S2013

Problem 5: Perturbing a Square Well

Consider a particle of mass m in a 1D infinite square well of width a,

$$V(x) = 0, \quad 0 \leq x \leq a \qquad V(x) = \infty, \quad x < 0, \quad x > a. \tag{1}$$

(a) [2 pts] Derive the eigenfunctions and eigenenergies of the particle in this potential. Be sure to normalize the states.

(b) [2 pts] Show that if the well is perturbed by a potential $V'(x) = \alpha\, x$, the energy of all the unperturbed states shift by the same amount to first order in α. Find an expression for this energy shift. Give a physical explanation for why this perturbation results in an equal first-order energy shift for all states.

(c) [3 pts] Next, instead of the perturbing potential from part (b), the well is perturbed by a potential

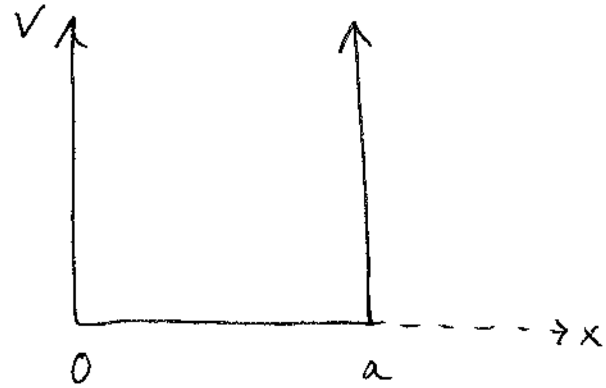
$$V'(x) = V_0, \quad \frac{a}{2} - \delta \leq x \leq \frac{a}{2} + \delta \qquad V'(x) = 0, \quad x < \frac{a}{2} - \delta, \quad x > \frac{a}{2} + \delta \tag{2}$$

Compute the energy shift to first order in α for the unperturbed energy eigenstates $\psi_n(x)$. Explain the limit of this result as n, the unperturbed energy level, gets large.

(d) [2 pts.] What is the energy shift of the states $\psi_n(x)$ to first order in δ as $\delta \to 0$? (V_0 is constant.) Give a physical explanation of this result. Note: You should be able to answer this question even if you did not get a solution to part (c).

(e) [1 pt] What is the energy shift of the states $\psi_n(x)$ as $\delta \to \frac{a}{2}$? (V_0 is constant.) Give a physical explanation of this result. Note: You should again be able to answer this question even if you did not get a solution to part (c).

(a)



The Schrödinger equation for this potential is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi,$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}.$$

The general solution is

$$\psi(x) = A\sin(kx) + B\cos(kx).$$

The boundary conditions require

$$\psi(0) = \psi(a) = 0.$$

So

$$\psi(0) = A\sin(0) + B\cos(0) = 0$$

and we must have $B = 0$.

(a), cont'd...

Then

$$\psi(x) = A\sin(kx).$$

So

$$\psi(a) = A\sin(ka) = 0,$$

which implies

$$ka = n\pi$$

$$k = \frac{n\pi}{a}, \qquad n = 1, 2, 3, \ldots$$

Normalizing...

$$A^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

$$A^2 \int_0^a \frac{1}{2}\left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right) dx = 1$$

$$\frac{A^2}{2}\left(x - \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)\right)\Big|_0^a = 1$$

$$\frac{A^2}{2}\left(a - \frac{a}{2n\pi}\sin(2n\pi)\right) = 1$$

$$A = \sqrt{\frac{2}{a}}$$

and

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), \; n = 1, 2, 3, \ldots}$$

(a), cont'd...

We have

$$k = \frac{n\pi}{a} = \frac{\sqrt{2mE}}{\hbar}$$

$$\sqrt{2mE} = \frac{n\pi\hbar}{a}$$

$$\boxed{E = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

(b)

The first order energy correction is given by

$$\begin{aligned}
E^{(1)} &= \langle n|V'|n\rangle \\
&= \langle n|\,\alpha x\,|n\rangle \\
&= \alpha\langle n|x|n\rangle \\
&= \alpha\int_0^a \psi^* x \psi\, dx \\
&= \frac{2\alpha}{a}\int_0^a x\sin^2\left(\frac{n\pi x}{a}\right)dx \\
&= \frac{2\alpha}{a}\int_0^a \frac{x}{2}\left(1-\cos\left(\frac{2n\pi x}{a}\right)\right)dx \\
&= \frac{\alpha}{a}\left[\int_0^a x\,dx - \int_0^a x\cos\left(\frac{2n\pi x}{a}\right)dx\right] \\
&= \frac{\alpha}{a}\left[\frac{1}{2}a^2 - \int_0^a x\cos\left(\frac{2n\pi x}{a}\right)dx\right]
\end{aligned}$$

(b), cont'd...

Let: $u = x$ $\qquad dv = \cos\left(\frac{2n\pi x}{a}\right)dx$

$du = dx \qquad v = \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)$.

