Physics 3610H: Assignment III

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September 25, 2025

Problem 1. Consider a particle in the infinite square well from $0 < x < a$. The eigenstates and eigenvalues of the T.D.S.E for this system are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$
$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

respectively. We also found that these states form an orthonormal set,

$$\int_{\mathbb{R}} \psi_n^*(x)\psi_m(x)dx = \delta_{mn}.$$

Suppose a particle in such a well is in the following state at $t = 0$:

$$\Psi(x, 0) = A(\psi_1(x) + 2\psi_2(x))$$

(a) Find A such that $\Psi(x, 0)$ is normalized.

(b) Draw $\Psi(x, 0)$ as a function of x.

(c) Where is the particle most likely to be found at $t = 0$? (Draw arrow(s) on your plot.)

(d) Where is the particle least likely to be found at $t = 0$? (Draw arrow(s) on your plot.)

(e) What is the probability of finding the particle in the left half of the well (i.e. $0 < x < a/2$) at $t = 0$?

(f) Find $\Psi(x, t)$.

(g) Show $\Psi(x, t)$ is normalized for all times t.

(h) What is the expectation value of x?

(i) If you measured the energy of this particle, what values might you get and what is the probability that you will get each of these values?

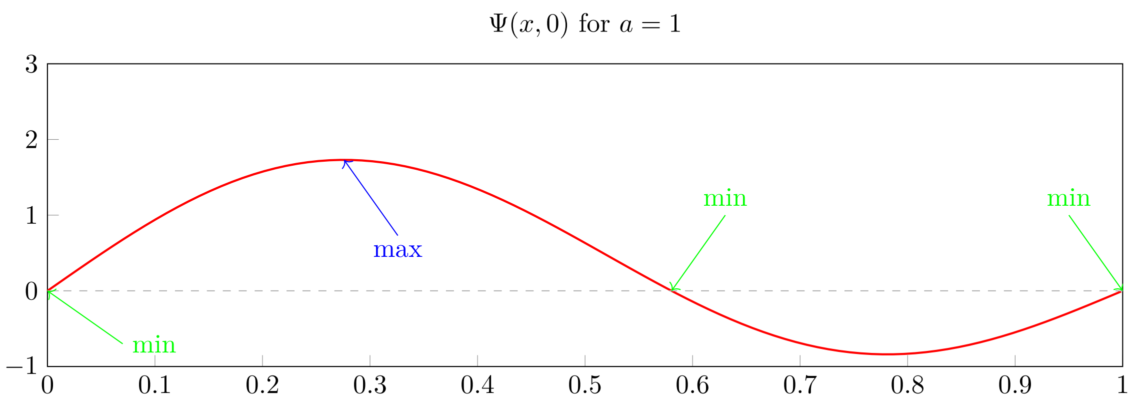
(j) What is the expectation value of the energy?

Solution 1.

(a) Here we force the integral over all space of $|\Psi|^2$ to be 1 and solve for an A which satisfies this. We can note that because we are dealing with an infinite well here the wavefunction is only nonzero within the well so we can trim down the bounds a bit,

$$\begin{aligned}
1 &= \int_0^a \Psi^*(x,0)\Psi(x,0)\,dx \\
&= |A|^2 \int_0^a (\psi_1^*(x) + 2\psi_2^*(x))(\psi_1(x) + 2\psi_2(x))\,dx \\
&= |A|^2 \int_0^a \psi_1^*(x)\psi_1(x) + 2\psi_2^*(x)\psi_1(x) + 2\psi_2(x)\psi_1^*(x) + 4\psi_2(x)\psi_2^*(x)\,dx \\
&= |A|^2 \int_0^a \psi_1^*(x)\psi_1(x) + 2\delta_{12} + 2\delta_{12} + 4\psi_2(x)\psi_2^*(x)\,dx \\
&= |A|^2 \left[\delta_{11} + \cancelto{0}{\delta_{12} + \delta_{12}} + 4\delta_{22}\right] \\
&= |A|^2 [1+4] \implies |A|^2 = 1/5 \implies A = \sqrt{1/5}
\end{aligned}$$

(b)



