PHASE SPACE DISTRIBUTIONS IN QUANTUM SYSTEMS

1. Phase space distributions in quantum systems

We now discuss a phase-space description of quantum mechanics due to Wigner, which reveals more directly the similarities and differences between the dynamics of classical and quantum systems. We will limit ourselves to the case of a single particle, noting that the formalism can be extended to many-body system in a straightforward, if cumbersome fashion. Some additional materials can be found e.g. in the lecture notes of A. Polkovnikov available online at `http://physics.bu.edu/~asp/teaching/lecture_notes_wigner_boulder_2013.pdf` and references therein.

1.1. **Description of a single particle in Wigner-Weyl formalism.** We consider a simple quantum system, with a single degree of freedom with no internal structure (such as spin etc.) for which the position and momentum eigenstates form a complete set of states on the Hilbert space, i.e. we have

$$1 = \int \mathrm{d}^d\mathbf{x}\ |\mathbf{x}\rangle\langle\mathbf{x}| = \int \frac{\mathrm{d}^d\mathbf{p}}{(2\pi\hbar)^d}|\mathbf{p}\rangle\langle\mathbf{p}| \ . \tag{1}$$

with position and momentum states related by

$$|\mathbf{p}\rangle = \int \mathrm{d}^d\mathbf{x}\ e^{i\mathbf{p}\mathbf{x}/\hbar}\ |\mathbf{x}\rangle \tag{2}$$

and normalized such that

$$\langle\mathbf{x}|\mathbf{x}'\rangle = \delta^{(d)}(\mathbf{x}-\mathbf{x}')\ , \qquad \langle\mathbf{p}|\mathbf{p}'\rangle = (2\pi\hbar)^d\delta^{(d)}(\mathbf{p}-\mathbf{p}')\ . \tag{3}$$

Now the challenge in defining a phase-space distribution derives from the fact that since $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$ do not commute with each other

$$[\hat{\mathbf{x}}^i, \hat{\mathbf{p}}^j] = i\hbar\delta^{ij}\ , \tag{4}$$

we can not measure the precise position and momentum of the particle at the same time due to the uncertainty principle. Now to retain as much information as possible, we define for any hermitian Schroedinger operator $\hat{O}$ acting on the Hilbert space, the Wigner-Weyl transform O_W as

$$O_W(\mathbf{x},\mathbf{p}) = \int \mathrm{d}^d\mathbf{s}\ e^{i\mathbf{p}\mathbf{s}/\hbar}\ \langle\mathbf{x}-\mathbf{s}/2|\hat{O}|\mathbf{x}+\mathbf{s}/2\rangle\ , \tag{5}$$

or equivalently

$$O_W(\mathbf{x},\mathbf{p}) = \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi\hbar)^d}\ e^{-i\mathbf{q}\mathbf{x}/\hbar}\ \langle\mathbf{p}-\mathbf{q}/2|\hat{O}|\mathbf{p}+\mathbf{q}/2\rangle \tag{6}$$

which is a function of the phase space variables $\mathbf{x}$ and $\mathbf{p}$. Specifically, for $\hat{O} = \hat{\rho}(t)$ the corresponding phase-space function $\rho_W(t,\mathbf{x},\mathbf{p})$ is referred to as the *Wigner function* or *Wigner distribution.* Since we cannot measure momentum and position precisely at the same time, the best we can hope for in terms of phase-space distribution $\rho_W(\mathbf{x},\mathbf{p})$ is that upon marginalizing the information over position (momentum), we obtain the corresponding momentum (position) distribution. Indeed it is easily checked that

$$\int \frac{\mathrm{d}^d\mathbf{p}}{(2\pi\hbar)^d}\ \rho_W(t,\mathbf{x},\mathbf{p}) \quad = \quad \langle\mathbf{x}|\hat{\rho}(t)|\mathbf{x}\rangle\ , \tag{7}$$

and similarly

$$\begin{aligned}\int \mathrm{d}^d\mathbf{x}\ \rho_W(t,\mathbf{x},\mathbf{p}) \quad &= \quad \int \mathrm{d}^d\mathbf{x}\int \mathrm{d}^d\mathbf{s}\ e^{i\mathbf{p}\mathbf{s}/\hbar}\ \langle\mathbf{x}-\mathbf{s}/2|\hat{\rho}(t)|\mathbf{x}+\mathbf{s}/2\rangle \\ &= \quad \left(\int \mathrm{d}^d(\mathbf{x}-\mathbf{s}/2)\ e^{-i\mathbf{p}(\mathbf{x}-\mathbf{s}/2)/\hbar}\ \langle\mathbf{x}-\mathbf{s}/2|\right)\hat{\rho}(t)\left(\int \mathrm{d}^d(\mathbf{x}+\mathbf{s}/2)\ e^{i\mathbf{p}(\mathbf{x}+\mathbf{s}/2)/\hbar}|\mathbf{x}+\mathbf{s}/2\rangle\right) \\ &= \quad \langle\mathbf{p}|\hat{\rho}(t)|\mathbf{p}\rangle\ . \end{aligned} \tag{8}$$

