3.9 Motion of Wave Packets: Ehrenfest's Theorem

According to Ehrenfest's theorem (1927), *the equations of motion of the expectation values of the position and momentum vectors for a wave packet are formally identical to Newton's equations of classical mechanics*. That is,

$$\frac{d}{dt}\langle \mathbf{r} \rangle = \frac{\langle \mathbf{p} \rangle}{m} \qquad \ldots(3.48)$$

$$\frac{d}{dt}\langle \mathbf{p} \rangle = -\langle \nabla V \rangle \qquad \ldots(3.49)$$

Proof of (6.48) $\frac{d}{dt}\langle \mathbf{r} \rangle = \frac{\langle \mathbf{p} \rangle}{m}$

Let us first consider the expectation value of the x-component of the position vector r. Assuming that the wave function Ψ representing the wave packet is normalized to unity, we have,

$$\langle x \rangle = \int \Psi^* x \Psi \, d\mathbf{r}$$

The time rate of change of $\langle x \rangle$ is

$$\frac{d}{dt}\langle x \rangle = \frac{d}{dt}\int \Psi^* x \Psi \, d\mathbf{r}$$

$$= \int \Psi^* x \frac{\partial \Psi}{\partial t} d\mathbf{r} + \int \frac{\partial \Psi^*}{\partial t} x \Psi d\mathbf{r}$$

The right-hand side can be transformed by using the Schrödinger equation and its complex conjugate.

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

We obtain,

$$\frac{d}{dt}\langle x \rangle = \frac{1}{i\hbar}\left[\int \Psi^* x \left(-\frac{\hbar^2}{2m}\nabla^2 \Psi + V\Psi\right) d\mathbf{r} - \int \left(-\frac{\hbar^2}{2m}\nabla^2 \Psi^* + V\Psi^*\right) x \Psi \, d\mathbf{r}\right.$$

$$= \frac{i\hbar}{2m}\int [\Psi^* x \, (\nabla^2 \Psi) - (\nabla^2 \Psi^*) x \, \Psi] \, d\mathbf{r} \qquad \ldots(3.50)$$

Let us consider the second part of the integral. Using Green's first identity

Green's first identity: If f and g are scalar functions of position, then

$$\int_V [f\,\nabla^2 g + (\nabla f)\cdot(\nabla g)]d\mathbf{r} = \int_S f(\nabla g)\cdot d\mathbf{S}$$

where V is the volume bounded by the closed surface S. For our case, take $f = x\Psi$ and $g = \Psi^*$.

We obtain,

$$\int (\nabla^2\Psi^*)x\Psi d\mathbf{r} = \int_S x\Psi(\nabla\Psi^*)\cdot d\mathbf{S} - \int (\nabla\Psi^*)\cdot\nabla(x\Psi)d\mathbf{r}$$

Since the volume under consideration is the entire space, the surface S in the first integral on the right is at infinity. Hence, this integral is zero because the wave function vanishes at large distances. Therefor,

$$\int (\nabla^2\Psi^*)x\Psi d\mathbf{r} = -\int (\nabla\Psi^*)\cdot\nabla(x\Psi)\ d\mathbf{r}$$

Using Green's first identity again, we get

$$-\int (\nabla\Psi^*)\cdot\nabla(x\Psi)d\mathbf{r} = -\int_S \Psi^*\nabla(x\Psi)\cdot d\mathbf{S} + \int \Psi^*\ \nabla^2(x\Psi)\ d\mathbf{r}$$

The surface integral again vanishes. Thus,

$$\int (\nabla^2\Psi^*)x\Psi d\mathbf{r} = \int \Psi^*\ \nabla^2(x\Psi)\ d\mathbf{r}$$

Substituting this back into (3.50), we obtain

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\int \Psi^*[x\nabla^2\Psi - \nabla^2(x\Psi)]d\mathbf{r}$$