(c) Here we take the derivative of the wavefunction $\Psi(x,0)$ and determine the turning points,

$$\begin{aligned}
0 &= \frac{d}{dx}\Psi(x,0) \\
&= A\left[\frac{d}{dx}(\psi_1(x) + 2\psi_2(x))\right] \\
&= A\left[\frac{d}{dx}\psi_1(x) + 2\frac{d}{dx}\psi_2(x)\right] \\
&= A\left[\frac{d}{dx}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + 2\frac{d}{dx}\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)\right] \\
&= A\sqrt{\frac{2}{a}}\left[\frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right) + \frac{4\pi}{a}\cos\left(\frac{2\pi x}{a}\right)\right] \\
&= A\frac{\pi}{a}\sqrt{\frac{2}{a}}\left[\cos\left(\frac{\pi x}{a}\right) + 4\cos\left(\frac{2\pi x}{a}\right)\right]
\end{aligned}$$

Which will be zero when

$$\cos\left(\frac{\pi x}{a}\right) = -4\cos\left(\frac{2\pi x}{a}\right).$$

This is a nasty expression to solve analytically so we force a computer to do it. I used SageMath but most advanced CAS software (or numerical optimization techniques, as it turns out) should be able to handle this

[2]:
```
a = 1
A = 1/sqrt(5)
x = var("x")
eqn = cos(pi*x/a) == -4*cos(2*pi*x/a) #
show(find_root(eqn, 0, a/2)) # Find roots on [0,a/2] because we need to force finding the
↪  maxima on the left rather than the minima on the right
```

[2]: 0.27587156664462037

Sadly even sage can't give me a nice analytical solution here (Interestingly, the open access version of Wolfram alpha actually can) so we'll have to resign ourselves to using a numerical value that has to be recalculated for new a. See blue mark on the plot for where this point lies.

(d) Here we recognize that as probability is $|\Psi|^2$ we lose the sign and so are looking for the smallest value. Because we have points where we cross zero those will remain the smallest even when taking the modulus and squaring it and so we can look for points

$$\Psi(x,0) = 0.$$

This are given by

$$A\sqrt{\frac{2}{a}}\left[\sin\left(\frac{\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right)\right] = 0$$

which reduces to

$$\sin\left(\frac{\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right) = 0.$$

which we can see will have "cheap" solutions at $x = a$ and $x = 0$. We expect from the graph however there to exist a third solution somewhere between these two. To find this we can again employ our CAS approach as before while restricting the solver to between $0+\epsilon$ and $a-\epsilon$ where ϵ is sufficiently small that the algorithm (whatever you chose) will skip the trivial endpoints. Doing this for our case of $a = 1$ gives $x = 0.5804306232551663$. This is, and the other two points, is marked in green on the original plot.

(e) Here we just integrate our probability density over $0 \to a/2$,

$$\begin{aligned}
P(0 < x \leq a/2) &= \int_0^{a/2} |\Psi(x,0)|^2\, dx \\
&= \int_0^{a/2} A\sqrt{\frac{2}{a}}\left[\sin\left(\frac{\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right)\right] A\sqrt{\frac{2}{a}}\left[\sin\left(\frac{\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right)\right]\, dx
\end{aligned}$$

we've skipped a bit here by not explicitly writing the conjugate (and assuming $|A| = A$) but that ends up being fine as the wavefunction a $t = 0$ is entirely real. Proceeding with the integration,

$$\begin{aligned}
&= \frac{2A^2}{a}\int_0^{a/2} \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{\pi x}{a}\right)2\sin\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right)2\sin\left(\frac{2\pi x}{a}\right)\, dx \\
&= \frac{2A^2}{a}\int_0^{a/2} \sin^2\left(\frac{\pi x}{a}\right) + 2\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{\pi x}{a}\right)2\sin\left(\frac{2\pi x}{a}\right) + 4\sin^2\left(\frac{2\pi x}{a}\right)\, dx \\
&= \frac{2A^2}{a}\left[\int_0^{a/2} \sin^2\left(\frac{\pi x}{a}\right)\, dx + 4\int_0^{a/2} \sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\, dx + 4\int_0^{a/2} \sin^2\left(\frac{2\pi x}{a}\right)\, dx\right] \\
&= \frac{2A^2}{a}\left[a/4 + \frac{8a}{3\pi} + a\right] \\
&= A^2/2 + \frac{16A^2}{3\pi} + 2A^2 \approx 84\%.
\end{aligned}$$

(f) Here we are going to be "undoing" the separation $\Psi(x,t) = \psi(x)\phi(t)$. Due to the completeness of the set of solutions to the T.D.S.E Ψ can be expressed as a weighted sum of the $\psi(x)\phi(t)$ terms. When we are considering

