Exercise 5.1: Moyal ⋆-product and the Harmonic Oscillator (12P)

In standard quantum mechanics, the ground state $|0\rangle$ and the first excited eigenstate $|1\rangle$ of the harmonic oscillator $\mathbf{H} = \frac{\mathbf{P}^2}{2m} + \frac{m\omega^2\mathbf{Q}^2}{2}$ can be represented by the wave functions

$$\psi_0(q) = \langle q|0\rangle = \frac{1}{\pi^{1/4}a^{1/2}} e^{-\frac{q^2}{2a^2}}\,, \quad \psi_1(q) = \langle q|1\rangle = \frac{\sqrt{2}}{\pi^{1/4}a^{3/2}}\, q\, e^{-\frac{q^2}{2a^2}}\,,$$

where $a = \sqrt{\frac{\hbar}{m\omega}}$ denotes the characteristic length scale of the oscillator.

(a) Compute the Moyal-Wigner functions $\rho_0(p,q)$ and $\rho_1(q,p)$ by applying the inverse Weyl transform to the pure density matrices $\hat{\rho}_0 = |0\rangle\langle 0|$ and $\hat{\rho}_1 = |1\rangle\langle 1|$. (2P)

(b) Check the normalization of the Wigner function $\rho_0(q,p)$. (1P)

(c) Determine the trajectory $\big(q(t),p(t)\big)$ of the *classical* harmonic oscillator for the initial condition $\big(q(0),p(0)\big)$ at $t=0$ by solving the Hamilton equations of motion. Invert the solution in order to express $\big(q(0),p(0)\big)$ in terms of $\big(q(t),p(t)\big)$. (2P)

(d) Since the Moyal-Wigner formalism takes place in phase space, it is near at hand that the time-dependent Wigner function $\rho(q,p,t)$ simply moves like classical particles according to the classical Hamiltonian flow. This means that we can make the ansatz

$$\rho\big(q(t),p(t),\,t\big) = \rho\big(q(0),p(0),\,0\big) \qquad \forall t\,,$$

where $q(t),p(t)$ is a classical solution. Use this ansatz and (c) to prove that (1P)

$$\rho(q,p,t) \;=\; \rho\Big(q\cos\omega t - \frac{p}{m\omega}\sin\omega t\,,\;\; p\cos\omega t + q\,m\omega\sin\omega t\,,\;\; 0\Big).$$

(e) Argue why the star commutator $[H,\rho]_\star$ for ρ computed in (d) is of the form (2P)

$$[H,\rho]_\star = i\hbar\Big((\partial_q H)(\partial_p \rho) - (\partial_q\rho)(\partial_p H)\Big) = i\hbar\{H,\rho\}_{\text{Poisson}}\,.$$

(f) Let us define the abbreviations (1P)

$$A = A(q,p,t) = \frac{\partial\rho(\tilde{q},\tilde{p},0)}{\partial\tilde{q}}\bigg|_{\tilde{q}=q\cos\omega t-\frac{p}{m\omega}\sin\omega t,\ \tilde{p}=p\cos\omega t+q\,m\omega\sin\omega t}$$

$$B = B(q,p,t) = \frac{\partial\rho(\tilde{q},\tilde{p},0)}{\partial\tilde{p}}\bigg|_{\tilde{q}=q\cos\omega t-\frac{p}{m\omega}\sin\omega t,\ \tilde{p}=p\cos\omega t+q\,m\omega\sin\omega t}$$

Compute the three partial derivatives $\partial_q\rho(q,p,t)$, $\partial_p\rho(q,p,t)$, and $\partial_t\rho(q,p,t)$.

(g) Use (d)-(f) to prove that for the harmonic oscillator the equation of motion $i\hbar\partial_t\rho = [H,\rho]_\star$ is satisfied, justifying *a posteriori* the ansatz made in (d). (1P)

(h) Show that the ground state function $\rho_0(q,p)$ computed in (a) is invariant along classical trajectories. (1P)

(i) Explain why all eigenstates of $\mathbf{H}$ are represented by constant density matrices $\hat{\rho}$ and constant Moyal-Wigner functions. (1P)

(j) Explain qualitatively the time dependence of a Moyal-Wigner function starting with a 'spatially shifted ground state' of the form

$$\rho_0(q,p) = 2\exp\Big(-\frac{(q-b)^2}{a^2} - \frac{a^2p^2}{\hbar^2}\Big)\,.$$

How does it look like as time evolves? (1P)

Sample Solution

(a) The inverse Weyl transformation maps an operator $\mathbf{F}$ to a phase space function

$$f(q,p) \;=\; 2\int_{-\infty}^{+\infty} \mathrm{d}q' e^{2ipq'/\hbar}\langle q-q'|\mathbf{F}|q+q'\rangle\,.$$

For $\mathbf{F} = \hat{\rho}_0 = |0\rangle\langle 0|$ this turns into

$$\begin{aligned} f(q,p) \;&=\; 2\int_{-\infty}^{+\infty} \mathrm{d}q' e^{2ipq'/\hbar}\,\psi_0(q-q')\psi_0^*(q+q') \\ &=\; \frac{2}{\pi^{1/2}a}\int_{-\infty}^{+\infty} \mathrm{d}q' e^{2ipq'/\hbar}\,\exp\Big(\underbrace{-\frac{(q-q')^2+(q+q')^2}{2a^2}}_{=-(q^2+q'^2)/a^2}\Big)\,. \end{aligned}$$

