Schrodinger Equation

Probability Density, Current and Momentum

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Introduction

- We will look at the conservation of probability
- We will see how this consideration leads to a statement of charge conservation
- We will also see how we can determine the quantum mechanical momentum operator

Conservation of Probability

- In quantum mechanics, we know that the wavefunction $\Psi(x,t)$ must be ***normalizable***, specifically $\int \|\Psi(x,t)\|^2 dx = 1$.
- It is important to know whether a wavefunction, once normalized, remains as such as it evolves over time. Mathematically this translates to: $\frac{\partial}{\partial t}\left[\int \|\Psi(x,t)\|^2 dx\right] = 0$.
- The time evolution of the wavefunction is dictated by the Schrodinger equation (Sch. eq) (when $v << c$ i.e. non-relativistic speeds). We'll use the equation to verify the conservation of probability

Conservation of Probability

Dropping the x and t dependence for ease of reading the equations, The Sch.eq and its complex conjugate are:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \tag{1}$$

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

The norm of the wavefunction is:

$$\|\Psi\|^2 = \Psi^*\Psi \tag{3}$$

Such that:

$$\frac{\partial}{\partial t}\left[\int \|\Psi(x,t)\|^2 dx\right] = \int \frac{\partial}{\partial t}\left[\Psi^*\Psi\right] dx \tag{4}$$

Using the product rule, we get:

$$\int \Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi^*}{\partial t} \tag{5}$$

The time derivatives can be obtained from equations (1) and (2)

Conservation of Probability

We rearrange equations (1 and 2):

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V\Psi \tag{6}$$

$$\frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V\Psi^* \tag{7}$$

Thus from equations (5), (6) and (7) we have:

$$\frac{\partial}{\partial t}[\Psi^*\Psi] = \Psi^*(\frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V\Psi) + \Psi(\frac{-i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V\Psi^*) \tag{8}$$

$$= \frac{i\hbar}{2m}\Psi^*\frac{\partial^2 \Psi}{\partial x^2} - \frac{i\hbar}{2m}\Psi\frac{\partial^2 \Psi^*}{\partial x^2} \tag{9}$$

$$= \frac{i\hbar}{2m}\left[\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right)\right] \tag{10}$$

N.B:*Notice how differentiating (10) wrt x yields (9), so the step in going from (9) to (10) is legal!*

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Hence, we see that the time-derivative of the probability density is:

$$\frac{\partial}{\partial t}\left[\int \left\|\Psi(x,t)\right\|^2 dx\right] = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right)\Big]_{-\infty}^{\infty} \tag{11}$$

Now recall that $\Psi \to 0$ as $x \to \infty$, in addition the derivative of Ψ is bounded, i.e. $\frac{\partial \Psi}{\partial x} < \infty$. Thus, the time-derivative of the normalization condition is zero.

Hence once a wavefunction normalized, it remains as such.

Charge Conservation

Back in equation 10, we got an important result. Hence let's look at it again:

$$\frac{\partial}{\partial t}[\Psi^*\Psi] = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \Psi\frac{\partial \Psi^*}{\partial x}\right)\right] \tag{12}$$

- We can set $\rho = \Psi^*\Psi$ and is called the *probability density*.
- Secondly, the term in square brackets can be simplified: If we denote the first term as the complex number z, the second is its conjugate z^*, and we realize that in the bracket we have $z - z^*$ and this is equal to $2iIm(z)$[1]. Hence the right-hand side of the equation becomes:

$$-\frac{\partial}{\partial x}\left[\frac{\hbar}{m}Im(\Psi^*\frac{\partial \Psi}{\partial x})\right] \tag{13}$$

[1] *Recall any complex number $z = a + ib$ has its conjugate $z^* = a - ib$, and $Re(z) = a$ and $Im(z) = b$. So $z - z^* = 2ib = 2iIm(z)$*

Charge Conservation

We now call the term in bracket $\boldsymbol{J}$, and equation (12) becomes:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \mathbf{J}}{\partial x} \tag{14}$$

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial \mathbf{J}}{\partial x} = 0} \tag{15}$$

It is useful to do some unit analysis to get a bit more insight on $\boldsymbol{J}$.

- Recall that Ψ has units of $[L^{1/2}]$. Hence, $\left(\Psi^* \frac{\partial \Psi}{\partial x}\right)$ has units of $[L^{-2}]$.
- Also, $\hbar$ has units of *energy* $\times$ $[T]$ specifically this corresponds to $[M] * [L^2] * [T^{-1}]$.
- The mass term in the denominator cancels out the mass term from $\hbar$. The length terms cancel from the Ψ terms and $\hbar$.
- We determine that $\boldsymbol{J}$ has units of $[T^{-1}]$. $\boldsymbol{J}$ is called the *probability current*.

Probability Current

The result we arrived at can also be extended in three dimensions. In the three dimensional case, equation (15) is written as:

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0} \tag{16}$$

Where $\nabla \cdot = (\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z})$ is the divergence. Hence, equations (15) in 1-D and (16) in 3-D tells us that if the probability density, in a region of space, is decreasing in time, this means that current diverges from this location, which we would expect for charge conservation.

Momentum

- Recall that classically, and in the absence of an electromagnetic field, the momentum of a particle is given by: $p = mv$, where m and v are the mass and velocity respectively.
- In order to obtain the quantum mechanical operator for momentum, we can:
  - try to find the expectation value of the velocity (the time derivative of the expectation value of position)
  - multiply the obtained expression by m.

Expectation Value of Velocity

the expectation value of velocity is $< v >$ is the time derivative of the expectation value of position $< v >= \frac{\mathrm{d} <x>}{\mathrm{d}t}$. Therefore, we have:

$$< v >= \int x \frac{\partial}{\partial t} (\Psi^* \Psi) dx \tag{17}$$

We have already taken the time derivative of the probability density, its result is equation (10). Thus, how integral becomes:

$$< v >= \frac{i\hbar}{2m} \int x \left[\frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \right] dx \tag{18}$$

Integrating by parts, we get:

$$= \frac{i\hbar}{2m} \left[\left[x \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \right]_{-\infty}^{\infty} - \int \frac{\partial x}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) dx \right] \tag{19}$$

The first term goes to zero, since $\Psi \to 0$ as $x \to \infty$. The $\frac{\partial x}{\partial x} = 1$. So our expression simplifies.

Expectation Value of Momentum

Our simplified expression is:

$$< v >= -\frac{i\hbar}{2m}\int\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)dx \tag{20}$$

Notice that there are two integrals in (20), each of which can be integrated by parts (*don't do that just yet!*). Notice also, that if we integrate by parts the second term, we get the first term back (try it!). That is we end up with:

$$< v >= -\frac{i\hbar}{2m}2\int\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)dx \tag{21}$$

Upon simplifying and multiplying by m to get the expectation value of momentum, we obtain:

$$< p >= -i\hbar\int\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)dx \tag{22}$$

Momentum Operator

The *momentum operator is*:

$$\boxed{p \to -i\hbar \frac{\partial}{\partial x}} \tag{23}$$