University of Alabama
Department of Physics and Astronomy

PH 253 / LeClair Fall 2010

Problem Set 6: Solutions

1. We found the wave functions and energies for a particle in an infinite potential well of width $2a$ to be

$$\psi^-(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad E_n^+ = \frac{\left(n-\frac{1}{2}\right)^2\pi^2\hbar^2}{2ma^2} \tag{1}$$

$$\psi^+(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{\left(n-\frac{1}{2}\right)\pi x}{a}\right) \qquad E_n^- = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2}$$

The + and − here indicate the even/odd solutions (i.e., an even or odd number of half-wavelengths fitting inside the well). Noting that $\langle p^2\rangle = 2mE_n^{\pm}$, calculate $\Delta p\,\Delta x$ for even and odd solutions, with $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$. How does the uncertainty behave for increasing n?

Solution: Here the well extends over the interval $[-a, a]$.

First, $\langle p\rangle = 0$ by symmetry for both + and − states – the particle goes to the left as much as it goes to the right, and overall the average momentum is zero. Similarly, $\langle x\rangle = 0$. Since the well is symmetric, the particle should have an average position in the middle at $x = 0$; this is readily verified. Since ψ is purely real, we don't need to worry about the complex conjugate, and the limits of the integral are from $-a$ to a since ψ is zero outside of the potential well:

$$\begin{aligned}\langle x_-\rangle &= \int_{-\infty}^{\infty} x|\psi|^2\,dx = \int_{-a}^{a}\frac{x}{a}\sin^2\left(\frac{n\pi x}{a}\right) = \left[-\frac{a}{8n^2\pi^2}\cos\left(\frac{2n\pi x}{a}\right) - \frac{x}{4n\pi}\sin\left(\frac{2n\pi x}{a}\right) + \frac{x^2}{4a}\right]_{-a}^{a} \\ &= -\frac{a}{8n^2\pi^2}\Big(\cos(2n\pi) - \cos(-2n\pi)\Big) - \frac{a}{4n\pi}\sin(2n\pi) - \frac{a}{4n\pi}\sin(-2n\pi) + \frac{a^2}{4a} - \frac{a^2}{4a} = 0\end{aligned}$$

We could have noted that cos and $x\sin$ are even functions of x, and the integration interval is symmetric, so the first two terms must give zero.

$$\langle x_+\rangle = \int_{-\infty}^{\infty} x|\psi|^2\,dx = \int_{-a}^{a}\frac{x}{a}\cos^2\left(\frac{\left(n-\frac{1}{2}\right)\pi x}{a}\right) \tag{3}$$

$$= \left[\frac{a}{8a\pi^2\left(n-\frac{1}{2}\right)^2}\cos\left(\frac{2\left(n-\frac{1}{2}\right)\pi x}{a}\right) + \frac{x}{8a\pi\left(n-\frac{1}{2}\right)}\sin\left(\frac{2\left(n-\frac{1}{2}\right)\pi x}{a}\right) + \frac{x^2}{4a}\right]_{-a}^{a}$$

$$= 0 \tag{4}$$

In both cases, noting that $\cos x = \cos(-x)$ and $\sin x = -\sin(-x)$ speeds things up considerably. In order to find Δx we need $\langle x^2 \rangle$ for both + and − solutions:

$$\begin{aligned}
\langle x_-^2 \rangle &= \int_{-\infty}^{\infty} x^2 |\psi|^2 \, dx = \int_{-a}^{a} \frac{x^2}{a} \sin^2\left(\frac{n\pi x}{a}\right) \\
&= \left[-\frac{ax}{4n^2\pi^2} \cos\left(\frac{2n\pi x}{a}\right) - \frac{1}{8n^2 p^3} \left(2n^2\pi^2 x^2 - a^2\right) \sin\left(\frac{2n\pi x}{a}\right) + \frac{x^3}{6a} \right]_{-a}^{a} \\
&= \left(\frac{-a}{2n^2\pi^2}\right) \Big(a\cos(2n\pi) + a\cos(-2n\pi) \Big) + 0 + \frac{a^2}{6} + \frac{a^2}{6} = a^2 \left(\frac{1}{3} - \frac{1}{n^2\pi^2}\right)
\end{aligned} \tag{5}$$

