Problem Set #1

Problem 1

For an infinite square well:

$$k_n = \frac{n\pi}{a},\ n = 1, 2, ... \tag{1.1}$$

$$E_n^o = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{1.2}$$

$$\Psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi}{a}x\right) \tag{1.3}$$

1 point given for correct wavefunction

(a) Use first-order time-independent perturbation theory to calculate the energy correction. The delta-function potential is:

$$H' = \alpha\delta\left(x - \frac{a}{2}\right) \tag{1.4}$$

1 point given for correct function

Using perturbation theory

$$E_n^{(1)} = \langle H' \rangle \tag{1.5}$$

1 point given for correct expression of first order energy correction

Evaluating this we find:

$$\langle H' \rangle = \int \Psi_n^*(x)\alpha\delta\left(x - \frac{a}{2}\right)\Psi_n(x)dx = \int |\Psi_n(x)|^2\alpha\delta\left(x - \frac{a}{2}\right)dx \tag{1.6}$$

$$\int |\Psi_n(x)|^2\alpha\delta\left(x - \frac{a}{2}\right)dx = \alpha|\Psi_n(\frac{a}{2})|^2 = \alpha \times \left(\frac{2}{a}\right) \sin^2\left(\frac{n\pi}{a}\frac{a}{2}\right) = 2\frac{\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right) \tag{1.7}$$

1 point given for correct answer

Note that this was calculated for any state in the square well. We find that for odd n: $E_n^{(1)} = \frac{2\alpha}{a}$ and for even n: $E_n^{(1)} = 0$

(b) The second-order correction to the ground state energy is:

$$E_1^{(2)} = \sum_{n\neq 1} \frac{|\langle\Psi_n|H'|\Psi_n\rangle|^2}{E_1 - E_n} \tag{1.8}$$

1 point given for correct second order energy correction expression

Since the perturbation is a delta function each term in the summation is the proportional to the overlap of one of the solutions with the ground state wavefunction. However, the solutions of the infinite square well alternate in parity so terms which have the same parity have an overlap of 0.

So the only the terms which have odd n are nonzero. Because of the periodicity of sine, the result for the overlap is the same as $|E_n^{(1)}|^2$.

$$\sum_{n\neq 1} \frac{|\langle \Psi_n|H'|\Psi_1\rangle|^2}{E_1 - E_n} = \sum_{n\neq 1,\ odd} \left(\frac{2\alpha}{a}\right)^2 \frac{1}{E_1 - E_n} \tag{1.9}$$

1 point given for correct calculation of numerator

Now plugging in the result for E_n:

$$\sum_{n\neq 1,\ odd} \left(\frac{2\alpha}{a}\right)^2 \frac{1}{E_1 - E_n} = \left(\frac{2\alpha}{a}\right)^2 \sum_{n\neq 1,\ odd} \frac{1}{1-n^2}\left(\left(\frac{\pi\hbar}{a}\right)^2 \frac{1}{2m}\right)^{-1} = \frac{8m\alpha^2}{\pi^2\hbar^2} \sum_{n\neq 1,\ odd} \frac{1}{1-n^2} \tag{1.10}$$

1 point given for correct substitution of energy in denominator

To evaluate this sum you can perform partial fraction decomposition.

$$\frac{1}{1-n^2} = \frac{A}{1-n} + \frac{B}{1+n} \tag{1.11}$$

$$1 = A(1+n) + B(1-n) = A + An + B - Bn = (A+B) + (A-B)n \tag{1.12}$$

Clearly $A = 1/2$ and $B = 1/2$. This gives:

$$\sum_{n\neq 1,\ odd} \frac{1}{1-n^2} = \frac{1}{2}\sum_{n\neq 1,\ odd} \frac{1}{1-n} + \frac{1}{2}\sum_{n\neq 1,\ odd} \frac{1}{1+n} \tag{1.13}$$

