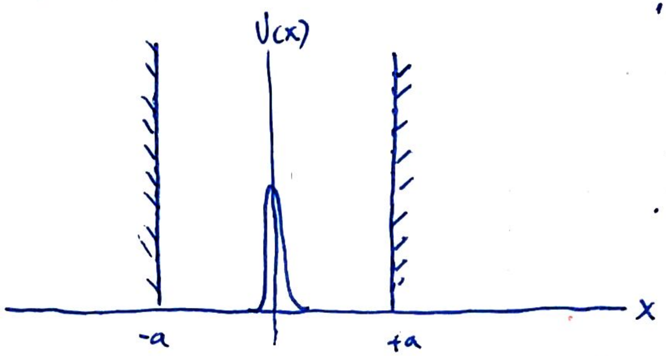
More Solving Schrödinger's Equation (Problem 2.44 in Griffith's QM 2nd Ed.)

Solve the time-independent Schrödinger equation for a centered infinite square well with a delta-function barrier in the middle:

$$V(x) = \begin{cases} \alpha\delta(x), & \text{for } -a < x < a \\ \infty, & \text{for } |x| \geq a \end{cases}$$

- Find the allowed energies.
- How do they compare with those in the absence of the delta function?
- Comment on the limiting cases $\alpha \to 0$, $\alpha \to \infty$.



S.E. $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \alpha\delta(x)\psi(x) = E\psi(x)$$

Remember to break your solutions up into <u>regions</u> around the delta function.

You already know the solutions for the infinite square well without the delta-function, we can use those in the regions on either side:

$-a < x < 0$: $\psi_1(x) = A\sin(kx) + B\cos(kx)$ $\qquad k = \frac{\sqrt{2mE}}{\hbar}$

$0 < x < a$: $\psi_2(x) = C\sin(kx) + B\cos(kx)$

* Important: Potential $V(x)$ is even. Can separate and treat even/odd solutions!

Even solutions: $\psi_1^e(x) = A\sin(Kx) + B\cos(Kx)$
$\psi_2^e(x) = -A\sin(Kx) + B\cos(Kx)$

Boundary conditions: $\psi_1^e(-a) = 0 = \psi_2^e(a)$

$$\psi_1^e(-a) = A\sin(-Ka) + B\cos(-Ka) = 0$$

$$-A\sin(Ka) + B\cos(Ka) = 0$$

$$\psi_2^e(a) = -A\sin(Ka) + B\cos(Ka) = 0$$

Same condition.

$$\Rightarrow \quad A\sin(Ka) = B\cos(Ka)$$

$$\Rightarrow \quad \tan(Ka) = \frac{B}{A}$$

Continuity: $\psi_1^e(0) = \psi_2^e(0)$

$$A\cancel{\sin(0)} + B\cancel{\cos(0)} = -A\cancel{\sin(0)} + \cancel{B}\cos(0) \quad ✓$$

Good to check.

What about the derivatives? $\frac{d\psi_1^e}{dx}$, $\frac{d\psi_2^e}{dx}$?

Recall: $$\left.\frac{d\psi}{dx}\right|_+ - \left.\frac{d\psi}{dx}\right|_- = \frac{2m\alpha}{\hbar^2}\psi(0)$$

$$\left.\frac{d\psi}{dx}\right|_+ \Rightarrow \frac{d}{dx}(\psi_2^e) = -AK\cos(Kx) - BK\sin(Kx)$$

$$\left.\frac{d\psi}{dx}\right|_- \Rightarrow \frac{d}{dx}(\psi_1^e) = AK\cos(Kx) - BK\sin(Kx)$$

$$\frac{d\psi_2^e}{dx} - \frac{d\psi_1^e}{dx} = -AK\cos(Kx) - \cancel{BK\sin(Kx)} - AK\cos(Kx) + \cancel{BK\sin(Kx)}$$

$$= -2AK\cos(Kx)$$

$$\lim_{x\to 0} -2AK\cos(Kx) = -2AK$$

$$-2AK = \frac{2m\alpha}{\hbar^2}\psi(0) \qquad \psi(0) = B$$

$$-\cancel{2}AK = \frac{\cancel{2}m\alpha}{\hbar^2} B \quad \Rightarrow \quad B = -\frac{K\hbar^2}{m\alpha} A$$

