqrt{1-\xi^2}-\frac{a\xi^4}{\sqrt{1-\xi^2}}\right)$ $\xi^2=\frac{m\omega^2}{2E}x^2$ $a=\frac{2E\lambda}{m^2\omega^4}$

(use the approximation: λ is small enough.)

$\therefore$ (*): $\pi(n+\frac{1}{2})\hbar=2\int_0^{x_2}\sqrt{2mE}\left(\sqrt{1-\xi^2}-\frac{a\xi^4}{\sqrt{1-\xi^2}}\right)dx=2\sqrt{\frac{2E}{m\omega^2}}\int_0^1\left(\sqrt{1-\xi^2}-\frac{a\xi^4}{\sqrt{1-\xi^2}}\right)d\xi\sqrt{2mE}$

$\overset{\xi=\sin\alpha}{=}\frac{4E}{\omega}\int_0^{\frac{\pi}{2}}\left(\sqrt{1-\sin^2\alpha}-\frac{a\sin^4\alpha}{\sqrt{1-\sin^2\alpha}}\right)d(\sin\alpha)=\frac{4E}{\omega}\int_0^{\frac{\pi}{2}}(\cos^2\alpha-a\sin^4\alpha)\,d\alpha$

$=\frac{4E}{\omega}\left(\frac{\pi}{4}-\frac{3}{16}\pi a\right)$ $\Rightarrow$ $E\left(1-\frac{3\lambda}{2m^2\omega^4}E\right)=(n+\frac{1}{2})\hbar\omega$.

$\therefore$ after some reasonable approximation: ~~$E_n=$~~ keep to the first order of λ:

$E_n=(n+\frac{1}{2})\hbar\omega\left[1+\frac{3\lambda}{2m^2\omega^4}(n+\frac{1}{2})\hbar\omega\right]$

$\therefore k_n(x)=\frac{1}{\hbar}\sqrt{2m\left(E_n-\frac{1}{2}m\omega^2x^2-\lambda x^4\right)}$ $\psi_n(x)=Ae^{i\int_0^x k_n(x')dx'}+Be^{-i\int_0^x k_n(x')dx'}$

energy of the ground state: (keep to first order of λ)

d) in a) $E_0\simeq\frac{1}{2}\hbar\omega+E_0^{(1)}=\frac{1}{2}\hbar\omega+3\left(\frac{\hbar}{2m\omega}\right)^2\lambda$

in b) $E_0\simeq\frac{1}{2}\hbar\omega+\frac{3\hbar^2}{4m^2\omega^2}\lambda$

in c) $E_0\simeq(0+\frac{1}{2})\hbar\omega\left[1+\frac{3\lambda}{2m^2\omega^4}(0+\frac{1}{2})\hbar\omega\right]=\frac{1}{2}\hbar\omega+\frac{3\hbar^2}{8m^2\omega^2}\lambda$

The results in a) b) are the same, but c)'s is different from a) and b)

However, the first order corrections only differ by a factor 2 between those results.

c) is only valid when energy is high, so for ground state, WKB could work ~~badly~~ poorly