Square Well with a Bump

$$\hat{H}_0 = \frac{\hat{p}^2}{2M} + V(\hat{x}) \quad \text{where} \quad V(x) = \begin{cases} \infty & L < x \\ 0 & 0 < x < L \\ \infty & x < 0 \end{cases}$$

$$\hat{H}' = V'(\hat{x}) \quad \text{where} \quad V'(x) = \begin{cases} 0 & (L+a)/2 < x \\ V & (L-a)/2 < x < (L+a)/2 \\ 0 & x < (L-a)/2 \end{cases}$$

The first-order **energy corrections** are

$$\begin{aligned}
E_n^{(1)} &= \langle \eta_n | \hat{H}' | \eta_n \rangle \\
&= \int_{(L-a)/2}^{(L+a)/2} \eta_n^*(x)\, V\, \eta_n(x)\, dx \\
&= \frac{2}{L} V \int_{(L-a)/2}^{(L+a)/2} \sin^2\left(n\pi \frac{x}{L}\right) dx \quad [\![\text{Use } u = n\pi x/L \text{ giving}\ldots]\!] \\
&= \frac{2}{L} V \int_{n\pi(1-a/L)/2}^{n\pi(1+a/L)/2} \sin^2 u\, \frac{L}{n\pi}\, dx \quad [\![\text{Use Dwight 430.20 giving}\ldots]\!] \\
&= \frac{2}{n\pi} V \left[\frac{1}{2} u - \frac{1}{4} \sin(2u) \right]_{n\pi(1-a/L)/2}^{n\pi(1+a/L)/2} \\
&= \frac{2}{n\pi} V \left[\frac{1}{2}\left(n\pi \frac{a}{L}\right) - \frac{1}{4}\left(\sin(n\pi(1+a/L)) - \sin(n\pi(1-a/L)) \right) \right] \quad [\![\text{Use Dwight 401.09 giving}\ldots]\!] \\
&= \frac{2}{n\pi} V \left[\frac{1}{2}\left(n\pi \frac{a}{L}\right) - \frac{1}{4}\left(2 \sin\left(\tfrac{1}{2}(n\pi 2a/L)\right) \cos\left(\tfrac{1}{2}(2n\pi)\right) \right) \right] \\
&= V \left[\frac{a}{L} - \frac{1}{n\pi} \sin(n\pi a/L)(-1)^n \right]
\end{aligned}$$

The first-order correction to an **energy eigenfunction** is

$$|n^{(1)}\rangle = \sum_{m \neq n} |m^{(0)}\rangle \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}.$$

In this case we're thinking about the ground state, $n = 1$, and

$$E_1^{(0)} - E_m^{(0)} = (1 - m^2) \frac{\pi^2 \hbar^2}{2ML^2}$$

where M is the mass and m is a summation index. Thus the correction is

$$\eta_1^{(1)}(x) = -\frac{2ML^2}{\pi^2 \hbar^2} \sum_{m=2}^{\infty} \eta_m(x) \frac{H'_{m1}}{m^2 - 1}.$$

We need

$$
\begin{aligned}
H'_{m1} &= \langle \eta_m | \hat{H}' | \eta_1 \rangle \\
&= \int_{(L-a)/2}^{(L+a)/2} \eta_m^*(x)\, V\, \eta_1(x)\, dx \\
&= \frac{2}{L} V \int_{(L-a)/2}^{(L+a)/2} \sin\left(m\pi \frac{x}{L}\right) \sin\left(\pi \frac{x}{L}\right)\, dx \quad [\![\text{Use } u = \pi x/L \text{ giving}\ldots]\!] \\
&= \frac{2}{L} V \int_{\pi(1-a/L)/2}^{\pi(1+a/L)/2} \sin(mu)\sin(u)\, \frac{L}{\pi}\, dx \quad [\![\text{Use Dwight 435 giving}\ldots]\!] \\
&= \frac{2}{\pi} V \left[\frac{\sin[(m-1)u]}{2(m-1)} - \frac{\sin[(m+1)u]}{2(m+1)} \right]_{\pi(1-a/L)/2}^{\pi(1+a/L)/2} \\
&= \frac{2}{\pi} V \left[\frac{\sin[(m-1)\pi(1+a/L)/2] - \sin[(m-1)\pi(1-a/L)/2]}{2(m-1)} \right. \\
&\qquad \left. - \frac{\sin[(m+1)\pi(1+a/L)/2] - \sin[(m+1)\pi(1-a/L)/2]}{2(m+1)} \right] \\
&\qquad\quad [\![\text{Use Dwight 401.09 giving}\ldots]\!] \\
&= \frac{2}{\pi} V \left[\frac{2\sin[(m-1)\pi(a/L)/2]\cos[(m-1)\pi/2]}{2(m-1)} - \frac{2\sin[(m+1)\pi(a/L)/2]\cos[(m+1)\pi/2]}{2(m+1)} \right].
\end{aligned}
$$

But

$$
\cos\frac{N\pi}{2} = \begin{cases} 0 & \text{when} \quad N \quad \text{odd} \\ +1 & \text{when} \quad N/2 \quad \text{odd} \\ -1 & \text{when} \quad N/2 \quad \text{even.} \end{cases}
$$

So, when m is even, H'_{m1} vanishes. (Challenge: Can you see this fact at a glance using symmetry under reflection?) When m is odd and $(m-1)/2$ is odd then

$$
\cos[(m-1)\pi/2] = +1 \quad \text{and} \quad \cos[(m+1)\pi/2] = -1.
$$

But when m is odd and $(m-1)/2$ is even then

$$
\cos[(m-1)\pi/2] = -1 \quad \text{and} \quad \cos[(m+1)\pi/2] = +1.
$$

So when m is odd

$$
H'_{m1} = \frac{2}{\pi} V \left[\frac{\sin[(m-1)\pi a/2L]}{m-1} + \frac{\sin[(m+1)\pi a/2L]}{m+1} \right] (-1)^{(m+1)/2}.
$$

All together,

$$
\eta_1^{(1)}(x) = \frac{4ML^2V}{\pi^3\hbar^2} \sum_{m=3,\ \text{odd}}^{\infty} \eta_m(x)(-1)^{(m-1)/2} \left[\frac{\sin[(m-1)\pi a/2L]}{(m-1)^2(m+1)} + \frac{\sin[(m+1)\pi a/2L]}{(m-1)(m+1)^2} \right].
$$

You can write out many different forms for this sum, but as far as I can see no one form is particularly "simpler" than any other, so I'll just let it rest as it stands.

Notice that while the perturbing bump is located only in a region of width a at the center of the well, the ground state wavefunction is affected both inside and outside of that region. How can the bump at the center affect the wavefunction outside of that region? How can the bump at one place affect the particle at some other place, a place where the bump is not?

Remember that in this energy eigenstate, the particle doesn't have a position. If you think something like "the bump over here can't affect the particle over there", then you're thinking that the particle has a position "over there", and that's wrong: The particle doesn't have a position.

In the case $a = L$, the bump is as wide as the well. Thus the problem is the infinite square well again, but with the minimum potential energy called V rather then called 0. The exact solution is easy: all the energy eigenfunctions remain as they were, and all the energy eigenvalues shift up by V.

What does first-order perturbation theory say in this case? The first-order energy corrections are exactly V, and the first-order corrections to the ground state vanish! So in these situations first-order perturbation theory gives the exact correct answer. Talk about luck!

⟦*Grading:* 4 points for energy correction, 5 points for wavefunction correction, 1 point for discussion.⟧