$<3|3> \ge 0$. You have thereby introduced the relationship of inequality and the rest is the algebra of bras, kets, and norms. Remember that inner products are scalars.

Let
$$|3\rangle = |1\rangle - \frac{\langle 2|1\rangle}{|1\rangle|^2} |2\rangle \Rightarrow \langle 3| = \langle 1| - \langle 2|\frac{\langle 2|1\rangle^*}{|1\rangle|^2}$$
. Then $\langle 3|3\rangle \ge 0$, so $\langle 1|1\rangle - \langle 1|2\rangle \frac{\langle 2|1\rangle}{|1\rangle|^2} - \langle 2|1\rangle \frac{\langle 2|1\rangle^*}{|1\rangle|^2} + \frac{\langle 2|1\rangle\langle 2|1\rangle^*\langle 2|2\rangle}{|1\rangle|^2} \ge 0$.

Now $<2 |2> = ||2>|^2$ and using $<2 |1>^* = <1 |2>$ selectively,

$$<1|1> - <2|1> \frac{<2|1>^{*}}{||2>|^{2}} - \frac{<2|1>}{||2>|^{2}} <1|2> + \frac{<2|1>/(1|2>)}{||2>|^{2}} \ge 0.$$

$$\Rightarrow <1|1> \ge \frac{<2|1><2|1>^{*}}{||2>|^{2}}$$

$$\Rightarrow ||1>|^{2}||2>|^{2} \ge |<2|1>|^{2}$$

where $<2|1><2|1>^* = |<2|1>|^2$. Taking a square root of both sides yields $||1>||2>| \ge |<2|1>|$.

15. Show that $[\mathcal{X}, \mathcal{P}] = i\hbar$ in position space.

A commutator that is equivalent to multiplication by $i\hbar$ is called a **canonical commutator**. If $[\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} = i\hbar$ then $[\mathcal{A}, \mathcal{B}]$ is a canonical commutator. The commutator relating position and momentum operators, $[\mathcal{X}, \mathcal{P}] = i\hbar$, is particularly useful. Note that $[\mathcal{P}, \mathcal{X}] = -i\hbar$ when the order of the operators is reversed.

A commutator is an operator so is given an arbitrary function, f(x), on which to operate, then

$$\left[\mathcal{X}, \mathcal{P}\right] f(x) = \left(\mathcal{X}\mathcal{P} - \mathcal{P}\mathcal{X}\right) f(x) = \mathcal{X}\mathcal{P}f(x) - \mathcal{P}\mathcal{X}f(x).$$

Using the forms of the position and momentum operators in position space developed earlier,

$$\left[\mathcal{X}, \mathcal{P}\right] f(x) = (x) \left(-i\hbar \frac{d}{dx}\right) f(x) - \left(-i\hbar \frac{d}{dx}\right) x f(x)$$

where we need to use the chain rule to evaluate the last term. Differentiating,

$$\left[\mathcal{X}, \mathcal{P}\right] f(x) = -i\hbar x \frac{df(x)}{dx} + i\hbar f(x) + i\hbar x \frac{df(x)}{dx} = i\hbar f(x).$$

Since f(x) is an arbitrary function, the effect of the the commutator is $[\mathcal{X}, \mathcal{P}] = i\hbar$.

Postscript: The quantity $i\hbar$ means $i\hbar \mathcal{I}$ in two or more dimensions.

Canonical commutators are fundamentally important operators. The postulates of quantum mechanics can be stated in terms of canonical commutators.

16. Show that a commutator of two Hermitian operators \mathcal{A} and \mathcal{B} of the form $[\mathcal{A}, \mathcal{B}] = i\mathcal{C}$ requires that \mathcal{C} is Hermitian.

This problem is an intermediate result used to derive the Heisenberg uncertainty relations. It is a short application of commutator algebra and the meaning of Hermiticity.

$$\left[\mathcal{A},\mathcal{B}\right]^{\dagger} = \left(\mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}\right)^{\dagger} = \left(\mathcal{A}\mathcal{B}\right)^{\dagger} - \left(\mathcal{B}\mathcal{A}\right)^{\dagger} = \mathcal{B}^{\dagger}\mathcal{A}^{\dagger} - \mathcal{A}^{\dagger}\mathcal{B}^{\dagger} = \mathcal{B}\mathcal{A} - \mathcal{A}\mathcal{B} = -\left[\mathcal{A},\mathcal{B}\right] = -i\mathcal{C}.$$

Then $\left[\mathcal{A}, \mathcal{B}\right]^{\dagger} = \left(i\mathcal{C}\right)^{\dagger} = i^{\dagger}\mathcal{C}^{\dagger} = -i\mathcal{C} \iff \mathcal{C} = \mathcal{C}^{\dagger} \Rightarrow \mathcal{C} \text{ is Hermitian.}$

- 17. Define a "hatted" operator $\widehat{\mathcal{A}} = \mathcal{A} \langle \mathcal{A} \rangle \mathcal{I}$. Show that
- (a) $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] = \left[\mathcal{A}, \mathcal{B}\right]$ and
- (b) that if \mathcal{A} is Hermitian, $\widehat{\mathcal{A}}$ is Hermitian,
- (c) and that for Hermitian \mathcal{A} and \mathcal{B} , $(\triangle \mathcal{A})^2 (\triangle \mathcal{B})^2 = \left| |\widehat{\mathcal{A}}\psi\rangle \right|^2 \left| |\widehat{\mathcal{B}}\psi\rangle \right|^2$.

The use of "hatted" operators is a convenience used only to reduce clutter. Simply expand the commutator in terms of the definition for part (a). Remember that the identity operator and a scalar, an expectation value is a scalar for instance, commute with everything. The definitions of a "hatted" operator and Hermiticity are key to both parts (b) and (c). The definitions of uncertainty and a norm are also needed for part (c).

