January 2008

Ehrenfest's Theorem

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(Dated: January 22, 2008)

I. SYNOPSIS

The idea that quantum mechanics "becomes" classical mechanics in the limit $h \to 0$ (and in the limit $c \to \infty$, but that's not treated here) is discussed using Ehrenfest's theorem.

II. THE MOMENTUM OPERATOR $p^x_{op} = -\imath\hbar\frac{\partial}{\partial x}$

How is it possible that a wave function can in some way imitate Newton's Second Law?

We start with a definition of momentum.

Assuming the Schrödinger Equation:

$$H\psi = \imath\hbar\frac{\partial\psi}{\partial t}$$

and

$$H\psi^* = -\imath\hbar\frac{\partial\psi^*}{\partial t}$$

where H, the Hamiltonian, has the form (for a one-dimensional particle subject to a potential function $V(x)$),

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

i.e., we are dealing with a conservative one dimensional system, then

$$\frac{d<x>}{dt} = \int \frac{d\psi^*}{dt}x\psi dx + \int \psi^* x\frac{d\psi}{dt}dx$$

which becomes

$$\frac{d<x>}{dt} = \int -\frac{1}{\imath\hbar}H\psi^* x\psi dx + \int \psi^* x\frac{1}{\imath\hbar}H\psi dx$$

$$\frac{d<x>}{dt} = \int -\frac{1}{\imath\hbar}\left\{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi^*\right\}x\psi dx + \int \psi^* x\frac{1}{\imath\hbar}\left\{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi\right\}dx$$

The integrals containing V cancel using the Hermitian property of V over ψ. We are left with

$$\frac{d<x>}{dt} = \int -\frac{1}{\imath\hbar}\left\{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi^*\right\}x\psi dx + \int \psi^* x\frac{1}{\imath\hbar}\left\{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi\right\}dx$$

which is

$$\imath\hbar\frac{2m}{\hbar^2}\frac{d<x>}{dt} = \int\left\{\left(\frac{\partial^2\psi^*}{\partial x^2}\right)x\psi\right\}dx - \int\left\{\psi^* x\left(\frac{\partial^2\psi}{\partial x^2}\right)\right\}dx$$

each of which can be integrated twice by parts, yielding for the first term

$$\imath\hbar\frac{2m}{\hbar^2}\frac{d<x>}{dt} = \int\left\{\left(\frac{\partial\frac{\partial\psi^*}{\partial x}}{\partial x}\right)x\psi\right\}dx - \int\left\{\psi^* x\left(\frac{\partial^2\psi}{\partial x^2}\right)\right\}dx$$

where we define u as $x\psi$ and dv as

$$dv = \frac{\partial\frac{\partial\psi^*}{\partial x}}{\partial x}dx = d\left(\frac{\partial\psi^*}{\partial x}\right)$$

so that $v = \frac{\partial\psi^*}{\partial x}$.

We integrate by parts, obtaining

$$= \frac{\partial\psi^*}{\partial x}x\psi\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial x}\frac{\partial(x\psi)}{\partial x}dx - \int_{-\infty}^{\infty}\left\{\psi^* x\left(\frac{\partial^2\psi}{\partial x^2}\right)\right\}dx$$

but the non integral parts of the above vanish, since the wave functions are required to have zero slope at plus and minus infinity.

$$= -\int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial x}\frac{\partial(x\psi)}{\partial x}dx - \int_{-\infty}^{\infty}\left\{\psi^* x\left(\frac{\partial^2\psi}{\partial x^2}\right)\right\}dx$$

We integrate again by parts, with $\frac{\partial\psi^*}{\partial x}dx$ as dv, and $\frac{\partial(x\psi)}{\partial x}$ as u, and obtain

$$- -\psi^*\frac{\partial(x\psi)}{\partial x}\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\psi^*\frac{\partial^2(x\psi)}{\partial x^2}dx$$

so, again declaring the first term to be zero, we have

$$\imath\hbar\frac{2m}{\hbar^2}\frac{d<x>}{dt} = +\int_{-\infty}^{\infty}\psi^*\frac{\partial^2(x\psi)}{\partial x^2}dx - \int_{-\infty}^{\infty}\psi^* x\frac{\partial^2(\psi)}{\partial x^2}dx$$

which is

$$\imath\hbar\frac{2m}{\hbar^2}\frac{d<x>}{dt} = \int_{-\infty}^{\infty}\frac{\partial\left(\frac{\partial(x\psi)}{\partial x} - x\frac{\partial\psi}{\partial x} + \frac{\partial\psi}{\partial x}\right)}{\partial x}dx$$

