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:

\[
\langle x \rangle (t) = \int \mathbb{R}^d \times 1 \, \Psi(x,t) \, |\Psi(x,t)|^2 \, dx \quad (\langle x \rangle(0) \in \mathbb{R}^d)
\]

\[
\langle p \rangle (t) = \frac{i}{\hbar} \int \mathbb{R}^d \, k \, |\Psi(k,t)|^2 \, dk
\]

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 equation)**

Let \( \Psi(x,t) \) be a classical solution of the Schrödinger equation. We also suppose that \( \int |\Psi(x,t)|^2 \, dx = 1 \), \( \int \nabla \Psi(x,t) \, \Psi(x,t)^* \, dx = 0 \), \( \int |\nabla \Psi(x,t)|^2 \, dx \leq C_0 \). Then

(a) \( \frac{\partial}{\partial t} \langle x \rangle (t) = \frac{\hbar}{2m} < p > (t) \)

(b) \( \frac{\partial}{\partial t} \langle p \rangle (t) = - \langle \nabla V(x) \rangle (t) \)

(c) \( \frac{\partial}{\partial t} \left( \frac{\hbar}{2m} \langle p \rangle (t) + \langle p \rangle (t) \right) = 0 \)

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

**Proof**: Essentially straightforward calculation. For (a),

\[
\frac{\partial}{\partial t} < x > (t) = \text{Im}(\frac{\partial}{\partial t} \int \mathbb{R}^d \frac{2}{\hbar} [\frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \Psi(x,t)] \, dx
\]

\[
\text{Sch. eq.} = \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

\[
\frac{\partial}{\partial t} < p > (t) = - \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

\[
\text{Im. eq.} = \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

For (b), we use Eq. (4) above.

\[
\frac{\partial}{\partial t} < p > (t) = \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

\[
= \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

\[
= \frac{i}{\hbar} \int \mathbb{R}^d \left[ - \frac{\hbar}{2m} \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

\[
= \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]

\[
= \frac{i}{\hbar} \int \mathbb{R}^d \left[ \frac{\partial}{\partial \phi} \frac{\partial}{\partial \phi} \phi(x,t) \frac{2}{\hbar} \Psi(x,t) \right] \, dx
\]
\[ \ldots = -\int \nabla \cdot (x) \cdot (x) \, dx = - (\nabla \cdot (x))(0). \]

Exercise 3: Prove Theorem 2.3 (c), (a) and (b) may help.

2.4. Uncertainty principles

The Heisenberg uncertainty principle states that a particle cannot be localized in space, and simultaneously have a definite momentum. It is also a nice inequality for 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 \( \|f\|_2 = 1 \), any \( x, k \in \mathbb{R}^d \), and any \( j = 1, \ldots, d \), we have

\[ \int_{\mathbb{R}^d} |x_j - (x)_j|^2 |\hat{f}(k)|^2 \, dx \cdot \frac{1}{\omega^d} \int_{\mathbb{R}^d} |x_j - (x)_j|^2 |\hat{f}(k)|^2 \, dk \geq \frac{1}{\pi}. \]

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

**Proof**: We can shift \( P \) so that \( x_0 = 0 \). We can add a phase so that \( k_0 = 0 \). It is then enough to prove the Theorem for \( x = k = 0 \).

\[ 1 = \int |P|^2 \, dx = -\int x_j \frac{\partial}{\partial x_j} |\hat{f}(k)|^2 \, dx = -\int x_j \frac{\partial}{\partial x_j} \int |\hat{f}(k)|^2 \, dk \, dx. \]

Then

\[ 1 \leq 2 \int |x_j| \int |\hat{f}(k)|^2 \, dk \, dx \leq 2 \left( \int |x_j|^2 |\hat{f}(k)|^2 \, dk \right)^{1/2} \left( \int \frac{\partial}{\partial x_j} \int |\hat{f}(k)|^2 \, dk \right)^{1/2}. \]

Combining

\[ 2 \left( \int |x_j|^2 |\hat{f}(k)|^2 \, dk \right)^{1/2} \leq 2 \left( \int \frac{\partial}{\partial x_j} \int |\hat{f}(k)|^2 \, dk \right)^{1/2}. \]

**Remark**: The inequality is saturated by Gaussian functions, i.e. there is equality iff \( \hat{f}(k) = \frac{A}{\sqrt{2\pi}} e^{-\frac{(x - \langle x \rangle)^2}{2}} \) with \( B > 0 \) and \( A \mu^* = (\frac{B}{\pi})^{1/2} \). The theorem somehow assumes that \( \int |\hat{f}(k)|^2 \, dk \) and \( \int \ln |\hat{f}(k)| \, dk \). 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 its general claim is obtained by continuity.