Evaluating the first few terms:

$$\frac{1}{2}\sum_{n\neq 1,\ odd} \frac{1}{1-n} = -\frac{1}{4} - \frac{1}{8} - \frac{1}{12} - \ldots \tag{1.14}$$

$$\frac{1}{2}\sum_{n\neq 1,\ odd} \frac{1}{1+n} = \frac{1}{8} + \frac{1}{12} + \ldots \tag{1.15}$$

Clearly the only term that will not be eliminated between the two sums is -1/4. This gives:

$$E_1^{(2)} = -\frac{1}{4} \times \frac{8m\alpha^2}{\pi^2\hbar^2} = \frac{-2m\alpha^2}{\pi^2\hbar^2} \tag{1.16}$$

1 point given for correct answer

(c) Which correction is larger depends on α,a,and m. Take the ratio of the two corrections:

$$\left|\frac{E_1^{(2)}}{E_1^{(1)}}\right| = \frac{\frac{2m\alpha^2}{\pi^2\hbar^2}}{\frac{2\alpha}{a}} = \frac{ma\alpha}{\pi^2\hbar^2} \tag{1.17}$$

Clearly, if $\alpha < (\pi^2\hbar^2)/(ma)$ then $E_1^{(2)} < E_1^{(1)}$. Perturbation theory says that the expansion parameter must be sufficiently small. Here we find that the expansion parameter α is sufficently small when it meets this condition.

1 point given for correct answer

Problem 2

(a) First write down the Hamiltonian describing this system:

$$H = \begin{bmatrix} E_a & t \\ t & E_b \end{bmatrix} \tag{2.1}$$

1 point given for correct Hamiltonian

Then diagonalize the matrix:

$$\det(H - EI) = (E_a - E)(E_b - E) - t^2 = E^2 - E(E_a + E_b) + (E_a E_b - t^2) \tag{2.2}$$

1 point given for diagonalizing matrix

$$E^2 - E(E_a + E_b) + (E_a E_b - t^2) = E^2 - 2EE_0 + (E_0^2 - t^2) = 0 \tag{2.3}$$

We find:

$$E = E_0 \pm t \tag{2.4}$$

1 point given for correct eigenenergies

(b)

$$\psi = \alpha\psi_a + \beta\psi_b \tag{2.5}$$

For $E = E_0 + t$:

$$\begin{pmatrix} -t & t \\ t & -t \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{2.6}$$

1 point given for correct substitution

$$\alpha = \beta \tag{2.7}$$

$$\psi_1 = \sqrt{\frac{1}{2}}\Big(\psi_a + \psi_b\Big) \tag{2.8}$$

1 point given for corrrect eigenfunction

For $E_2 = E_0 - t$:

$$\begin{pmatrix} t & t \\ t & t \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{2.9}$$

1 point given for correct substitution

$$\alpha = -\beta \tag{2.10}$$

$$\psi_2 = \frac{\psi_a - \psi_b}{\sqrt{2}} \tag{2.11}$$

1 point given for correct eigenfunction

(c)

$$\begin{pmatrix} E_0 + \Delta - E & t \\ t & E_0 - \Delta - E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = H - E \tag{2.12}$$

$$(E_0 + \Delta - E)(E_0 - \Delta - E) - t^2 = 0 \tag{2.13}$$

1 point given for correct characteristic equation

$$E^2 - 2E_0 E + E_0^2 - \Delta^2 - t^2 = 0 \tag{2.14}$$

$$E = \frac{2E_0 + \pm\sqrt{4E_0^2 - 4(E_0^2 - \Delta^2 - t^2)}}{2} = E_0 \pm \sqrt{\Delta^2 + t^2} \tag{2.15}$$

1 point given for correct eigenenergies

For state 1, where $E = E_0 + \sqrt{\Delta^2 + t^2}$:

$$\begin{pmatrix} \Delta - \sqrt{\Delta^2 + t^2} & t \\ t & -\Delta - \sqrt{\Delta^2 + t^2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{2.16}$$

For state 2:

$$\begin{pmatrix} \Delta + \sqrt{\Delta^2 + t^2} & t \\ t & +\Delta - \sqrt{\Delta^2 + t^2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{2.17}$$

2 points given (1 for each correct matrix)