$$\begin{aligned}
\langle x_+^2 \rangle &= \int_{-\infty}^{\infty} x^2 |\psi|^2 \, dx = \int_{-a}^{a} \frac{x^2}{a} \cos^2\left(\frac{\left(n - \frac{1}{2}\right)\pi x}{a}\right) \\
&= \frac{1}{48a\left(n - \frac{1}{2}\right)^3 \pi^3} \left[-3a \left(2a^2 - 4\left(n - \frac{1}{2}\right)^2 \pi^2 x^2 \right) \sin\left(\frac{2\left(n - \frac{1}{2}\right)\pi x}{a}\right) \right. \\
&\qquad \left. + 12a^2 \pi x \left(n - \frac{1}{2}\right) \cos\left(\frac{2\left(n - \frac{1}{2}\right)\pi x}{a}\right) + 8\left(n - \frac{1}{2}\right)^3 \pi^3 x^3 \right]_{-a}^{a} \\
&= \frac{a^2}{2\pi^2\left(n - \frac{1}{2}\right)^2} + \frac{a^2}{6} + \frac{a^2}{6} = a^2 \left(\frac{1}{3} + \frac{1}{2\pi^2\left(n - \frac{1}{2}\right)^2} \right)
\end{aligned} \tag{6}$$

For large n, we have $\langle x_-^2 \rangle \approx \langle x_+^2 \rangle \approx a^2/3$. The uncertainty in position is then $\Delta x = \sqrt{\langle x^2 \rangle}$ for both + and − solutions, since $\langle x \rangle$ is zero for both.

We now need only $\langle p^2 \rangle$, since $\langle p \rangle = 0$ for both odd and even states. From the energy formulas given,

$$\langle p_-^2 \rangle = 2mE_n^+ = \frac{n^2\pi^2\hbar^2}{a^2} \tag{7}$$

$$\langle p_+^2 \rangle = 2mE_n^- = \frac{\left(n - \frac{1}{2}\right)^2 \pi^2\hbar^2}{a^2} \tag{8}$$

Since $\langle p \rangle = 0$ for both solutions, $\Delta p = \sqrt{\langle p^2 \rangle}$. The uncertainty relationship is then

$$\Delta x_- \Delta p_- = \sqrt{a^2\left(\frac{1}{3} - \frac{1}{n^2\pi^2}\right)} \sqrt{\frac{n^2\pi^2\hbar^2}{a^2}} = \hbar\sqrt{\frac{1}{3}n^2\pi^2 - 1} \tag{9}$$

$$\Delta x_+ \Delta p_+ = \sqrt{a^2\left(\frac{1}{3} + \frac{1}{2\pi^2\left(n - \frac{1}{2}\right)^2}\right)} \sqrt{\frac{\left(n - \frac{1}{2}\right)^2 \pi^2\hbar^2}{a^2}} = \hbar\sqrt{\frac{1}{3}\left(n - \frac{1}{2}\right)^2 \pi^2 + \frac{1}{2}} \tag{10}$$

We see that in general uncertainty grows with n (linearly with n for large n), and that for any n the uncertainty relationship $\Delta x\,\Delta p \geqslant \hbar/2$ is satisfied.

2. The state of a free particle is described by the following wave function

$$\psi(x) = \begin{cases} 0 & x < -b \\ A & -b \leqslant x \leqslant 2b \\ 0 & x > 2b \end{cases} \tag{11}$$

(a) Determine the normalization constant A.
(b) What is the probability of finding the particle in the interval $[0, b]$?
(c) Determine $\langle x \rangle$ and $\langle x^2 \rangle$ for this state.
(d) Find the uncertainty in position $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$.

Solution: As above, we can normalize the wavefunction by integrating its square over all space. Conveniently, the wavefunction is zero except over the interval $[-b, 2b]$

$$\int |\psi(x)|^2\,dx = \int_{-b}^{2b} A^2\,dx = 3bA^2 = 1 \qquad \Longrightarrow \qquad A = \frac{1}{\sqrt{3b}} \tag{12}$$

The probability of finding the particle in $[0, b]$ means integrating the probability density, $|\psi|^2$ over that interval:

$$P(x \in [0, b]) = \int_0^b A^2\,dx = \int_0^b \frac{1}{3b}\,dx = \frac{1}{3} \tag{13}$$

Finding $\langle x \rangle$ proceeds as above, though now we integrate over all space. As with the normalization integral above, we need only integrate over the interval where ψ is nonzero:

$$\langle x \rangle = \int_{-b}^{2b} \frac{x}{3b}\,dx = \frac{1}{3b}\left[\frac{1}{2}x^2\right]_{-b}^{2b} = \frac{1}{6b}\left(4b^2 - b^2\right) = \frac{b}{2} \tag{14}$$

Similarly,

$$\langle x^2 \rangle = \int_{-b}^{2b} \frac{x^2}{3b}\,dx = \frac{1}{3b}\left[\frac{1}{3}x^3\right]_{-b}^{2b} = \frac{1}{9b}\left[8b^3 + b^3\right] = b^2 \tag{15}$$

