Chapter 2 Problems

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Problem 2.1

Prove the following theorems:

(a) For normalizable solutions, the separation constant E must be *real*

Assume E is complex, meaning $E = a + ib$ for some $a, b \in \mathbb{R}$. For a separable solution $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$, we have that

$$\begin{aligned}
|\Psi(x,t)|^2 &= |\psi|^2 \left| e^{-i(a+ib)t/\hbar} \right|^2 \\
&= |\psi|^2 \left| e^{-iat/\hbar} e^{bt/\hbar} \right|^2 \\
&= |\psi|^2 e^{2bt/\hbar}
\end{aligned}$$

For $t = 0$, we know that $\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1$ so

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = \int_{-\infty}^{\infty} |\psi|^2 e^0 dx = \int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

Now for any $t > 0$, we have

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} |\psi|^2 e^{2bt/\hbar} dx = e^{2bt/\hbar} \int_{-\infty}^{\infty} |\psi|^2 dx = e^{2bt/\hbar} = 1$$

Taking the natural log of both sides we see

$$2bt/\hbar = 0$$

and hence $b = 0$ and E is composed of only the real component.

(b) The time independenent wave function ψ can always be taken to be *real* (unlike Ψ which is necessarily complex). That doesn't mean that every solution to the time-independent Schroedinger equation is real; what it says is that if you've got one that is not, it can always be expressed as a linear combination of solutions (with the same energy) that are real. So you might as well stick to ψs that are real.

Assume $\psi = a + ib$ is a solution to the time-independent Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \psi V = \psi E$$

Since both ψ and ψ^* solve this, we can plug both in to this equation:

$$\begin{aligned}
-\frac{\hbar^2}{2m}\left(\frac{\partial^2 a}{\partial x^2} + i\frac{\partial^2 b}{\partial x^2}\right) + (a+ib)V = (a+ib)E \\
-\frac{\hbar^2}{2m}\left(\frac{\partial^2 a}{\partial x^2} - i\frac{\partial^2 b}{\partial x^2}\right) + (a-ib)V = (a-ib)E
\end{aligned}$$

Adding these equations together we get

$$\begin{aligned}
-\frac{\hbar^2}{2m}\left(2\frac{\partial^2 a}{\partial x^2} + i\frac{\partial^2 b}{\partial x^2} - i\frac{\partial^2 b}{\partial x^2}\right) + (2a + ib - ib)V \quad &= (a + ib - ib)E \\
-\frac{\hbar^2}{2m}\left(2\frac{\partial^2 a}{\partial x^2}\right) + 2aV = 2aE \\
-\frac{\hbar^2}{2m}\left(\frac{\partial^2 a}{\partial x^2}\right) + aV = aE
\end{aligned}$$

And hence $a = \frac{1}{2}(\psi + \psi^*)$ is also a solution, and has no imaginary component. It is worth noting that we should probably use $\frac{1}{\sqrt{2}}(\psi + \psi^*)$ instead, so that we still have a normalized solution.

(c) If $V(x)$ is an even function, then ψ can always be taken to be either even or odd.

Assume we have some solution $\psi(x)$. Let $\gamma(x) = \psi(-x)$. We then have

$$\begin{aligned}
\frac{\partial \gamma}{\partial x}(x) &= -\frac{\partial \psi}{\partial x}(-x) \\
\frac{\partial^2 \gamma}{\partial x^2}(x) &= \frac{\partial^2 \psi}{\partial x^2}(-x)
\end{aligned}$$

If we look at γ in the time-independent equation we get

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2 \gamma}{\partial x^2}(x) + \gamma(x)V(x) = \gamma(x)E \\
-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}(-x) + \psi(-x)V(x) = \psi(-x)E \\
-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}(-x) + \psi(-x)V(-x) = \psi(-x)E
\end{aligned}$$

Where the last equation uses the evenness of V. This equation also holds since the time independent equation holds for all $x \in \mathbb{R}$. Thus, $\psi(-x)$ is also a solution if V is even.

