Physics 4310 Homework #11

4 problems

Solutions

▷ **1.**

[Ch 6] Consider an infinite square well with a slightly tilted floor:

$$V(x) = \begin{cases} \epsilon x & 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$$

Find expressions for the approximate (first-order) ground state energy *and* eigenstate of this potential; write them in closed form if possible.

Answer:

The solutions of the unperturbed Hamiltonian (the infinite square well) are

$$\psi_{n0}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad \text{and} \quad E_{n0} = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

The correction to the energy is

$$\begin{aligned} E_{n1} &= \langle \psi_{n0} | H' | \psi_{n0} \rangle \\ &= \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \epsilon x \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \, dx \\ &= \frac{2}{a}\epsilon \int_0^a x \sin^2\left(\frac{n\pi}{a}x\right) \, dx \\ &= \frac{2}{a}\epsilon\frac{a^2}{4} = \boxed{\epsilon\frac{a}{2}} \end{aligned}$$

The correction is independent of n, which is interesting. The total energy is

$$E_n \approx \frac{\pi^2\hbar^2}{2ma^2}n^2 + \epsilon\frac{a}{2}$$

The correction for the wavefunction is

$$\psi_{n1} = \sum_{m \ne n} \frac{\langle \psi_{m0} | H' | \psi_{n0} \rangle}{(E_{n0} - E_{m0})} \psi_{m0}$$

The matrix element is

$$\begin{aligned}\langle\psi_{m0}|H'|\psi_{n0}\rangle &= \frac{2}{a}\epsilon\int_0^a x\sin\left(\frac{n\pi}{a}x\right)\sin\left(\frac{m\pi}{a}x\right)\,dx \\ &= -a^2\frac{2mn(1-(-1)^{m+n})}{(m^2-n^2)^2\pi^2} \\ &= -a^2\frac{4mn}{(m^2-n^2)^2\pi^2},\ m+n \text{ odd}\end{aligned}$$

but zero if $m+n$ is even. Substituting into the sum,

$$\begin{aligned}\psi_{n1} &= \sum_{m\neq n}\frac{\langle\psi_{m0}|H'|\psi_{n0}\rangle}{(E_{n0}-E_{m0})}\psi_{m0} \\ &= \sum_{\substack{m\neq n \\ m+n\,\mathrm{odd}}}\left(-a^2\epsilon\frac{4mn}{(m^2-n^2)^2\pi^2}\right)\left(\frac{2Ma^2}{\pi^2\hbar^2(n^2-m^2)}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{m\pi}{a}x\right) \\ &= \frac{8\sqrt{2}Ma^{7/2}\epsilon}{\pi^4\hbar^2}\sum_{\substack{m\neq n \\ m+n\,\mathrm{odd}}}\frac{mn}{(n^2-m^2)^3}\sin\left(\frac{m\pi}{a}x\right)\end{aligned}$$

where M is the mass. I sincerely doubt this sum can be evaluated, but it can be approximated. Write $m=n+2j$ where j is an integer. Then

$$\frac{mn}{(n^2-m^2)^3}=\frac{(n+2j)n}{(n^2-n^2-4nj-4j^2)^3}=-\frac{n(n+2j)}{64j^3(1+j)^3}$$

As j increases, this coefficient dies off as $\frac{1}{j^5}$ which is pretty fast, so it would be reasonable to only keep a couple terms of m on either side of n. For example,

$$\begin{aligned}\psi_{(n=1)1} &\approx \frac{8\sqrt{2}Ma^{7/2}\epsilon}{\pi^4\hbar^2}\left[\frac{3(1)}{(1-9)^3}\sin\left(\frac{3\pi x}{a}\right)+\frac{5(1)}{(1-25)^3}\sin\left(\frac{5\pi x}{a}\right)+\dots\right] \\ &\approx -\frac{8\sqrt{2}Ma^{7/2}}{\pi^4\hbar^2}\left[0.0059\sin\left(\frac{3\pi x}{a}\right)+0.00036\sin\left(\frac{5\pi x}{a}\right)+\dots\right]\end{aligned}$$

and so

$$\psi_1\approx\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)-\frac{8\sqrt{2}Ma^{7/2}\epsilon}{\pi^4\hbar^2}\left[0.0059\sin\left(\frac{3\pi x}{a}\right)+0.00036\sin\left(\frac{5\pi x}{a}\right)+\dots\right]$$

If ϵ is small too, then you'd even be okay by saying $\psi_1\approx\psi_{01}$ and dropping the extra terms all together.