It can be easily shown that

$$\nabla^2(x\Psi) = x\nabla^2\Psi + 2\frac{\partial\Psi}{\partial x}$$

Therefore,

$$\begin{aligned}\frac{d}{dt}\langle x\rangle &= -\frac{i\hbar}{m}\int \Psi^*\ \frac{\partial\Psi}{\partial x}\ d\mathbf{r} \\ &= \frac{1}{m}\int \Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi\ d\mathbf{r} \\ &= \frac{\langle p_x\rangle}{m}\end{aligned}$$

Similarly, we can prove that

H.W. $$\frac{d}{dt}\langle y\rangle = \frac{\langle p_y\rangle}{m},\quad \frac{d}{dt}\langle z\rangle = \frac{\langle p_z\rangle}{m}$$

Proof of (6.49) $\frac{d}{dt}\langle \mathbf{p}\rangle = -\langle \nabla V\rangle$

Let us calculate the time rate of change of the expectation value of the x-component of the momentum of the particle. We have

$$\frac{d}{dt}\langle p_x\rangle = -i\hbar\,\frac{d}{dt}\int \Psi^* \frac{\partial \Psi}{\partial t}\,d\mathbf{r}$$

$$= -i\hbar\left[\int \Psi^* \frac{\partial}{\partial x}\frac{\partial \Psi}{\partial t}\,d\mathbf{r} + \int \frac{\partial \Psi^*}{\partial t}\frac{\partial \Psi}{\partial x}\,d\mathbf{r}\right]$$

by using the Schrödinger equation and its complex conjugate.

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

To replace $\frac{\partial \Psi}{\partial t}$ and $\frac{\partial \Psi^*}{\partial t}$, respectively, we get,

$$\frac{d}{dt}\langle p_x\rangle = -\int \Psi^* \frac{\partial}{\partial x}\left(-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi\right)d\mathbf{r} + \int\left(-\frac{\hbar^2}{2m}\nabla^2\Psi^* + V\Psi^*\right)\frac{\partial \Psi}{\partial x}\,d\mathbf{r}$$

$$= \frac{\hbar^2}{2m}\int\left[\Psi^*\left(\nabla^2\frac{\partial \Psi}{\partial x}\right) - (\nabla^2\Psi^*)\frac{\partial \Psi}{\partial x}\right]d\mathbf{r} - \int \Psi^*\left[\frac{\partial}{\partial x}(V\Psi) - V\frac{\partial \Psi}{\partial x}\right]d\mathbf{r}$$

Using Green's second identity,

> Green's second identity: If f and g are scalar functions of position, then
>
> $$\int_V [f\,\nabla^2 g - g\,\nabla^2 f]\,d\mathbf{r} = \int_S [f\,\nabla g - g\,\nabla f]\cdot d\mathbf{S}$$
>
> where V is the volume bounded by the closed surface S.

The first integral on the right is zero because Ψ and $\frac{\partial \Psi}{\partial t}$ vanish at large distances. The second integral gets simplified as

$$-\int \Psi^*\left[\frac{\partial}{\partial x}(V\Psi) - V\frac{\partial \Psi}{\partial x}\right]d\mathbf{r} = -\int \Psi^*\frac{\partial V}{\partial x}\Psi\,d\mathbf{r}$$

$$= -\left\langle \frac{\partial V}{\partial x}\right\rangle$$

Thus,

$$\frac{d}{dt}\langle p_x \rangle = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

Similarly we can prove that

H.W. $$\frac{d}{dt}\langle p_y \rangle = -\left\langle \frac{\partial V}{\partial y} \right\rangle, \quad \frac{d}{dt}\langle p_z \rangle = -\left\langle \frac{\partial V}{\partial z} \right\rangle$$

Thus, the proof of Ehrenfest's theorem is complete.

3.10 Exact Statement and Proof of the Position-Momentum Uncertainty Relation

The uncertainty relation defines as, *the root-mean-square deviation (also called the standard deviation) from the mean (i.e. the expectation) value*.

