Problem 1

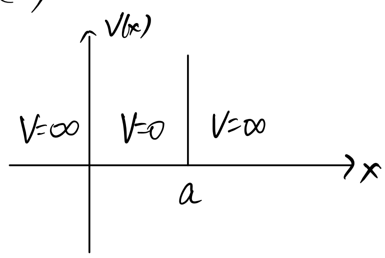
Consider an unperturbed Hamiltonian corresponding to the square well of width a with infitely high walls (hard walls). A particle of mass m is in this well. Now, as a perturbation, introduce a delta function potential in the middle of the well of strength α.

(a) What is the first-order correction to the energy of the ground state?

(b) The second-order correction to the energy of the ground state can be expressed as an infinite series that can be summed exactly. Write down the expression for the second-order correction as a sum and then sum it exactly to provide a compact expression for the second-order correction.

(c) Which is larger — the first-order or second-order correction? Does the answer of which is larger depend on the parameters of the square well?

(a)



in the well: $E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)$. $V(x)=0$.

boundary condition: $\begin{cases} \psi(x=0)=0 \\ \psi(x=a)=0. \end{cases}$

the well has infinitely walls. so there is no tunneling effect

$$\begin{cases} \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0, \quad E \geq 0. \\ \psi(x=a)=0. \quad \psi(x=0)=0 \end{cases}$$

let $\psi = e^{\lambda x}$. so $\psi' = \lambda e^{\lambda x}$. $\psi'' = \lambda^2 e^{\lambda x}$

$$\Rightarrow \lambda^2 e^{\lambda x} + \frac{2mE}{\hbar^2} e^{\lambda x} = 0$$

$$\lambda = \pm\sqrt{\frac{-2mE}{\hbar^2}} = \pm i\sqrt{\frac{2mE}{\hbar^2}}, \quad \text{so} \begin{cases} \psi_1(x) = \exp\left(-i\sqrt{\frac{2mE}{\hbar^2}}\,x\right) \\ \psi_2(x) = \exp\left(i\sqrt{\frac{2mE}{\hbar^2}}\,x\right) \end{cases}$$

because of the linear properity.

$\psi(x) = C_1\psi_1(x) + C_2\psi_2(x)$ is another solution to the eq.

So $\psi(x=0) = C_1\psi_1(0) + C_2\psi_2(0) = C_1 + C_2 = 0$

$\psi(x) = C_1\psi_1(x) - C_1\psi_2(x) = -2iC_1 \sin\sqrt{\frac{2mE}{\hbar^2}}\, x = D\sin\sqrt{\frac{2mE}{\hbar^2}}\, x$

Boundary condition: $\psi(a) = 0 \Rightarrow D\sin\sqrt{\frac{2mE}{\hbar^2}}\, a = 0$

So $\sqrt{\frac{2mE}{\hbar^2}}\, a = n\pi \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ $(n=1,2,\cdots)$

$\int_0^a |\psi_n(x)|^2 dx = 1 \Rightarrow D = \sqrt{\frac{2}{a}} \Rightarrow \psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$ $(n=1,2,\cdots)$

A delta function potential in the middle of the well of strength α:

$V(x) = \alpha\delta(x-\frac{a}{2})$

from the perturbation theory, the 1st order correction to the energy of the ground state: $n=1$

$E_1^{(1)} = \langle\psi_1|V(x)|\psi_1\rangle = \int \psi_1^*(x)\,\alpha\delta(x-\frac{a}{2})\,\psi_1(x)\,dx$

$= \frac{2}{a}\int_0^a \sin^2\frac{\pi}{a}x \cdot \alpha\delta(x-\frac{a}{2})\,dx = \frac{2}{a}\alpha\cdot\sin^2\frac{\pi}{a}\cdot\frac{a}{2} = \frac{2\alpha}{a}$