Now, since any linear combination of solutions is also a solution, we can use the even combination $\psi(x) + \psi(-x)$ or the odd combination $\psi(x) - \psi(-x)$ in order to get an even or odd solution to the equation.

Problem 2.2

Prove that E must exceed the minimum value of $V(x)$ at some point.
Assume $E < V(x)$ for all x. Then we can solve for $\frac{\partial^2\psi}{\partial x^2}$ to see that

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2m}{\hbar^2}\psi\left(V(x) - E\right)$$

This says that ψ and $\frac{\partial^2\psi}{\partial x^2}$ always have the same sign, taking ψ as a real solution. Assuming ψ is C^2, if it ever takes a positive value, then it must continue to curve upwards in the positive direction and hence would grow unbounded. Symmetrically if ψ takes on some negative value, it will grow unboundedly negative in the negative direction. Hence, since $\psi \neq 0$ we have a contradiction and $E > V(x)$ for some x.

Problem 2.3

Calculate $\langle x\rangle, \langle x^2\rangle, \langle p\rangle, \langle p^2\rangle, \sigma_x$, and σ_p for the n-th stationary state of the infinite square well. Check that the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

Recall that

$$\psi_n = \sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}x)$$

Thus we compute

$$\begin{aligned}
\langle x^2\rangle &= \int_0^a x^2|\psi_n|^2 dx \\
&= \left[\frac{1}{12}\left(\frac{3\left(a^2 - 2\pi^2n^2x^2\right)\sin\left(\frac{2\pi nx}{a}\right) - 6\pi anx\cos\left(\frac{2\pi nx}{a}\right)}{\pi^3n^3} + \frac{4x^3}{a}\right)\right]_0^a \\
&= \frac{a^2\left(4\pi^3n^3 + 3\sin(2\pi n) - 6\pi n(\pi n\sin(2\pi n) + \cos(2\pi n))\right)}{12\pi^3n^3} \\
&= \frac{a^2(4\pi^3n^3 - 6\pi n)}{12\pi^3n^3} \\
&= \frac{a^2}{3} - \frac{a^2}{2\pi^2n^2} \\
\langle x\rangle &= \int_0^a x|\psi_n|^2 dx \\
&= \left[\frac{a\left(-2\pi^2n^2 + 2\pi n\sin(2\pi n) + \cos(2\pi n) - 1\right)}{4\pi^2n^2}\right] \\
&= \frac{a}{2} \text{ (I used mathematica)}
\end{aligned}$$

Thus we have

$$\begin{aligned}
\sigma_x^2 &= \left\langle x^2 \right\rangle - \left\langle x \right\rangle^2 \\
&= \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2} - \frac{a^2}{4} \\
&= a^2 \left(\frac{1}{12} - \frac{1}{2n^2\pi^2} \right)
\end{aligned}$$

It makes sense that the standard deviation would scale linearly with the area.

$$\begin{aligned}
\langle p \rangle &= \int_0^a \psi^* \left[-i\hbar \frac{\partial \psi}{\partial x} \right] dx \\
&= \int_0^a \frac{-2\hbar i n\pi \cos(\frac{n\pi x}{a}) \sin(\frac{n\pi x}{a})}{a^2} dx \\
&= \left[\frac{\hbar i \cos(\frac{2n\pi x}{a})}{2a} \right]_0^a \\
&= 0 \\
\left\langle p^2 \right\rangle &= \int_0^a \psi^* \left[-\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \right] dx \\
&= \int_0^a \frac{1}{a^3} 2\hbar^2 n^2 \pi^2 \sin^2(\frac{n\pi x}{a}) \\
&= \frac{\hbar^2 n^2 \pi^2}{a^2}
\end{aligned}$$

Thus $\sigma_p^2 = \left\langle p^2 \right\rangle = \frac{\hbar^2 n^2 \pi^2}{a^2}$