This integral can be evaluated by completion of the square, rendering a Gaussian integral. The result reads:

$$\rho_0(q,p) = 2\exp\Big(-\frac{q^2}{a^2} - \frac{a^2p^2}{\hbar^2}\Big)\,.$$

Similarly we can compute the first excited state:

$$\rho_1(q,p) = \Big(\frac{4q^2}{a^2} + \frac{4a^2p^2}{\hbar^2} - 2\Big)\,\exp\Big(-\frac{q^2}{a^2} - \frac{a^2p^2}{\hbar^2}\Big)\,.$$

(b) The normalization can be checked by another Gaussian integration:

$$||\rho_0|| \;=\; \frac{1}{2\pi\hbar}\int \mathrm{d}q\int \mathrm{d}p\, 2\,\exp\Big(-\frac{q^2}{a^2} - \frac{a^2p^2}{\hbar^2}\Big) \;=\; 1.$$

Note: Similarly it can be verified that ρ_1 is properly normalized.

(c) The Hamilton equations of motion $\dot{q} = \partial_p H, \dot{p} = -\partial_q H$ yield the solution

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & \frac{1}{m\omega}\sin\omega t \\ -m\omega\sin\omega t & \cos\omega t \end{pmatrix}\begin{pmatrix} q_0 \\ p_0 \end{pmatrix}$$

By inverting the matrix (or, equivalently, by solving for (q_0,p_0)) we obtain

$$\begin{pmatrix} q_0 \\ p_0 \end{pmatrix} = \begin{pmatrix} \cos\omega t & -\frac{1}{m\omega}\sin\omega t \\ m\omega\sin\omega t & \cos\omega t \end{pmatrix}\begin{pmatrix} q(t) \\ p(t) \end{pmatrix}$$

(d) Insert (c) on the r.h.s. of the ansatz; this yields:

$$\rho\big(q(t),p(t),\,t\big) = \rho\Big(q(t)\cos\omega t - \frac{p(t)}{m\omega}\sin\omega t\,,\;\; p(t)\cos\omega t + q(t)\,m\omega\sin\omega t\,,\,0\Big).$$

Since this relation is valid for all trajectories which are solutions of the Hamilton equations of motion, we can replace $q(t)\to q$ and $p(t)\to p$, arriving at the desired equation.

(e) Regardless of the specific form of the Hamilton function $H(q,p)$, we can use the fact that $\rho(q,p,t)$ given in (d) depends only linearly on q and p. Thus the quadratic and all higher orders in the Taylor expansion of the exponential in the star operator do not contribute. Moreover, the zeroth order in the commutator cancels anyway. Thus we are left with the first order which gives identical contributions in both terms, i.e. $H \star \rho = -\rho \star H$. Hence

$$[H,\rho]_\star = 2H \star \rho = i\hbar\Big((\partial qH)(\partial_p \rho) - (\partial_q \rho)(\partial_p H)\Big)\,.$$

(f) Just apply the chain rule, the two abbreviations are the outer derivatives:

$$\begin{aligned}
\partial_q \rho(q,p,t) &= A\cos\omega t + Bm\omega \sin\omega t \\
\partial_p \rho(q,p,t) &= -A\frac{1}{m\omega}\sin\omega t + B\cos\omega t \\
\partial_t \rho(q,p,t) &= A\Big(-\omega q\sin\omega t - \frac{p}{m}\cos\omega t\Big) + B\Big(-p\omega\sin\omega t + qm\omega^2\cos\omega t\Big)
\end{aligned}$$

(g) For the harmonic oscillator we have $\partial_q H = m\omega^2 q, \partial_p H = p/m$, hence

$$\begin{aligned}
[H,\rho]_\star = i\hbar\Big[m\omega^2 q\Big(A(-\frac{1}{m\omega}\sin\omega t) + B\cos\omega t\Big) - \frac{p}{m}\Big(A\cos\omega t + Bm\omega\sin\omega t\Big)\Big] \\
= i\hbar A(-\omega q\sin\omega t - \frac{p}{m}\cos\omega t\Big) + i\hbar B\Big(m\omega^2 q\cos\omega t - p\omega\sin\omega t\Big) = i\hbar\partial_t\rho
\end{aligned}$$

(h) Taking a classical trajectory computed in (c), we know that the energy $E = H = p2/2m + m\omega^2 q^2/2$ is conserved along the trajectory. The solution for ρ_0 computed in (a) can be recast as

$$\rho_0(q,p) = 2\exp\Big(\frac{2H(q,p)}{\hbar\omega}\Big)$$

Therefore, it is clear that $\rho_0(q(t),p(t))$ is constant along a classical trajectory.

(i) A ket eigenstate $|n\rangle$ evolves in time by an oscillating phase $e^{-\frac{i}{\hbar}E_n t}$ while the corresponding bra eigenstate $\langle n|$ oscillates with the conjugate phase. Thus, the density matrix $|n\rangle\langle n|$ is constant. The same applies of course to the Wigner-Moyal function which is derived from $|n\rangle\langle n|$.

(j) In this exercise we have seen that the Moyal-Wigner functions just move along the classical Hamiltonian flow. The shifted initial condition looks initially like a Gaussian bell shape curve displaced from the origin by the distance b. Since the classical trajectories of the harmonic oscillator are circles (ellipses) with the same frequency ω, we expect that this Gaussian bell patch simple moves cyclically in phase space around the origin.

($\Sigma = 12$P)