PHY 615-2012
Problem Set #8

Problem 1

(i) Eigenstates localized in the left well are

$$\psi_{l,n}(x) = \begin{cases} \sqrt{\frac{4}{L}}\sin\left(\frac{2\pi n x}{L}\right) & -\frac{1}{2} < x < 0 \\ 0 & x > 0 \end{cases}$$

while those localized to the right are.

$$\psi_{r,n}(x) = \begin{cases} 0 & x < 0 \\ \sqrt{\frac{4}{L}}\sin\left(\frac{2\pi n x}{L}\right) & 0 < x < \frac{1}{2} \end{cases}$$

$\psi_{l,n}, \psi_{r,n}$ have the ~~same~~ eigenvalues

$$E_n = \frac{2\pi^2 n^2}{m L^2}.$$

Each state is 2-fold degenerate. The ground state energy is

$$E_0 = \frac{2\pi^2}{m L^2}$$

Denote the degenerate states by $|l0\rangle$ and $|r0\rangle$

(ii) Consider the perturbation

$$H_1 = \begin{cases} V_0 & -a/2 < x < a/2 \\ 0 & \text{otherwise} \end{cases}$$

To calculate the perturbed energy levels need to diagonalize the matrix

$$\begin{bmatrix} \langle \ell 0 | H_1 | \ell 0 \rangle & \langle \ell 0 | H_1 | r0 \rangle \\ \langle r0 | H_1 | \ell 0 \rangle & \langle r0 | H_1 | r0 \rangle \end{bmatrix}$$

Consider

$$\langle \ell 0 | H_1 | r0 \rangle = V_0 \int_{-a/2}^{a/2} dx \, \psi_{\ell 0}^*(x) \psi_{r0}(x)$$

However this integral vanishes, since in

$-a/2 < x < 0$ $\quad \psi_{r0} = 0$

while $\quad 0 < x < a/2 \quad \psi_{\ell 0} = 0$

Thus $\quad \psi_{\ell 0}^*(x) \psi_{r0}(x) = 0$ in $-a/2 \leq x \leq a/2$

Similarly $\quad \langle r0 | H_1 | \ell 0 \rangle = 0$

Thus H_1 is already diagonal in the degenerate subspace.

Eigenvalues of H_1 are

$$E_\ell^{(1)} = V_0 \int_{-a/2}^{0} dx\, \psi_{\ell 0}^*(x)\psi_{\ell 0}(x)$$

$$= \frac{V_0 a}{4} - \frac{V_0 L}{8\pi}\sin\left(\frac{2\pi a}{L}\right) \equiv \bar{E}^{(1)}$$

$$E_r^{(1)} = V_0 \int_{0}^{a/2} dx\, \psi_{r0}^*(x)\psi_{r0}(x)$$

$$= \frac{V_0 a}{2} - \frac{V_0 L}{8\pi}\sin\left(\frac{2\pi a}{L}\right) = \bar{E}^{(1)}$$

Thus degeneracy is not lifted

(iv) For $H_2 = \begin{cases} -V_0 & -\frac{a}{2} \le x \le 0 \\ V_0 & 0 \le x \le a/2 \end{cases}$

We clearly have

$$E_\ell^{(1)} = -\bar{E}^{(1)}$$

$$E_r^{(1)} = \bar{E}^{(1)}$$

Thus new energy levels are

$$\frac{2\pi^2}{ML^2} \pm \bar{E}^{(1)}$$ degeneracy is lifted

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(~~iv~~) For either perturbation there cannot be any degeneracy in the exact solution

Suppose in a 1 dim QM problem there are two states $\psi_1(x)$, $\psi_2(x)$ with the same energy.

Then

$$\frac{d^2\psi_1}{dx^2} + 2m(E - V(x))\psi_1 = 0$$

$$\frac{d^2\psi_2}{dx^2} + 2m(E - V(x))\psi_2 = 0$$

Then the Wronskian W is a constant

$$W = \psi_1 \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_1}{dx}$$

Since this is a constant we may evaluate this at any value of x, eg at ~~x = 0~~ any $x > L/2$. Here $W = 0$

Thus

$$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2}$$

$\Rightarrow$ $\psi_1(x) \propto \psi_2(x)$ $\Rightarrow$ they are not

Problem 2:

There are four states with $n=2$ which are degenerate. Denote these by

$$|1\rangle = |2,1,1\rangle$$
$$|2\rangle = |2,1,-1\rangle$$
$$|3\rangle = |2,1,0\rangle$$
$$|4\rangle = |2,0,0\rangle$$

where the notation is $|n,l,m\rangle$.