Thus,

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{b^2 - \frac{b^2}{4}} = \pm\frac{b\sqrt{3}}{2} \tag{16}$$

3. A particle of mass m is confined to a one-dimensional box of width L, that is, the potential energy of the particle is infinite everywhere except in the interval $0 < x < L$, where its potential energy is zero. The particle is in its ground state. What is the probability that a measurement of the particle's position will yield a result in the left quarter of the box? The wavefunction for a particle in a 1D box may be written

$$\psi(x) = A\sin\left(Bnx\right) \tag{17}$$

where A and B are constants you will need to find, and n is an integer. *Hint: normalize and apply boundary conditions.*

Solution: *UA physics graduate qualifying exam, 2002.* Our boundary conditions are that the wavefunction vanish at the boundaries of the box $x = 0$ and $x = L$, since the potential is infinite outside of that region.[i] This allows us to determine B already:

$$\psi(0) = A\sin 0 = 0 \tag{18}$$

$$\psi(L) = A\sin BnL = 0 \qquad \Longrightarrow \qquad BnL = n\pi \qquad \Longrightarrow \qquad B = \frac{\pi}{L} \tag{19}$$

Thus, $\psi(x) = A\sin\left(\frac{n\pi x}{L}\right)$. We need only determine the overall constant A, which can be done by enforcing normalization (i.e., the probability density integrated over all space must give unity). Since the wavefunction vanishes outside $[0, L]$, we need only integrate over that interval.

$$1 = \int_0^L |\psi(x)|^2\,dx = \int_0^L A^2\sin^2\left(\frac{n\pi x}{L}\right)dx = \frac{1}{2}A^2L \qquad \Longrightarrow \qquad A = \sqrt{\frac{2}{L}} \tag{20}$$

Thus,

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \tag{21}$$

[i] We also require that the derivative of the wavefunction vanish at the boundaries, but this does not help us in the present case.

The probability that the particle will be found in the left quarter of the box is determined by integrating the probability density over that interval:

$$P(x \in [0, L/4]) = \int_0^{L/4} \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) dx = \int_0^{n\pi/4} \frac{2}{L}\left(\frac{L}{n\pi}\right)\left(\frac{1}{2}\right)(1 - \cos 2u)\ du \qquad \left(\text{let } u = \frac{n\pi x}{L}\right)$$
$$= \frac{1}{n\pi}\left[u - \frac{1}{2}\sin 2u\right]_0^{L/4} = \frac{1}{n\pi}\left[\frac{n\pi}{4} - \frac{1}{2}\right] = \frac{1}{4} - \frac{1}{2n\pi} \tag{22}$$

For the ground state, $n=1$, and $P = \frac{1}{4} - \frac{1}{2\pi} \approx 0.091$.

4. Given the wave function

$$\psi(x) = \frac{N}{x^2 + a^2} \tag{23}$$

(a) Find N needed to normalize ψ.
(b) Find $\langle x \rangle$, $\langle x^2 \rangle$, and Δx.
(c) What is the probability that the particle is found in the interval $[-a, a]$?

Solution: Normalize by enforcing unit probability that the particle is *somewhere*, i.e, integrate $|\psi|^2$ over all space and set the result equal to one.[ii]

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{\infty} \frac{N^2}{(x^2 + a^2)^2}\, dx = \frac{N^2}{2a^3}\left[\frac{ax}{x^2 + a^2} + \tan^{-1}\left(\frac{x}{a}\right)\right]_{-\infty}^{\infty} \tag{24}$$

$$1 = \frac{N^2}{2a^3}\left[0 - 0 + \frac{\pi}{2} - \frac{-\pi}{2}\right] = \frac{\pi N^2}{2a^3} \tag{25}$$

$$\Longrightarrow \qquad N = \sqrt{\frac{2a^3}{\pi}} \tag{26}$$

The average position is

$$\langle x \rangle = \int_{-\infty}^{\infty} x\, |\psi|^2\, dx = \int_{-\infty}^{\infty} \frac{N^2 x}{(x^2 + a^2)^2}\, dx = \left.\frac{-1}{2\,(a^2 + x^2)}\right|_{-\infty}^{\infty} = 0 \tag{27}$$

Since ψ is an even function and x an odd function, the integral is zero as we expect. The rms position is

[ii] This function is a well-known one, and you will probably encounter it again. See http://mathworld.wolfram.com/LorentzianFunction.html.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi|^2 \, dx = \int_{-\infty}^{\infty} \frac{N^2 x^2}{(x^2+a^2)^2} \, dx = N^2 \left[\frac{1}{2a} \tan^{-1}\left(\frac{x}{a}\right) - \frac{x}{2(x^2+a^2)} \right]_{-\infty}^{\infty} \tag{28}$$

$$= \frac{N^2}{2a} \left(\frac{\pi}{2} - \frac{-\pi}{2} + 0 - 0 \right) = \frac{N^2 \pi}{2a} = \frac{2a^3}{\pi} \frac{\pi}{2a} = a^2 \tag{29}$$