But we know $B = A\tan(Ka)$

$$\Rightarrow \quad \cancel{A}\tan(Ka) = -\frac{K\hbar^2}{m\alpha}\cancel{A}$$

$$\text{so} \quad \tan(Ka) = -\frac{K\hbar^2}{m\alpha}$$

From what you've seen in class, this equation usually gives you K, and hence E.

In this case, the solutions aren't so obvious!

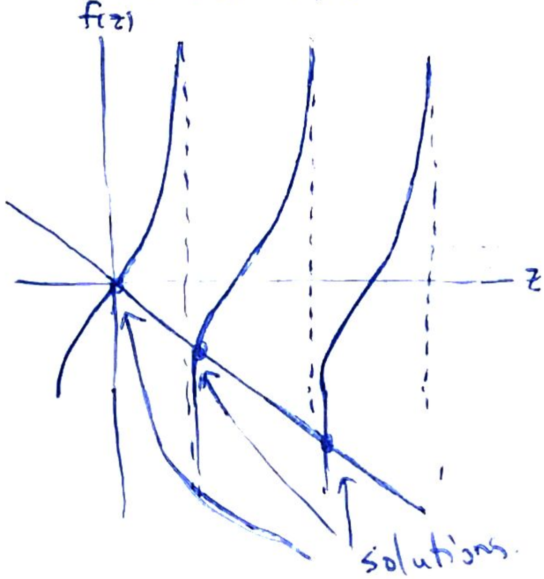
Let $z \equiv Ka$ and multiply by a/a on R.H.S.

$$\tan(Ka) = -Ka\frac{\hbar^2}{m\alpha a}$$

$$\Rightarrow \quad \tan(z) = -\frac{\hbar^2}{m\alpha a} z$$

Solve numerically/graphically for z.

What does this mean in English? The solutions are where $\tan(z)$ and $(\#) z$ intersect. For now let $\frac{\hbar^2}{m\alpha a} = 1$



Only care about $z > 0$, since $K > 0$, $a > 0$.

Infinite solutions!

Odd Solutions: $\psi_1^o(x) = A\sin(Kx) + B\cos(Kx)$

$\psi_2^o(x) = A\sin(Kx) - B\cos(Kx)$

Continuity. $\psi_1^o(0) = \psi_2^o(0)$

$B = -B \Rightarrow B = 0.$

So, $\psi_1^o(x) = \psi_2^o(x)$ and derivative automatically is continuous.

Boundary Conditions:

$\psi_1^o(a) = A\sin(Ka) = 0$

$Ka = n\pi, \quad n = 0, 1, 2, \ldots$

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

$\Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ Write in terms of $L \equiv 2a$.

$E_n = \frac{(2n)^2\pi^2\hbar^2}{2mL^2}$ } only even energy levels stay the same (because odd wavefunctions are unaffected)

Limiting cases: $\alpha \to 0$:

$\lim_{\alpha\to 0} \tan(z) = \lim_{\alpha \to 0} \frac{-\hbar^2}{m\alpha a} z = \infty \Rightarrow z \to (2n+1)\frac{\pi}{2}$

$n = 0, 1, 2, \ldots$

so, $z = Ka = (2n+1)\pi/2$

$\Rightarrow E_n = \frac{(2n+1)^2\pi^2\hbar^2}{2mL^2}$ } We get back the odd energy levels.

$\alpha \to \infty$: $\lim_{\alpha\to\infty} \tan(z) = 0 \Rightarrow z = n\pi, \quad n = 0, 1, 2, \ldots$

so $z = Ka = n\pi$

$\Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ } Normal energy levels in half-width.