The perturbation to the H-atom hamiltonian is

$$H_1 = eEz$$

Clearly

$$\langle nlm|z|nlm\rangle = 0$$

by parity considerations

Now consider

$$\langle nlm|z|nl'm'\rangle$$

Since $[z, L_z] = 0$, the state

$$L_z\left(z|nl'm'\rangle\right) = m'\left(z|nl'm'\right)$$

Since states with different L_z have no overlap

$$\langle n\,l\,m|z|n\,l'\,m'\rangle = A_{l,l'} B_m \delta_{mm'}$$

This means that the nonzero matrix elements for $n=2$ are

$$\langle 3|H_1|4\rangle = \langle 4|H_1|3\rangle^*$$

$$\langle 3|H_1|4\rangle = eE\int dr\, r^2 \sin\theta\, d\theta\, d\phi\; u^*_{210}(r,\theta,\phi)\, r\cos\theta\; u_{200}(r,\theta,\phi)$$

Using

$$u_{210}(r,\theta,\phi) = \left(\frac{1}{32\pi a_0^3}\right)^{1/2} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$$

$$u_{200}(r,\theta,\phi) = \left(\frac{1}{32\pi a_0^3}\right)^{1/2} \left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$$

we get

$$\langle 3|H_1|4\rangle = \frac{2\pi eE}{32\pi a_0^3}\frac{1}{a_0}\int dr\, r^4 \left(2-\frac{r}{a_0}\right) e^{-r/a_0} \int_0^{\pi} d\theta\, \sin\theta\cos^2\theta$$

$$= -\frac{eE}{16 a_0^4}\, 72\, a_0^5 \cdot \frac{2}{3} = -3eEa_0$$

$$\langle 4|H_1|3\rangle = -3eEa_0$$

In usual degenate perturbation theory we need to start with a state

$$|\psi\rangle = \sum_{i=1}^{4} a_i |i\rangle$$

Then the first order perturbation theory leads to the equations

$$\sum_i \left[\langle j|H_1|i\rangle - E^{(1)} \delta_{ij} \right] a_j = 0$$

where $E^{(1)}$ is the correction this gives

$$0 = \begin{pmatrix} -E^{(1)} & 0 & 0 & 0 \\ 0 & -E^{(1)} & 0 & 0 \\ 0 & 0 & -E^{(1)} & -3eEa_0 \\ 0 & 0 & -3eEa_0 & -E^{(1)} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

Thus

$$(E^{(1)})^2 \left((E^{(1)})^2 - (3eEa_0)^2 \right) = 0$$

Thus

$$E^{(1)} = 0, 0, 3eEa_0, -3eEa_0$$

Thus the degeneracy is only partly lifted to this order.

Problem 3:

(i) The unperturbed wavefunctions are plane waves

$$\psi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{L^3}} e^{i\vec{k}\cdot\vec{x}}$$

Since $\psi_{\vec{k}}(\vec{x})$ is periodic we must have

$$\vec{k} = \frac{2\pi \vec{n}}{L}$$

where $\vec{n}$ is an integer valued vector

(ii) Since $V(\vec{x} + a\hat{e}) = V(\vec{x})$

$$\vec{g} = \frac{\vec{m}}{a}$$

where $\vec{m}$ is an integer valued vector.

Clearly this is consistent with periodicity across the box, since

$$e^{2\pi i g_x L} = e^{\frac{2\pi i m_x L}{a}} = e^{2\pi i N m_x} = 1$$

(iii) The matrix element of the perturbation is

$$\langle \vec{k}' | V | \vec{k} \rangle = \sum_{\vec{g}} V(\vec{g}) \frac{1}{L^3} \int d^3x\, e^{i(\vec{k}-\vec{k}'+2\pi\vec{g})\cdot\vec{x}}$$

$$= \sum_{\vec{g}} V(\vec{g})\, \delta(2\pi g - \vec{k}' + \vec{k})$$

$$= V\left(\frac{1}{2\pi}(\vec{k}'-\vec{k})\right) \equiv V(\vec{g}_0).$$

From usual perturbation theory the first order correction to the state $|\vec{k}\rangle$ is

$$\frac{1}{\sqrt{L^3}} \sum_{\vec{k}' \neq \vec{k}} \frac{\langle k'|V|k\rangle}{E_k - E_{k'}} |k'\rangle$$

$$\psi_k^{(1)}(\vec{x}) = \frac{1}{\sqrt{L^3}} \sum_{\vec{g}\neq 0} \frac{V(\vec{g})}{\vec{k}^2 - (\vec{k}+2\pi\vec{g})^2} \cdot \frac{2m}{\hbar^2} e^{i(\vec{k}+2\pi\vec{g})\cdot\vec{x}}$$

$$= \frac{1}{\sqrt{L^3}} \frac{2m}{\hbar^2} \sum_{g\neq 0} \frac{V(\vec{g})\, e^{i(\vec{k}+2\pi\vec{g})\cdot\vec{x}}}{\vec{k}^2 - (\vec{k}+2\pi\vec{g})^2}$$

The first order correction to the energy is

$$E_k^{(1)} = \langle k|V|k\rangle = V(0).$$

The second order correction is

$$\frac{2m}{\hbar^2} \sum_{\vec{g} \neq 0} \frac{|V(\vec{g})|^2}{\vec{k}^2 - (\vec{k}+2\pi\vec{g})^2}$$

This works for generic $\vec{k}$.

