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Quantum Mechanics I
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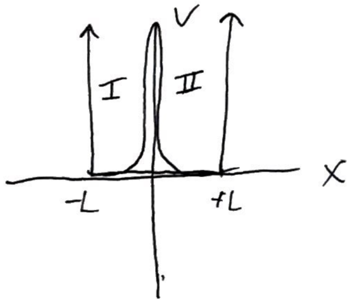
HW 6 Solutions

1. Infinite well with delta function barrier:

Let's first shift the well to be centered. We can do this because for this problem statement, we only care about the energies & sketching the wavefunction, but we'd have to be more careful if we wanted the actual wavefunctions.



$$V(x) = \begin{cases} \alpha\,\delta(x) & -L < x < L \\ \infty & \text{else} \end{cases}$$

We wanted a centered well because now it is easy to see that the potential is even, $V(x) = V(-x)$.

So we can use our knowledge from HW4 Bonus problem: the solutions must be either even or odd.

For both regions $-L < x < 0$ & $0 < x < L$, $V = 0$, so Schrödinger eqn reads:

$$\frac{\partial^2\psi}{\partial x^2} = -\underbrace{\frac{2mE}{\hbar^2}}_{k^2}\psi \quad \rightarrow \quad \begin{aligned} \psi_I &= A\sin(kx) + B\cos(kx) \\ \psi_{II} &= C\sin(kx) + D\cos(kx) \end{aligned}$$

Even solutions

The even solutions require $\psi(x) = \psi(-x)$, so $\psi_I(x) = \psi_{II}(-x)$:

$$A\sin(kx) + B\cos(kx) = C\sin(-kx) + D\cos(-kx) = -C\sin(kx) + D\cos(kx)$$

Matching terms, $A = -C$ & $B = D$

BC @ $x=-L$, continuity: $\psi_I(-L) = 0$

$$0 = A\sin(-kL) + B\cos(kL) \rightarrow A = B\frac{\cos(kL)}{\sin(kL)} = B\cot(kL) \Rightarrow \boxed{\begin{aligned} \psi_I &= B[\sin(kx)\cot(kL) + \cos(kx)] \\ \psi_{II} &= B[-\sin(kx)\cot(kL) + \cos(kx)] \end{aligned}}$$

BC @ $x=0$, discontinuity of derivative:

Start from Schrödinger eqn @ $x=0$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \alpha\,\delta(x)\psi = E\psi \longrightarrow \text{integrate from } -\epsilon \text{ to } \epsilon: \quad \underbrace{-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{\partial^2\psi}{\partial x^2}dx}_{-\frac{\hbar^2}{2m}\left(\frac{\partial\psi}{\partial x}\Big|_{0^+} - \frac{\partial\psi}{\partial x}\Big|_{0^-}\right)} + \underbrace{\alpha\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)dx}_{\alpha\psi(0)} = \underbrace{E\int_{-\epsilon}^{\epsilon}\psi(x)dx}_{0 \text{ because}}$$

taking the limit as $\epsilon \to 0$:

$\left(\frac{\partial\psi}{\partial x}\Big|_{0^+} - \frac{\partial\psi}{\partial x}\Big|_{0^-}\right)$: $\Delta\frac{\partial\psi}{\partial x}$

plugging 0 into ψ_I, $\psi(0) = B$

0 because ψ normalizable, so at any given point, integral is infinitesimal

$$\Rightarrow \Delta\frac{\partial\psi}{\partial x} = +\frac{2m\alpha}{\hbar^2}B \quad (\star)$$

