INFINITE SQUARE WELL - CENTERED COORDINATES

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.36.

We've analyzed the infinite square well potential in the case where the potential is

$$V(x)=\begin{cases}0 & 0<x<a\\ \infty & \text{otherwise}\end{cases} \tag{1}$$

A variant on this is the potential

$$V(x)=\begin{cases}0 & -a<x<a\\ \infty & \text{otherwise}\end{cases} \tag{2}$$

This is an even potential, with a width twice that of the original potential. Because it's even, solutions of the Schrödinger equation can be taken as either even or odd. Where the potential is infinite, the wave function is zero, so we are left with finding solutions in the central region $-a<x<a$, where we must solve

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{3}$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \tag{4}$$

$$\text{with } k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{5}$$

An even solution is

$$\psi_e(x)=A\cos(kx) \tag{6}$$

Since the solution is even, the boundary conditions at the two ends of the well give the same equation. Also, since the potential is infinite at the boundaries, we cannot impose continuity of ψ', so the only condition comes from the continuity of ψ itself. This gives

$$A\cos(ka)=0 \tag{7}$$

From this we obtain a condition on k and thus on the energy:

$$k = (2n+1)\frac{\pi}{2a} \tag{8}$$

$$E = \frac{(2n+1)^2\hbar^2\pi^2}{2m(2a)^2} \tag{9}$$

If we compare this with the energies for the original square well, which are

$$E=\frac{n^2\pi^2\hbar^2}{2ma^2} \tag{10}$$

we see that we have the *odd* quantum numbers represented for a well of width $2a$.

If we make the coordinate substitution $x'=(x+a)/2$ (so $x=2x'-a$) which transforms our double-width square well back to the single-widthoriginal, our even solution becomes

$$\psi_e(x') = A\cos\left((2n+1)\frac{\pi}{a}x'-(2n+1)\frac{\pi}{2}\right) \tag{11}$$

$$= (-1)^n A\sin\left((2n+1)\frac{\pi}{a}x'\right) \tag{12}$$

This corresponds to the odd-numbered solutions we got for the original square well (we can get A by normalization as usual; the extra factor of $(-1)^n$ cancels out when we take the square modulus so doesn't affect the physical content of the solution).

We can do a similar analysis with the odd solution. We have

$$\psi_o(x)=B\sin(kx) \tag{13}$$

The boundary condition (again there is only one such condition that gives a unique equation) gives us

$$B\sin(ka)=0 \tag{14}$$

from which we get

$$k = \frac{\pi n}{a} \tag{15}$$

$$= \frac{2n\pi}{2a} \tag{16}$$

$$E = \frac{(2n)^2 \hbar^2 \pi^2}{2m(2a)^2} \tag{17}$$

We've inserted the extra factor of 2 into the numerator and denominator in the second line to show that, for a well of width $2a$, we get the *even* numbered quantum states.

Using the same variable substitution on the wave function, we get

$$\psi_o(x') = B\sin\left(\frac{2n\pi}{a}x' - n\pi\right) \tag{18}$$

$$= (-1)^n B\sin\left(\frac{2n\pi}{a}x'\right) \tag{19}$$

We recover the original wave functions, apart from a different normalization.

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