Quantum Mechanics II

Exercise 2: Wigner Representation

Wigner representation of quantum states is equivalent to the one by density operators.

1. The Wigner function for a system in the state $\hat{\rho}$ defined in the *phase space* (x,p) is given by

$$W(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ipy/\hbar}\langle x - y/2|\hat{\rho}|x + y/2\rangle \, dy.$$

a) Using the identity

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ip(x-a)}\, dp = \delta(x-a)$$

show that the integral of the Wigner function over p is a probability distribution for x and vise versa.

Solution:

$$\begin{aligned}
\int_{-\infty}^{\infty} W(x,p)dp &= \int_{-\infty}^{\infty}\left(\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ipy/\hbar}\langle x - y/2|\hat{\rho}|x + y/2\rangle \, dy\right) dp \\
&= \int_{-\infty}^{\infty}\langle x - y/2|\hat{\rho}|x + y/2\rangle \, dy \, \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ipy/\hbar} dp \\
&= \int_{-\infty}^{\infty}\langle x - y/2|\hat{\rho}|x + y/2\rangle \, dy \, \frac{1}{2\pi\hbar} 2\pi\hbar\, \delta(y) \\
&= \langle x|\hat{\rho}|x\rangle = \rho(x,x),
\end{aligned}$$

which are diagonal elements of the density matrix of $\hat{\rho}$ in x - representation. We know that the density operator is hermitian and trace one, therefore

$$\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} W(x,p)\, dp\right) dx = \int_{-\infty}^{\infty}\rho(x,x)dx = \mathrm{Tr}\,\hat{\rho} = 1,$$

which verifies the requirements to a probability distribution.

In order to prove the same for the integral over x we have to change the representation of the density matrix operator:

$$\begin{aligned}
&\int_{-\infty}^{\infty} W(x,p)dx = \int_{-\infty}^{\infty}\left(\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ipy/\hbar}\langle x - y/2|\hat{\rho}|x + y/2\rangle \, dy\right) dx \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \, e^{ipy/\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dp'\, dp'' \,\langle x - y/2|p'\rangle\langle p'|\hat{\rho}|p''\rangle\langle p''|x + y/2\rangle \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dy \, e^{ipy/\hbar}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dp'\, dp'' \,\frac{e^{ip'(x-y/2)/\hbar}}{\sqrt{2\pi\hbar}}\langle p'|\hat{\rho}|p''\rangle\frac{e^{-ip''(x+y/2)/\hbar}}{\sqrt{2\pi\hbar}}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{\infty} dy\, e^{ipy/\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dp'\, dp''\, \langle p'|\hat\rho|p''\rangle e^{-i(p'+p'')y/(2\hbar)} \underbrace{\int_{-\infty}^{\infty} dx e^{ix(p'-p'')/\hbar} dx}_{2\pi\hbar\delta(p'-p'')} \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dy\, e^{ipy/\hbar}\int_{-\infty}^{\infty} dp'\, \langle p'|\hat\rho|p'\rangle e^{-i(p'+p')'y/(2\hbar)} \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp'\, \langle p'|\hat\rho|p'\rangle \underbrace{\int_{-\infty}^{\infty} dy\, e^{i(p-p')y/\hbar}}_{2\pi\hbar\delta(p-p')} \\
&= \langle p|\hat\rho|p\rangle = \rho(p,p)\,\blacksquare
\end{aligned}
$$

b) Verify that the expectation value of the operator of kinetic energy $\hat{T} = \hat{p}^2/(2m)$ is given by

$$
\langle \hat{T}\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} T(p)W(x,p)\, dx\, dp,
$$

where $T(p)$ is a function of p.

Solution: We have in full generality

$$
\langle \hat{T}\rangle = \mathrm{Tr}\left[\frac{\hat{p}^2}{2m}\hat\rho\right] = \mathrm{Tr}\left[\int_{-\infty}^{\infty} dp\, |p\rangle \frac{p^2}{2m}\langle p|\hat\rho\right] = \int_{-\infty}^{\infty} dp\, \frac{p^2}{2m}\langle p|\hat\rho|p\rangle = \int_{-\infty}^{\infty}\frac{p^2}{2m}\rho(p,p)dp.
$$

On the other hand

$$
\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{p^2}{2m}W(x,p)\, dx\, dp = \int_{-\infty}^{\infty}\frac{p^2}{2m}dp\int_{-\infty}^{\infty}W(x,p)\, dx = \int_{-\infty}^{\infty}\frac{p^2}{2m}\rho(p,p)dp.
$$