For state 1, performing the matrix multiplication we get a system of 2 equations:

$$(\Delta - \sqrt{\Delta^2 + t^2})\alpha + t\beta = 0 \tag{2.18}$$

$$t\alpha - (\Delta + \sqrt{\Delta^2 + t^2})\beta = 0 \tag{2.19}$$

We solve these and find:

$$\beta = \frac{\Delta + \sqrt{\Delta^2 + t^2}}{t}\alpha \tag{2.20}$$

Likewise for state 2 we get:

$$\alpha = \frac{-t}{\Delta + \sqrt{\Delta^2 + t^2}}\beta \tag{2.21}$$

Alternatively, the whole problem can be solved in Pauli matrices:

$$H = E_0 I + t\sigma_x + \Delta\sigma_z = E_0 I + \sqrt{\Delta^2 + t^2}\hat{n} \cdot \vec{\sigma} \tag{2.22}$$

where $\hat{n}$ is the direction of the splitting Hamiltonian, i.e. $\frac{t\hat{x} + \Delta\hat{z}}{\sqrt{\Delta^2 + t^2}}$. The eigenenergies are thus $E_0 \pm \sqrt{\Delta^2 + t^2}$, and the eigenstates are

$$\psi_+ = \begin{pmatrix} \cos\frac{1}{2}\arctan\frac{t}{\Delta} \\ \sin\frac{1}{2}\arctan\frac{t}{\Delta} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{2}\left(1 + \frac{\Delta}{\sqrt{\Delta^2+t^2}}\right)} \\ \sqrt{\frac{1}{2}\left(1 - \frac{\Delta}{\sqrt{\Delta^2+t^2}}\right)} \end{pmatrix} \tag{2.23}$$

$$\psi_- = \begin{pmatrix} \sin \frac{1}{2} \arctan \frac{t}{\Delta} \\ -\cos \frac{1}{2} \arctan \frac{t}{\Delta} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{2}\left(1 - \frac{\Delta}{\sqrt{\Delta^2+t^2}}\right)} \\ -\sqrt{\frac{1}{2}\left(1 + \frac{\Delta}{\sqrt{\Delta^2+t^2}}\right)} \end{pmatrix} \tag{2.24}$$

1 point were given for each correct eigenfunction, including normalization (2 total)

(d)

$$\frac{\Delta}{t} = \frac{4}{3} \tag{2.25}$$

1 point given for the correct answer

Problem 3

(a) The equation for the probability amplitude of the first excited state in time-dependent perturbation theory is:

$$c_2^{(1)} = \frac{-i}{\hbar} \int_{-\inf}^{t} H'_{ba}(t') e^{i\omega_0 t'} dt' \tag{3.1}$$

1 point given for the correct expression

Since $H_{ba}(t') = 0$ for $t' < 0$, $H_{ba}(t') = \int_0^{a/2} \psi_2 * (x) V_0 \psi_1(x) dx = 4V_0/(3\pi)$ for $t' > 0$.

1 point given for the correct time bound for the perturbation

1 point given for correctly evaluating $H'_{ba}(t')$

$$c_2^{(1)} = \frac{-i}{\hbar} \left(\frac{4V_0}{3\pi}\right) \int_0^t e^{i\omega_0 t'} dt' = \frac{4V_0 i}{3\hbar\pi} \frac{e^{i\omega_0 t}}{i\omega_0}\bigg|_0^T = \frac{-4V_0}{3\hbar\pi\omega_0}\left(e^{i\omega_0 T} - 1\right) \tag{3.2}$$

1 point given for correctly evaluating the time integral

Take the square to calculate the probability:

$$\left|c_2^{(1)}(T)\right|^2 = \frac{32V_0^2}{9\hbar^2\omega_0^2\pi^2}\Big(1 - \cos(\omega_0 T)\Big) \tag{3.3}$$

1 point given for evaluating the squared norm to find the probability

1 point given for the correct answer

(b) At $T = 2\pi/\omega_0$, $|c_2^{(1)}|^2 = 0$ for the first time since $T = 0$.

1 point given for the correct answer