$\Psi(x,0)$ the $\phi_n(t) = \exp(-iE_nt/\hbar)$ terms just become 1 and drop out. Combining both of these facts it's safe to say that

$$\Psi(x,t) = A(\psi_1(x)\exp(-iE_1t/\hbar) + 2\psi_2(x)\exp(-iE_2t/\hbar)).$$

Is there a more formal way of putting this together or do we just say "yeah, that's how it is"

(g) Again we integrate over all space. Now however we have A and are checking that the integral returns a value independent of time. We want the value independent of time because it implies that the total probability (of finding the particle at all) will never change.

$$\begin{aligned}
&= \int_0^a |\Psi(x,t)|^2\,dx \\
&= \int_0^a \Psi^*(x,t)\Psi(x,t)\,dx \\
&= \int_0^a |A|(\psi_1^*(x)\exp(iE_1t/\hbar) + 2\psi_2^*(x)\exp(iE_2t/\hbar))|A|(\psi_1(x)\exp(-iE_1t/\hbar) + 2\psi_2(x)\exp(-iE_2t/\hbar))\,dx \\
&= |A|^2 \int_0^a \psi_1^*(x)\exp(iE_1t/\hbar)\psi_1(x)\exp(-iE_1t/\hbar) \\
&\qquad + 2\psi_2^*(x)\exp(iE_2t/\hbar)\psi_1(x)\exp(-iE_1t/\hbar) \\
&\qquad + \psi_1^*(x)\exp(iE_1t/\hbar)2\psi_2(x)\exp(-iE_2t/\hbar) \\
&\qquad + 2\psi_2^*(x)\exp(iE_2t/\hbar)2\psi_2(x)\exp(-iE_2t/\hbar)\,dx \\
&= |A|^2 \left[\int_0^a \psi_1^*(x)\psi_1(x)\cancelto{1}{\exp(iE_1t/\hbar)\exp(-iE_1t/\hbar)}\,dx \right. \\
&\qquad + \int_0^a 2\psi_2^*(x)\psi_1(x)\exp(iE_2t/\hbar)\exp(-iE_1t/\hbar)\,dx \\
&\qquad + \int_0^a 2\psi_1^*(x)\psi_2(x)\exp(iE_1t/\hbar)\exp(-iE_2t/\hbar)\,dx \\
&\qquad \left. + \int_0^a 4\psi_2^*(x)\psi_2(x)\cancelto{1}{\exp(iE_2t/\hbar)\exp(-iE_2t/\hbar)}\,dx \right] \\
&= |A|^2 \left[\cancelto{1}{\delta_{11}} + 2\cancelto{0}{\delta_{21}}\int_0^a \exp(iE_2t/\hbar)\exp(-iE_1t/\hbar)\,dx + 2\cancelto{0}{\delta_{21}}\int_0^a \exp(iE_1t/\hbar)\exp(-iE_2t/\hbar)\,dx + 4\cancelto{1}{\delta_{22}} \right] \\
&= |A|^2 [1 + 4] = \frac{1}{5}\cdot 5 = 1.
\end{aligned}$$

This is, as we hoped, both normalized and time independent, meaning $\Psi(x,t)$ will remain normalized for all times.