(iv) when $\vec{k}^2 = (\vec{k}+2\pi\vec{g})^2$

ie $0 = 4\pi \vec{g}\cdot\vec{k} + 4\pi^2 \vec{g}^2$

This breaks down since the unperturbed states with $\vec{k}$, $\vec{k}+2\pi\vec{g}$ are degenerate

We then need to choose the correct linear combination which diagonalizes. Let this be

$$|\psi\rangle = a|\vec{k}\rangle + b|\vec{k}+2\pi\vec{g}\rangle$$

Then

$$0 = \begin{bmatrix} \langle k|V|k\rangle - E^{(1)} & \langle \vec{k}|V|\vec{k}+2\pi\vec{g}\rangle \\ \langle \vec{k}+2\pi\vec{g}|V|\vec{k}\rangle & \langle k+2\pi\vec{g}|V|k+2\pi\vec{g}\rangle - E^{(1)} \end{bmatrix}$$

ie

$$\det \begin{bmatrix} V_0 - E^{(1)} & V(\vec{g}) \\ V^*(\vec{g}) & V_0 - E^{(1)} \end{bmatrix} = 0$$

$$\Rightarrow \quad (V_0 - E^{(1)})^2 = |V(\vec{g})|^2$$

$$E^{(1)} = V_0 \pm |V(\vec{g})|$$

The wavefns are

$$\psi_\pm = \frac{1}{\sqrt{2L^3}} \left[e^{i\vec{k}\cdot\vec{x}} \pm e^{i(\vec{k}+2\pi\vec{g})\cdot\vec{x}} \right]$$

Problem 34 (18.2.1)

$$H'(t) = -\frac{eEx}{1+(t/\tau)^2}$$

Then

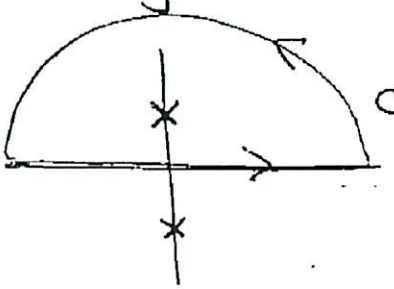
$$d_n(\infty) = -\frac{i}{\hbar}(-eE)\int_{-\infty}^{\infty} dt\, e^{i\omega t n}\frac{\langle n|x|0\rangle}{1+(t/\tau)^2}$$

$$d_1(\infty) = \frac{ieE}{\hbar}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\int_{-\infty}^{\infty}\frac{dt\, e^{i\omega t}}{1+(t/\tau)^2}$$

$$= \frac{ieE}{\hbar}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\tau\int_{-\infty}^{\infty}\frac{d\eta\, e^{i\nu\eta}}{1+\eta^2}\Bigg| \quad (\nu=\omega\tau)$$

For $\nu > 0$ the integral may be evaluated by closing contour in UHP.

$$\int_C \frac{d\eta\, e^{i\nu\eta}}{1+\eta^2} =$$



$$= \frac{2\pi i}{2i}e^{-\nu} = \pi e^{-\omega\tau}$$

Thus

$$d_1(\infty) = \frac{ieE}{\hbar}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\pi\tau e^{-\omega\tau}$$

$$\Rightarrow$$

$$P_{0\to 1} = \frac{e^2E^2\pi^2\tau^2}{2m\omega\hbar}e^{-2\omega\tau}$$

Problem 5 (18.2.3)

For a particle in a box of size L, the ground state energy is

$$E_0 = \frac{\pi^2 \hbar^2}{2mL^2}$$

Thus the average momentum is

$$p = \sqrt{2mE} = \frac{\pi\hbar}{L}$$

Time taken by particle to go across box is

$$T = \frac{Lm}{p} = \frac{mL^2}{\pi\hbar}$$

This is the time scale of problem.

If box is increased to $2L$ in a time $\tau \ll T$, the system remains in ground state of the original box, ie., at time $t=0$ when the change is made

$$\psi(x,0) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right) & -L/2 \le x \le L/2 \\ 0 & L/2 \le x \le L \\ & -L \le x \le -L/2 \end{cases}$$

The ground state wavefn in box of size 2L is

$$\psi'(x) = \sqrt{\frac{1}{L}}\cos\left(\frac{\pi x}{2L}\right) \quad -L \leq x \leq L$$

Thus the overlap is

$$\frac{\sqrt{2}}{L}\int_{-L/2}^{L/2} dx \cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{2L}\right) = \frac{8}{3\pi}$$

Thus $P_{sub} = \left(\frac{8}{3\pi}\right)^2$