We can use this to check the uncertainty principle:

$$\begin{aligned}
\sigma_x \sigma_p &= \left(\frac{\hbar n \pi}{a} \right) \left(a \sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} \right) \\
&> \hbar n \pi \frac{1}{2\sqrt{3}} \\
&> \hbar/2
\end{aligned}$$

This quantity is minimized for $n = 1$

Problem 2.5

A particle in the infinite square well has its initial wave function an even mixture of the first two stationary states:

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

(a) Normalize $\Psi(x,0)$:

$$\begin{aligned}1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx &= \int_{-\infty}^{\infty} A^2(\psi_1^*\psi_1 + \psi_1^*\psi_2 + \psi_2^*\psi_1 + \psi_2^*\psi_2)dx \\ &= A^2\left(\int_{-\infty}^{\infty} |\psi_1|^2 dx + \int_{-\infty}^{\infty} |\psi_2|^2 dx\right) \\ &= 2A^2\end{aligned}$$

Thus $A = 1/\sqrt{2}$.

(b) Find $\Psi(x,t), |\Psi(x,t)|^2$. Express the latter as a sinusoidal function of time, as in example 2.1. Let $\omega = \pi^2\hbar/2ma^2$.

We have that $c_1, c_2 = 1/\sqrt{2}$. Thus we have

$$\Psi(x,t) = \frac{1}{\sqrt{a}}\left[\sin\left(\frac{\pi x}{a}\right)e^{-i\omega t} + \sin\left(\frac{2\pi x}{a}\right)e^{-4i\omega t}\right]$$

See the attached mathematica notebook in which we compute that

$$|\Psi(x,t)|^2 = \frac{\sin^2\left(\frac{\pi x}{a}\right)\left(4\cos\left(\frac{\pi x}{a}\right)\cos(3t\omega) + 2\cos\left(\frac{2\pi x}{a}\right) + 3\right)}{a}$$

(c) Compute $\langle x\rangle$. Notice that it oscillates in time. What is the angular frequency of the oscillation? What is the amplitude of the oscillation?

Using mathematica we see that

$$\langle x\rangle = \frac{a}{2} - \frac{16a\cos(3t\omega)}{9\pi^2}$$

The amplitude of this oscillation is $16a/9\pi^2$ and it's frequency is 3ω.

(d) Compute $\langle p\rangle$.

Here we can use that $\langle p\rangle = m\frac{d}{dt}\langle x\rangle$:

$$\begin{aligned}\langle p\rangle &= m\frac{16a\omega}{3\pi^2}\sin(3t\omega) \\ &= \frac{8\hbar}{3a}\sin(3t\omega)\end{aligned}$$

(e) If you measured the energy of this particle, what possible values could it's energy be and with what probabilities? Find the expectation value of H. How does it compare with E_1, E_2.

The two possible values we could get are $E_1 = \omega, E_2 = 4\omega$. Since $c_1, c_2 = 1/\sqrt{2}$, we get either E_1 or E_2 with probability $1/2$.

$$
\begin{aligned}
\langle H \rangle &= \int_{-\infty}^{\infty} \Psi^* \hat{H} \Psi dx \\
&= \int_{-\infty}^{\infty} \Psi^* \frac{1}{\sqrt{2}} \left(E_1\psi_1 + E_2\psi_2\right) dx \\
&= \frac{1}{2} \int_{-\infty}^{\infty} \left[E_1\psi_1^*\psi_1 + E_1\psi_2^*\psi_1 + E_2\psi_1^*\psi_2 + E_2\psi_2^*\psi_2\right] dx \\
&= \frac{1}{2} \left(E_1 \int_{-\infty}^{\infty} \psi_1^*\psi_1 dx + E_2 \int_{-\infty}^{\infty} \psi_2^*\psi_2 dx \right) \\
&= \frac{E_1 + E_2}{2}
\end{aligned}
$$

Which, as we would expect is $\langle E \rangle$.

Problem 2.7