2.3 Evolution of a particle with external potential. Ehrenfest equation

Given a solution $\psi(x,t)$ of the Schrödinger equation, we write its mean position and mean momentum as follows:

$$\langle X\rangle(t) = \int_{\mathbb{R}^d} x\,|\psi(x,t)|^2\,dx \qquad (\langle X\rangle(t)\in\mathbb{R}^d)$$

$$\langle P\rangle(t) = \frac{\hbar}{(2\pi)^d}\int_{\mathbb{R}^d} k\,|\hat{\psi}(k,t)|^2\,dk$$

More generally, if f is a function $\mathbb{R}^d\to\mathbb{C}$, we write

$$\langle f(X)\rangle(t) = \int_{\mathbb{R}^d} f(x)\,|\psi(x,t)|^2\,dx.$$

Theorem 2.3 (Ehrenfest equations)

Let $\psi(x,t)$ be a classical solution of the Schrödinger equation. We also suppose that $\int|\psi(x,t)|^2dx=1$, $\int\|x\|\,|\psi|^2<\infty$, $\int\|k\|\,|\hat\psi(k,t)|^2dk<\infty$, $\int\|\nabla V(x)\|\,|\psi(x,t)|^2dx<\infty$. Then

(a) $\frac{d}{dt}\langle X\rangle(t) = \frac{1}{m}\langle P\rangle(t)$

(b) $\frac{d}{dt}\langle P\rangle(t) = -\langle\nabla V(X)\rangle(t)$

(c) $\frac{d}{dt}\left(\frac{1}{2m}\langle P^2\rangle(t) + \langle V(X)\rangle(t)\right) = 0$

The first two equations are the counterparts of Hamilton's equations for a classicle particle, and (c) is the conservation of energy. Notice that a natural guess for (b) could have been $\frac{d}{dt}\langle P\rangle(t) = -\nabla V(\langle X\rangle(t))$, but this turns out to be incorrect.

Proof: Essentially straightforward calculations. For (a),

$$\frac{d}{dt}\langle X_j\rangle(t) \overset{\text{Thm 2.27 in Folland}}{=} \int_{\mathbb{R}^d}\frac{\partial}{\partial t}\left[x_j\,\overline{\psi(x,t)}\,\psi(x,t)\right]dx$$

$$= \int x_j\left(\frac{\partial\overline{\psi}}{\partial t}\psi + \overline{\psi}\frac{\partial\psi}{\partial t}\right)dx$$

$$\overset{\text{Schr. eq.}}{=} i\int x_j\left[\left(-\frac{\hbar}{2m}\Delta\overline{\psi} + \frac{1}{\hbar}V\overline{\psi}\right)\psi - \overline{\psi}\left(-\frac{\hbar}{2m}\Delta\psi + \frac{1}{\hbar}V\psi\right)\right]dx$$

$$= i\frac{\hbar}{2m}\int\left(-x_j\Delta\overline{\psi}\,\psi + x_j\overline{\psi}\Delta\psi\right)dx$$

$$\overset{\text{by parts}}{=} i\frac{\hbar}{2m}\int\left(\nabla(x_j\psi)\cdot\nabla\overline{\psi} - \nabla(x_j\overline{\psi})\cdot\nabla\psi\right)dx$$

$$= i\frac{\hbar}{2m}\int\nabla x_j\cdot\left[\nabla\overline{\psi}\,\psi - \overline{\psi}\nabla\psi\right]dx$$

$$= i\frac{\hbar}{2m}\int\left(\frac{\partial\overline{\psi}}{\partial x_j}\psi - \overline{\psi}\frac{\partial\psi}{\partial x_j}\right)dx$$

$$(*) \qquad \overset{\text{by parts}}{=} \frac{i\hbar}{m}\int\frac{\partial\overline{\psi}}{\partial x_j}\psi\,dx$$

$$\overset{\text{Plancherel}}{=} \frac{1}{(2\pi)^d}\frac{i\hbar}{m}\int\widehat{\overline{\frac{\partial\psi}{\partial x_j}}}\,\hat{\psi}\,dk$$

$$= \frac{1}{(2\pi)^d}\frac{\hbar}{m}\int k_j\,|\hat\psi(k,t)|^2\,dk$$

$$= \frac{1}{m}\langle P_j\rangle(t).$$

For (b), we use Eq. (*) above.