(a)
$$\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] = \widehat{\mathcal{A}}\widehat{\mathcal{B}} - \widehat{\mathcal{B}}\widehat{\mathcal{A}} = \left(\mathcal{A} - \langle \mathcal{A} \rangle \mathcal{I}\right) \left(\mathcal{B} - \langle \mathcal{B} \rangle \mathcal{I}\right) - \left(\mathcal{B} - \langle \mathcal{B} \rangle \mathcal{I}\right) \left(\mathcal{A} - \langle \mathcal{A} \rangle \mathcal{I}\right)$$

 $= \mathcal{A}\mathcal{B} - \mathcal{A} \langle \mathcal{B} \rangle \mathcal{I} - \langle \mathcal{A} \rangle \mathcal{I}\mathcal{B} + \langle \mathcal{A} \rangle \mathcal{I} \langle \mathcal{B} \rangle \mathcal{I}$
 $- \mathcal{B}\mathcal{A} + \mathcal{B} \langle \mathcal{A} \rangle \mathcal{I} + \langle \mathcal{B} \rangle \mathcal{I}\mathcal{A} - \langle \mathcal{B} \rangle \mathcal{I} \langle \mathcal{A} \rangle \mathcal{I}$
 $= \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} + \left(-\langle \mathcal{B} \rangle \mathcal{I}\mathcal{A} + \langle \mathcal{B} \rangle \mathcal{I}\mathcal{A}\right) + \left(-\langle \mathcal{A} \rangle \mathcal{I}\mathcal{B} + \langle \mathcal{A} \rangle \mathcal{I}\mathcal{B}\right)$
 $+ \left(\langle \mathcal{A} \rangle \langle \mathcal{B} \rangle \mathcal{I}^{2} - \langle \mathcal{A} \rangle \langle \mathcal{B} \rangle \mathcal{I}^{2}\right)$ where all the terms grouped in

parentheses sum to zero, therefore, $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} = \left[\mathcal{A}, \mathcal{B}\right].$

(b) The definition $\widehat{\mathcal{A}} = \mathcal{A} - \langle \mathcal{A} \rangle \mathcal{I} \Rightarrow \widehat{\mathcal{A}}^{\dagger} = \left(\mathcal{A} - \langle \mathcal{A} \rangle \mathcal{I}\right)^{\dagger} = \mathcal{A}^{\dagger} - \langle \mathcal{A} \rangle^{*} \mathcal{I}^{\dagger}$. Now $\mathcal{I}^{\dagger} = \mathcal{I}$ because of the nature of the identity, and $\mathcal{A}^{\dagger} = \mathcal{A}$ because it is given to be Hermitian.

The expectation value $\langle A \rangle$ is an expectation value of a Hermitian operator so is a real number meaning $\langle A \rangle^* = \langle A \rangle$, so

$$\widehat{\mathcal{A}}^{\dagger} = \mathcal{A}^{\dagger} - \langle \mathcal{A} \rangle^{*} \mathcal{I}^{\dagger} = \mathcal{A} - \langle \mathcal{A} \rangle \mathcal{I} = \widehat{\mathcal{A}}, \text{ therefore, if } \mathcal{A} \text{ is Hermitian, then } \widehat{\mathcal{A}} \text{ is Hermitian.}$$

(c) Consider the product of uncertainties

$$(\triangle \mathcal{A})^{2} (\triangle \mathcal{B})^{2} = \langle \psi | (\mathcal{A} - \langle \mathcal{A} \rangle \mathcal{I})^{2} | \psi \rangle \langle \psi | (\mathcal{B} - \langle \mathcal{B} \rangle \mathcal{I})^{2} | \psi \rangle$$

$$= \langle \psi | \widehat{\mathcal{A}}^{2} | \psi \rangle \langle \psi | \widehat{\mathcal{B}}^{2} | \psi \rangle$$

$$= \langle \psi | \widehat{\mathcal{A}} \widehat{\mathcal{A}} | \psi \rangle \langle \psi | \widehat{\mathcal{B}} \widehat{\mathcal{B}} | \psi \rangle$$

$$= \langle \psi | \widehat{\mathcal{A}}^{\dagger} \widehat{\mathcal{A}} | \psi \rangle \langle \psi | \widehat{\mathcal{B}} \widehat{\mathcal{B}} | \psi \rangle$$

$$= \langle \psi | \widehat{\mathcal{A}}^{\dagger} \widehat{\mathcal{A}} | \psi \rangle \langle \psi | \widehat{\mathcal{B}} \widehat{\mathcal{B}} | \psi \rangle$$

$$= \langle \psi \widehat{\mathcal{A}} | \widehat{\mathcal{A}} \psi \rangle \langle \psi \widehat{\mathcal{B}} | \widehat{\mathcal{B}} \psi \rangle = \left| | \widehat{\mathcal{A}} \psi \rangle \right|^{2} \left| | \widehat{\mathcal{B}} \psi \rangle \right|^{2}.$$

- 18. (a) Show that $\widehat{\mathcal{A}}\widehat{\mathcal{B}} = \frac{1}{2} \left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_{+} + \frac{1}{2} \left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]$ in general.
- (b) Show that $(\triangle \mathcal{A})^2 (\triangle \mathcal{B})^2 \ge \frac{1}{4} < \psi | [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_+ | \psi >^2 + \frac{1}{4} < \psi | \mathcal{C} | \psi >^2$ given that \mathcal{A} and \mathcal{B} are Hermitian and that $[\mathcal{A}, \mathcal{B}] = i\mathcal{C}$.

This problem introduces the anti–commutator defined $[\mathcal{A}, \mathcal{B}]_{+} = \mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A}$. Part (a) is simply an algebra problem using this definition and the additive identity. This result is used in part (b). Start with the last result of problem 17 for part (b). Apply the Schwarz inequality to get

$$(\triangle \mathcal{A})^2 (\triangle \mathcal{B})^2 \ge \frac{1}{4} | \langle \psi | [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_+ + i \mathcal{C} | \psi \rangle |^2.$$

Use the relation from part (a), the meanings of Hermiticity and the norm, and results from problems 16 and 17 to arrive at the result.