Comparison of the right hand sides of two equations above proves the desired equality with $T(p) = p^2/(2m)$.

c) Verify that the expectation value of operator of potential energy $\hat{U} = U(\hat{x})$ is given by

$$
\langle \hat{U}\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} U(x)W(x,p)\, dx\, dp.
$$

The solution follows the lines of the solution for question 1b)

2. Quantum superposition and mixture of two Gaussian states. Use here $\hbar = 1$.

Let two (non-normalized) Gaussian states are given by the wave functions:

$$
\begin{aligned}
\psi_1(x) &= \exp\left[-(x-5)^2\right], \\
\psi_2(x) &= \exp\left[-(x+5)^2\right].
\end{aligned}
$$

a) Find (up to a constant) the Wigner function of a (equiprobable) statistical mixture of the two states.

Solution: The wave functions $\psi_1(x)$ and $\psi_2(x)$ define pure states $|\psi_1\rangle$ and $|\psi_2\rangle$. which are equivalently given by density operators, which are projectors:

$$
\rho_1 = |\psi_1\rangle\langle\psi_1| \text{ and } \rho_2 = |\psi_2\rangle\langle\psi_2|.
$$

The equiprobable statistical mixture of these states is $\hat{\rho}_{1+2} = \frac{1}{2}\rho_1 + \frac{1}{2}\rho_2$. By linearity of the matrix element and the integral in the definition of the Wigner function the statistical mixture results in the same convex combination of Wigner functions of the constituent operators.

$$W_{1+2}(x,p) = \frac{1}{2}(W_1(x,p) + W_2(x,p))$$

Let us find first the Wigner function of the first state.

$$\begin{aligned}
W_1(x,p) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle x - y/2|\rho_1|x + y/2\rangle\, e^{ipy}\, dy \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle x - y/2|\psi_1\rangle\langle\psi_1|x + y/2\rangle\, e^{ipy}\, dy \\
&= \int_{-\infty}^{\infty} C_1\psi_1(x - y/2)\psi_1^*(x + y/2)\, e^{ipy}\, dy \\
&= C_1\int_{-\infty}^{\infty} e^{-(x-5-y/2)^2} e^{-(x-5+y/2)^2}\, e^{ipy}\, dy \\
&= C_1\int_{-\infty}^{\infty} e^{-2(x-5)^2-y^2/2+ipy}\, dy \\
&= C_1\int_{-\infty}^{\infty} e^{-\frac{1}{2}(y^2-2ipy+4(x-5)^2)}\, dy \\
&= C_1\int_{-\infty}^{\infty} e^{-\frac{1}{2}(y^2-2ipy-p^2+p^2+4(x-5)^2)}\, dy \\
&= C_1\int_{-\infty}^{\infty} e^{-\frac{1}{2}(y-ip)^2} + e^{-\frac{1}{2}(4(x-5)^2+p^2)}\, dy \\
&= C_1\sqrt{2\pi}e^{-\frac{1}{2}(4(x-5)^2+p^2)},
\end{aligned}$$

where C_1 is the square of the normalization constant of $\phi_1(x)$. The Wigner function has Gaussian shape.

Similar result for $W_2(x,p)$ can be obtained by replacement of $x-5$ by $x+5$ and C_1 by C_2. In addition, looking at functions $\psi_1(x)$ and $\psi_2(x)$ we can see that they differ only by a shift of the argument, therefore both normalization constants are the same $C_1 = C_2 = C$, because the normalization here implies integration with infinite limits. Then

$$W_{1+2} = C\sqrt{\frac{\pi}{2}}\left(e^{-\frac{1}{2}(4(x-5)^2+p^2)} + e^{-\frac{1}{2}(4(x+5)^2+p^2)}\right).$$

b) Find (up to a constant) the Wigner function of the superposition of the two states given by equal amplitudes.