$$\frac{d}{dt}\langle P_j\rangle(t) = i\hbar\int\left[\left(\frac{\partial}{\partial x_j}\frac{\partial}{\partial t}\overline{\psi(x,t)}\right)\psi + \frac{\partial\overline{\psi}}{\partial x_j}\frac{\partial\psi}{\partial t}\right]dx$$

$$= i\int\Bigg[i\Bigg(-\frac{\hbar^2}{2m}\frac{\partial}{\partial x_j}\Delta\overline{\psi} + \underbrace{\frac{\partial}{\partial x_j}V\overline{\psi}}_{=\frac{\partial V}{\partial x_j}\overline{\psi}+V\frac{\partial\overline{\psi}}{\partial x_j}}\Bigg)\psi - i\frac{\partial\overline{\psi}}{\partial x_j}\left(-\frac{\hbar^2}{2m}\Delta\psi + V\psi\right)\Bigg]dx$$

$$= \dots = -\int \frac{\partial V}{\partial x_j}(x)\, |\psi(x,t)|^2 dx = -\langle (\nabla V)_j (X) \rangle (t).$$

Exercise 3: Prove Theorem 2.3 (c). (a) and (b) may help. $\square$

2.4. Uncertainty principles

The Heisenberg uncertainty principle states that a particle cannot be localised in space, and simultaneously have a definite momentum. It is also a nice inequality of Fourier analysis. We first state the standard result. We also present another result that is valid in $d=1$ only but which has far-reaching consequences. In the next chapter we shall see a different generalisation based on properties of operators.

Theorem 2.4

For any $f \in L^2(\mathbb{R}^d)$ with $\|f\| = 1$, any $x_0, k_0 \in \mathbb{R}^d$, and any $j = 1, \dots, d$, we have

$$\int_{\mathbb{R}^d} |x_j - (x_0)_j|^2 |f(x)|^2 dx \cdot \frac{1}{(2\pi)^d} \int |k_j - (k_0)_j|^2 |\hat{f}(k)|^2 dk \geq \frac{1}{4}.$$

If we denote $\langle \Delta X \rangle = (\langle (X - \langle X \rangle)^2 \rangle)^{1/2}$ the mean deviation of X, and similarly for P, the theorem says that $\langle \Delta X \rangle \langle \Delta P \rangle \geq \frac{\hbar}{2}$.

Proof: We can shift f so that $x_0 = 0$. We can add a phase so that $k_0 = 0$. It is then enough to prove the theorem for $x_0 = k_0 = 0$.

$$1 = \int |f|^2 \overset{\text{by parts}}{=} -\int_{\mathbb{R}^d} x_j \frac{\partial}{\partial x_j} |f(x)|^2 dx$$
$$= -\int x_j \frac{\partial \bar{f}}{\partial x_j} f\, dx - \int x_j \bar{f} \frac{\partial f}{\partial x_j} dx.$$

Then

$$1 \leq 2 \int |x_j|\, |f(x)|\, \left|\frac{\partial f}{\partial x_j}(x)\right| dx$$
$$\overset{\text{Cauchy-Schwarz}}{\leq} 2 \left(\int x_j^2 |f(x)|^2 dx \right)^{1/2} \underbrace{\left(\int \left|\frac{\partial f}{\partial x_j}\right|^2 dx \right)}_{= \frac{1}{(2\pi)^d} \int k_j^2 |\hat{f}|^2 dk}^{1/2}.$$

$\square$

Remarks:
- The inequality is saturated by gaussian functions, i.e. there is equality iff $f(x) = A\, e^{i(x-x_0)k_0} e^{-B(x-x_0)^2}$ with $B > 0$ and $|A|^2 = \left(\frac{B}{\pi}\right)^{d/2}$.
- The theorem somehow assumes that $\int \|x\|^2 |f|^2 < \infty$ and $\int \|k\|^2 |\hat{f}| < \infty$. The left side is understood to be infinite otherwise.
- In the proof we also assumed that $f \in C^1$. But we have proved the inequality for a dense set of functions, and the general claim is obtained by continuity.