▷ **2.**

[Ch 6] Consider a two-dimensional infinite square well, with potential $V(x,y)=0$ if $0\le x\le a$ and $0\le y\le a$ and ∞ otherwise. The energy eigenstates are

$$\psi_{n_x n_y}(x,y)=\left(\frac{2}{a}\right)\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right),\ n_x,n_y=1,2,3,\dots$$

with energy $E=\frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2)$. Notice that the second-lowest energy $E=\frac{\pi^2\hbar^2}{2ma^2}(4+1)$ has a twofold degeneracy: $(n_x,n_y)=(1,2)$ and $(2,1)$. To break this degeneracy, we add a perturbation to the Hamiltonian:

$$H'=\begin{cases}V_0, & 0\le x\le \frac{a}{2} \quad\text{and}\quad 0\le y\le\frac{a}{2}\\ 0, & \text{otherwise}\end{cases}$$

Find the approximate energies $E_\pm$ and eigenstates $\psi_\pm$ once the degeneracy is broken.

Answer:

To figure this out, we need the matrix

$$W_{pq}=\langle\psi_p(x,y)|H'|\psi_q(x,y)\rangle$$

where p and q are either $\vec{a}=(1,2)$ or $\vec{b}=(2,1)$. The integrals are

$$W_{aa}=\int_0^{a/2}\int_0^{a/2}\left(\frac{2}{a}\right)^2\sin\left(\frac{a_x\pi x}{a}\right)\sin\left(\frac{a_y\pi y}{a}\right)V_0\sin\left(\frac{a_x\pi x}{a}\right)\sin\left(\frac{a_y\pi y}{a}\right)dx\,dy$$

$$=\frac{4V_0}{a^2}\int_0^{a/2}\sin\left(\frac{1\pi x}{a}\right)\sin\left(\frac{1\pi x}{a}\right)dx\int_0^{a/2}\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{2\pi y}{a}\right)dy$$

$$=\frac{4V_0}{a^2}\left(\frac{a}{4}\right)\left(\frac{a}{4}\right)=\frac{1}{4}V_0$$

$$W_{ab}=\frac{4V_0}{a^2}\int_0^{a/2}\sin\left(\frac{1\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx\int_0^{a/2}\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{1\pi y}{a}\right)dy$$

$$=\frac{4V_0}{a^2}\left(\frac{2a}{3\pi}\right)\left(\frac{2a}{3\pi}\right)=\frac{16}{9\pi^2}V_0$$

$$W_{ba}=\frac{4V_0}{a^2}\int_0^{a/2}\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{1\pi x}{a}\right)dx\int_0^{a/2}\sin\left(\frac{1\pi y}{a}\right)\sin\left(\frac{2\pi y}{a}\right)dy$$

$$=\frac{4V_0}{a^2}\left(\frac{2a}{3\pi}\right)\left(\frac{2a}{3\pi}\right)=\frac{16}{9\pi^2}V_0$$

$$W_{bb}=\frac{4V_0}{a^2}\int_0^{a/2}\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx\int_0^{a/2}\sin\left(\frac{1\pi y}{a}\right)\sin\left(\frac{1\pi y}{a}\right)dy$$

$$=\frac{4V_0}{a^2}\left(\frac{a}{4}\right)\left(\frac{a}{4}\right)=\frac{1}{4}V_0$$

(The bits in red are the factors corresponding to the second term.) The matrix W is thus

$$W = V_0 \begin{pmatrix} 1/4 & 16/9\pi^2 \\ 16/9\pi^2 & 1/4 \end{pmatrix}$$

The corrections to the initial energy $E = \frac{5\pi^2\hbar^2}{2ma^2}$ are the eigenvalues of this matrix:

$$E_\pm = \frac{5\pi^2\hbar^2}{2ma^2} + \frac{1}{4}V_0 \pm \frac{16}{9\pi^2}V_0$$

The eigenvectors of this matrix are $v_\pm = \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$ which tells us how to mix our initial states to get the "good" eigenstates. We have

$$\begin{aligned} \psi_\pm &= \frac{1}{\sqrt{2}}\left[\psi_a \pm \psi_b\right] \\ &= \frac{2}{a\sqrt{2}}\left[\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right) \pm \sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\right] \end{aligned}$$

▷ **3.**
[Ch 7] Use a gaussian trial function (Eq. 7.2) to obtain the lowest upper bound you can on the ground state energy of the linear potential $V(x) = \alpha|x|$ and the quartic potential $V(x) = \alpha x^4$. Compare your bounds to the exact ground state energy of the potential $V(x) = \alpha x^2$.