(a) $\begin{aligned}
\widehat{\mathcal{A}}\widehat{\mathcal{B}} &= \frac{1}{2}\,\widehat{\mathcal{A}}\widehat{\mathcal{B}} + \frac{1}{2}\,\widehat{\mathcal{A}}\widehat{\mathcal{B}} \\
&= \frac{1}{2}\,\widehat{\mathcal{A}}\widehat{\mathcal{B}} + \frac{1}{2}\,\widehat{\mathcal{A}}\widehat{\mathcal{B}} + \frac{1}{2}\,\widehat{\mathcal{B}}\,\widehat{\mathcal{A}} - \frac{1}{2}\,\widehat{\mathcal{B}}\,\widehat{\mathcal{A}} \\
&= \frac{1}{2}\,\Big(\widehat{\mathcal{A}}\widehat{\mathcal{B}} + \widehat{\mathcal{B}}\,\widehat{\mathcal{A}}\Big) + \frac{1}{2}\,\Big(\widehat{\mathcal{A}}\widehat{\mathcal{B}} - \widehat{\mathcal{B}}\,\widehat{\mathcal{A}}\Big) = \frac{1}{2}\,\big[\,\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\,\big]_{+} + \frac{1}{2}\,\big[\,\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\,\big]_{+} \\
\end{aligned}$

(b) Applying the Schwarz inequality to the relation from part (c) of problem 17 means

$$(\Delta \mathcal{A})^{2} (\Delta \mathcal{B})^{2} = \left| |\widehat{\mathcal{A}}\psi\rangle \right|^{2} \left| |\widehat{\mathcal{B}}\psi\rangle \right|^{2} \ge \left| \langle\psi|\widehat{\mathcal{A}}\widehat{\mathcal{B}}|\psi\rangle \right|^{2}$$
$$\Rightarrow (\Delta \mathcal{A})^{2} (\Delta \mathcal{B})^{2} \ge \left| \langle\psi|\frac{1}{2}[\widehat{\mathcal{A}},\widehat{\mathcal{B}}]_{+} + \frac{1}{2}[\widehat{\mathcal{A}},\widehat{\mathcal{B}}]|\psi\rangle \right|^{2}$$

$$\Rightarrow \quad \left(\bigtriangleup \mathcal{A} \right)^2 \left(\bigtriangleup \mathcal{B} \right)^2 \geq \frac{1}{4} \left| < \psi \left| \left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}} \right]_+ + i \, \mathcal{C} \left| \psi \right> \right|^2 \right.$$

since $[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}] = [\mathcal{A}, \mathcal{B}] = i\mathcal{C}$. The anti-commutator is Hermitian, *i.e.*, $[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_{+}^{\dagger} = [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_{+}^{\dagger}$. A Hermitian operator is analogous to a real number. And since \mathcal{C} is previously shown to be Hermitian it also analogous to a real number. The right side of the last equation is an operator expression analogous to a complex number of the form a + ib. The right side of the last equation concerns the norm of a quantity analogous to a complex number. The norm of a complex number is $|a + ib|^2 = a^2 + b^2$. Extending this argument to the right side of the last equation,

$$\left(\bigtriangleup\mathcal{A}\right)^{2}\left(\bigtriangleup\mathcal{B}\right)^{2} \geq \frac{1}{4} < \psi \left| \left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_{+} \right| \psi >^{2} + \frac{1}{4} < \psi \left| \mathcal{C} \right| \psi >^{2}$$

Postscript: The result of part (b) is a statement of the **general uncertainty relation**.

19. Given canonically conjugate operators \mathcal{A} and \mathcal{B} , show that $(\triangle \mathcal{A})(\triangle \mathcal{B}) \geq \frac{1}{2}\hbar$.

This problem is a derivation of the relation commonly known as the **Heisenberg uncertainty** relation or the **Heisenberg uncertainty principle**. The relation between canonically conjugate operators is $[\mathcal{A}, \mathcal{B}] = i\hbar = i\hbar \mathcal{I}$. The result of part (b) of the last problem relies on the relation $[\mathcal{A}, \mathcal{B}] = i\mathcal{C}$. Let $\mathcal{C} = \hbar \mathcal{I}$. The first term on the right side of the general uncertainty principle is Hermitian so its magnitude is real and we can conclude it is greater than or equal to zero, *i.e.*,

$$\frac{1}{4} < \psi \left| \left[\mathcal{A}, \mathcal{B} \right]_+ \right| \psi >^2 \ge 0.$$

Since this term can never be less than zero, we can surmise that

$$(\bigtriangleup \mathcal{A})^2 (\bigtriangleup \mathcal{B})^2 \geq \frac{1}{4} < \psi \, | \, \mathcal{C} \, | \, \psi \! >^2$$

Substitute $\hbar \mathcal{I}$ for \mathcal{C} and assume an orthonormal basis to arrive at the desired result.

$$\begin{aligned} \left(\bigtriangleup \mathcal{A} \right)^{2} \left(\bigtriangleup \mathcal{B} \right)^{2} &\geq \frac{1}{4} < \psi \, | \, \mathcal{C} \, | \, \psi >^{2} \\ \Rightarrow \quad \left(\bigtriangleup \mathcal{A} \right)^{2} \left(\bigtriangleup \mathcal{B} \right)^{2} &\geq \frac{1}{4} < \psi \, | \, \hbar \, \mathcal{I} \, | \, \psi >^{2} \\ \Rightarrow \quad \left(\bigtriangleup \mathcal{A} \right)^{2} \left(\bigtriangleup \mathcal{B} \right)^{2} &\geq \frac{1}{4} \left(\hbar \right)^{2} < \psi \, | \, \mathcal{I} \, | \, \psi >^{2} \\ \Rightarrow \quad \left(\bigtriangleup \mathcal{A} \right)^{2} \left(\bigtriangleup \mathcal{B} \right)^{2} &\geq \frac{1}{4} \, \hbar^{2} < \psi \, | \, \psi >^{2} \\ \Rightarrow \quad \left(\bigtriangleup \mathcal{A} \right)^{2} \left(\bigtriangleup \mathcal{B} \right)^{2} &\geq \frac{1}{4} \, \hbar^{2}, \end{aligned}$$

assuming that the basis is orthonormal $\Rightarrow \langle \psi | \psi \rangle = 1$. A square root of both sides yields

$$(\triangle \mathcal{A})(\triangle \mathcal{B}) \geq \frac{1}{2}\hbar$$

for canonically conjugate commutators in an orthonormal basis.

Postscript: The most common application is to the fundamental canonical commutator,

$$\left[\left. \mathcal{X}, \mathcal{P} \right.
ight] = i\hbar \quad \Rightarrow \quad \left(\bigtriangleup \mathcal{X} \right) \left(\bigtriangleup \mathcal{P} \right) \; \ge \; rac{1}{2} \, \hbar \, .$$

This is stated in terms of the uncertainties of operators. It is a much more general statement than the relation $\Delta x \Delta p \ge \hbar/2$ stated in terms of the uncertainties of real scalars in position space.

20. Use the Heisenberg uncertainty principle to show that the Bohr model of the hydrogen atom is technically flawed.

The statement $\Delta x \Delta p \ge \hbar/2$ in position space is often used to demonstrate implausibility or impossibility, as seen in this problem.