Since the Wigner-Weyl transformation can be inverted, according to

$$\int \frac{\mathrm{d}^d\mathbf{p}}{(2\pi\hbar)^d}\ e^{-i\mathbf{p}\mathbf{s}/\hbar}\ O_W(\mathbf{x},\mathbf{p}) = \langle\mathbf{x}-\mathbf{s}/2|\hat{O}|\mathbf{x}+\mathbf{s}/2\rangle\ , \tag{9}$$

or equivalently

$$\int \mathrm{d}^d\mathbf{x}\; e^{i\mathbf{q}\mathbf{x}/\hbar}\; O_W(\mathbf{x},\mathbf{p}) = \langle \mathbf{p}-\mathbf{q}/2|\hat{O}|\mathbf{p}+\mathbf{q}/2\rangle \;, \tag{10}$$

to yield all possible operator matrix elements, it contains by definition all information about the action of the Schroedinger operator on the Hilbert space, and is therefore fully equivalent to the conventional operator formulation.

1.2. **Expectation values.** Based on the Wigner-Weyl foramlism, we can now also calculate expectation values of hermitian operators $\hat{O}$, which in the standard operator formalism are given by

$$\langle \hat{O}(t)\rangle = \mathrm{tr}\Big[\hat{O}\hat{\rho}(t)\Big] \;, \tag{11}$$

Evaluating the trace in position space one finds

$$\begin{aligned}
\langle \hat{O}(t)\rangle &= \int \mathrm{d}^d\mathbf{x} \int \mathrm{d}^d\mathbf{x}' \langle \mathbf{x}|\hat{O}|\mathbf{x}'\rangle\langle \mathbf{x}'|\hat{\rho}(t)|\mathbf{x}\rangle && (12)\\
&= \int \mathrm{d}^d\mathbf{x} \int \mathrm{d}^d\mathbf{s} \langle \mathbf{x}-\mathbf{s}/2|\hat{O}|\mathbf{x}+\mathbf{s}/2\rangle\langle \mathbf{x}+\mathbf{s}/2|\hat{\rho}(t)|\mathbf{x}-\mathbf{s}/2\rangle \;, && (13)\\
&= \int \mathrm{d}^d\mathbf{x} \int \mathrm{d}^d\mathbf{s} \int \frac{\mathrm{d}^d\mathbf{p}}{(2\pi\hbar)^d} e^{-i\mathbf{p}\mathbf{s}/\hbar}\; O_W(\mathbf{x},\mathbf{p}) \int \frac{\mathrm{d}^d\mathbf{p}'}{(2\pi\hbar)^d} e^{+i\mathbf{p}'\mathbf{s}/\hbar} \rho_W(\mathbf{x},\mathbf{p}') \;, && (14)\\
&= \int \mathrm{d}^d\mathbf{x} \int \frac{\mathrm{d}^d\mathbf{p}}{(2\pi\hbar)^d}\; O_W(\mathbf{x},\mathbf{p})\; \rho_W(\mathbf{x},\mathbf{p}) \;. && (15)
\end{aligned}$$

which is analogous to the coresponding expression in the classical ensemble. Clearly, one may wonder at this stage, how a classical phase-space distribution such as the Wigner function $\rho_W(t,\mathbf{x},\mathbf{p})$ can describe the properties of a quantum system. One crucial difference to the classical probabilistic phase-space picture is however, that the distribution $\rho_W(t,\mathbf{x},\mathbf{p})$ is in general *not positive semi-definite*, i.e. in contrast to the classical phase-space distribution the quantum mechanical Wigner function does not necessarily have a probabilistic interpretation.

1.3. **Evolution of the Wigner function.** We now proceed to investigate the quantum dynamics in phase-space, by considering the evolution equation of the Wigner function based on the von-Neumann equation

$$i\hbar\partial_t\rho_W(t,\mathbf{x},\mathbf{p}) = \int \mathrm{d}^d\mathbf{s}\; e^{i\mathbf{p}\mathbf{s}/\hbar}\; \langle \mathbf{x}-\mathbf{s}/2|\;\Big[\hat{H},\hat{\rho}(t)\Big]\;|\mathbf{x}+\mathbf{s}/2\rangle \;. \tag{16}$$

