

Molecular quantum dynamics: Exercise series 6

Read Tannor 5.2.

Problem 1: Properties of the Wigner function

In class, we defined the Wigner function $\rho_W(q, p)$ of a wave function $\psi(q)$ as

$$\rho_W(q, p) := \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \psi\left(q - \frac{s}{2}\right) \psi^*\left(q + \frac{s}{2}\right) e^{ips/\hbar} ds.$$

(a) Prove that

$$\int \rho_W(q, p) dp = |\psi(q)|^2.$$

(b) Prove that

$$\int \rho_W(q, p) dq = \left| \tilde{\psi}(p) \right|^2.$$

where $\tilde{\psi}(p) = (2\pi\hbar)^{-1/2} \int \psi(q) \exp(-ipq/\hbar) dq$ is the wave function in momentum representation.

Note: By solving this exercise, you will have shown that the Wigner function behaves like a quasiprobability distribution function. By integrating over q or p , you obtain the probability density in p or q , respectively! So Wigner function provides a very elegant phase space picture of quantum mechanics, which is *exactly* equivalent to the wave function picture.

Hints: (a) is easy, you will only need to use the following property of the delta function,

$$\int e^{ipq/\hbar} dq = 2\pi\hbar \delta(p).$$

Part (b) is a bit harder. In (b), start from the Dirac notation

$$\rho_W(q, p) := \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \left\langle q - \frac{s}{2} \right| \psi \rangle \langle \psi \left| q + \frac{s}{2} \right\rangle e^{ips/\hbar} ds.$$

Then insert resolutions of identity $1 = \int dp_1 |p_1\rangle \langle p_1|$ and $1 = \int dp_2 |p_2\rangle \langle p_2|$ in appropriate places. The rest is a simplification of various integrals by using the Dirac notation properties discussed in the beginning of the course, and the delta function property mentioned above (you will actually need it several times).