One fundamental premise of the Bohr atom is that "orbits" are quantized such that $pr = n\hbar$, for $n = 1, 2, 3, \ldots$ We expect that $\Delta x \ll r$, (or $\Delta r \ll r$), and $\Delta p \ll p$ in these precisely defined orbits. Rewriting these relations

$$\frac{\Delta x}{r} \ll 1$$
, and $\frac{\Delta p}{p} \ll 1 \Rightarrow \frac{\Delta x \Delta p}{rp} \ll 1.$ (1)

The premise $pr = n\hbar \Rightarrow \hbar = pr/n$, so the uncertainty principle states

$$\triangle x \, \triangle p \geq \frac{\hbar}{2} = \frac{pr}{2n} \quad \Rightarrow \quad \frac{\triangle x \, \triangle p}{rp} \geq \frac{1}{2n}$$

which is inconsistent with statement (1) except for large n. Since hydrogen appears to be stable in its ground state, n = 1, the Heisenberg uncertainty principle indicates that the Bohr model of the hydrogen atom is technically flawed.

21. Show that the general uncertainty relation becomes an equality when both

$$\langle \psi | [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_{+} | \psi \rangle = 0$$
 and $\widehat{\mathcal{A}} | \psi \rangle = \beta \widehat{\mathcal{B}} | \psi \rangle_{2}$

where β is a scalar. \mathcal{A} and \mathcal{B} are given to be Hermitian.

This problem is intended to deepen your grasp on the general uncertainty relation. For Hermitian \mathcal{A} and \mathcal{B} , $[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}] = [\mathcal{A}, \mathcal{B}]$, however, $[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_+ \neq [\mathcal{A}, \mathcal{B}]_+$, in general (see problem 36). Thus, it is appropriate to work with "hatted" operators. The assumption $\langle \psi | [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_+ | \psi \rangle = 0$ is implied in the derivation of the uncertainty relation for the fundamental canonical commutator since only the $\frac{1}{4} \langle \psi | \mathcal{C} | \psi \rangle^2$ term is retained to conclude $(\Delta \mathcal{A})(\Delta \mathcal{B}) \geq \frac{1}{2}\hbar$. The "hatted" anti-commutator is Hermitian, therefore, the expectation value is real. This allows a conclusion about the square of the expectation value and its impact on the argument leading to the general uncertainty relation. The substance of the problem is the rearrangement of the second condition

using bra/ket algebra. Use adjoint quantities to attain the product of the squares of the norms of $\mathcal{A} | \psi \rangle$ and $\mathcal{B} | \psi \rangle$, substitute the right side of the second condition, and use the definition of a norm. You should find that the square of the right side of the Schwarz inequality emerges under a relationship of equality. The condition of *proportionality* allows the minimum in the product of uncertainties, $(\Delta \mathcal{A})(\Delta \mathcal{B}) = \frac{1}{2}\hbar$.

The anti-commutator $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_+$ is a Hermitian operator. A Hermitian operator has real eigenvalues. The expectation value $\langle \psi | [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_+ | \psi \rangle$ is therefore a real scalar which means that $\langle \psi | [\widehat{\mathcal{A}}, \widehat{\mathcal{B}}]_+ | \psi \rangle^2 \geq 0$. Since this quantity is greater than or equal to zero,

$$\frac{1}{4} < \psi \,|\, \widehat{\mathcal{A}}, \, \widehat{\mathcal{B}} \,]_{+} \,|\, \psi >^{2} + \frac{1}{4} \,< \psi \,|\, \mathcal{C} \,|\, \psi >^{2} = \frac{1}{4} \,< \psi \,|\, \mathcal{C} \,|\, \psi >^{2},$$

if and only if

$$\psi | \hat{\mathcal{A}}, \hat{\mathcal{B}}]_+ | \psi \rangle^2 = 0 \quad \Rightarrow \quad \langle \psi | [\hat{\mathcal{A}}, \hat{\mathcal{B}}]_+ | \psi \rangle = 0.$$

Then $\widehat{\mathcal{A}} \mid \psi > = \beta \, \widehat{\mathcal{B}} \mid \psi > \Rightarrow \langle \psi \mid \widehat{\mathcal{A}} = \langle \psi \mid \widehat{\mathcal{B}} \, \beta^*$. The product of the norms squared is

$$\begin{split} \left| \left| \widehat{\mathcal{A}}\psi \right\rangle \right|^{2} \left| \left| \widehat{\mathcal{B}}\psi \right\rangle \right|^{2} &= \left| \left| \beta \widehat{\mathcal{B}}\psi \right\rangle \right|^{2} \left| \left| \widehat{\mathcal{B}}\psi \right\rangle \right|^{2} \\ &= \langle \psi \widehat{\mathcal{B}}\beta \left| \beta \widehat{\mathcal{B}}\psi \right\rangle \langle \psi \widehat{\mathcal{B}} \left| \widehat{\mathcal{B}}\psi \right\rangle \\ &= \left| \beta \right|^{2} \langle \psi \widehat{\mathcal{B}} \left| \widehat{\mathcal{B}}\psi \right\rangle \langle \psi \widehat{\mathcal{B}} \right| \widehat{\mathcal{B}}\psi \rangle \\ &= \langle \psi \widehat{\mathcal{B}}\beta \left| \widehat{\mathcal{B}}\psi \right\rangle \langle \psi \widehat{\mathcal{B}} \right| \beta \widehat{\mathcal{B}}\psi \rangle \\ &= \langle \psi \widehat{\mathcal{A}} \left| \widehat{\mathcal{B}}\psi \right\rangle \langle \psi \widehat{\mathcal{B}} \right| \beta \widehat{\mathcal{A}}\psi \rangle \\ &= \langle \psi \widehat{\mathcal{A}} \left| \widehat{\mathcal{B}}\psi \right\rangle \langle \psi \widehat{\mathcal{A}} \right| \widehat{\mathcal{B}}\psi \rangle^{*} \\ &= \left| \langle \psi \right| \widehat{\mathcal{A}}\widehat{\mathcal{B}} \left| \psi \right\rangle \right|^{2}, \end{split}$$

after considering the result of problem 17 (c), $(\triangle A)^2 (\triangle B)^2 = ||\widehat{A}\psi \rangle |^2 ||\widehat{B}\psi \rangle |^2$. The relation of equality is thus appropriate for the Schwarz inequality used in problem 18 (b) so that the relation of equality is appropriate for the general uncertainty relation that results.