Thus, the uncertainty in position is

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{a^2 - 0} = a \tag{30}$$

The probability of finding the particle in the interval $[-a, a]$ is

$$P(\text{in } [-a,a]) = \int_{-a}^{a} |\psi(x)|^2 \, dx = \frac{2a^3}{\pi} \int_{-a}^{a} \frac{1}{(x^2+a^2)^2} \, dx = \frac{1}{\pi} \left[\frac{ax}{x^2+a^2} + \tan^{-1}\left(\frac{x}{a}\right) \right]_{-a}^{a} \tag{31}$$

$$= \frac{1}{\pi} \left[\frac{a^2}{2a^2} + \tan^{-1} 1 - \frac{(-a^2)}{2a^2} - \tan^{-1}(-1) \right] = \frac{1}{\pi} \left(1 + \frac{\pi}{2} \right) \approx 0.818 \tag{32}$$

5. In electromagnetic theory, the conservation of charge is represented by the continuity equation (in one dimension)

$$\frac{\partial \vec{j}}{\partial x} = -e \frac{\partial \rho}{\partial t} \tag{33}$$

where $\vec{j}$ is current density and ρ charge density.

Identifying $|\psi(x)|^2$ as a ‘probability density,’ the quantum-mechanical analog of charge density is

$$j(x) = -\frac{i\hbar e}{2m} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \tag{34}$$

(a) Show that the continuity equation above is satisfied with this definition of current density.
(b) For a bound-state wave function (a wave that isn’t traveling), ψ can be chosen to be perfectly real, and $\psi^* = \psi$. What does this imply about the current density for bound states?
(c) Verify that the wave function from problem 4 gives zero current density everywhere.

Solution: The probability density is $|\psi(x)|^2$, and its time derivative is

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial t} |\psi(x)|^2 = \frac{\partial}{\partial t} (\psi^* \psi) = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \tag{35}$$

The time-dependent Schrödinger equation tells us

$$\frac{\partial\psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{i}{\hbar}V\psi \tag{36}$$

Taking the complex conjugate (replacing all i's with $-i$'s), we have

$$\frac{\partial\psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^* \tag{37}$$

Replacing the time derivatives in Eq. 35,

$$\frac{\partial P}{\partial t} = \left(\frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - \frac{i}{\hbar}V\psi\right)\psi + \left(-\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^*\right)\psi = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right) \tag{38}$$

Using the proposed equation for current density, Eq. 34,

$$\frac{\partial j}{\partial x} = -\frac{i\hbar e}{2m}\left(\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} + \psi^*\frac{\partial^2\psi}{\partial x^2} - \frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right) = -\frac{i\hbar e}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right) \tag{39}$$

Comparing, we see that $\partial j/\partial x$ only differs from $\partial P/\partial t$ by a factor $-e$, and thus

$$\frac{\partial\vec{j}}{\partial x} = -e\frac{\partial\rho}{\partial t} \tag{40}$$

There is also a derivation of the continuity equation here: `http://en.wikipedia.org/wiki/Probability_current`.

If ψ is perfectly real, as is the case for a bound state, then $\psi^* = \psi$, and the same is true of their derivatives, so j must be zero. Bound states are just what they sound like – bound – and do not flow out of a region.

The function in problem 4 is purely real, so $\psi^* = \psi$ and $\partial\psi^*/\partial x = \partial\psi/\partial x$ and the identity holds.

6. A particle is in a stationary state in the potential $V(x)$. The potential function is now increased over all x by a constant value V_o. What is the effect on the quantized energy? Show that the spatial wave function of the particle remains unchanged.

Solution: Changing the overall value of the potential by V_o is equivalent to changing the zero of potential energy by V_o. Since we can only measure differences in potential energy, all this does is globally shift our energy readings by V_o, and the measured energies must also then increase by V_o.

The time-independent Schrödinger equation in 1D reads

$$E\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \tag{41}$$

Adding V_o to the potential energy gives

$$E\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + (V(x) + V_o)\,\psi \tag{42}$$

$$(E - V_o)\,\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \tag{43}$$

$$\tag{44}$$

Thus, the same time-independent Schrödinger equation is obeyed, with the energies are shifted upward by V_o. The spatial part of the wave function remains unchanged, since $\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$ is still just equal to a constant times ψ.