PH3102: QM Assignment 09

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Q1. Perturbing the Infinite square well

The unperturbed problem is $H_0 = \frac{\hat{p}^2}{2m} + V'(x)$, where $V'(x)$ and the perturbation $V(x)$ is

$$V'(x) = \begin{cases} 0 & x : 0 < x < a \\ \infty & \text{elsewhere} \end{cases} \quad ; \quad V(x) = \begin{cases} V_0 & x : \frac{a}{2} < x < \frac{3a}{2} \\ 0 & \text{elsewhere} \end{cases} \tag{1}$$

The energy eigenvalues and eigenfunctions to H_0 are given as

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , \quad \psi_n^{(0)} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

Answer 1.1

Considering the nature of the perturbation, the ground state energy should increase to accomodate the perturbation. Since $V_0 > 0$, the particle in its ground state should have higher energy. The peak of the ground state takes place at $x = a/2$. Since there is a higher potential at $x = a/2$, the peak which is proportional to the pdf at $x = a/2$, will decrease since the addition of a higher potential near it would decrease the pdf and thereafter the peak.

Answer 1.2

We now calculate the first order correction to the ground state energy. The first order correction is given as

$$E_1^{(1)} = \left\langle \psi_1^{(0)} \middle| V \middle| \psi_1^{(0)} \right\rangle = \frac{2}{a}V_0 \int_{\frac{a}{3}}^{\frac{2a}{3}} \sin^2\left(\frac{\pi x}{a}\right) dx = \left[\frac{2\pi + 3^{\frac{3}{2}}}{6\pi}\right] V_0 = \left[\frac{1}{3} + \frac{\sqrt{3}}{2\pi}\right] V_0 \tag{2}$$

Answer 1.3

The perturbation V_0 is invariant under parity transformation about $x = a/2$. Thus there will only be mixing with among the states of same parity. The ground state has even parity about $x = a/2$. Thus it will mix with only the states that have even parity around $a/2$ which have $n = 3, 5, 7...$ which are odd eigenstates. The lowest excited state with which it will mix is ψ_3

$$\begin{aligned} E_1^{(2)} \mid_{n=3} &= \frac{\left|\left(\left\langle \psi_3^{(0)} \middle| V_0 \middle| \psi_1^{(0)} \right\rangle\right)\right|^2}{E_1^{(0)} - E_3^{(0)}} \\ &= -\frac{ma^2}{4a\hbar^2\pi^2}\left|\frac{2}{a}V_o \int_{\frac{a}{3}}^{\frac{2a}{3}} \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right) dx\right|^2 \\ \Rightarrow E_1^{(0)} \mid_{n=3} &= -\frac{27ma^2V_0^2}{64\pi^4\hbar^2} \end{aligned} \tag{3}$$

The complete corrected ground state function upto the corrections upto a certain order we calculated is given by

$$E_1 = E_1^{(0)} + E_1^{(1)} + E_1^{(2)} \; |_{n=3} = \frac{\pi^2\hbar^2}{2ma^2} + V_0\left(\frac{1}{3} + \frac{\sqrt{3}}{2\pi}\right) - \frac{27ma^2V_0^2}{64\pi^4\hbar^2} \tag{4}$$

Answer 1.4

We want to find the first order correction to the ground state due to mixing with lowest excited state which is given as

$$\begin{aligned} \left|\psi_1^{(1)}\right\rangle \; |_{n=3} &= \frac{\left\langle\psi_3^{(0)}\middle|V_0\middle|\psi_1^{(0)}\right\rangle}{E_1^{(0)} - E_3^{(0)}}|\psi_3\rangle = \frac{3\sqrt{3}V_0}{4\pi}\frac{ma^2}{4\hbar^2\pi^2}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right) \\ &= \frac{3\sqrt{6}V_0ma^{\frac{3}{2}}}{16\pi^3\hbar^2}\sin\left(\frac{3\pi x}{a}\right) \end{aligned} \tag{5}$$