(b). from perturbation theory, the 2nd order correction to the ground state energy:

$$E_1^{(2)} = \sum_{n\neq 1} \frac{|\langle \varphi_n | V(x) | \varphi_1 \rangle|^2}{E_1 - E_n} = \sum_{n\neq 1} \frac{|V_{n,1}|^2}{E_1 - E_n} = \sum_{n\neq 1} \frac{\left(\frac{2\alpha}{a}\sin\frac{n\pi}{2}\right)^2}{\frac{\pi^2\hbar^2}{2ma^2} - \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

$$= \frac{8m\alpha^2}{\pi^2\hbar^2} \sum_{k=1} \frac{1}{1-(2k+1)^2} = \frac{2m\alpha^2}{\pi^2\hbar^2} \sum_{k=1} \frac{1}{-k^2-k} = \frac{-2m\alpha^2}{\pi^2\hbar^2} \sum_{k=1} \left(\frac{1}{k} - \frac{1}{k+1}\right)$$

$$= \frac{-2m\alpha^2}{\pi^2\hbar^2}$$

(C). $E_1^{(1)} = \frac{2\alpha}{a}$, $E_1^{(2)} = \frac{-2m\alpha^2}{\pi^2\hbar^2}$

if $\alpha > 0$. $E_1^{(1)}$ is positive, while $E_1^{(2)}$ is negative. So $E_1^{(1)} > E_1^{(2)}$

$$\frac{|E_1^{(1)}|}{|E_1^{(2)}|} = \frac{2\alpha}{a} \cdot \frac{\pi^2\hbar^2}{2m\alpha^2} = \frac{\pi^2\hbar^2}{ma\alpha} \quad \text{if } |E_1^{(1)}| > |E_1^{(2)}| \Leftrightarrow \alpha < \frac{\pi^2\hbar^2}{ma}$$

if $|E_1^{(1)}| < |E_1^{(2)}| \Leftrightarrow \alpha > \frac{\pi^2\hbar^2}{ma}$

Problem 2

Consider two potential wells for an electron, well a and well b (these could, for example, be atomic nuclei). Each well binds an electron into a state with energy $E_a = E_b = E_0$ in the absence of the other well. When the two wells are brought close together there is a matrix element $\langle a|H|b\rangle = t$. t is real and increases as the distance between the wells decreases. Solve non-perturbatively.

(a) Find the two solutions for the energy of the electron in terms of E_0 and t.

(b) If the two unperturbed wave functions are ψ_a and ψ_b, find the two solutions for the eigenfunctions and indicate which corresponds to which energy.

(c) Now apply an electric field to the system and approximate the effect of the electric field as changing E_a to $E_0 + \Delta$ and E_b to $E_0 - \Delta$. Find the energies and wave functions of the new eigenstates.

(d) (Numerical) How large must Δ/t be for one of the wave functions to be localized in well a with 90% probability?

(a) well a : $\hat{H}_a|a\rangle = E_a|a\rangle$.

well b : $\hat{H}_b|b\rangle = E_b|b\rangle$.

Since each well binds an electron into a state with energy $E_a = E_b = E_0$. in the absence of the other well. so we may assume these two eigenfunctions are orthogonal. $\langle a|b\rangle = 0$. hence $|a\rangle$ and $|b\rangle$ are orthonormal basis.

and we have : $\langle a|H|b\rangle = t$.

$$H = \begin{pmatrix} E_0 & \langle a|H|b\rangle \\ \langle a|H|b\rangle & E_0 \end{pmatrix}$$. then diagonalization : $\hat{H}|\psi\rangle = \hat{E}\,\mathbb{1}|\psi\rangle$

$$(H - E\mathbb{1})|\psi\rangle = 0 \Rightarrow \det(H - E\mathbb{1}) = 0 \Rightarrow \begin{vmatrix} E_0 - E & t \\ t & E_0 - E \end{vmatrix} = 0$$

so $(E_0 - E)^2 - t^2 = 0 \Rightarrow E = E_0 \pm t$

$\int |\psi|^2 dx = 1$ $\int c_1^2 (\psi_a + \psi_b)^2 dx = 1$

$c_1^2 \left(\int |\psi_a|^2 dx + \int |\psi_b|^2 dx + \int 2\psi_a\psi_b\, dx \right) = 1$

(b) for linear property of the equation. $\psi = C_1\psi_a + C_2\psi_b$ is an solution.

when $E = E_0 + t$.