Typeset by REVTEX

or

$$\imath\hbar\frac{2m}{\hbar^2}\frac{d<x>}{dt} = \int_{-\infty}^{\infty}\frac{\partial\left(\frac{\partial(\psi)}{\partial x} + \cancel{x\frac{\partial\psi}{\partial x}} - \cancel{x\frac{\partial\psi}{\partial x}} + \frac{\partial\psi}{\partial x}\right)}{\partial x}dx$$

which becomes

$$\imath\frac{2m}{\hbar}\frac{d<x>}{dt} = \int_{-\infty}^{\infty}\frac{\partial\left(2\frac{\partial(\psi)}{\partial x}\right)}{\partial x}dx = 2\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx$$

which is

$$m\frac{d<x>}{dt} = \frac{\hbar}{\imath}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx$$

$$m\frac{d<x>}{dt} = \int_{-\infty}^{\infty}\psi^*\left(\frac{\hbar}{\imath}\frac{\partial}{\partial x}\right)\psi dx$$

or

$$m\frac{d<x>}{dt} = \int_{-\infty}^{\infty}\psi^*\left(-\imath\,\hbar\frac{\partial}{\partial x}\right)\psi dx$$

or, once again:

$$m\frac{d<x>}{dt} = \int_{-\infty}^{\infty}\psi^* p_{op}^x\psi dx$$

which identifies the operator which we normally associate with the linear momentum. So, Ehrenfest's first theorem recovers the operator definition of the linear momentum.

III. NEWTON'S SECOND LAW RECOVERED

Now we repeat the above computation, but instead look at the time rate of change of momentum, looking to recover Newton's 2'nd Law. We have

$$\frac{d<p>}{dt} = -i\hbar\frac{d\int\psi^*\frac{\partial\psi}{\partial x}}{dt}dx$$

which we are also going to integrate (by parts).

We have

$$-\frac{1}{\imath\hbar}\frac{d<p>}{dt} = \int\frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x}dx + \int\psi^*\frac{d\frac{\partial\psi}{\partial x}}{dt}dx$$

which is

$$-\frac{1}{\imath\hbar}\frac{d<p>}{dt} = \int\frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x}dx + \int\psi^*\frac{d\frac{\partial\psi}{\partial t}}{dx}dx$$
$$= \int\frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x}dx + \frac{1}{\imath\hbar}\int\psi^*\frac{dH\psi}{dx}dx$$

or

$$-\frac{1}{\imath\hbar}\frac{d<p>}{dt} = \int\frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x}dx$$
$$+\frac{1}{\imath\hbar}\int\psi^*\frac{d\left(\frac{-\hbar^2}{2\mu}\frac{\partial^2\psi}{\partial x^2} + V(x)\right)\psi}{dx}dx$$
$$-\frac{1}{\imath\hbar}\frac{d<p>}{dt} = \int\left(\frac{1}{-\imath\hbar}\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2\psi^*}{\partial x^2}\right.\right.$$
$$\left.\left.+V\psi^*\right)\right)\frac{\partial\psi}{\partial x}dx$$
$$+\frac{1}{\imath\hbar}\int\psi^*\frac{d\left(\frac{-\hbar^2}{2\mu}\frac{\partial^2\psi}{\partial x^2} + V(x)\right)\psi}{dx}dx$$

and again, when integrating by parts, the two terms related to the kinetic energy operator cancel. We are left with

$$-\frac{d<p>}{dt} = \left(-\int V\psi^*\frac{\partial\psi}{\partial x}dx + \int\psi^*\left(\frac{dV(x)\psi}{dx}\right)dx\right)$$

$$\frac{d<p>}{dt} = -\left(-\int\left(V\psi^*\right)\frac{\partial\psi}{\partial x}dx + \right.$$
$$\left.\int\left(\psi^*\left(\frac{dV(x)}{dx}\psi + V(x)\frac{d\psi}{dx}\right)dx\right)\right)$$

which is

$$\frac{d<p>}{dt} = +\int\left(\psi^*\left(\frac{dV(x)}{dx}\psi\right)\right)dx$$

Clearly, we have obtained something akin to Newton's second law.