Considering a wave packet moving along the *x* direction, we have

$$\Delta x = \left\langle (x - \langle x \rangle)^2 \right\rangle^{1/2}, \quad \mathbf{\Delta} p = \left\langle (p - \langle p \rangle)^2 \right\rangle^{1/2} \qquad \ldots(3.51)$$

Let us put

and

$$\left.\begin{aligned} A &= x - \langle x \rangle \\ B &= p - \langle p \rangle = i\hbar\left[\frac{d}{dx} - \left\langle \frac{d}{dx} \right\rangle\right] \end{aligned}\right\} \qquad \ldots(3.52)$$

Then

$$(\mathbf{\Delta} x)^2 \ (\mathbf{\Delta} p)^2 = \int_{-\infty}^{\infty} \Psi^* \ A^2 \ \Psi dx \ \int_{-\infty}^{\infty} \Psi^* \ B^2 \Psi \ dx$$

$$= \int_{-\infty}^{\infty} (A^* \Psi^*) \ (A\Psi) \ dx \ \int_{-\infty}^{\infty} (B^* \ \Psi^*) \ (B\Psi) dx \qquad \ldots(3.53)$$

The last step follows from the fact that *A* and *B* are Hermitian operators, as the relation

$$\int \Psi^* \hat{A} \Psi \, d\mathbf{r} = \int (\hat{A}\Psi)^* \ \Psi \, d\mathbf{r}$$

It can also be verified directly by partial integration and remembering that Ψ vanishes at infinity.

We shall use the *Schwarz* inequality

$$\int |f|^2 \ dx \ \int |g|^2 \ dx \geq \left| \int f^* g \, dx \right|^2 \qquad \ldots(3.54)$$

where f and g are arbitrary functions and the equality is valid only if $f = \alpha g$, where α is a constant. Taking $f = A\Psi$ and $g = B\Psi$, Equation (3.53) becomes

$$(\Delta x)^2(\Delta p)^2 \geq \left|\int (A^*\Psi^*)(B\Psi)\,dx\right|^2 = \left|\int \Psi^* AB\Psi\,dx\right|^2 \qquad \ldots(3.55)$$

The expression on the right-hand side can be written as

$$\left|\int \Psi^*\left[\frac{1}{2}(AB - BA) + \frac{1}{2}(AB + BA)\right]\Psi dx\right|^2$$

$$= \frac{1}{4}\left|\int \Psi^*(AB - BA)\Psi\,dx\right|^2 + \frac{1}{4}\left|\int \Psi^*(AB + BA)\Psi\,dx\right|^2 \qquad \ldots(3.56)$$

Here we have omitted the cross terms which can be shown to vanish by using the relation

$$\left[\int \Psi^* AB\Psi\,dx\right]^* = \int \Psi A^* B^* \Psi^*\,dx$$

$$= \int B^*\Psi^* A\Psi\,dx$$

$$= \int \Psi^* BA\,\Psi\,dx$$

Now from (3.52)

$$(AB - BA)\Psi = -i\hbar\left[x\frac{d\Psi}{dx} - \frac{d}{dx}(x\Psi)\right]$$

$$= -i\hbar\left[x\frac{d\Psi}{dx} - \Psi - x\frac{d\Psi}{dx}\right]$$

$$= i\hbar\,\Psi$$

Therefore,

$$\int \Psi^*(AB - BA)\Psi\,dx = i\hbar \int \Psi^*\,\Psi\,dx$$

$$= i\hbar \qquad \ldots(3.57)$$

as Ψ is normalized.

From (3.55), (3.56) and (3.57) we obtain

$$(\Delta x)^2(\Delta p)^2 \geq \hbar^2/4$$

$$\boxed{\Delta x\,\Delta p \geq \hbar/2} \qquad \ldots(3.58)$$

Equation (3.58) is the exact statement of the position-momentum uncertainty relation, where the uncertainties in x and p are defined as root-mean-square deviations from the expectation values $\langle x\rangle$ and $\langle p\rangle$,respectively.