

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 $v \ll c$ i.e. non-relativistic velocities). 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:

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

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

The norm of the wavefunction is:

$$\|\Psi\|^2 = \Psi^* \Psi \quad (3)$$

Such that:

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

Using the product rule, we get:

$$\int \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \quad (5)$$

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

Conservation of Probability

We rearrange equations (1 and 2):

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

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

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

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

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

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

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

Continued

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

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

Now recall that $\Psi \rightarrow 0$ as $x \rightarrow \infty$, 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 is normalized, it remains as such.

Charge Conservation

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

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

- We can set $\rho = \Psi^* \Psi$ and is 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 $z - z^*$. This is equal to $2i\text{Im}(z)$ ¹. Hence the right-hand side of the equation becomes:

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

¹ Recall any complex number $z = a + ib$ has its conjugate $z^* = a - ib$, and $\text{Re}(z) = a$ and $\text{Im}(z) = b$. So $z - z^* = 2ib = 2i\text{Im}(z)$.

Charge Conservation

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

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \mathbf{J}}{\partial x} \quad (14)$$

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

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

- Recall that Ψ has units of $[L^{1/2}]$. Hence, $(\Psi^* \frac{\partial \Psi}{\partial x})$ 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 \mathbf{J} has units of $[T^{-1}]$. \mathbf{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:

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

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 $\langle v \rangle$ is the time derivative of the expectation value of position $\langle v \rangle = \frac{d\langle x \rangle}{dt}$. Therefore, we have:

$$\langle v \rangle = \int x \frac{\partial}{\partial t} (\Psi^* \Psi) dx \quad (17)$$

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

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

Integrating by parts, we get:

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

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

Expectation Value of Momentum

Our simplified expression is:

$$\langle v \rangle = -\frac{i\hbar}{2m} \int \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) dx \quad (20)$$

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:

$$\langle v \rangle = -\frac{i\hbar}{2m} 2 \int \left(\psi^* \frac{\partial \psi}{\partial x} \right) dx \quad (21)$$

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

$$\langle p \rangle = -i\hbar \int \left(\psi^* \frac{\partial \psi}{\partial x} \right) dx \quad (22)$$

Momentum Operator

The *momentum operator* is:

$$p \rightarrow -i\hbar \frac{\partial}{\partial x} \quad (23)$$