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- Integrals you might need:

$$\int_0^{\pi} du\, \sin^2 u = \frac{\pi}{2}\,, \qquad \int_0^{\pi} du\, u \sin^2 u = \frac{\pi^2}{4}\,, \qquad \int_0^{\pi} du\, u^2 \sin^2 u = \frac{\pi^3}{6} - \frac{\pi}{4}\,.$$

- Suggestions for this assignment:
  (1) (Re-)read the section on Expectation Values (3.5) in Nash's notes.
  (2) Read about spin-1/2 systems. A couple of links appear on the module webpage.

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1. A particle is confined in the one-dimensional region between $x = 0$ to $x = L$. It is in the stationary state $\psi = \sqrt{\frac{2}{L}}\sin(\pi x/L)$.

   (a) Show that the wavefunction is normalized.

   Hint/Solution/Discussion →
   The square of the norm of the wavefunction is

$$\langle\psi|\psi\rangle \;=\; \int_0^L dx\, \big|\psi(x)\big|^2$$

The integral runs only from $x = 0$ to $x = L$ because the particle is confined in the region between $x = 0$ and $x = L$. You can think of this as being due to the fact that $\psi(x)$ vanishes everywhere outside this region:

$$\begin{aligned}\langle\psi|\psi\rangle \;&=\; \int_{-\infty}^{\infty} dx\, \big|\psi(x)\big|^2 \\ &=\; \int_{-\infty}^{0} dx\, \big|\psi(x)\big|^2 \;+\; \int_0^L dx\, \big|\psi(x)\big|^2 \;+\; \int_L^{\infty} dx\, \big|\psi(x)\big|^2 \\ &=\; 0 \;+\; \int_0^L dx\, \big|\psi(x)\big|^2 \;+\; 0 \;=\; \int_0^L dx\, \big|\psi(x)\big|^2.\end{aligned}$$

We are supposed to check that the given wavefunction is normalized, i.e, that $\langle\psi|\psi\rangle = 1$. So let's check:

$$\int_0^L dx\,\left|\psi(x)\right|^2 = \frac{2}{L}\int_0^L dx\,\sin^2\left(\frac{\pi x}{L}\right) = \frac{2}{L}\int_{u=0}^{u=L}\frac{Ldu}{\pi}\,\sin^2(u)$$
$$= \frac{2}{\pi}\int_{u=0}^{u=\pi} du\,\sin^2(u) = \frac{2}{\pi}\frac{\pi}{2} = 1.$$

The integral was done above using the variable substitution $x = Lu/\pi$. Hopefully you are able to do the integral in other ways, for example, by plotting the integrand and examining the symmetries of your plot. (Discussed in class.)

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(b) Find $\langle\hat{x}\rangle$, the expectation value of the position of the particle. (You should be able to guess the answer before doing the calculation.)

Hint/Solution/Discussion →
Let's guess first. The wavefunction is spread between $x = 0$ and $x = L$. So the average value of x is probably the midpoint of this interval. Do we expect $x = L/2$? Let's see:

$$\langle\hat{x}\rangle = \langle\psi|\,\hat{x}\,|\psi\rangle = \int_0^L dx\,\psi^*(x)\hat{x}\psi(x)$$
$$= \int_0^L dx\,\psi^*(x)x\psi(x) = \int_0^L dx\,x\left|\psi(x)\right|^2$$
$$= \frac{2}{L}\int_0^L dx\,x\sin^2\left(\frac{\pi x}{L}\right) = \frac{2}{L}\left(\frac{L}{\pi}\right)^2\int_0^\pi du\,u\sin^2 u$$
$$= \frac{2}{L}\left(\frac{L}{\pi}\right)^2\frac{\pi^2}{4} = \frac{L}{2}$$

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(c) Find the uncertainty of the position, i.e., $\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$.