22. Assume that $\langle \psi | [\mathcal{X}, \mathcal{P}]_+ | \psi \rangle = 0$ and $\mathcal{P} | \psi \rangle = \beta \mathcal{X} | \psi \rangle$ where $\beta = i\hbar/\alpha^2$. Show that these conditions require that the wavefunction in position space is Gaussian.

This problem joins the Gaussian wavefunction and the uncertainty principle to canonical operators under conditions that require the relation of equality in the general uncertainty principle. Act with $\langle x |$ to establish the second condition in position space. Use the position space representations of \mathcal{X} and \mathcal{P} . This results in a variables separable differential equation $\Rightarrow \psi(x) = e^{i\beta x^2/2\hbar}$. Substitute the expression given for β to realize a Gaussian function.

Acting with $\langle x |$ to establish the second condition in position space, and using the position space representations of \mathcal{X} and \mathcal{P} ,

$$\langle x | \mathcal{P} | \psi \rangle = \langle x | \beta \mathcal{X} | \psi \rangle \quad \Rightarrow \quad -i\hbar \frac{d}{dx} \langle x | \psi \rangle = \beta x \langle x | \psi \rangle$$

$$\Rightarrow -i\hbar \frac{d}{dx} \psi(x) = \beta x \psi(x) \Rightarrow \frac{d\psi(x)}{dx} = \frac{i}{\hbar} \beta x \psi(x) \Rightarrow \frac{d\psi(x)}{\psi(x)} = \frac{i}{\hbar} \beta x dx$$

$$\Rightarrow \ln \psi(x) = \frac{i}{\hbar} \beta \frac{x^2}{2} \Rightarrow \psi(x) = e^{i\beta x^2/2\hbar}$$
and $\beta = i \frac{\hbar}{\alpha^2} \Rightarrow \psi(x) = e^{-\hbar x^2/2\hbar\alpha^2} \Rightarrow \psi(x) = e^{-x^2/2\alpha^2}$

which is the unnormalized t = 0 Gaussian wavefunction.

23. Assuming that the wave function $|\psi\rangle$ is a function of time and that the operator \mathcal{A} is time independent, show that

$$\langle \dot{\mathcal{A}} \rangle = rac{i}{\hbar} \langle \left[\mathcal{H}, \mathcal{A} \right] \rangle$$
.

This problem derives **Ehrenfest's theorem**. Quantum mechanics must yield the results of classical mechanics in a classical regime. That the relations of quantum mechanics reduce to the relations of classical mechanics for large quantum numbers is Bohr's correspondence principle. Paul Ehrenfest replaces the dynamical variables of classical mechanics with the expectation values of quantum mechanics to attain an alternative viewpoint.

Start with the expectation value of a time-independent operator, $\langle \mathcal{A} \rangle = \langle \psi | \mathcal{A} | \psi \rangle$, and take a time derivative. The chain rule is necessary because the wavefunction is assumed to be a function of time. \mathcal{A} is assumed to be time independent so its time derivative is zero. Employ the time-dependent Schrodinger equation which introduces both $| \dot{\psi} \rangle$ and \mathcal{H} . Finally, realize that \mathcal{H} is Hermitian so you can attain a form for $\langle \dot{\psi} |$ from the adjoint.

$$<\!\mathcal{A}\!> = <\!\psi \,|\,\mathcal{A}\,|\,\psi\!> \quad \Rightarrow \quad \frac{d}{dt} <\!\mathcal{A}\!> = <\!\dot{\psi}\,|\,\mathcal{A}\,|\,\psi\!> + <\!\psi \,|\,\dot{\mathcal{A}}\,|\,\psi\!> + <\!\psi \,|\,\mathcal{A}\,|\,\dot{\psi}\!> \;.$$

Since the operator is assumed to be time independent, the middle term is zero so

$$\frac{d}{dt} < \mathcal{A} > = \langle \dot{\psi} | \mathcal{A} | \psi > + \langle \psi | \mathcal{A} | \dot{\psi} \rangle .$$
(1)

The time-dependent Schrodinger equation is

$$\mathcal{H} | \psi \rangle = i\hbar | \dot{\psi} \rangle \quad \Rightarrow \quad | \dot{\psi} \rangle = \frac{1}{i\hbar} \mathcal{H} | \psi \rangle = -\frac{i}{\hbar} \mathcal{H} | \psi \rangle . \quad \text{The adjoint is} \quad \langle \dot{\psi} | = \langle \psi | \mathcal{H}^{\dagger} \left(\frac{i}{\hbar} \right),$$

and since the Hamiltonian is Hermitian, $\langle \dot{\psi} | = \frac{i}{\hbar} \langle \psi | \mathcal{H}$. Using these in equation (1),

$$\begin{aligned} \frac{d}{dt} < \mathcal{A} > &= \frac{i}{\hbar} < \psi \,|\, \mathcal{H} \,\mathcal{A} \,|\, \psi > -\frac{i}{\hbar} < \psi \,|\, \mathcal{A} \,\mathcal{H} \,|\, \psi > \\ &= \frac{i}{\hbar} \left(< \psi \,|\, \mathcal{H} \,\mathcal{A} \,|\, \psi > - < \psi \,|\, \mathcal{A} \,\mathcal{H} \,|\, \psi > \right) \\ &= \frac{i}{\hbar} < \psi \,|\, \left[\,\mathcal{H} , \,\mathcal{A} \,\right] \,|\, \psi > \quad \text{or} \quad <\dot{\mathcal{A}} > = \frac{i}{\hbar} < \left[\,\mathcal{H} , \,\mathcal{A} \,\right] > \quad \text{which is Ehrenfest's theorem.} \end{aligned}$$

24. Given that the potential energy is a function of position, calculate $\langle \dot{\mathcal{X}} \rangle$.

This problem applies Ehrenfest's theorem and exercises commutator algebra. Substitute \mathcal{X} for \mathcal{A}

$$\Rightarrow \langle \dot{\mathcal{X}} \rangle = \frac{i}{\hbar} \langle \left[\mathcal{H}, \mathcal{X} \right] \rangle \text{ Use the Hamiltonian for a particle } \mathcal{H} = \frac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X})$$
$$\Rightarrow \langle \dot{\mathcal{X}} \rangle = \frac{i}{\hbar} \langle \left[\frac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X}), \mathcal{X} \right] \rangle = \frac{i}{\hbar} \langle \left[\frac{\mathcal{P}^2}{2m}, \mathcal{X} \right] + \left[\mathcal{V}(\mathcal{X}), \mathcal{X} \right] \rangle \text{ .}$$

Use the fact that a commutator containing an operator that is a sum can be split into the sum of two commutators as shown. We demonstrate that this is true when addressing angular momentum. Since $\mathcal{V}(\mathcal{X})$ is a function of position, it commutes with \mathcal{X} making the second commutator easy to evaluate. Expand the first commutator and then add zero in the form of $\mathcal{P}\mathcal{X}\mathcal{P} - \mathcal{P}\mathcal{X}\mathcal{P}$.