The corrected ground state with first order corrections upto the first order with the mixing of the ground state with the lowest excited state is given by

$$|\psi_1\rangle = \left|\psi_1^{(0)}\right\rangle + \left|\psi_1^{(1)}\right\rangle \; |_{n=3} = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \frac{3\sqrt{6}V_0ma^{\frac{3}{2}}}{16\pi^3\hbar^2}\sin\left(\frac{3\pi x}{a}\right) \tag{6}$$

Answer 1.5

To infer results for $V_0 < 0$ in the perturbation, we map $V_0 \longrightarrow -V_0$. The energy eigenvalues and eigenstates are given as

$$\begin{aligned} E_1 &= \frac{\pi^2\hbar^2}{2ma^2} - V_0\left(\frac{1}{3} + \frac{\sqrt{3}}{2\pi}\right) - \frac{27ma^2V_0^2}{64\pi^4\hbar^2} \\ |\psi_1\rangle &= \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) - \frac{3\sqrt{6}V_0ma^{\frac{3}{2}}}{16\pi^3\hbar^2}\sin\left(\frac{3\pi x}{a}\right) \end{aligned} \tag{7}$$

Answer 1.6

The plots for the unperturbed ground state and perturbed ground states with $V_0 > 0$ and $V_0 < 0$ are plotted below,

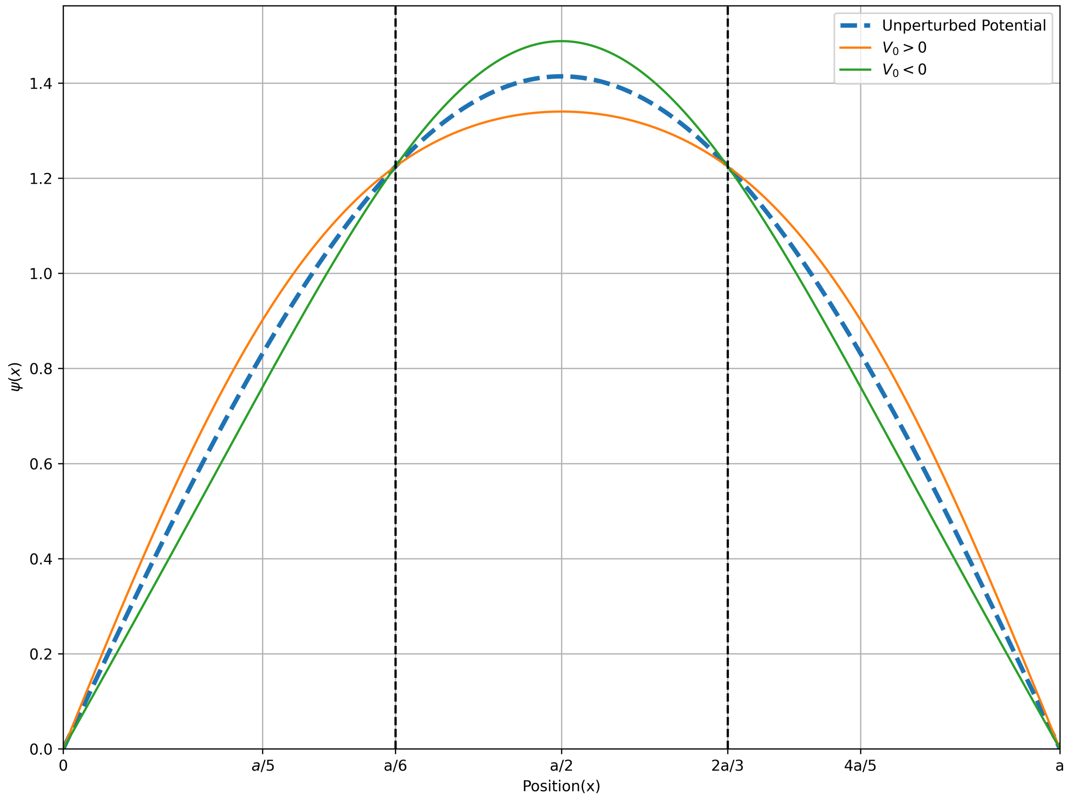

Figure 1: Sketches of the ground state wavefunctions

Q2. Perturbation theory for a 3-level problem

Answer 2.1

The Hamiltonian of the 3-level system is given as

$$\widehat{H} = \begin{bmatrix} -u & v & 0 \\ v & u & 0 \\ 0 & 0 & u' \end{bmatrix} \quad ; u', u, v > 0$$