Now we can also calculate $\Delta\frac{\partial\psi}{\partial x}$ from our ψ solutions:

$$\underset{(+0\text{ side})}{\frac{\partial\psi_{II}}{\partial x}(0)} - \underset{(-0\text{ side})}{\frac{\partial\psi_I}{\partial x}(0)} = B\left[\left(-k\underbrace{\cos(k0)}_{1}\cot(kL) - k\underbrace{\sin(k0)}_{0}\right) - \left(k\underbrace{\cos(k0)}_{1}\cot(kL) - k\underbrace{\sin(k0)}_{0}\right)\right] = -2Bk\cot(kL)$$

minus

Plugging this into ☆,

rewriting so have same variable in both sides

$$-2Bk\cot(kL) = +\frac{2m\alpha}{\hbar^2}B \Rightarrow \cot(kL) = -\frac{m\alpha}{k\hbar^2} \Rightarrow \tan(kL) = -\frac{k\hbar^2}{m\alpha} = -\frac{\hbar^2}{m\alpha L}kL$$

This equation, $\boxed{\tan(kL) = -\left(\frac{\hbar^2}{m\alpha L}\right)kL}$ is a transcendental equation whose solutions give us k.

The energies are then $\boxed{E_n^{even} = \frac{\hbar^2 k_n^2}{2m}}$.

<u>Odd Solutions</u>

We now find the odd ψ's, $\psi_I(x) = -\psi_{II}(-x)$

$$\Rightarrow A\sin(kx) + B\cos(kx) = -C\sin(-kx) - D\cos(-kx) = C\sin(kx) - D\cos(kx)$$

$\Rightarrow A = C,\ D = -B$

BC: continuity @ $x=0$: $\psi_I(0) = \psi_{II}(0)$

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

So for both sides of the well we have the same solution, $\boxed{\psi_I = \psi_{II} = A\sin(kx)}$
(we see that it is already continuous on the derivative at $x=0$!)

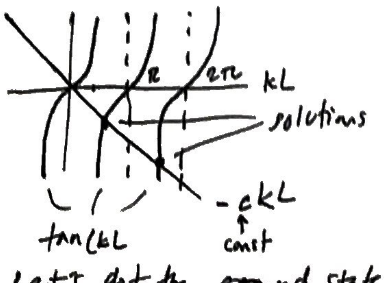
BC: continuity @ $x=L$: $\psi_{II}(L) = 0 \to$ bc ψ goes to infinity @ L

$$\Rightarrow A\sin(kL) = 0 \Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L},\ n = 1, 2, \cdots$$

Thus the energies are, $\boxed{E_n^{odd} = \frac{\hbar^2\pi^2 n^2}{2mL^2}}$

Now let's try to figure out how these energies compare to the plain infinite square well.
We can rewrite $E_n^{odd} = \frac{\hbar^2\pi^2(2n)^2}{2m(2L)^2}$, which are just the even-n solutions to the inf. well with width $2L$ (as we have here). So these are just the regular ~~odd~~ wavefunctions.

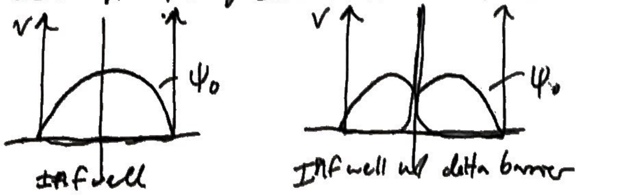
For the even energies, let's sketch the transcendental equation:



We see that the lowest-k solution falls between $\frac{\pi}{2} < kL < \pi$,
so $E_1 = \frac{\hbar^2(k_1 L)^2}{2mL^2} \Rightarrow \frac{\hbar^2\pi^2}{2m(2L)^2} < E_1 < \frac{4\hbar^2\pi^2}{2m(2L)^2}$.

The lower bound is the ground state energy of the regular well!
So adding the delta function barrier $\boxed{\text{increases the ground state energy}}$.

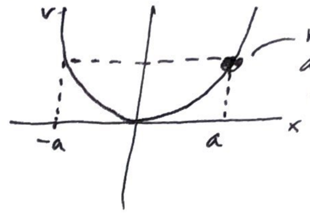
Let's plot the ground state wavefunctions:



When $\alpha \to \infty$, it divides the well into 2; we get $\tan(kL) \to 0 \Rightarrow kL = n\pi \to k = \frac{n\pi}{L}$, so for the ground state $n=1$, $E_1 = \frac{\hbar^2\pi^2}{2mL^2}$ — the ground state energy of a well of width L (half the original width).