Using the given and commentary conditions in Ehrenfest's theorem,

$$\langle \dot{\mathcal{X}} \rangle = \frac{i}{\hbar} \langle \left[\frac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X}), \mathcal{X} \right] \rangle = \frac{i}{\hbar} \langle \left[\frac{\mathcal{P}^2}{2m}, \mathcal{X} \right] + \left[\mathcal{V}(\mathcal{X}), \mathcal{X} \right] \rangle.$$

The second commutator in the expectation value is zero because $\mathcal{V}(\mathcal{X})$ commutes with \mathcal{X} . The

time derivative of the position operator is $\langle \dot{\mathcal{X}} \rangle = \frac{i}{\hbar} \langle \left[\frac{\mathcal{P}^2}{2m}, \mathcal{X}\right] \rangle = \frac{i}{2m\hbar} \langle \left[\mathcal{P}^2, \mathcal{X}\right] \rangle$. (1)

The commutator, $\left[\mathcal{P}^2, \mathcal{X}\right] = \mathcal{P}^2 \mathcal{X} - \mathcal{X} \mathcal{P}^2 = \mathcal{P} \mathcal{P} \mathcal{X} - \mathcal{X} \mathcal{P} \mathcal{P}$. Adding and subtracting $\mathcal{P} \mathcal{X} \mathcal{P}$,

$$\begin{bmatrix} \mathcal{P}^{2}, \mathcal{X} \end{bmatrix} = \mathcal{P}\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\mathcal{P} + \mathcal{P}\mathcal{X}\mathcal{P} - \mathcal{P}\mathcal{X}\mathcal{P} = \mathcal{P}\mathcal{P}\mathcal{X} - \mathcal{P}\mathcal{X}\mathcal{P} + \mathcal{P}\mathcal{X}\mathcal{P} - \mathcal{X}\mathcal{P}\mathcal{P} \\ = \mathcal{P}\left(\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\right) + \left(\mathcal{P}\mathcal{X} - \mathcal{X}\mathcal{P}\right)\mathcal{P} = \mathcal{P}\left[\mathcal{P}, \mathcal{X}\right] + \left[\mathcal{P}, \mathcal{X}\right]\mathcal{P} \\ = \mathcal{P}\left(-i\hbar\right) + \left(-i\hbar\right)\mathcal{P} = -2i\hbar\mathcal{P}, \end{cases}$$

having recognized the fundamental canonical commutator. Using this in equation (1),

$$\langle \dot{\mathcal{X}} \rangle = \frac{i}{2m\hbar} \langle (-2i\hbar \mathcal{P}) \rangle = \frac{i}{2m\hbar} (-2i\hbar) \langle \mathcal{P} \rangle = \frac{\langle \mathcal{P} \rangle}{m}.$$

Postscript: Classically, the time derivative of position is velocity, momentum divided by mass. The equation $\langle \dot{\mathcal{X}} \rangle = \langle \mathcal{P} \rangle / m$ is a quantum mechanical analogy of this classical statement. It is one of Ehrenfest's equations. Problem 38 addresses the other Ehrenfest equation.

25. Using a Gaussian wave packet, find the expectation value of the time rate of change of position in position space assuming that potential energy is a function of position.

The fact that the Gaussian wave packet is an excellent model is sometimes overlooked in the relatively strenuous mathematics. The Gaussian wave packet is the assumed standard in the absence of additional information. The normalized Gaussian wave packet can be described

$$\psi(x) = \frac{e^{ip_0 x/\hbar} e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}} \quad \text{and you remember that in one spatial dimension} \quad \mathcal{P} = -i\hbar \frac{d}{dx},$$

so using the result of problem 25, $\langle \dot{\mathcal{X}} \rangle = \frac{\langle \mathcal{P} \rangle}{m}$, the desired expectation value is

$$\langle \dot{\mathcal{X}} \rangle = \frac{\langle \mathcal{P} \rangle}{m} = \frac{1}{m} \int_{-\infty}^{\infty} \psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \psi(x) \, dx \, .$$

This becomes a Gaussian integral and the integral of an odd function between symmetric limits.

Using the result from problem 25,

$$\begin{aligned} <\dot{\mathcal{X}}> &= \frac{-i\hbar}{m} \int_{-\infty}^{\infty} \frac{e^{-ip_0 x/\hbar} e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}} \left(\frac{d}{dx}\right) \frac{e^{ip_0 x/\hbar} e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}} \, dx \\ &= \frac{-i\hbar}{m\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-ip_0 x/\hbar} e^{-x^2/2\alpha^2} \left(\frac{d}{dx}\right) e^{ip_0 x/\hbar} e^{-x^2/2\alpha^2} \, dx \\ &= \frac{-i\hbar}{m\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-ip_0 x/\hbar} e^{-x^2/2\alpha^2} \left(\frac{ip_0}{\hbar} e^{ip_0 x/\hbar} e^{-x^2/2\alpha^2} - \frac{x}{\alpha^2} e^{ip_0 x/\hbar} e^{-x^2/2\alpha^2}\right) \, dx \\ &= \frac{-i\hbar}{m\alpha\sqrt{\pi}} \frac{ip_0}{\hbar} \int_{-\infty}^{\infty} e^{-x^2/\alpha^2} \, dx + \frac{i\hbar}{m\alpha\sqrt{\pi}} \frac{1}{\alpha^2} \int_{-\infty}^{\infty} x \, e^{-x^2/\alpha^2} \, dx \\ &= \frac{p_0}{m\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\alpha^2} \, dx + \frac{i\hbar}{m\alpha^3\sqrt{\pi}} \int_{-\infty}^{\infty} x \, e^{-x^2/\alpha^2} \, dx. \end{aligned}$$

The second integrand is the product of an odd and even function so is an odd function. The integral of an odd function evaluated between symmetric limits is zero. The first integral is Gaussian and is $\sqrt{\pi \alpha^2} = \alpha \sqrt{\pi}$. The expectation value then, is

 $\langle \dot{\mathcal{X}} \rangle = \frac{p_0}{m\alpha\sqrt{\pi}} \ \alpha\sqrt{\pi} = \frac{p_0}{m} = \frac{mv_0}{m} = v_0$, which you recognize from introductory physics.