Then

$$\int_0^a x\cos\left(\frac{2n\pi x}{a}\right)dx = \frac{a}{2n\pi}x\sin\left(\frac{2n\pi x}{a}\right)\Big|_0^a - \int_0^a \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)dx$$

$$= \frac{a^2}{4n^2\pi^2}\cos\left(\frac{2n\pi x}{a}\right)\Big|_0^a$$

$$= \frac{a^2}{4n^2\pi^2}.$$

So

$$E^{(1)} = \frac{\alpha}{a}\left[\frac{1}{2}a^2 - \frac{a^2}{4n^2\pi^2}\right]$$

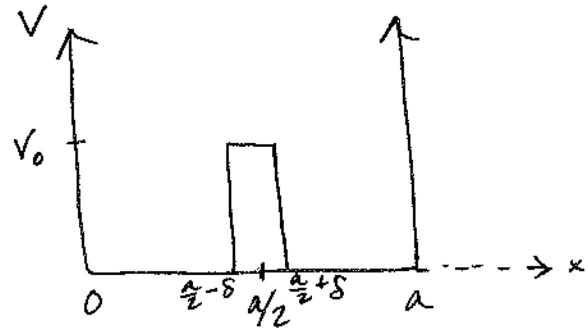
$$\boxed{E^{(1)} = \frac{\alpha}{2}a - \frac{\alpha a}{4n^2\pi^2}},$$

which is our first-order energy shift for all states $|n\rangle$. If we compare the terms, we see that the second is much smaller than the first, so we effectively have

$$E^{(1)} \approx \frac{\alpha}{2}a,$$

which is the same for all n.

(c)



The first order correction is given by

$$E^{(1)} = \langle n | V' | n \rangle$$

$$= \langle n | V_0 | n \rangle$$

$$= V_0 \int_{\frac{a}{2}-\delta}^{\frac{a}{2}+\delta} \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{2V_0}{a} \int_{\frac{a}{2}-\delta}^{\frac{a}{2}+\delta} \frac{1}{2} \left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right) dx$$

$$= \frac{V_0}{a} \left[\int_{\frac{a}{2}-\delta}^{\frac{a}{2}+\delta} dx - \int_{\frac{a}{2}-\delta}^{\frac{a}{2}+\delta} \cos\left(\frac{2n\pi x}{a}\right) dx \right]$$

$$= \frac{V_0}{a} \left[x - \frac{a}{2n\pi} \sin\left(\frac{2n\pi x}{a}\right) \right] \Bigg|_{\frac{a}{2}-\delta}^{\frac{a}{2}+\delta}$$

$$= \frac{V_0}{a} \left[\left(\cancel{\frac{a}{2}} + \delta - \frac{a}{2n\pi} \sin\left(\frac{2n\pi\left(\frac{a}{2}+\delta\right)}{a}\right) \right) - \left(\cancel{\frac{a}{2}} - \delta - \frac{a}{2n\pi} \sin\left(\frac{2n\pi\left(\frac{a}{2}-\delta\right)}{a}\right) \right) \right]$$

$$= \frac{V_0}{a} \left[2\delta - \frac{a}{2n\pi} \sin\left(\frac{2n\pi\left(\frac{a}{2}+\delta\right)}{a}\right) + \frac{a}{2n\pi} \sin\left(\frac{2n\pi\left(\frac{a}{2}-\delta\right)}{a}\right) \right]$$

$$= \frac{V_0}{a} \left[2\delta - \frac{a}{2n\pi} \left(\cancel{\sin(n\pi) \cos\left(\frac{2n\pi\delta}{a}\right)} + \cos(n\pi) \sin\left(\frac{2n\pi\delta}{a}\right) \right) + \frac{a}{2n\pi} \left(\cancel{\sin(n\pi) \cos\left(\frac{2n\pi\delta}{a}\right)} - \cos(n\pi) \sin\left(\frac{2n\pi\delta}{a}\right) \right) \right]$$

$$\boxed{E^{(1)} = \frac{V_0}{a} \left[2\delta - \frac{a}{n\pi} \cos(n\pi) \sin\left(\frac{2n\pi\delta}{a}\right) \right]}$$

As $n \to \infty$, we have $E^{(1)} = \frac{2V_0\delta}{a}$.

(d)

As $\delta \to 0$, we have

$$V'(x) = V_0\, \delta\left(x - \frac{a}{2}\right).$$

So our energy correction to first order is

$$E^{(1)} = \langle n | V' | n \rangle$$

$$= \langle n | V_0\, \delta\left(x - \frac{a}{2}\right) | n \rangle$$

$$= V_0 \int_0^a \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right) \delta\left(x - \frac{a}{2}\right) dx$$

$$= \frac{2V_0}{a} \sin^2\left(\frac{n\pi (a/2)}{a}\right)$$

$$= \frac{2V_0}{a} \sin^2\left(\frac{n\pi}{2}\right)$$

$$\boxed{E^{(1)} = \frac{2V_0}{a} \begin{cases} 0 , & n \in \text{evens} \\ 1 , & n \in \text{odds} \end{cases}}$$

This result makes sense given that our wavefunction has a node in the center of the well (at $x = a/2$) for even values of n. Thus, I would expect no effect from the perturbation for $n \in$ evens.

(e)

As $\delta \to a/2$, we have a constant perturbation of V_0 for $0 < x < a$. So

$$E^{(1)} = \langle n | V_0 | n \rangle$$
$$= V_0 \int_0^a \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right) dx$$
$$= \frac{2V_0}{a} \int_0^a \frac{1}{2} \left(1 - \cos\left(\frac{2n\pi x}{a}\right)\right) dx$$
$$= \frac{V_0}{a} \left[x - \frac{a}{2n\pi} \sin\left(\frac{2n\pi x}{a}\right) \right] \Big|_0^a$$

$$\boxed{E^{(1)} = V_0}$$

This is to be expected since the perturbation is constant throughout the well.