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Problems set # 6 | **Physics 400** | March 21, 2019

1. Starting with Schrödinger equation derive the one-dimensional *continuity equation*

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0\,, \tag{1}$$

where

$$\rho \equiv |\psi(x,t)|^2 \tag{2}$$

and

$$j \equiv -\frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right]\,. \tag{3}$$

What does this equation imply in terms of conservation of probability?

2. Let $\hat{A}$ and $\hat{B}$ be Hermitian operators *(i)* Show that $\hat{A}\hat{B} = [\hat{A},\hat{B}]/2 + \{\hat{A},\hat{B}\}/2$ where $\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is the anticommutator. *(ii)* Show that the anticommutator is Hermitian and the commutator is anti- Hermitian (that is, $[\hat{A},\hat{B}]^\dagger = -[\hat{A},\hat{B}]$). *(iv)* We know that expectation values of Hermitian operators are real. What can you say about the expectation value of an anti-Hermitian operator?

3. We have seen that the Heisenberg uncertainty principle captures the difference between classical and quantum states, and sets a limit on the precision of incompatible quantum measurements. It has been introduced in the early days of quantum mechanics, but its form has evolved with the understanding and formulation of quantum physics throughout the years. In particular, Robertson and Schrödinger presented a lower bound for the product of the dispersion of two non-commuting observables. This lower bound is more general than the one given in class $\Delta x\, \Delta p \geq h$. Let A and B be Hermitian operators. Define the "uncertainty" in A by the square root of the mean square deviation from the mean:

$$\Delta A = \sqrt{\langle(\hat{A} - \langle A\rangle)^2} \tag{4}$$

Show that

$$\Delta A \Delta B \geq \tfrac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|\,. \tag{5}$$

Recall that the commutator of $\hat{x}$ and $\hat{p}_x$ is $i\hbar$, so from (5) we have $\Delta x\, \Delta p_x \geq \hbar/2$. [*Hint*: Use the Schwarz inequality.]

4. Its often the case that we want to find the component of a function parallel to another function. We just take the dot product with the second function, but then we also need to multiply by the second function. A handy notation is $|\psi\rangle\langle\psi|$. This *projector operator* projects onto ψ. Operating on $|\phi\rangle$, we get $|\psi\rangle\langle\psi|\phi\rangle$, which is what we want. Remember $\langle\psi|\phi\rangle$ is just a number and $|\psi\rangle$ is the vector. Similarly, operating on $\langle\phi|$ we get $\langle\phi|\psi\rangle\langle\psi|$ which is the desired expression for the adjoint vector. Suppose you have a complete set of orthonormal basis vectors $|\psi_n\rangle$. What is a compact expression for transforming an arbitrary vector $|\phi\rangle$ into this basis set? (This is much easier to write down than to ask!)

5. If $p(x) = xe^{-x/\lambda}$ is a probability density function over the interval $0 < x < \infty$, find: *(i)* the mean, *(ii)* the standard deviation, and *(iii)* the most probable value (i.e., where probability density is maximum) of x.

SOLUTIONS

1. Perhaps the most direct solution is to begin with the continuity equation (1), substitute in the definitions of ρ and j, and then prove the equality. First, calculate the partial derivatives:

$$\frac{\partial j}{\partial x} = -\frac{i\hbar}{2m}\left(\frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x} + \psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi - \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x}\right) = -\frac{i\hbar}{2m}\left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi\right) \tag{6}$$

and

$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}\,. \tag{7}$$

The connection between the time and space derivatives is given by rearranging the Schrödinger equation and its complex conjugate

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar}V\psi \quad \text{and} \quad \frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^*\,. \tag{8}$$

Substituting (8) into (7)

$$\frac{\partial \rho}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2}\psi + \frac{i}{\hbar}V\psi^*\psi + \frac{i\hbar}{2m}\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{h}V\psi^*\psi = -\frac{\partial j}{\partial x}\,. \tag{9}$$

The continuity equation is equivalent to conservation of probability. One way to see this is to integrate the continuity equation over x, with the added restriction that ψ and $\partial\psi/\partial x$ go to zero as $x \to \pm\infty$,

$$0 = \int_{-\infty}^{+\infty} dx \left(\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x}\right) = \frac{\partial}{\partial t}\int_{-\infty}^{+\infty} dx|\psi|^2 + \int_{-\infty}^{+\infty} dx\frac{\partial j}{\partial x} = \frac{\partial}{\partial t}\int_{-\infty}^{+\infty} dx|\psi|^2 + j(x)\Big|_{-\infty}^{+\infty} = \frac{\partial}{\partial t}\int_{-\infty}^{+\infty} dx|\psi|^2\,. \tag{10}$$

The last integral is the total probability (otherwise known as the normalization), and is shown to be constant with respect to time.