By inserting a complete set of position states $\frac{1}{2^d}\int \mathrm{d}^d\mathbf{s}'|\mathbf{x}+\mathbf{s}'/2\rangle\langle \mathbf{x}+\mathbf{s}'/2|$ we readily obtain

$$i\hbar\partial_t\rho_W(t,\mathbf{x},\mathbf{p}) = \frac{1}{2^d}\int \mathrm{d}^d\mathbf{s} \int \mathrm{d}^d\mathbf{s}'\; e^{i\mathbf{p}\mathbf{s}/\hbar}\; \Big[\langle \mathbf{x}-\mathbf{s}/2|\hat{H}|\mathbf{x}+\mathbf{s}'/2\rangle\langle \mathbf{x}+\mathbf{s}'/2|\hat{\rho}(t)|\mathbf{x}+\mathbf{s}/2\rangle - (\hat{H}\leftrightarrow\hat{\rho})\Big]$$

By changing integration variables from $\mathbf{s}$ and $\mathbf{s}'$ to

$$\mathbf{x}' = \frac{\mathbf{s}'-\mathbf{s}}{4} \;, \qquad \mathbf{x}'' = \frac{\mathbf{s}'+\mathbf{s}}{4} \;, \tag{17}$$

accompanied by the Jacobian $\det(\frac{\partial(\mathbf{x}',\mathbf{x}'')}{\partial(\mathbf{s},\mathbf{s}')}) = \frac{1}{8^d}$, and re-expressing the matrix elements of $\hat{H}$ and $\hat{\rho}(t)$ in terms of the Wigner transforms

$$\begin{aligned}
\langle \mathbf{x}-\mathbf{s}/2|\hat{H}|\mathbf{x}+\mathbf{s}'/2\rangle &= \int \frac{\mathrm{d}^d\mathbf{p}'}{(2\pi\hbar)^d} H_W(\mathbf{x}+\mathbf{x}',\mathbf{p}+\mathbf{p}')e^{-2i(\mathbf{p}+\mathbf{p}')\mathbf{x}''/\hbar} && (18)\\
\langle \mathbf{x}+\mathbf{s}'/2|\hat{\rho}(t)|\mathbf{x}+\mathbf{s}/2\rangle &= \int \frac{\mathrm{d}^d\mathbf{p}''}{(2\pi\hbar)^d} \rho_W(\mathbf{x}+\mathbf{x}'',\mathbf{p}+\mathbf{p}'')e^{+2i(\mathbf{p}+\mathbf{p}'')\mathbf{x}'/\hbar} && (19)
\end{aligned}$$

we obtain

$$\begin{aligned}
i\hbar\partial_t\rho_W(t,\mathbf{x},\mathbf{p}) = 4^d \int \mathrm{d}^d\mathbf{x}' \int \mathrm{d}^d\mathbf{x}'' \int \frac{\mathrm{d}^d\mathbf{p}'}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d\mathbf{p}''}{(2\pi\hbar)^d}\; e^{2i\mathbf{p}(\mathbf{x}''-\mathbf{x}')/\hbar}\; e^{-2i(\mathbf{p}+\mathbf{p}')\mathbf{x}''/\hbar}\; e^{+2i(\mathbf{p}+\mathbf{p}'')\mathbf{x}'/\hbar} \\
\Big[H_W(\mathbf{x}+\mathbf{x}',\mathbf{p}+\mathbf{p}')\rho_W(\mathbf{x}+\mathbf{x}'',\mathbf{p}+\mathbf{p}'') - \rho_W(\mathbf{x}+\mathbf{x}',\mathbf{p}+\mathbf{p}')H_W(\mathbf{x}+\mathbf{x}'',\mathbf{p}+\mathbf{p}'')\Big] && (20)
\end{aligned}$$

By accounting for the cancelation in the phase-factors, and performing a change of variables $(\mathbf{x}',\mathbf{p}')\leftrightarrow(\mathbf{x}'',\mathbf{p}'')$ for the second term, we obtain

$$\partial_t\rho_W(t,\mathbf{x},\mathbf{p}) = 4^d \int \mathrm{d}^d\mathbf{x}' \int \mathrm{d}^d\mathbf{x}'' \int \frac{\mathrm{d}^d\mathbf{p}'}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d\mathbf{p}''}{(2\pi\hbar)^d}\; 2\sin\left(\frac{2}{\hbar}(\mathbf{p}''\mathbf{x}'-\mathbf{p}'\mathbf{x}'')\right) H_W(\mathbf{x}+\mathbf{x}',\mathbf{p}+\mathbf{p}')\rho_W(\mathbf{x}+\mathbf{x}'',\mathbf{p}+\mathbf{p}'') \;. \tag{21}$$