To apply perturbation theory to this we seperate $\widehat{H}$ into $H_0 + V$ where H_0 is the zeroth Hamiltonian and V is the perturbation.

We define H_0 and V to be

$$H_0 = \begin{bmatrix} -u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u' \end{bmatrix} \qquad V = \begin{bmatrix} 0 & v & 0 \\ v & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad [8]$$

Answer 2.2

We want to find the energy eigenvalues $E_1^{(0)}, E_2^{(0)}, E_3^{(0)}$ and the energy eigenstates $\left|\psi_1^{(0)}\right\rangle, \left|\psi_2^{(0)}\right\rangle, \left|\psi_3^{(0)}\right\rangle$ of the zeroth Hamiltonian. The eigenvalues of a diagonal matrix like H_0 are the diagonal entries themselves. So the energy eigenvalues are

$$\begin{aligned} E_1^{(0)} &= -u & E_2^{(0)} &= u & E_3^{(0)} &= u' \\ \left|\psi_1^{(0)}\right\rangle &= \begin{pmatrix}1\\0\\0\end{pmatrix} & \left|\psi_2^{(0)}\right\rangle &= \begin{pmatrix}0\\1\\0\end{pmatrix} & \left|\psi_3^{(0)}\right\rangle &= \begin{pmatrix}0\\0\\1\end{pmatrix} \end{aligned} \tag{9}$$

Answer 2.3

We calculate the energy corrections upto the second order. The first order and second energy corrections are given by

$$\begin{aligned} E_n^{(1)} &= \left\langle \psi_n^{(0)} \middle| V \middle| \psi_n^{(0)} \right\rangle \\ E_n^{(2)} &= \left\langle \psi_n^{(0)} \middle| V \middle| \psi_n^{(1)} \right\rangle = \sum_{k\neq n} \frac{\left|\left\langle \psi_k^{(0)} \middle| V \middle| \psi_n^{(0)} \right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} \end{aligned} \tag{10}$$

To find them we represent the perturbation V in the eigenbasis of H_0 that is in terms of $\left|\psi_1^{(0)}\right\rangle, \left|\psi_2^{(0)}\right\rangle, \left|\psi_3^{(0)}\right\rangle$.

$$V = \begin{bmatrix} \left\langle \psi_1^{(0)} \middle| V \middle| \psi_1^{(0)} \right\rangle & \left\langle \psi_1^{(0)} \middle| V \middle| \psi_2^{(0)} \right\rangle & \left\langle \psi_1^{(0)} \middle| V \middle| \psi_3^{(0)} \right\rangle \\ \left\langle \psi_2^{(0)} \middle| V \middle| \psi_1^{(0)} \right\rangle & \left\langle \psi_2^{(0)} \middle| V \middle| \psi_2^{(0)} \right\rangle & \left\langle \psi_2^{(0)} \middle| V \middle| \psi_3^{(0)} \right\rangle \\ \left\langle \psi_3^{(0)} \middle| V \middle| \psi_1^{(0)} \right\rangle & \left\langle \psi_3^{(0)} \middle| V \middle| \psi_2^{(0)} \right\rangle & \left\langle \psi_3^{(0)} \middle| V \middle| \psi_3^{(0)} \right\rangle \end{bmatrix} = \begin{bmatrix} 0 & v & 0 \\ v & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{11}$$