Practice Problems

26. Show that the normalization constant of a Gaussian function is $1/(\pi \alpha^2)^{1/4}$.

This is a straightforward application of the normalization condition. See problem 4.

27. (a) What are the possible outcomes of a measurement of momentum of a free particle? Calculate the probability of each possible outcome.

- (b) Explain why you can assume the orthornormality of eigenstates.
- (c) Assume $\langle E | \mathcal{P} | E \rangle = \langle p | \mathcal{P} | p \rangle$ to use $\langle E | \mathcal{P} | E \rangle$ to find the expectation value of momentum for a free particle.

- (d) Explain why you can assume that $\langle E | \mathcal{P} | E \rangle = \langle p | \mathcal{P} | p \rangle$.
- (e) Use $\langle A \rangle = \sum P(\alpha_i) \alpha_i$ to verify your result from part (c).

This problem amplifies problem 2. Postulate 1 says that $|E\rangle = c_1 |+p^2/2m\rangle + c_2 |-p^2/2m\rangle$. Postulate 3 describes possibilities. Probabilities are calculated using postulate 4,

$$P(\alpha) \propto | < \alpha | \psi > |^2$$
 or $P(\alpha) = \frac{| < \alpha | \psi > |^2}{< \psi | \psi >}$.

You should find $P(+p) = \frac{|c_1|^2}{|c_1|^2 + |c_2|^2}$ and $P(-p) = \frac{|c_2|^2}{|c_1|^2 + |c_2|^2}$ for part (a). Refer to postulate 2 for part (b). Remember that \mathcal{H} and \mathcal{P} commute for part (d). You should find that the expectation value is $\langle \mathcal{P} \rangle = |c_1|^2 (+p) + |c_2|^2 (-p)$.

28. Normalize $|E\rangle = c_1 |\alpha\rangle + c_2 |\beta\rangle + c_3 |\gamma\rangle$, given that α , β , and γ are energy eigenvalues.

Energy is an observable quantity so the operator constructed from the eigenvectors $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$ is Hermitian. If the operator is Hermitian, its eigenvectors are orthogonal. If the eigenvectors are orthogonal, they can be made orthonormal. You should find that the normalized state vector is $\frac{|E\rangle}{\sqrt{|c_1|^2 + |c_2|^2 + |c_3|^2}}$. Use procedures similar to those in problem 27.

29. Solve the Schrödinger equation for a free particle in momentum space.

This problem is largely an exercise in representation. For a free particle, $V(x) = 0 \Rightarrow \mathcal{V}(\mathcal{X}) = 0$, so the Hamiltonian is $\mathcal{P}^2/2m$. In momentum space, $\mathcal{P} \to p$. Use this to form the Hamiltonian, then use your Hamiltonian in the Schrödinger equation. Act on both sides of the of your resulting Schrödinger equation with $|\langle p \rangle|$ to arrive at a momentum space representation. You should find

$$\frac{p^{2}}{2m}\,\widehat{\psi}\left(p,t\right) \;=\; i\hbar\,\frac{\partial}{\partial t}\,\widehat{\psi}\left(p,t\right).$$

Recognize that the solution is $\hat{\psi}(p,t) = A e^{-iEt/\hbar}$. Substitute this into your Schrodinger equation and do the requisite differentiation to demonstrate that it is a solution. The procedure for finding the eigenvalues is similar to the argument used to find eigenvalues in position space in problem 3.

30. Show that Gaussian wavefunction

$$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}} \left(1 + \frac{i\hbar}{m\alpha^2}t\right)^{-1/2} \exp\left[-\frac{x^2}{2\left(\alpha^2 + \frac{i\hbar}{m}t\right)}\right] \quad \text{is normalized.}$$

The given equation is the result of problem 8. This problem shows that the Gaussian wavefunction used throughout this chapter is normalized. The problem amounts to integrating $|\psi(x,t)|^2$, the probability density, over all space. You may want to start with the result of problem 10 (a). $|\psi(x,t)|^2$ is Gaussian in x which is the parameter over which you want to integrate. The integral of the probability density over all space is 1 meaning that the wavefunction is normalized.

31. What is the uncertainty in position if $\psi(x) = e^{-x^2/2a^2 + x/2b}$?

Problem 9 provides the simplest and most useful form of a Gaussian function, but you will also likely encounter the Gaussian forms in problem 11 and this problem. (a) Normalize the wave function, (b) calculate $\langle x \rangle$, (c) calculate $\langle x^2 \rangle$, and then (d) calculate $\Delta x = (\langle x^2 \rangle - \langle x \rangle^2)^{1/2}$. Normalization is a practical necessity in this case. You need the basic Gaussian integral, form 3.323.2 from Gradshteyn and Ryzhik (see problem 6), and 3.462.2 from Gradshteyn and Ryzhik,

$$\int_{-\infty}^{\infty} x^n e^{-px^2 + 2qx} dx = \frac{1}{2^{n-1}p} \sqrt{\frac{\pi}{p}} \frac{d^{n-1}}{dq^{n-1}} q e^{q^2/p}, \quad p > 0$$

You need to use this integral with n = 1 for part (b) and with n = 2 for part (c). The n = 2 case requires differentiation. If you are not familiar with generation by differentiation, consider

$$\frac{d^{2-1}}{dq^{2-1}} q e^{q^2/p} = \frac{d}{dq} q e^{q^2/p} = e^{q^2/p} + q\left(\frac{2q}{p}\right) e^{q^2/p} = \left(1 + \frac{2q^2}{p}\right) e^{q^2/p}$$

which is an example for the case n = 2. Then substitute appropriate constants p and q. You should find that the uncertainty is the same as the uncertainties in problems 9 and 11.

- 32. Given $\psi(x) = \frac{e^{ik_0x} e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}},$
- (a) find $\widehat{\psi}(p)$,
- (b) show that this result is consistent with problem 13,
- (c) and show that your $\widehat{\psi}(p)$ is dimensionality correct.

The Gaussian wavefunction that includes the factor e^{ik_0x} has a wave packet centered at k_0 or p_0 instead of zero which is realism. Including the factor e^{ik_0x} , however, makes the math sufficiently formidable that it can detract from the physics. The $k_0 = 0$ form was used in problem 13 to best emphasize the concepts. This is the $k_0 \neq 0$ version.