2. HO: prob. of finding particle outside classical region?

For a classical oscillator, the energy is $E = T + V$, where T is the kinetic energy and $V = \frac{1}{2}kx^2$ (can be found from $F = -\frac{\partial V}{\partial x}$, and we know $F = -kx$, for a HO). The particle will be at its maximum amplitude in the oscillation "a" when all of the energy is potential (its turning around so $V=0$), so $E = \frac{1}{2}ka^2$. with $\omega = \sqrt{\frac{k}{m}} \Rightarrow k = m\omega^2$, we have $E = \frac{1}{2}m\omega^2 a^2$. Solving for a, $a = \sqrt{\frac{2E}{m\omega^2}}$, so the classically allowed region is $-\sqrt{\frac{2E}{m\omega^2}} < x < \sqrt{\frac{2E}{m\omega^2}}$ $(-a < x < a)$.



Let's first find the probability that, in the <u>ground state of the HO</u>, the particle is outside to the left:

$$P(x<-a) = \int_{-\infty}^{-a} |\psi_0|^2 dx = \alpha^2 \int_{-\infty}^{-a} e^{-\frac{m\omega}{\hbar}x^2} dx \quad \text{where } \alpha = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$$

Now for the ground state, $E_0 = \frac{1}{2}\hbar\omega$, so $a = \sqrt{\frac{2E_0}{m\omega^2}} = \sqrt{\frac{2(\frac{1}{2}\hbar\omega)}{m\omega^2}} = \sqrt{\frac{\hbar}{m\omega}}$, so $\frac{m\omega}{\hbar} = \frac{1}{a^2}$.

$$\Rightarrow P(x<-a) = \alpha^2 \int_{-\infty}^{-a} e^{-x^2/a^2} dx.$$

Now let's change variables to get the form of the integral to be that of the standard Normal Distribution:

$$\frac{x^2}{a^2} = \frac{t^2}{2} \Rightarrow x = \frac{1}{\sqrt{2}}at, \quad dx = \frac{1}{\sqrt{2}}a\,dt, \quad t = \sqrt{2}\frac{x}{a}, \quad \text{so boundary } -a \to \sqrt{2}\left(\frac{-a}{a}\right) = -\sqrt{2}, \quad -\infty \to -\infty$$

$$\Rightarrow P(x<-a) = \alpha^2 \int_{-\infty}^{-\sqrt{2}} e^{-t^2/2}\left(\frac{1}{\sqrt{2}}a\,dt\right) = \frac{1}{\sqrt{2}}a\alpha^2 \int_{-\infty}^{-\sqrt{2}} e^{-t^2/2} dt$$

We can look up this integral in a table (e.g. "standard Normal Table" on wikipedia), and see that $\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{-\sqrt{2}} e^{-\frac{t^2}{2}} dt = 0.0793$. Plugging it all in:

$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{\hbar}{m\omega}}\right)\left(\sqrt{\frac{m\omega}{\pi\hbar}}\right)\left[\sqrt{2\pi}\cdot 0.0793\right] = 0.0793$$

everything else cancels

So, given that the potential is even, $P(x>a) = 0.0793$ also, and

$$\boxed{P(\text{outside classical}) = P(x<-a) + P(x>a) = 2\cdot 0.0793 = \boxed{0.159}}$$

$\psi_0 = \alpha e^{-\frac{1}{2}\xi^2}$ $\psi_1 = \alpha\sqrt{2}\,\xi e^{-\frac{1}{2}\xi^2}$, $\alpha = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$, $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$

3. HO Potential: $\psi(x,0) = A[3\overbrace{\psi_0(x)} + 4\overbrace{\psi_1(x)}]$

a) $1 = \int|\psi(x,0)|^2dx = A^2\int\Big[9\underbrace{|\psi_0|^2}_{1} + 16\underbrace{|\psi_0|^2}_{1} + 12\underbrace{\psi_0^*\psi_1}_{0} + 12\underbrace{\psi_1^*\psi_0}_{0}\Big]dx$

by orthogonality under the integral:

$= A^2 \cdot 25 \Rightarrow A^2 = \frac{1}{25} \Rightarrow \boxed{A = \frac{1}{5}}$

b) $\boxed{\psi(x,t)} = \sum_n c_n \psi_n e^{-itE_n/\hbar}$, $E_n = (n+\frac{1}{2})\hbar\omega$ for HO

$= \boxed{\frac{1}{5}\left[3\psi_0 e^{-\frac{1}{2}i\omega t} + 4\psi_1 e^{-\frac{3}{2}i\omega t}\right]}$

$\boxed{|\psi(x,t)|^2} = \frac{1}{25}\left[9|\psi_0|^2 + 16|\psi_1|^2 + 12\psi_0^*\psi_1 e^{-i\omega t} + 12\psi_1^*\psi_0 e^{i\omega t}\right]$

$= \boxed{\frac{1}{25}\left[9|\psi_0|^2 + 16|\psi_1|^2 + 24\psi_0\psi_1\cos(\omega t)\right]}$ using euler's identity & fact that ψ_0, ψ_1 are real

c) $\langle x\rangle = \int_{-\infty}^{\infty} x|\psi(x,t)|^2dx$

$= \frac{1}{25}\int_{-\infty}^{\infty}\Big[\underbrace{9|\psi_0|^2x}_{I_1} + \underbrace{16|\psi_1|^2x}_{I_2} + 24\underbrace{\psi_0\psi_1 x}_{I_3}\cos(\omega t)\Big]dx$

$I_1 = \alpha^2\int_{-\infty}^{\infty} x e^{-\xi^2}dx = \alpha^2\int_{-\infty}^{\infty} x e^{-\frac{m\omega}{\hbar}x^2} = 0$ because integrand is odd func (x) · even func (e^{-x^2}) = odd func

$I_2 = 2\alpha\int_{-\infty}^{\infty}\xi^2 x e^{-\xi^2}dx = 2\alpha^2\left(\frac{m\omega}{\hbar}\right)\int x^3 e^{-\frac{m\omega}{\hbar}x^2} = 0$ by same reason, here x^3 is odd

$I_3 = \sqrt{2}\alpha^2\int_{-\infty}^{\infty}\xi x e^{-\xi^2}dx = \sqrt{2}\alpha^2\sqrt{\frac{m\omega}{\hbar}}\underbrace{\int_{-\infty}^{\infty}x^2 e^{-\frac{m\omega}{\hbar}x^2}dx}$

use integrals given in previous HW: $\frac{\hbar}{2m\omega}\int_{-\infty}^{\infty}e^{-\frac{m\omega}{\hbar}x^2}dx = \frac{\hbar}{2m\omega}\sqrt{\frac{\pi\hbar}{m\omega}}$

$= \sqrt{2}\alpha^2\left(\frac{\hbar}{2m\omega}\right)\sqrt{\pi} = \sqrt{2}\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\pi}\left(\frac{\hbar}{2m\omega}\right) = \sqrt{\frac{\hbar}{2m\omega}}$

$\Rightarrow \boxed{\langle x\rangle = \frac{1}{25}\left(24\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t)\right) = \frac{24}{25}\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t)}$

$\boxed{\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -\frac{24}{25}m\sqrt{\frac{\hbar}{2m\omega}}\,\omega\sin(\omega t) = -\frac{24}{25}\sqrt{\frac{\hbar m\omega}{2}}\sin(\omega t)}$

d) $E_0 = \frac{1}{2}\hbar\omega$ with probability $|c_0|^2 = \left(\frac{3}{5}\right)^2 = \boxed{\frac{9}{25}}$

$E_1 = \frac{3}{2}\hbar\omega$ with probability $|c_1|^2 = \left(\frac{4}{5}\right)^2 = \boxed{\frac{16}{25}}$