Let us calculate $E_n^{(1)}$ using the gram-matrix elements of V using the eigenbasis of H_0

$$E_1^{(1)} = E_2^{(2)} = E_3^{(3)} = 0 \tag{12}$$

We know calculate $E_n^{(2)}$ using the matrix elements of V in the eigenbasis of H_0

$$\begin{aligned} E_1^{(2)} &= \frac{\left|\left\langle \psi_2^{(0)} \middle| V \middle| \psi_1^{(0)} \right\rangle\right|^2}{E_1^{(0)} - E_2^{(0)}} = -\frac{v^2}{2u} \\ E_2^{(2)} &= \frac{\left|\left\langle \psi_1^{(0)} \middle| V \middle| \psi_2^{(0)} \right\rangle\right|^2}{E_2^{(0)} - E_1^{(0)}} = \frac{v^2}{2u} \\ E_3^{(2)} &= 0 \end{aligned} \tag{13}$$

Answer 2.4

We use the expression for the corrections to the eigenstates as $\left|\psi_n^{(j)}\right\rangle = \sum_{k\neq n} c_{nk}^{(j)} \left|\psi_n^{(0)}\right\rangle$ to find the first order corrections to the eigenstates. To find out $c_{nk}^{(1)}$ we use,

$$c_{nk}^{(1)} = \frac{\left\langle \psi_k^{(0)} \middle| V \middle| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} \tag{14}$$

Let us write the matrix of the coefficients of first order corrections C as $C_{ij} = c_{ij}^{(1)}$. The matrix is

$$C = \begin{bmatrix} 0 & \frac{v}{2u} & 0 \\ -\frac{v}{2u} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{15}$$

The first order correction to the eigenstates are $\left|\psi_1^{(1)}\right\rangle, \left|\psi_2^{(1)}\right\rangle, \left|\psi_3^{(1)}\right\rangle$, are

$$\begin{aligned} \left|\psi_1^{(1)}\right\rangle &= C_{12}|\psi_2^0\rangle + C_{13}|\psi_3^0\rangle = -\frac{v}{2u}\left|\psi_2^{(0)}\right\rangle = -\frac{v}{2u}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\ \left|\psi_2^{(1)}\right\rangle &= C_{21}|\psi_1^0\rangle + C_{23}|\psi_3^0\rangle = \frac{v}{2u}\left|\psi_1^{(0)}\right\rangle = \frac{v}{2u}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \\ \left|\psi_3^{(1)}\right\rangle &= C_{32}|\psi_2^0\rangle + C_{31}|\psi_1^0\rangle = 0 \end{aligned} \tag{16}$$

Answer 2.5

We now solve the problem by diagonalising the matrix H. The matrix H is diagonalizable because it is a symmetric matrix and symmetric matrics are normal. By Spectral Theorem, there exists an orthogonal eigenbasis of the matrix. After diagonalizing, we get

$$\begin{aligned} H = \begin{bmatrix} -u & v & 0 \\ v & u & 0 \\ 0 & 0 & u' \end{bmatrix} &= \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} \begin{bmatrix} -\sqrt{u^2+v^2} & 0 & 0 \\ 0 & \sqrt{u^2+v^2} & 0 \\ 0 & 0 & u' \end{bmatrix} \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}^{\mathsf{T}} \\ &= \begin{bmatrix} -\frac{\sqrt{u^2+v^2}+u}{v} & \frac{\sqrt{u^2+v^2}-u}{v} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -\sqrt{u^2+v^2} & 0 & 0 \\ 0 & \sqrt{u^2+v^2} & 0 \\ 0 & 0 & u' \end{bmatrix} \begin{bmatrix} -\frac{\sqrt{u^2+v^2}+u}{v} & 1 & 0 \\ \frac{\sqrt{u^2+v^2}-u}{v} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned} \tag{17}$$

The energy eigenvalues that we get from diagonalising the matrix are

$$\boxed{\lambda_1 = -\sqrt{u^2+v^2} \quad ; \quad \lambda_2 = \sqrt{u^2+v^2} \quad ; \quad \lambda_3 = u'} \tag{18}$$