$$(H - EI)|\psi\rangle = 0 \Rightarrow \begin{pmatrix} -t & t \\ t & -t \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \Rightarrow \begin{cases} -tC_1 + tC_2 = 0 \\ tC_1 - tC_2 = 0 \end{cases} \Rightarrow C_1 = C_2$$

normalization: $\int |\psi|^2 dx = 1 \Rightarrow \int (C_1\psi_a + C_1\psi_b)^2 dx = 1 \Rightarrow C_1^2\left(\int \psi_a^2 dx + \int \psi_b^2 dx + \int 2\psi_a\psi_b dx\right) = 1$

$$2C_1^2 = 1 \Rightarrow C_1 = C_2 = \frac{1}{\sqrt{2}}, \text{ so } \psi_1 = \frac{1}{\sqrt{2}}(\psi_a + \psi_b).$$

when $E = E_0 - t$.

$$\begin{pmatrix} t & t \\ t & t \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \Rightarrow C_1 = -C_2 = \frac{1}{\sqrt{2}}, \text{ so } \psi_2 = \frac{1}{\sqrt{2}}(\psi_a - \psi_b).$$

(c) $H = \begin{pmatrix} E_0 + \Delta & \langle a|H|b\rangle \\ \langle a|H|b\rangle & E_0 - \Delta \end{pmatrix}$

So. $(H - EI)|\psi\rangle = 0 \Rightarrow \det(H - EI) = 0 \Rightarrow \begin{vmatrix} E_0 + \Delta - E & t \\ t & E_0 - \Delta - E \end{vmatrix} = 0$

$$(E_0 + \Delta - E)(E_0 - \Delta - E) - t^2 = 0 \Rightarrow (E_0 - E)^2 - \Delta^2 - t^2 = 0$$

$$E^2 - 2E_0E + E_0^2 - \Delta^2 - t^2 = 0 \Rightarrow E = \frac{2E_0 \pm \sqrt{(2E_0)^2 - 4(E_0^2 - \Delta^2 - t^2)}}{2}$$

hence. $E = E_0 \pm \sqrt{\Delta^2 + t^2}$

substitute $E=E_0+\sqrt{\Delta^2+t^2}$ in $(H-EL)|\psi\rangle=0$:

$$\begin{pmatrix}\Delta-\sqrt{\Delta^2+t^2} & t \\ t & -\Delta-\sqrt{\Delta^2+t^2}\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix}=0$$

$$\Rightarrow \begin{cases}(\Delta-\sqrt{\Delta^2+t^2})c_1+tc_2=0\\ tc_1+(-\Delta-\sqrt{\Delta^2+t^2})c_2=0\end{cases}$$ so we have $$\begin{cases}c_1=\dfrac{t}{\sqrt{\Delta^2+t^2}-\Delta}c_2\\ c_2=\dfrac{t}{\Delta+\sqrt{\Delta^2+t^2}}c_1\end{cases}$$

normalization: $\int|\psi|^2dx=1 \Rightarrow \int|c_1\psi_a+c_2\psi_b|^2dx=1$

so $c_1^2\int|\psi_a|^2dx+c_2^2\int|\psi_b|^2dx=1$

$$c_2^2\frac{t^2}{(\sqrt{\Delta^2+t^2}-\Delta)^2}+c_2^2=1 \Rightarrow c_2=\frac{\sqrt{\Delta^2+t^2}-\Delta}{\sqrt{2(t^2+\Delta^2-\Delta\sqrt{\Delta^2+t^2})}}$$

$$c_1^2+c_2^2=1 \Rightarrow c_1=\frac{t}{\sqrt{2(t^2+\Delta^2-\Delta\sqrt{\Delta^2+t^2})}}$$

so $\psi=c_1\psi_a+c_2\psi_b$.

when $E=E_0-\sqrt{\Delta^2+t^2}$

$$\begin{pmatrix}\Delta+\sqrt{\Delta^2+t^2} & t \\ t & \sqrt{\Delta^2+t^2}-\Delta\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix}=0$$

$$\Rightarrow \begin{cases}(\Delta+\sqrt{\Delta^2+t^2})c_1+tc_2=0\\ tc_1+(\sqrt{\Delta^2+t^2}-\Delta)c_2=0\end{cases}$$ so we have $$\begin{cases}c_1=-\dfrac{t}{\Delta+\sqrt{\Delta^2+t^2}}c_2\\ c_2=\dfrac{t}{\Delta-\sqrt{\Delta^2+t^2}}c_1\end{cases}$$

$$\Rightarrow C_1 = \frac{t}{\sqrt{2(t^2+\Delta^2+\Delta\sqrt{\Delta^2+t^2})}}, \quad C_2 = \frac{-\sqrt{\Delta^2+t^2}-\Delta}{\sqrt{2(t^2+\Delta^2+\Delta\sqrt{\Delta^2+t^2})}}$$

