HW 4 Solutions

TA: Kate Storey-Fisher
Prof: Javad Shabani
Quantum Mechanics I
Fall 2021

1. Let's consider the Schrödinger eqn:

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

There are multiple ways to think about this problem; we'll show 2 here:

Method I

Let's multiply the whole Schrödinger eqn by ψ^* and integrate from $-\infty$ to ∞:

$$\underbrace{-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi^*\frac{d^2\psi}{dx^2}dx}_{I_T} + \underbrace{\int\psi^* V\psi\,dx}_{I_V} = \underbrace{\int\psi^* E\psi\,dx}_{I_E}$$

I_T: notice that we can write the integral as $\int_{-\infty}^{\infty}\psi^*\frac{p^2}{2m}\psi\,dx = \frac{1}{2m}\int_{-\infty}^{\infty}(p^*\psi^*)(p\psi)\,dx$ where $p = -i\hbar\frac{\partial}{\partial x}$. Now $p^*\psi^*$ must equal $p\psi$, and $|p\psi|^2$ must be positive, because ~~square~~ the norm must always be positive (the $*$'s get rid of any i issues). So $I_T \geq 0$

I_V: The potential V will be greater than or equal to the minimum, ~~velocity~~ potential V_0 at all points (by definition), so the integral will also be $\geq V_0$:

$$I_V \geq \int\psi^* V_0\psi\,dx = V_0\underbrace{\int\psi^*\psi\,dx}_{1} = V_0 \implies I_V \geq V_0$$

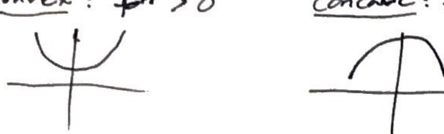
I_E: Here we just get the energy back because it's just a number: $I_E = E\overbrace{\int\psi^*\psi\,dx}^{1} = E$

So: If $I_T \geq 0$ & $I_V \geq V_0$, then $I_T + I_V \geq V_0$. $I_T + I_V = I_E = E$, so $\boxed{E \geq V_0}$; the energy is always greater than the minimum of the potential $V(x)$, V_0.
For this proof we assumed we could normalize ψ, $\int\psi^*\psi\,dx = 1$, so this only holds for normalizeable solutions.

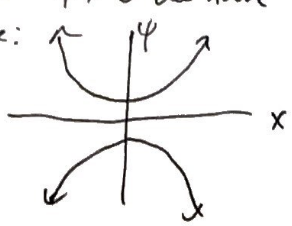
Method II

Looking at our 2nd version of the Schrödinger eqn above, we see that if we ever have $E < V$, then we will have $\frac{d^2\psi}{dx^2} = k^2\psi$ where $k^2 > 0$. This means that ψ & $\frac{d^2\psi}{dx^2}$ have the same sign. Recall the definitions of convexity & concavity:

convex: $f'' > 0$ concave: $f'' < 0$



So if for $\psi > 0$ we have $\psi'' > 0$ and for $\psi < 0$ we have $\psi'' < 0$, our wavefunction must look like:



But look, this isn't a normalizeable wavefunction, it goes to ∞ at $x \to \pm\infty$! So for solutions to Schröd to be normalizeable, we cannot have $E < V$; rather, we need $\boxed{E > V_0}$ $\rightarrow$ V_0 is minimum of potential.

2. Particle in infinite square well: $\psi(x,0) = A[\psi_1(x) + \psi_2(x)]$

a) Normalize: $1 = \int_{-\infty}^{\infty} |\psi|^2 dx = A^2 \int_{-\infty}^{\infty} [\underbrace{\psi_1^*\psi_1}_{1} + \underbrace{\psi_2^*\psi_2}_{1} + \underbrace{\psi_1^*\psi_2}_{0} + \underbrace{\psi_2^*\psi_1}_{0}] dx$ → when integrate over all space, because eigenstates are orthogonal!