(h) Here we are searching for $\langle \hat{x} \rangle$ which is given by

$$
\begin{aligned}
&= \int_0^a \Psi^* \hat{x} \Psi \, dx \\
&= A^2 \int_0^a (\psi_1^*(x) \exp(iE_1 t/\hbar) + 2\psi_2^*(x) \exp(iE_2 t/\hbar)) x (\psi_1(x) \exp(-iE_1 t/\hbar) + 2\psi_2(x) \exp(-iE_2 t/\hbar)) \, dx \\
&= A^2 \int_0^a x\psi_1^*(x) \exp(iE_1 t/\hbar) \psi_1(x) \exp(-iE_1 t/\hbar) \\
&\quad + 2x\psi_2^*(x) \exp(iE_2 t/\hbar) \psi_1(x) \exp(-iE_1 t/\hbar) \\
&\quad + x\psi_1^*(x) \exp(iE_1 t/\hbar) 2\psi_2(x) \exp(-iE_2 t/\hbar) \\
&\quad + 2x\psi_2^*(x) \exp(iE_2 t/\hbar) 2\psi_2(x) \exp(-iE_2 t/\hbar) \, dx \\
&= A^2 \int_0^a x\psi_1^*(x) \psi_1(x) \\
&\quad + 2x\psi_2^*(x) \psi_1(x) \exp(iE_2 t/\hbar) \exp(-iE_1 t/\hbar) \\
&\quad + x\psi_1^*(x) 2\psi_2(x) \exp(iE_1 t/\hbar) \exp(-iE_2 t/\hbar) \\
&\quad + 4x\psi_2^*(x) \psi_2(x) \, dx \\
&= A^2 \Bigg[\int_0^a x\psi_1^*(x) \psi_1(x) \, dx \\
&\quad + 2 \exp(iE_2 t/\hbar) \exp(-iE_1 t/\hbar) \int_0^a x\psi_2^*(x) \psi_1(x) \, dx \\
&\quad + 2 \exp(iE_1 t/\hbar) \exp(-iE_2 t/\hbar) \int_0^a x\psi_1^*(x) \psi_2(x) \, dx \\
&\quad + 4 \int_0^a x\psi_2^*(x) \psi_2(x) \, dx \Bigg] \\
&= A^2 \Bigg[\int_0^a x \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \, dx \\
&\quad + 2 \exp(iE_2 t/\hbar) \exp(-iE_1 t/\hbar) \int_0^a x \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \, dx \\
&\quad + 2 \exp(iE_1 t/\hbar) \exp(-iE_2 t/\hbar) \int_0^a x \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \, dx \\
&\quad + 4 \int_0^a x \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \, dx \Bigg] \\
&= \frac{2A^2}{a} \Bigg[\int_0^a x \sin^2\left(\frac{\pi x}{a}\right) \, dx \\
&\quad + 2 \int_0^a x \sin\left(\frac{2\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) \, dx \left(\exp\left(\frac{it}{\hbar} [E_2 - E_1] \right) \right. \\
&\quad \left. + \exp\left(\frac{it}{\hbar} [E_1 - E_2] \right) \right) \\
&\quad + 4 \int_0^a x \sin^2\left(\frac{2\pi x}{a}\right) \, dx \Bigg] \\
&= \frac{2A^2}{a} \left[\frac{a^2}{4} - \frac{16a^2}{9\pi^2} \left(\exp\left(\frac{it}{\hbar} [E_2 - E_1] \right) + \exp\left(\frac{it}{\hbar} [E_1 - E_2] \right) \right) + a^2 \right] \\
&= \frac{a}{2} - \frac{32a}{45\pi^2} \left(\exp\left(\frac{it}{\hbar} [E_2 - E_1] \right) + \exp\left(\frac{it}{\hbar} [E_1 - E_2] \right) \right)
\end{aligned}
$$

(i) Because energy is quantized here we would expect to only see energy values corresponding to the states we have, so E_1 and E_2. For the probabilities that a measurement would yield one of these energies we can begin by recalling that

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n \exp(-iE_n t/\hbar)$$

where $|c_n|^2$ is the probability that a measurement would find the particle in state n. I'm not sure how to prove this fact but the text states it and we've shown in class that it sure behaves a lot like a probability so I'm fairly comfortable with trusting that it is, though I wish I had something more formal to justify it with. Knowing that our Ψ can be expressed in this form with c_n having a meaning we can look back to our original function and note that we had

$$\Psi(x,0) = \frac{1}{\sqrt{5}} (\psi_1 + 2\psi_2)$$

which looks like the fixed-time version of the linear combination we had above. Again this is an area where I'm kind of trusting what I've been told without really being able to justify it to a level I'm comfortable with beyond potential coincidence but things still work. If we say that this *is* a specific form linear combination we had above for this system we can note that then

$$c_1 = \frac{1}{\sqrt{5}} \qquad \text{and} \qquad c_2 = \frac{2}{\sqrt{5}}.$$

That would mean that the probability of finding the particle with energy E_1 would be $|c_1|^2 = 1/5 = 20\%$ and the probability of E_2 would be $|c_2|^2 = 4/5 = 80\%$ which does align with the total probability being 1.

(j) We could make the elaborate derivation of the expectation value of the Hamiltonian here or, if we were short on time (hypothetically), we could note that

$$\langle \hat{H} \rangle = \langle E \rangle$$

and because we just have a set of E_ns with associated probabilities $|c_n|^2$ and we know that the expectation value of some probabilistic measurement is

$$\langle A \rangle = \sum_n P(A_n) A_n$$

we can say that

$$\langle E \rangle \sum_n |c_n|^2 E_n$$

which for our case of two energies become

$$\langle E \rangle = \frac{1}{5} \cdot E_1 + \frac{4}{5} \cdot E_2 = \frac{\hbar^2 \pi^2}{10ma^2} + \frac{8\hbar^2\pi^2}{10ma^2} = \frac{9\hbar^2\pi^2}{10ma^2}.$$