The third energy eigenvalue is not disturbed by the perturbation V. Let us focus on the other ones. In the regime where $v/u \ll 1$, we expand eigenvalues as a power series in terms of $\frac{v}{u}$

$$\begin{aligned} \lambda_1 &= -u\sqrt{1+\frac{v^2}{u^2}} = -u - \frac{v^2}{2u} - O\left(\frac{v^4}{u^2}\right) = -u - \frac{v^2}{2u} = E_1 \\ \lambda_2 &= u\sqrt{1+\frac{v^2}{u^2}} = u + \frac{v^2}{2u} + O\left(\frac{v^4}{u^2}\right) = u + \frac{v^2}{2u} = E_2 \end{aligned}$$

Thus we can see that this result matches that of perturbative result which we have calculated ignoring terms with $O\left(\frac{v^4}{u^2}\right)$. The eigenvectors are

$$v_1 = \begin{pmatrix} -\frac{\sqrt{u^2+v^2}+u}{v} \\ 1 \\ 0 \end{pmatrix}, v_2 = \begin{pmatrix} \frac{\sqrt{u^2+v^2}-u}{v} \\ 1 \\ 0 \end{pmatrix}, v_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{19}$$

Let us take the first two eigenvectors and again in the regime of $v/u \ll 1$ let us expand into a power series

$$
\begin{aligned}
v_1 &= \begin{pmatrix} -\frac{u}{v}\left(1+\sqrt{1+\frac{v^2}{u^2}}\right) \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{-2u}{v} \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{v}{2u} \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} - \frac{v}{2u}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \left|\psi_1^{(0)}\right\rangle + \left|\psi_1^{(1)}\right\rangle = |\psi_1\rangle \\
v_2 &= \begin{pmatrix} \frac{u}{v}\left(\sqrt{1+\frac{v^2}{u^2}}-1\right) \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{v}{2u} \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + \frac{v}{2u}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \left|\psi_2^{(0)}\right\rangle + \left|\psi_2^{(1)}\right\rangle = |\psi_s\rangle \\
v_2 &= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |\psi_3\rangle
\end{aligned}
\tag{20}
$$

Here we have used the approximations $v/u \approx 0$ and $\sqrt{1+v^2/u^2} \approx 1 + v^2/2u^2$. We see that the eigenfunctions of the total hamiltonian match the eigenstates we obtained from our perturbation calculations upto to certain order.

Answer 2.6

We calculate the wavefunction renormalization as Z of the ground state which is given by

$$
Z = \left| \left\langle \psi_1^{(0)} \middle| \psi_1 \right\rangle_N \right|^2 \tag{21}
$$

We apply the corrections we obtained from the perturation theory results, to the ground state

$$
\begin{aligned}
|\psi_1\rangle &= \left|\psi_1^{(0)}\right\rangle - \frac{v}{2u}\left|\psi_2^{(0)}\right\rangle = \begin{pmatrix} 1 \\ -\frac{v}{2u} \\ 0 \end{pmatrix} \\
\Rightarrow |\psi_1\rangle_N &= \frac{1}{\sqrt{1+\frac{v^2}{4u^2}}}\begin{pmatrix} 1 \\ -\frac{v}{2u} \\ 0 \end{pmatrix} \\
\Rightarrow Z &= \frac{1}{1+\frac{v^2}{4u^2}}\left|(1\ \ 0\ \ 0)\begin{pmatrix} 1 \\ -\frac{v}{2u} \\ 0 \end{pmatrix}\right|^2 = \frac{1}{1+\frac{v^2}{4u^2}}
\end{aligned}
\tag{22}
$$

The regime of validity of this perturbation problem is $v/u \ll 1$. We can see this regime validity appearing in the renormalization problem. Going beyond the regime of this problem, we get

$$
Z = \frac{1}{1+v^2/4u^2} \longrightarrow 0, \quad as \quad \frac{v}{u} \longrightarrow \infty
$$