(d). $E = E_0 + \sqrt{\Delta^2+t^2}$ has more overlap, so:

set $C_1^2 \geq 90\% \Rightarrow \frac{t^2}{2(t^2+\Delta^2-\Delta\sqrt{\Delta^2+t^2})} \geq 0.9 \Rightarrow \frac{\Delta}{t} \geq \frac{4}{3}$

Problem 3

Consider the hard wall square well of width a. A particle of mass m is in the ground state of this well. At time 0 a perturbation begins, in which a potential V_0 becomes present in the left half of the well.

(a) At time $T > 0$, the energy of the particle is measured. What is the probability that the energy of the particle is measured to be that of the first excited state $n=2$ in the quantum well? Treat the calculation perturbatively (*e.g.* do not consider excitations to other states that then lead to population of first excited state ...).

(b) What is the first time after $T = 0$ that the probability is zero?

(a). the eigenvalue and eigenfunction of a particle in an infinite well:

$$\begin{cases} E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (n=1,2,\cdots) \\ \psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi}{a}x \quad (n=1,2,\cdots) \end{cases}$$

from time-dependent perturbation theory

$$\dot{C}_f^1(t) = \frac{1}{i\hbar}\langle f^{(0)}|\hat{H}_1(t)|i^{(0)}\rangle e^{i\omega_{fi}t}, \quad \text{where } \omega_{fi} = \frac{E_f^{(0)}-E_i^{(0)}}{\hbar}$$

$$H_{fi}(t') = \langle f^{(0)} | \hat{H}_1(t) | i^{(0)} \rangle = \langle \varphi_2(x) | V_0 | \varphi_1(x) \rangle = \int_0^{\frac{a}{2}} \varphi_2^*(x) V_0 \varphi_1(x) \, dx = \frac{4V_0}{3\pi}$$

$$\omega_{fi} = \frac{E_2 - E_1}{\hbar} = (4-1) \frac{\pi^2 \hbar^2}{2ma^2 \hbar} = \frac{3\pi^2 \hbar}{2ma^2}$$

$$C_f^1(t) = \frac{1}{i\hbar} \int_0^t H_{fi}(t') \exp(i \omega_{fi} t') \, dt' = \frac{1}{i\hbar} \int_0^t \frac{4V_0}{3\pi} \exp\left(i \frac{3\pi^2 \hbar}{2ma^2} t'\right) dt'$$

$$= \frac{4V_0}{i\hbar 3\pi} \int_0^t \exp\left(i \frac{3\pi^2 \hbar}{2ma^2} t'\right) dt' = \frac{4V_0}{i\hbar 3\pi} \frac{2ma^2}{3i\pi^2 \hbar} \exp\left(i \frac{3\pi^2 \hbar}{2ma^2} t'\right) \Big|_0^t$$

$$= \frac{-8V_0 m a^2}{9\pi^3 \hbar^2} \left[\exp\left(i \frac{3\pi^2 \hbar}{2ma^2} T\right) - 1 \right]$$

$|C_f^1(t)|^2$ is the probability of finding $|\varphi_2^{(0)}\rangle$ at t.

so $$|C_f^1(t)|^2 = \left\{ \frac{-8V_0 m a^2}{9\pi^3 \hbar^2} \left[\exp\left(i \frac{3\pi^2 \hbar}{2ma^2} T\right) - 1 \right] \right\}^2$$

(b). considering $e^{ix} = \cos x + i \sin x$. when $e^{ix} = 1 \Rightarrow x = 2\pi n$, $n = 0, 1, 2 \cdots$

so the first time after $T=0$ is $\frac{3\pi^2 \hbar}{2ma^2} T = 2\pi \Rightarrow T = \frac{4ma^2}{3\pi\hbar}$