1.3.5. Ehrenfest's Theorem & Classical Mechanics

By further studying expectation values, we will determine under what circumstances we recover classical mechanics from our quantum mechanical laws of motion.

Recall the continuity equation

$$\frac{\partial}{\partial t}(\psi^*\psi) + \vec{\nabla}\cdot\frac{\hbar}{2im}(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\psi) = 0.$$

Multiply this by $\vec{r}$ and integrate over all space

$$\frac{d}{dt}\int d^3r\,\psi^*\vec{r}\,\psi$$

$$= \frac{i\hbar}{2m}\int d^3r\,\vec{r}\,\vec{\nabla}\cdot(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\psi).$$

The RHS is integrated by parts using

$$\int d^3r\,\vec{\nabla}\cdot(x_i\vec{F}) = \int d^3r\,F_i + \int d^3r\,x_i\vec{\nabla}\cdot\vec{F}$$

$$\|$$

$$\oint d\vec{S}\cdot(x_i\vec{F})$$

But as $S \to \infty$ $\psi \to 0$ sufficiently rapidly so that we can neglect the surface terms, hence

$$\frac{d}{dt}\int d^3r\, \psi^* \vec{r}\, \psi = \frac{-i\hbar}{2m}\int d^3r \left[\psi^* \vec{\nabla}\psi - \vec{\nabla}\psi^* \psi\right].$$

Now again integrating the second term on the RHS by parts and ignoring surface terms

$$\int d^3r\, (\vec{\nabla}\psi^*)\,\psi = -\int d^3r\, \psi^* \vec{\nabla}\psi + \int_{S\to\infty} d\vec{S}\, \cancelto{0}{\psi^*\psi}$$

we find

$$\frac{d}{dt}\int d^3r\, \psi^* \vec{r}\, \psi = \int d^3r\, \psi^* \left(\frac{-i\hbar}{m}\vec{\nabla}\psi\right).$$

But $\langle \vec{r} \rangle = \int d^3r\, \psi^* \vec{r}\, \psi$

$\langle \vec{p} \rangle = \int d^3r\, \psi^* \frac{\hbar}{i}\vec{\nabla}\, \psi$,

Thus $$\frac{d}{dt}\langle \vec{r} \rangle = \frac{1}{m}\langle \vec{p} \rangle,$$

The expectation values of position

and momentum of the particle obey the classical relation between momentum and velocity.

Similarly we have

$$\frac{d}{dt}\langle \vec{p}\rangle = \int d^3r \, \frac{\hbar}{i}\left(\frac{\partial}{\partial t}\psi^* \vec{\nabla} \psi + \psi^* \vec{\nabla} \frac{\partial}{\partial t}\psi\right).$$

We can now use the quantum mechanical laws of dynamics, the Schrödinger equation

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

and its complex conjugate

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

Thus the integrand on the RHS becomes

$$\left(-i\hbar\frac{\partial}{\partial t}\psi^*\vec{\nabla}\psi - \psi^*\vec{\nabla}\, i\hbar\frac{\partial}{\partial t}\psi\right)$$

$$= -\frac{\hbar^2}{2m}\nabla^2\psi^*\vec{\nabla}\psi + V\psi^*\vec{\nabla}\psi$$

$$+ \frac{\hbar^2}{2m}\psi^*\vec{\nabla}\nabla^2\psi - \psi^*\vec{\nabla}(V\psi)$$

$$= -\frac{\hbar^2}{2m}\frac{\partial}{\partial x_i}\left[\frac{\partial}{\partial x_i}\psi^* \vec{\nabla}\psi - \psi^*\frac{\partial}{\partial x_i}\vec{\nabla}\psi\right]$$

$$- \psi^*\psi\,\vec{\nabla}V$$

Thus we find

$$\frac{d}{dt}\langle\vec{p}\rangle = \int d^3r\,(-\vec{\nabla}V)|\psi|^2$$

$$-\frac{\hbar^2}{2m}\int d^3r\,\frac{\partial}{\partial x_i}\left[\frac{\partial}{\partial x_i}\psi^*\vec{\nabla}\psi - \psi^*\frac{\partial}{\partial x_i}\vec{\nabla}\psi\right].$$

The second term on the RHS vanishes for $\psi \to 0$ as $S \to \infty$ sufficiently rapidly.

Hence we obtain

$$\frac{d}{dt}\langle\vec{p}\rangle = -\langle\vec{\nabla}V\rangle,$$

For a sufficiently localized state (so we can drop surface terms) it follows that Newton's second law is valid for expectation values of the momentum and force.