Hint/Solution/Discussion →
Let's try guessing first. The wavefunction extends from 0 to L, i.e., the possible values of the particle position extends along this region. So the uncertainty in position should be of the order L. In other words, it is some constant value times L. This constant value could be 1 or 2 or 1/2 or π or some combination thereof. It's difficult (impossible?) to say what this constant is without explicitly calculating Δx. But we can infer, even before calculation, that the form is a constant times L.
To calculate Δx, we need both $\langle \hat{x}^2 \rangle$ and $\langle \hat{x} \rangle$. We've already calculated $\langle \hat{x} \rangle$ to be $\langle \hat{x} \rangle = L/2$. Let's calculate the expectation value of $\hat{x}^2$:

$$\begin{aligned}
\langle \hat{x}^2 \rangle &= \langle \psi | \hat{x}^2 | \psi \rangle = \int_0^L dx\, \psi^*(x) \hat{x}^2 \psi(x) \\
&= \int_0^L dx\, x^2 \big|\psi(x)\big|^2 = \frac{2}{L} \int_0^L dx\, x^2 \sin^2\left(\frac{\pi x}{L}\right) \\
&= \frac{2}{L}\left(\frac{L}{\pi}\right)^3 \int_0^\pi du\, u^2 \sin^2 u = \frac{2L^2}{\pi^3}\left(\frac{\pi^3}{6} - \frac{\pi}{4}\right) = \frac{L^2}{3} - \frac{L^2}{2\pi^2}
\end{aligned}$$

Putting this all together

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

Thus the position uncertainty is

$$\Delta x = \sqrt{\frac{1}{12} - \frac{1}{2\pi^2}}\, L$$

This is consistent with our guess: a dimensionless constant times L. The constant multiplying L appears to be quite small:

$$\left(\frac{1}{12} - \frac{1}{2\pi^2}\right)^{1/2} \approx 0.181$$

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(d) Find the expectation value of the momentum of the particle.
Warning: $\psi^*(x)\hat{p}\psi(x) \neq \hat{p}|\psi(x)|^2$. Why not?
(You should be able to guess the answer before doing the calculation.)

Hint/Solution/Discussion $\rightarrow$
Guessing: The particle is confined to a region. If it had a nonzero average momentum, surely it would move away from this region, and not be confined. So we expect the momentum expectation value to be zero.
To calculate the expectation value of the momentum, first recall that the momentum operator is given by

$$\hat{p} \;=\; -\,i\hbar\frac{d}{dx} \;=\; \frac{\hbar}{i}\frac{d}{dx} \;=\; -\,i\hbar\partial_x \;=\; \frac{\hbar}{i}\partial_x$$

Here ∂_x is shorthand for the derivative operator $\frac{d}{dx}$. If the wavefunction depends on other variables, e.g., time, you would also be justified in writing the operator as $\frac{\partial}{\partial x}$. i.e., whether it is a full derivative or a partial derivative depends on the context. Making this distinction is usually not important in quantum mechanics, so it doesn't matter much which of these notations you use.
The expectation value is

$$\begin{aligned} \langle\hat{p}\rangle \;=\; \langle\psi|\,\hat{p}\,|\psi\rangle \;&=\; \int_0^L dx\,\psi^*(x)\hat{p}\psi(x) \\ &=\; \int_0^L dx\,\psi^*(x)\left(\frac{\hbar}{i}\partial_x\right)\psi(x) \;=\; \frac{\hbar}{i}\int_0^L dx\,\psi^*(x)\,\partial_x\psi(x) \\ &=\; \frac{\hbar}{i}\int_0^L dx\,\psi^*(x)\,\psi'(x) \end{aligned}$$

Note: Please convince yourself that
$\psi^*(x)\hat{p}\psi(x)$ is NOT equal to $\hat{p}|\psi(x)|^2$.

Notation comment: the asterisk means complex conjugation, while the prime means taking the derivative. Some of you prefer an over-bar for complex conjugation, instead of an asterisk. That's perfectly okay, of course.

Using $\psi(x) = \sqrt{\frac{2}{L}}\sin(\pi x/L)$ we get for the given wavefunction

$$\begin{aligned}\langle\hat{p}\rangle &= \frac{\hbar}{i}\int_0^L dx\sqrt{\frac{2}{L}}\sin(\pi x/L)\sqrt{\frac{2}{L}}\frac{\pi}{L}\cos(\pi x/L) \\ &= \frac{\hbar}{i}\frac{2\pi}{L^2}\int_0^L dx\,\sin(\pi x/L)\,\cos(\pi x/L) \;=\; \frac{\hbar}{i}\frac{\pi}{L^2}\int_0^L dx\,\sin\left(\frac{2\pi x}{L}\right) \\ &\qquad\qquad = \frac{\hbar}{i}\frac{\pi}{L^2}\frac{L}{2\pi}\int_0^{2\pi} du\,\sin(0) \;=\; 0.\end{aligned}$$

We ended up with an integral of the sine function over a full period, which is zero. (Plot the sine function to make sure you see this visually.)