2. *(ii)* $[\hat{A},\hat{B}]/2 + \{\hat{A},\hat{B}\}/2 = (\hat{A}\hat{B} - \hat{B}\hat{A})/2 + (\hat{A}\hat{B} + \hat{B}\hat{A})/2 = \hat{A}\hat{B}$. *(iii)* $\{\hat{A},\hat{B}\}^\dagger = (\hat{A}\hat{B})^\dagger + (\hat{B}\hat{A})^\dagger = \hat{B}^\dagger\hat{A}^\dagger + \hat{A}^\dagger\hat{B}^\dagger = \{\hat{A},\hat{B}\}$, so the anticommutator is hermitian. $[\hat{A},\hat{B}]^\dagger = (\hat{A}\hat{B})^\dagger - (\hat{B}\hat{A})^\dagger = \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = -(\hat{A}\hat{B} - \hat{B}\hat{A}) = -[\hat{A},\hat{B}]$, so the commutator is anti-Hermitian. *(iv)* An anti-hermitian operator is equal to the negative of its hermitian conjugate, that is $\hat{A}^\dagger = -\hat{A}$. In inner products this means $\langle\phi|\hat{A}\psi\rangle = \langle\hat{A}^\dagger\phi|\psi\rangle = -\langle\hat{A}\phi|\psi\rangle$. The expectation value of an anti-hermitian operator is: $\langle\psi|\hat{A}\psi\rangle = \langle\hat{A}^\dagger\psi|\psi\rangle = -\langle\hat{A}\psi|\psi\rangle = -\langle A\rangle^*$. But $\langle\psi|\hat{A}\psi\rangle = \langle A\rangle$, so $\langle A\rangle = -\langle A\rangle^*$, which means the expectation value must be pure imaginary.

3. Define new Hermitian operators $\hat{A}' = \hat{A} - \langle\hat{A}\rangle$ and $\hat{B}' = \hat{B} - \langle\hat{B}\rangle$. Then, using the Schwarz's inequality we obtain $\langle\hat{A}'^2\rangle\langle\hat{B}'^2\rangle \geq |\langle\hat{A}'\hat{B}'\rangle|^2$, or $\Delta A\,\Delta B \geq |\langle\hat{A}'\hat{B}'\rangle| = |\langle[\hat{A}',\hat{B}']\rangle/2 + \langle\{\hat{A}',\hat{B}'\}\rangle/2 \geq |\langle[\hat{A}',\hat{B}']\rangle|/2$. Since the expectation value of the commutator is imaginary and the anticommutator is real, each makes a positive contribution to the absolute value, and the anticommutator can be dropped without changing the inequality in the last step. So, $\Delta A\,\Delta B \geq |\langle[\hat{A}',\hat{B}']\rangle|/2 = |\langle[\hat{A},\hat{B}] - [\hat{A},\langle\hat{B}\rangle] - [\langle\hat{A}\rangle,\hat{B}] + [\langle\hat{A}\rangle,\langle\hat{B}\rangle]\rangle|/2 = |\langle[\hat{A},\hat{B}]\rangle|/2$. Note that $\langle\hat{A}\rangle$ and $\langle\hat{B}\rangle$ are just numbers, so they commute with the operators and the commutators involving them are 0.

4. We want to project $|\phi\rangle$ onto each basis vector (this gives the expansion coefficients) and then sum the coefficients times the basis vectors: $|\phi\rangle = (\sum_n \psi_n\rangle\langle\psi_n|)\,|\phi\rangle$.

5. *(i)* The mean value of x is

$$\overline{x} = \frac{\int_0^\infty x\,p(x)\;dx}{\int_0^\infty p(x)\,dx} = \frac{\int_0^\infty x^2\,e^{-x/\lambda}dx}{\int_0^\infty x\,e^{-x/\lambda}dx} = \lambda\frac{\Gamma(3)}{\Gamma(2)} = 2\lambda.$$

(ii) The standard deviation is defined by $\sigma^2 = \overline{x^2} - (\overline{x})^2$, so

$$\overline{x^2} = \frac{\int_0^\infty x^2\,p(x)\,dx}{\int_0^\infty p(x)\,dx} = \frac{\int_0^\infty x^3 e^{-x/\lambda}dx}{\int_0^\infty x e^{-x/\lambda}dx} = \lambda^2\frac{\Gamma(4)}{\Gamma(2)} = 6\lambda^2\,.$$

Therefore, $\sigma^2 = 6\lambda^2 - 4\lambda^2 = 2\lambda^2$, which implies $\sigma = \sqrt{2}\,\lambda$. *(iii)* The probability density is an extremum when

$$p'(x) = e^{-x/\lambda} - \frac{x}{\lambda}e^{-x/\lambda} = 0,$$

that is at $x = \lambda$ or as $x \to \infty$. Note that $\lambda > 0$ if $p(x)$ is to be finite in $0 < x < \infty$. Since

$$p'(x) = -\frac{2}{\lambda}e^{-x/\lambda} + \frac{x}{\lambda^2}e^{-x/\lambda}$$

we have

$$p''(\lambda) = -\frac{1}{\lambda}e^{-1} < 0 \quad \text{and} \quad \lim_{x\to\infty} p''(x) = 0,$$

so the probability density is a maximum at $x = \lambda$. Hence, the most probable value of x is λ.