Solution: The superposition $\psi_{12} = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle$ is equivalently given density operator ρ_{12}, which is a projector:

$$\rho_{12} = |\psi_{12}\rangle\langle\psi_{12}|.$$

Then

$$
\begin{aligned}
W_{12}(x,p) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle x-y/2|\rho_{12}|x+y/2\rangle\, e^{ipy}\, dy \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle x-y/2|\psi_{12}\rangle\langle\psi_{12}|x+y/2\rangle\, e^{ipy}\, dy \\
&= \frac{C}{2}\int_{-\infty}^{\infty}\Big((\psi_1(x-y/2)\psi_1^*(x+y/2)+\psi_2(x-y/2)\psi_2^*(x+y/2) \\
&+ \psi_1(x-y/2)\psi_2^*(x+y/2)+\psi_2(x-y/2)\psi_1^*(x+y/2)\Big)\, e^{ipy}\, dy \\
&= \frac{1}{2}(W_1(x,y)+W_2(x,y)) \\
&+ \frac{C}{2}\int_{-\infty}^{\infty}\left(e^{-(x-5-y/2)^2}e^{-(x+5+y/2)^2}+e^{-(x+5-y/2)^2}e^{-(x-5+y/2)^2}\right)e^{ipy}\, dy.
\end{aligned}
$$

Already here we observe that the Wigner function of the superposition differs from the Wigner function of the mixture by the cross terms, which are not the Wigner functions themselves. Let us start with the first cross term.

$$
\begin{aligned}
&\frac{C}{2}\int_{-\infty}^{\infty} e^{-(x-5-y/2)^2}e^{-(x+5+y/2)^2}\, e^{ipy}\, dy \\
&= \frac{C}{2}\int_{-\infty}^{\infty} e^{-2(x^2+(5+y/2)^2)}\, e^{ipy}\, dy, \quad 5+y/2=y' \\
&= \frac{C}{2}e^{-2x^2}\int_{-\infty}^{\infty} e^{-2y'^2+ip(2y'-10)}\, dy \\
&= \frac{C}{2}e^{-2x^2}e^{-10ip}\int_{-\infty}^{\infty} e^{-2(y'^2-ipy'+(ip/2)^2-(ip/2)^2)}\, dy' \\
&= \frac{C}{2}e^{-2x^2+2(ip/2)^2}e^{-10ip}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(y'-ip/2)^2}\, dy' \\
&= C\sqrt{\frac{\pi}{2}}e^{-\frac{1}{2}(4x^2+p^2)}e^{-10ip}.
\end{aligned}
$$

The calculation of the second cross term is follows the same lines. The only difference comes from replacement $5\to -5$ in the first line, which implies the change of the variable of integration $y'=y/2-5$ in the second line. Then, in third line, the only change is in the factor $(2y'-10)$, which is replaced by $(2y'+10)$. The only effect of this in the fourth line is complex conjugation of e^{-10ip}, while the integral is left unchanged. Finally the second cross term is the complex conjugation of the first one so that their sum is real.

Summing up all terms we obtain

$$
W_{12}(x,p)=C\sqrt{\frac{\pi}{2}}\left(e^{-\frac{1}{2}(4(x-5)^2+p^2)}+e^{-\frac{1}{2}(4(x+5)^2+p^2)}+2e^{-\frac{1}{2}(4x^2+p^2)}\cos 10p\right).
$$

c) Comparer the two Wigner functions. In which case the Wigner function shows non-classical features the state?

Answer: The two Wigner functions differ by an oscillating term:

$$W_{12}(x,p) = W_{1+2}(x,p) + C\sqrt{2\pi}e^{-\frac{1}{2}(4x^2+p^2)}\cos 10p.$$

This term makes a crucial difference. The Wigner function W_{1+2} of the mixture is always positive being a convex combination of two positive Gaussian functions. Such states can be considered as "classical". The cross term in $W_{12}(x'p)$ may have negative values. The constants C are the same for all three terms in $W_{12}(x,p)$. The exponential functions in all three terms are obtained from the same function by different argument shifts along x-axis. Therefore, the maximum of the amplitude of the oscillating term is equal to the sum of the maxima of two others. As the terms are shifted differently along x-axis the whole expression for $W_{12}(x,p)$ may then take negative values. This illustrates non-classical correlations which exist in quantum superposition of Gaussian states and which are absent in the "classical" mixture.

Why the Wigner function is called *quasi probability* distribution?

Answer: In particulr, because it may take negative values.

3. *Coherent state* is an eigenstate of the annihilation operator. Use here $\hbar = 1$.

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \qquad \text{where} \quad \hat{a} = (\hat{x} + i\hat{p})/\sqrt{2}.$$

The (complex) eigenvalue α is related to the phase space variables x et p as

$$\begin{aligned} x &= \sqrt{2}\,\mathrm{Re}(\alpha), \\ p &= \sqrt{2}\,\mathrm{Im}(\alpha). \end{aligned}$$

a) Find the average value of the number of particles in the coherent state.