Now to make this expression look more classical it is useful to re-express the change of coordinates in terms of the action of the derivative operator

$$H_W(\mathbf{x}+\mathbf{x}',\mathbf{p}+\mathbf{p}') = e^{\mathbf{x}'\frac{\partial}{\partial \mathbf{x}}} e^{\mathbf{p}'\frac{\partial}{\partial \mathbf{p}}} H_W(\mathbf{x},\mathbf{p}) \; . \tag{22}$$

one can then perform the various integrations in Eq. (20), according to

$$4^d \int \mathrm{d}^d\mathbf{x}' \int \mathrm{d}^d\mathbf{x}'' \int \frac{\mathrm{d}^d\mathbf{p}'}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d\mathbf{p}''}{(2\pi\hbar)^d} H_W(\mathbf{x},\mathbf{p}) e^{\mathbf{x}'\frac{\overleftarrow{\partial}}{\partial \mathbf{x}}} e^{\mathbf{p}'\frac{\overleftarrow{\partial}}{\partial \mathbf{p}}} e^{\mathbf{x}''\frac{\overrightarrow{\partial}}{\partial \mathbf{x}}} e^{\mathbf{p}''\frac{\overrightarrow{\partial}}{\partial \mathbf{p}}} e^{2i(\mathbf{p}''\mathbf{x}'-\mathbf{p}'\mathbf{x}'')/\hbar} \rho_W(\mathbf{x},\mathbf{p}) \tag{23}$$

$$= 4^d \int \mathrm{d}^d\mathbf{x}' \int \mathrm{d}^d\mathbf{x}'' \int \frac{\mathrm{d}^d\mathbf{p}'}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d\mathbf{p}''}{(2\pi\hbar)^d} H_W(\mathbf{x},\mathbf{p}) \; e^{\frac{+2i}{\hbar}\mathbf{x}'\left(\mathbf{p}''-\frac{i\hbar}{2}\frac{\overleftarrow{\partial}}{\partial \mathbf{x}}\right)} e^{\frac{-2i}{\hbar}\mathbf{x}''\left(\mathbf{p}'+\frac{i\hbar}{2}\frac{\overrightarrow{\partial}}{\partial \mathbf{x}}\right)} e^{\mathbf{p}'\frac{\overleftarrow{\partial}}{\partial \mathbf{p}}} e^{\mathbf{p}''\frac{\overrightarrow{\partial}}{\partial \mathbf{p}}} \rho_W(\mathbf{x},\mathbf{p}) \tag{24}$$

$$= H_W(\mathbf{x},\mathbf{p}) \; \exp\left[i\frac{\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial \mathbf{x}}\frac{\overrightarrow{\partial}}{\partial \mathbf{p}} - \frac{\overrightarrow{\partial}}{\partial \mathbf{x}}\frac{\overleftarrow{\partial}}{\partial \mathbf{p}}\right)\right] \; \rho_W(\mathbf{x},\mathbf{p}) \; , \tag{25}$$

for the first term and similary for the second term. Dividing by $i\hbar$ and collecting the contribution from both terms

$$\partial_t \rho_W(t,\mathbf{x},\mathbf{p}) = H_W(\mathbf{x},\mathbf{p}) \; \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial \mathbf{x}}\frac{\overrightarrow{\partial}}{\partial \mathbf{p}} - \frac{\overrightarrow{\partial}}{\partial \mathbf{x}}\frac{\overleftarrow{\partial}}{\partial \mathbf{p}}\right)\right] \; \rho_W(\mathbf{x},\mathbf{p}) \tag{26}$$

where the operator on the right hand side defines the *Moyal bracket* denoted as

$$\{\{f,g\}\} = f(\mathbf{x},\mathbf{p}) \; \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial \mathbf{x}}\frac{\overrightarrow{\partial}}{\partial \mathbf{p}} - \frac{\overrightarrow{\partial}}{\partial \mathbf{x}}\frac{\overleftarrow{\partial}}{\partial \mathbf{p}}\right)\right] \; g(\mathbf{x},\mathbf{p}) \; , \tag{27}$$

such that in analogy to the classical equation of motion for the phase space density, the equation of motion for the Wigner function takes the form

$$\partial_t \rho_W = \{\{H_W, \rho_W\}\} \tag{28}$$

where the Poisson-Bracket in the classical theory is replaced by the Moyal bracket in the quantum theory. Noteably, the classical equation of motion can be recovered by expanding the result to leading order in $\hbar$, yielding

$$\{\{f,g\}\} = \{f,g\} + \mathcal{O}(\hbar^2) \; . \tag{29}$$

Note that there are certain situations (e.g. for the evolution of a harmonic oscillator) where all terms of order $\hbar^2$ and higher vanish identically and the phase-space quantum dynamics can be described exactly by classical equations of motion. However, even in such situations quantum corrections may still enter via the initial conditions or via the observables.