Answer:
We need to calculate the average energy for the trial function $\psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}$.

$$\begin{aligned} \langle H \rangle &= \langle \psi(x)|H|\psi(x)\rangle \\ &= \langle \psi(x)|(T+V)|\psi(x)\rangle \end{aligned}$$

where $T = -\frac{\hbar^2}{2m}\nabla^2$ and V is one of the potentials given above. Griffiths already calculated the average of T part of the Hamiltonian:

$$\langle T \rangle = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\frac{d^2}{dx^2}e^{-bx^2}\,dx = \frac{\hbar^2 b}{2m}$$

And

$$\begin{aligned}\langle V \rangle &= \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} e^{-2bx^2} \alpha |x|^n \, dx \\ &= \alpha \frac{1}{\sqrt{\pi}} (2b)^{-\frac{1}{2}n} \Gamma\left(\frac{n+1}{2}\right)\end{aligned}$$

where $n = 1$ or 4. The total energy is thus

$$E(b) = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{\pi}} (2b)^{-\frac{1}{2}n} \Gamma\left(\frac{n+1}{2}\right)$$

Let's write this as $E(b) = Ab + Bb^{-n/2}$. We want to find b which minimizes the energy:

$$\begin{aligned} 0 = E'(b) &= A - \frac{n}{2} B b^{-n/2-1} \\ \implies A &= \frac{1}{2} n B b^{-n/2-1} \\ \implies b^{\frac{n+2}{2}} &= \frac{1}{2} n \frac{B}{A} \\ b &= \left(\frac{nB}{2A}\right)^{\frac{2}{n+2}} \\ \implies E_{\min} &= A \left(\frac{nB}{2A}\right)^{\frac{2}{n+2}} + B \left[\left(\frac{nB}{2A}\right)^{\frac{2}{n+2}}\right]^{-n/2} \\ &= A \left(\frac{nB}{2A}\right)^{\frac{2}{n+2}} + B \left(\frac{nB}{2A}\right)^{-\frac{n}{n+2}} \end{aligned}$$

where the ratio

$$\frac{nB}{2A} = \frac{1}{2A} nB = \frac{nm}{\hbar^2} \frac{\alpha}{\sqrt{\pi}} 2^{-n/2} \Gamma\left(\frac{n+1}{2}\right)$$

Asking Mathematica, the minimum energy for $n = 1$ is

$$E_{\min} = \frac{3}{2(2\pi)^{1/3}} \alpha \left(\frac{\hbar^2}{m\alpha}\right)^{1/3}$$

For $n = 4$,

$$E_{\min} = \frac{3^{4/3}}{4^{4/3}} \alpha \left(\frac{\hbar^2}{m\alpha}\right)^{2/3}$$

The ground state of the harmonic oscillator $V(x) = \alpha x^2$ is $\frac{1}{2}\hbar\omega$ where $\alpha = \frac{1}{2}m\omega^2 \implies \omega = \sqrt{\frac{2\alpha}{m}}$. Thus the energy is

$$E = \frac{1}{2}\hbar\sqrt{\frac{2\alpha}{m}} = \frac{1}{\sqrt{2}} \left(\frac{\hbar^2 \alpha}{m}\right)^{1/2} = \frac{1}{\sqrt{2}} \alpha \left(\frac{\hbar^2}{m\alpha}\right)^{1/2}$$

▷ **4.**
[Ch 8] Consider the potential

$$V(x) = \begin{cases} V_0(1 - \frac{x^2}{a^2}), & -a < x < a \\ 0, & otherwise \end{cases}$$

where V_0 and a are constants. Use the WKB approximation to find the scattering solution to the Schrodinger equation for this potential, with $E \gg V_0$.

Answer:
When the energy is much greater than the potential, the momentum $p(x) = 2m(E - V(x))$ is real, and the scattering solutions are

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int \sqrt{2m(E - V_0(1 - x^2/a^2))}\, dx}$$

Let's see if we can do the integral

$$\begin{aligned} \int p(x)\, dx &= \int \sqrt{2m\left(E - V_0(1 - \frac{x^2}{a^2})\right)}\, dx \\ &= \int \sqrt{2m(E - V_0) + \frac{2mV_0}{a^2} x^2}\, dx \\ &= x\sqrt{\frac{m}{2}}\sqrt{E - V_0\left(1 - \frac{x^2}{a^2}\right)} + a(E - V_0)\sqrt{\frac{m}{2V_0}} \ln\left(am\sqrt{V_0}\sqrt{E - V_0\left(1 - \frac{x^2}{a^2}\right)} + mV_0 x\right) \end{aligned}$$

The answer is "yes, but it's not terribly pretty" so the answer

$$\psi(x) \approx \frac{C}{\sqrt{2m(E - V_0(1 - x^2/a^2))}} e^{\pm \frac{i}{\hbar} \int \sqrt{2m(E - V_0(1 - x^2/a^2))}\, dx}$$

is satisfactory.