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(e) Find the uncertainty of the momentum.

Hint/Solution/Discussion →
To calculate

$$\Delta p \;=\; \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2} \;=\; \sqrt{\langle\hat{p}^2\rangle - 0} \;=\; \sqrt{\langle\hat{p}^2\rangle}$$

we need to calculate $\langle\hat{p}^2\rangle$, i.e., the expectation value of the operator

$$\hat{p}^2 \;=\; \hat{p}\hat{p} \;=\; \frac{\hbar}{i}\partial_x\frac{\hbar}{i}\partial_x \;=\; -\hbar^2\partial_x^2$$

Here ∂_x^2 is shorthand for the double-derivative operator $\frac{d^2}{dx^2}$.
Let's calculate the expectation value of this operator:

$$\begin{aligned}\langle\hat{p}^2\rangle \;=\; \langle\psi|\,\hat{p}^2\,|\psi\rangle \;&=\; -\hbar^2\int_0^L dx\,\psi^*(x)\partial_x^2\psi(x) \\ &= -\hbar^2\int_0^L dx\,\psi^*(x)\psi''(x)\end{aligned}$$

Using $\psi(x) = \sqrt{\frac{2}{L}}\sin(\pi x/L)$ we get

$$\begin{aligned}\langle \hat{p}^2\rangle &= -\hbar^2\int_0^L dx\,\sqrt{\frac{2}{L}}\sin(\pi x/L)\,\sqrt{\frac{2}{L}}\frac{\pi^2}{L^2}\big(-\sin(\pi x/L)\big)\\ &= +\hbar^2\frac{2\pi^2}{L^3}\int_0^L dx\,\sin^2(\pi x/L) \;=\; \frac{2\pi^2\hbar^2}{L^3}\frac{L}{\pi}\int_0^\pi du\,\sin^2(u)\\ &\qquad\qquad\qquad = \frac{2\pi^2\hbar^2}{L^3}\frac{L}{\pi}\frac{\pi}{2} \;=\; \frac{\pi^2\hbar^2}{L^2}\end{aligned}$$

As discussed before, the integral is $\pi/2$.
Thus

$$\Delta p = \sqrt{\langle \hat{p}^2\rangle - 0^2} = \frac{\pi\hbar}{L}$$

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(f) How does the position uncertainty depend on L? Could you have expected this?

Hint/Solution/Discussion →

This is discussed in the question where we calculated Δx. We guessed/argued that Δx should be a dimensionless constant times L, i.e., proportional to L. Restating the argument:

The particle is confined in the region $(0, L)$, hence a position measurement can give any value between 0 and L. We therefore expect the uncertainty in a position measurement to be proportional to L.

We cannot however predict the constant of proportionality from a physical argument like this; an explicit calculation is required. Indeed we have found above that Δx is a cumbersome number times L.

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(g) Does the momentum uncertainty increase or decrease, if L is increased? Explain whether/how this is consistent with the Heisenberg uncertainty principle.

Hint/Solution/Discussion $\rightarrow$
The momentum uncertainty Δp varies inversely with L, i.e., is proportional to $1/L$.
The Heisenberg uncertainty principle predicts that

$$\Delta x \Delta p \gtrsim \hbar \qquad \Longrightarrow \qquad \Delta p \gtrsim \frac{\hbar}{\Delta x}$$

The $\sim$ part of $\gtrsim$ indicates that these inequalities become precise with some constant, which we don't know or can't be bothered with at the moment. For microscopic states, we can replace the $\gtrsim$ by $\sim$:

$$\Delta p \sim \frac{\hbar}{\Delta x}$$

Since $\Delta x \sim L$, we expect

$$\Delta p \sim \frac{\hbar}{L}$$

i.e., Δp is a dimensionless constant times $\hbar/L$.
Indeed we have found Δp to be π times $\hbar/L$.