Perform a quantum mechanical Fourier transform to change the wave function from position space to momentum space using the same integral used in problem 13. This should be easier than the classical Fourier transform of problem 13 because time is not an independent variable here, or equivalently, the given ψ is $\psi(x, 0)$. You should find that

$$\widehat{\psi}\left(p\right) = \frac{\alpha}{\sqrt{\hbar} \,\left(\alpha^2 \pi\right)^{1/4}} \, e^{-(p-p_0)^2 \alpha^2 / 2\hbar^2}$$

Since $\psi(x) = \psi(x,0)$ is being modeled in this problem, you can use t = 0 to simplify $\widehat{\psi}(p,t)$ from problem 13 to complete part (b). Part (c) is intended to amplify the useful concept of dimensions. The argument of an exponential must be dimensionless. The units for a wavefunction in one dimension in momentum space must be some form of $1/\sqrt{\text{momentum}}$.

33. Show that the Schwarz inequality becomes an equality when $|v_i\rangle = c |v_j\rangle$.

Vectors that are proportional saturate the Schwarz inequality. Start with the intermediate result

$$<1|1> \ge \frac{<2|1><2|1>^{*}}{||2>|^{2}}$$

from problem 14. Let $|1\rangle = c |2\rangle$ and you will find $\langle 2|2\rangle \geq \langle 2|2\rangle$ which means the inequality is no longer necessary. Remember that $\langle 2|2\rangle = \langle 2|2\rangle^*$.

34. Show that $[\mathcal{X}, \mathcal{P}] = i\hbar$ in momentum space.

A statement in abstract Hilbert space must be true in any representation. Follow problem 15 which provides an interpretation in position space. Remember that in momentum space,

$$\mathcal{X} \to i\hbar \frac{\partial}{\partial p} \text{ and } \mathcal{P} \to p.$$

A commutator is an operator and needs something on which to operate. An arbitrary function of momentum, f(p), may be a good choice while working in momentum space.

35. Show that $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_{+}^{\dagger} = \left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_{+}$, if the operators \mathcal{A} and \mathcal{B} are Hermitian.

The anti-commutator is Hermitian if the operators are Hermitian. This fact was stated without proof and used in the derivation of the general uncertainty relation. This problem addresses that detail. Simply expand the anti-commutator, remember that $(\Lambda \Omega)^{\dagger} = \Omega^{\dagger} \Lambda^{\dagger}$ from part 2 of chapter 1, and that the "hatted" operators are Hermitian per problem 17.

36. Show that $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_{+} \neq \left[\mathcal{A}, \mathcal{B}\right]_{+}$ in general.

Follow the derivation of $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] = \left[\mathcal{A}, \mathcal{B}\right]$.

- 37. Given $\psi(x) = \frac{e^{ik_0 x} e^{-x^2/2\alpha^2}}{(\pi \alpha^2)^{1/4}}$, calculate
- (a) the expectation value of position,

- (b) the expectation value of position squared,
- (c) the uncertainty in position,
- (d) the expectation value of momentum,
- (e) the expectation value of the square of the momentum,
- (f) the uncertainty in momentum, and
- (g) the product of the uncertainties in position and momentum.

You should recognize that the $\psi(x)$ given is a normalized Gaussian wavefunction in position space. This problem is intended to convey the fact that the product of the uncertainties is a minimum for a Gaussian wave function, *i.e.*, $\Delta x \Delta p = \hbar/2$. Use the de Broglie relation, $k = p/\hbar$, to establish momentum in the wavefunction explicitly. Then use the position space representation of the momentum operator, $\mathcal{P} = -i\hbar \frac{d}{dx}$, in the integral of the expectation value for part (d). You need to conclude the differentiation before integrating. Integrate the square of the same momentum operator to find the second moment for part (e). The chain rule is necessary for this differentiation. Form 3.461.2 from Gradshteyn and Ryzhik,

$$\int_0^\infty x^{2n} e^{-px^2} dx = \frac{(2n-1)!!}{2(2p)^n} \sqrt{\frac{\pi}{p}}$$

may be useful for parts (b) and (e). Remember the arguments concerning even/odd functions integrated between symmetric limits. You should find $\langle p \rangle = p_0$ and $\langle p^2 \rangle = p_0^2 + \hbar^2/2\alpha^2$.

38. Show that $\langle \dot{\mathcal{P}} \rangle = -\langle \frac{dV(x)}{dx} \rangle$ given that the potential energy is a function of position.

This problem arrives at the second Ehrenfest equation which is the quantum mechanical equivalent of Newton's second law. Substitute \mathcal{P} for \mathcal{A} in Ehrenfest's theorem,

$$\langle \dot{\mathcal{P}} \rangle = \frac{i}{\hbar} \langle \left[\mathcal{H}, \mathcal{P} \right] \rangle = \frac{i}{\hbar} \langle \left[\frac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X}), \mathcal{P} \right] \rangle = \frac{i}{\hbar} \langle \left[\mathcal{V}(\mathcal{X}), \mathcal{P} \right] \rangle,$$

using the fact that the momentum operator commutes with itself and powers of itself. Represent the last expression in position space, *i.e.*,

$$\frac{i}{\hbar} < \left[\left. \mathcal{V} \left(\mathcal{X} \right), \, \mathcal{P} \right] > \rightarrow \frac{i}{\hbar} < \left[\left. V \left(x \right), \, -i\hbar \, \frac{d}{dx} \right] \right\} = \frac{i}{\hbar} \left(\psi \left(x \right) \left[\left. V \left(x \right), \, -i\hbar \, \frac{d}{dx} \right] \psi \left(x \right) \right) \,,$$

and expand the commutator. Express your result as an expectation value after completing the derivatives to arrive at the desired result.

Postscript: This procedure is technically suspect because $\langle \dot{\mathcal{P}} \rangle$ remains in abstract Hilbert space. This result is occasionally used to justify the representation $\langle \dot{\mathcal{P}} \rangle = -\langle \frac{d\mathcal{V}(\mathcal{X})}{d\mathcal{X}} \rangle$ in abstract Hilbert space, and generalizing from the specific to the abstract is more seriously suspect. Nevertheless, Ehrenfest's equations expressed in terms of the quantum mechanical Hamiltonian in abstract Hilbert space bear a striking resemblance to Hamilton's equations of classical mechanics.