$= A^2 \cdot 2 \Rightarrow A^2 = \frac{1}{2} \rightarrow \boxed{A = \frac{1}{\sqrt{2}}}$

b) $\psi(x,t) = \sum_n c_n \psi_n e^{-itE_n/\hbar}$

We can "read off" the c_n's from $\psi(x,0)$: $c_1 = \frac{1}{\sqrt{2}}$, $c_2 = \frac{1}{\sqrt{2}}$,

From the inf sq. well, we know $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ & $E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}$, so:

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x) e^{-itE_1/\hbar} + \psi_2(x) e^{-itE_2/\hbar}\right] = \frac{1}{\sqrt{a}}\left[\sin\left(\frac{\pi x}{a}\right) e^{-it\frac{\hbar\pi^2}{2ma^2}} + \sin\left(\frac{2\pi x}{a}\right) e^{-it\frac{4\hbar\pi^2}{2ma^2}}\right]}$$

c) $\langle x \rangle = \int_0^a x \psi^* \psi \, dx = \frac{1}{a}\int \Big[\underbrace{x\sin^2\left(\frac{\pi x}{a}\right)}_{I_1} + \underbrace{x\sin^2\left(\frac{2\pi x}{a}\right)}_{I_2} + \underbrace{\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\left[e^{-it\frac{3\hbar\pi^2}{2ma^2}} + e^{it\frac{3\hbar\pi^2}{2ma^2}}\right]}_{I_3}\Big]$

outside of box, $\psi = 0$!

$I_1 = \int_0^a \left(\frac{1}{2}x - \frac{1}{2}x\cos\left(\frac{2\pi x}{a}\right)\right) dx = \left[\frac{1}{4}x^2 - \frac{x}{2}\left(\frac{a}{2\pi}\right)\sin\left(\frac{2\pi x}{a}\right) - \left(\frac{a}{2\pi}\right)^2 \cos\left(\frac{2\pi x}{a}\right)\right]_0^a = \frac{a^2}{4}$ (because $\sin(2\pi) = 0$, $\sin(0) = 0$, & $\cos(2\pi) = \cos(0)$)

using $\sin^2\theta = \frac{1}{2} - \frac{1}{2}\cos(2\theta)$; using $\int x\cos(bx)dx = \frac{x}{b}\sin(bx) + \frac{1}{b^2}\cos(bx)$

$I_2 = \frac{a^2}{4}$, because we can see the same thing will happen as in I_1

$I_3 = f(x) g(t)$; $f(x) = \int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right) dx = \frac{1}{2}\int\left[x\cos\left(\frac{\pi x}{a}\right) - x\cos\left(\frac{3\pi x}{a}\right)\right] dx$

using $\sin x \sin y = \frac{1}{2}[\cos(x-y) - \cos(x+y)]$

$= \frac{1}{2}\left[x\frac{a}{\pi}\sin\left(\frac{\pi x}{a}\right) + \left(\frac{a}{\pi}\right)^2\cos\left(\frac{\pi x}{a}\right) - x\left(\frac{a}{3\pi}\right)\sin\left(\frac{3\pi x}{a}\right) - \left(\frac{a}{3\pi}\right)^2\cos\left(\frac{3\pi x}{a}\right)\right]_0^a$

$= \frac{1}{2}\left[\left(\frac{a}{\pi}\right)^2(-1) - \left(\frac{a}{3\pi}\right)^2(-1)\right] - \left[\left(\frac{a}{\pi}\right)^2(1) - \left(\frac{a}{3\pi}\right)^2(1)\right] = \frac{a^2}{2\pi^2}\left[-1 + \frac{1}{9} - 1 + \frac{1}{9}\right] = \frac{-16a^2}{18\pi^2} = \frac{8a^2}{9\pi^2}$

$g(t) = e^{-it\frac{3\hbar\pi^2}{2ma^2}} + e^{it\frac{3\hbar\pi^2}{2ma^2}} = 2\cos\left(t\frac{3\hbar\pi^2}{2ma^2}\right)$

$$\Rightarrow \boxed{\langle x \rangle = \frac{1}{a}\left[\frac{a^2}{4} + \frac{a^2}{4} - \frac{16a^2}{9\pi^2}\cos\Big(t\,\underbrace{\frac{3\hbar\pi^2}{2ma^2}}_{\omega}\Big)\right] = \frac{a}{2} - \frac{16a}{9\pi^2}\cos(3\omega t)}$$

d) $$\boxed{\langle p \rangle = m\frac{d\langle x \rangle}{dt} = -\frac{16ma}{9\pi^2}(3\omega)\sin(3\omega t) = -\frac{16ma\omega}{3\pi^2}\sin(3\omega t)}$$

$= -\frac{16ma}{3\pi^2}\left(\frac{\hbar\pi^2}{2ma^2}\right)\sin(3\omega t) = -\frac{8\hbar}{3a}\sin\left(3t\frac{\hbar\pi^2}{2ma^2}\right)$