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(h) If the energy (Hamiltonian) operator is $\hat{H} = \frac{\hat{p}^2}{2m}$, find the expectation value and the uncertainty of the energy.

Hint/Solution/Discussion →
The expectation value is

$$\langle \hat{H} \rangle = \langle \frac{\hat{p}^2}{2m} \rangle = \frac{\langle \hat{p}^2 \rangle}{2m}$$

(Perhaps silly) question: why can't you replace $\langle \hat{p}^2 \rangle$ by $\langle \hat{p} \rangle^2$?

Good thing we already calculated $\langle \hat{p}^2 \rangle$ to be $\pi^2\hbar^2/L^2$.

$$\langle \hat{H} \rangle = \frac{\pi^2\hbar^2/L^2}{2m} = \frac{\pi^2\hbar^2}{2mL^2}$$

From your study of the infinite square well, you might have known this answer. The given wavefunction is the ground state wavefunction of the infinite square well whose Hamiltonian is $\hat{H} = \frac{\hat{p}^2}{2m}$ within the well. Hence the expectation value of $\hat{H}$ in this state gives us the ground state energy, which has the expression above.

Could we have otherwise guessed the energy, at least up to a constant? Use dimensional analysis. You can figure out that the only combination of $\hbar$, mass and distance which has the dimension of energy is $\hbar/(mL^2)$. This implies that energy is expected to be some constant times $\hbar/(mL^2)$.

The uncertainty of the energy is left as an exercise. For this calculation you have to evaluate $\langle \hat{p}^4 \rangle$, which is very similar to the calculation of $\langle \hat{p}^2 \rangle$ that we already did.

Explain physically why the uncertainty of the energy is expected to be zero for the given wavefunction.

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2. Recall for a spin-1/2 system:

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Each of these matrices have two eigenvalues, in each case $+\hbar/2$ and $-\hbar/2$.

(a) Why does it make sense physically that the three operators have the same set of eigenvalues? (What's the connection between measurement results and eigenvalues?)

Hint/Solution/Discussion →
The choice of which direction to call x, y or z is arbitrary. Thus. the three components should have the same possible values in physical measurement. Hence the three operators should have the same set of eigenvalues.

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(b) For S_x, verify the statement about eigenvalues above i.e., calculate eigenvalues of the S_x matrix.

Hint/Solution/Discussion →
Eigenvalues of $S_x = \begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix}$ are the solutions of the determinant equation

$$\left| \begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = 0 \qquad \Longrightarrow \qquad \begin{vmatrix} -\lambda & \hbar/2 \\ \hbar/2 & -\lambda \end{vmatrix} = 0$$

$$\Longrightarrow \qquad (-\lambda)^2 - \left(\frac{\hbar}{2}\right)^2 = 0 \qquad \Longrightarrow \qquad \lambda^2 = \left(\frac{\hbar}{2}\right)^2$$

The eigenvalues are therefore $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$.
If you are not 100% comfortable with calculating eigenvalues fast, please review the technique asap. For practice, calculate the eigenvalues of the matrix $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$.

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(c) The eigenvector of S_x corresponding to the eigenvector $+\hbar/2$ is $|x,+\rangle = \begin{pmatrix}\alpha\\ \alpha\end{pmatrix}$. Calculate α so that the state is normalized. You can choose α to be real and positive.

Hint/Solution/Discussion →

$$2|\alpha|^2 = 1 \qquad \Longrightarrow \qquad \alpha = \frac{1}{\sqrt{2}}$$

Taking α to be real and positive.
You should of course check that $|x,+\rangle$ is indeed an eigenvector of S_x as claimed, by calculating the matrix-vector product $S_x\,|x,+\rangle$.

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(d) Calculate the expectation value of S_x in the state $|x,+\rangle$, i.e., calculate $\langle S_x\rangle = \langle x,+|\,S_x\,|x,+\rangle$. (You should be able to predict the answer before doing the calculation.)