These argements can be generalized to the time derivative of expectation values of arbitrary functions of $\vec{r}$ and $\vec{p}$,

$$\langle F \rangle \equiv \int d^3r\, \psi^*(\vec{r},t)\, F(\vec{r}, \tfrac{\hbar}{i}\vec{\nabla}, t)\, \psi(\vec{r},t)$$

with ψ normalized to unity.

$$\frac{d}{dt}\langle F \rangle = \int d^3r \left[\frac{\partial \psi^*}{\partial t} F \psi + \psi^* F \frac{\partial \psi}{\partial t} + \psi^* \frac{\partial F}{\partial t} \psi \right].$$

We again apply the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi \equiv H\psi$$

and its complex conjugate

$$-i\hbar \frac{\partial}{\partial t}\psi^* = (H\psi)^*$$

to the above

$$\frac{d}{dt}\langle F \rangle = \left\langle \frac{\partial F}{\partial t} \right\rangle + \frac{i}{\hbar}\int d^3r \left[+(H\psi)^* F\psi - \psi^* F (H\psi) \right]$$

Since H is a Hermitian operator, we have

$$\frac{d}{dt}\langle F\rangle = \left\langle \frac{\partial F}{\partial t}\right\rangle + \frac{i}{\hbar}\int d^3r\, \psi^*(HF - FH)\psi$$

$$= \frac{i}{\hbar}\int d^3r\, \psi^*[H,F]\psi + \left\langle \frac{\partial F}{\partial t}\right\rangle .$$

Thus we secure

$$\boxed{\frac{d}{dt}\langle F\rangle = \frac{i}{\hbar}\langle [H,F]\rangle + \left\langle \frac{\partial F}{\partial t}\right\rangle ,}$$

Ehrenfest's Theorem.

To recover our earlier results we have $\vec{F} = \vec{r}$ ($\frac{\partial F}{\partial t} = 0$ unless there is explicit time dependence in F, as, for example, in the case of a time varying external field)

$$\frac{d}{dt}\langle \vec{r}\rangle = \frac{i}{\hbar}\langle [H,\vec{r}]\rangle$$

$$= \frac{i}{\hbar}\left\langle \left[\frac{\vec{p}^{\,2}}{2m} + V(\vec{r}), \vec{r}\right]\right\rangle$$

$$= \frac{i}{\hbar 2m}\langle [\vec{p}^{\,2}, \vec{r}]\rangle$$

But using $[AB,C] = A[B,C] + [A,C]B$

we have
$$[\vec{P}^2, x_j] = P_i[P_i, x_j] + [P_i, x_j]P_i$$
$$= -i\hbar\, 2P_j \text{ by the CCR.}$$

Hence $\frac{d}{dt}\langle\vec{r}\rangle = \frac{1}{m}\langle\vec{P}\rangle$ as before.

Further
$$\frac{d}{dt}\langle\vec{P}\rangle = \frac{i}{\hbar}\langle[H,\vec{P}]\rangle$$
$$= \frac{i}{\hbar}\langle[\frac{\vec{P}^2}{2m} + V, \vec{P}]\rangle$$
$$= \frac{i}{\hbar}\langle[V, -i\hbar\vec{\nabla}]\rangle$$
$$= -\langle\vec{\nabla}V\rangle.$$

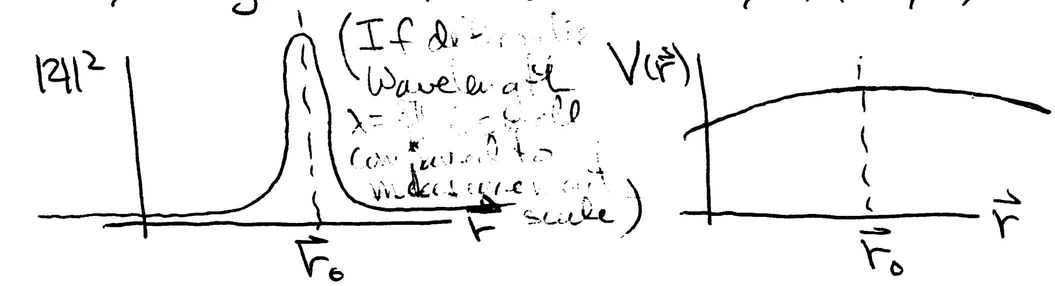
We can apply these results of Ehrenfest's theorem to the case in which
1) the wavefunction of the particle is sufficiently localized and
2) all potentials are sufficiently slowly varying

so that $\langle\vec{r}\rangle$, $\langle\vec{\nabla}V\rangle$ can be expanded about the peaked value of position $\vec{r}_0$,

$$\langle \vec{r} \rangle = \int d^3r\, \vec{r}\, \psi^*(\vec{r},t)\psi(\vec{r},t) \approx \vec{r}_0$$

$$\langle \vec{\nabla} V \rangle = \int d^3r\, \vec{\nabla} V(\vec{r})\psi^*(\vec{r},t)\psi(\vec{r},t) \approx \vec{\nabla} V(\vec{r}_0)$$

i.e.



Then $\langle \vec{p} \rangle \approx m\dot{\vec{r}}_0$; $\frac{d}{dt}\langle \vec{p} \rangle \approx m\ddot{\vec{r}}_0$

$$\frac{d}{dt}\langle \vec{p} \rangle \approx -\vec{\nabla} V(\vec{r}_0) \quad \text{and}$$

we obtain a local Newton's law $m\ddot{\vec{r}}_0 = -\vec{\nabla} V(\vec{r}_0)$.

1.3.6. The Heisenberg Uncertainty Principle

The expectation values of position and momentum can be used to define their root mean square deviations (consider 1-dimension for simplicity)

$$\Delta x \equiv \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$

$$\Delta p \equiv \sqrt{\langle (p - \langle p \rangle)^2 \rangle} .$$

The Heisenberg uncertainty principle