Hint/Solution/Discussion →

$$\begin{aligned}\langle S_x\rangle \;=\; \langle x,+|\,S_x\,|x,+\rangle \;&=\; \begin{pmatrix}\alpha^* & \alpha^*\end{pmatrix}\begin{pmatrix}0 & \hbar/2\\ \hbar/2 & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \alpha\end{pmatrix}\\ &=\; \begin{pmatrix}\alpha^* & \alpha^*\end{pmatrix}\begin{pmatrix}\alpha\hbar/2\\ \alpha\hbar/2\end{pmatrix} \;=\; 2|\alpha|^2\frac{\hbar}{2} \;=\; \frac{\hbar}{2}\end{aligned}$$

Since $|x,+\rangle$ is an eigenstate of S_x, a measurement of this observable will give the corresponding eigenvalue, i.e., we are sure to get the result $+\hbar/2$ in a measurement of the x-component of spin. So, the expectation value of the S_x operator should be $+\hbar/2$, as we found, and the uncertainty should be zero (next problem).

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(e) Calculate the uncertainty of S_x in the state $|x,+\rangle$. (You should be able to guess the answer before doing the calculation.)

Hint/Solution/Discussion →
We need to calculate $\sqrt{\langle S_x^2\rangle - \langle S_x\rangle^2}$.
Note that the operator (or matrix) S_x^2 is obtained by a matrix multiplication.

$$S_x^2 = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

Please note that this is NOT the same as squaring each element of S_x, i.e.,

$$S_x^2 \neq \begin{pmatrix}0 & \hbar^2/4\\ \hbar^2/4 & 0\end{pmatrix}$$

Therefore

$$\begin{aligned}\langle S_x^2\rangle &= \langle x,+|\, S_x^2\, |x,+\rangle = \frac{\hbar^2}{4}\begin{pmatrix}\alpha^* & \alpha^*\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\alpha\\ \alpha\end{pmatrix}\\ &= \frac{\hbar^2}{4}\begin{pmatrix}\alpha^* & \alpha^*\end{pmatrix}\begin{pmatrix}\alpha\\ \alpha\end{pmatrix} = \frac{\hbar^2}{4}2|\alpha|^2 = \frac{\hbar^2}{4}\end{aligned}$$

Thus the uncertainty is

$$\sqrt{\langle S_x^2\rangle - \langle S_x\rangle^2} = \sqrt{\frac{\hbar^2}{4} - \left(\frac{\hbar}{2}\right)^2} = 0$$

as expected.

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(f) Calculate the expectation value of S_z in the state $|x,+\rangle$. (You might be able to guess the answer before doing the calculation.)

Hint/Solution/Discussion →
What do we expect? $|x,+\rangle$ is an eigenstate of S_x, not of S_z. It's reasonable to assume that the $|x,+\rangle$ state does not prefer either a $+\hbar/2$ or a $-\hbar/2$ as the result for a measurement of S_z. (These are the only two outcomes of a S_z measurement.) So, one expects equal

probabilites for these two possible outcomes, if S_z is measured in the $|x,+\rangle$ state. One can thus expect the expectation value of S_z to be the average of these two values, i.e., 0. Let's see if this works:

$$\begin{aligned}\langle S_z\rangle &= \langle x,+|\, S_z\, |x,+\rangle = \begin{pmatrix}\alpha^* & \alpha^*\end{pmatrix}\begin{pmatrix}\hbar/2 & 0\\ 0 & -\hbar/2\end{pmatrix}\begin{pmatrix}\alpha\\ \alpha\end{pmatrix}\\ &= \begin{pmatrix}\alpha^* & \alpha^*\end{pmatrix}\begin{pmatrix}\alpha\hbar/2\\ -\alpha\hbar/2\end{pmatrix} = |\alpha|^2\frac{\hbar}{2} - |\alpha|^2\frac{\hbar}{2} = 0\end{aligned}$$

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(g) Calculate the uncertainty of S_z in the state $|x,+\rangle$.

Hint/Solution/Discussion →
One expects this to be nonzero, since outcomes $+\hbar/2$ and $-\hbar/2$ are equally probably. I can't however predict the exact value without doing the calculation.
Note that $S_z^2 = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = S_x^2$. Thus

$$\langle S_z^2\rangle = \langle S_x^2\rangle = \frac{\hbar^2}{4}$$

The uncertainty is

$$\Delta S_z = \sqrt{\langle S_z^2\rangle - \langle S_z\rangle^2} = \sqrt{\frac{\hbar^2}{4} - 0^2} = \frac{\hbar}{2}$$

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