Solution: The number operator is $\hat{N} = \hat{a}^\dagger\hat{a}$. By definition of the coherent state we have

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \;\Rightarrow\; \langle\alpha|\hat{a}^\dagger = \langle\alpha|\alpha^*.$$

Then

$$\langle\hat{N}\rangle_\alpha = \langle\alpha|\hat{N}|\alpha\rangle = \langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle = \langle\alpha|\alpha^*\alpha|\alpha\rangle = |\alpha|^2\langle\alpha|\alpha\rangle = |\alpha|^2.$$

b) Find the representation of the coherent state in the eigen basis of the number operator. What is the representation in this basis coherent state for $\alpha = 0$?

Solution: Let $|n\rangle$ be the eigenvectors of the number operator: $\hat{N}|n\rangle = n|n\rangle$. The representation of the coherent state in the basis formed by these vectors is

$$|\alpha\rangle = \sum_{n=0}^{\infty}|n\rangle\langle n|\alpha\rangle.$$

The number states $|n\rangle$ can be obtained from the vacuum state

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle.$$

The overlap of the coherent state with such number state is

$$\langle n|\alpha\rangle = \frac{1}{\sqrt{n!}}\langle 0|\hat{a}^m|\alpha\rangle = \frac{\alpha^m}{\sqrt{n!}}\langle 0|\alpha\rangle.$$

In order to find the overlap in the right hand side we use normalization

$$1 = \langle\alpha|\alpha\rangle = \sum_{n=0}^{\infty}\langle\alpha|n\rangle\langle n\alpha\rangle = \sum_{n=0}^{\infty}\frac{|\alpha^n|^2}{n!}|\langle 0|\alpha\rangle|^2,$$

which leads to

$$\langle 0|\alpha\rangle = \left(\sum_{n=0}^{\infty}\frac{|\alpha^n|^2}{n!}\right)^{-1/2} = e^{-\frac{|\alpha|^2}{2}},$$

where the choice of the phase of the square root corresponds to the choice of the global phase of $|\alpha\rangle$. Finally, we have

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle,$$

and therefore, the coherent state for $\alpha = 0$ coinsides with the vacuum state, which contains no particles (excitations).

c) Find the wave function of the coherent state in x-representation $\varphi_\alpha(x) = \langle x|\alpha\rangle$ using the representation of the annihilation operator in terms of position and momentum as given above. Remember that In the position representation we have

$$\begin{aligned}\hat{x} &= \int_{-\infty}^{\infty}|x\rangle x\langle x|\,dx\\ \hat{p} &= -i\int_{-\infty}^{\infty}|x\rangle\frac{d}{dx}\langle x|\,dx.\end{aligned}$$

Solution: The eigenvalue equation for the annihilation operator can be rewritten in terms of $\hat{x}$ and $\hat{p}$ operators :

$$\left.\begin{array}{l}\hat{a}|\alpha\rangle = \alpha|\alpha\rangle\\ \hat{a} = \frac{1}{\sqrt{2}}(\hat{x}+i\hat{p})\end{array}\right\} \Rightarrow (\hat{x}+i\hat{p})|\alpha\rangle = \sqrt{2}\alpha|\alpha\rangle.$$

In the position representation we have

$$\int_{-\infty}^{\infty}dx'\,|x'\rangle\left(x'+i\left(-i\frac{d}{dx'}\right)\right)\langle x'|\alpha\rangle = \sqrt{2}\alpha|\alpha\rangle.$$

Projecting this equation on arbitrary $\langle x|$ we obtain

$$\int_{-\infty}^{\infty} dx' \underbrace{\langle x|x'\rangle}_{\delta(x-x')} \left(x' + i\left(-i\frac{d}{dx'}\right)\right) \underbrace{\langle x'|\alpha\rangle}_{\varphi_\alpha(x')} = \sqrt{2}\alpha \underbrace{\langle x|\alpha\rangle}_{\varphi_\alpha(x)}.$$

So that we arrive at the differential equation

$$\left(x + \frac{d}{dx}\right)\varphi_\alpha(x) = \sqrt{2}\alpha\varphi_\alpha(x),$$

Let us look for solution in the form $\varphi_\alpha(x) = C_\alpha e^{f(x)}$, where C_α is normalization constant. Then we have

$$\begin{aligned}
& xC_\alpha e^{f(x)} + f'(x)C_\alpha e^{f(x)} = \sqrt{2}\alpha C_\alpha e^{f(x)}, \\
\Rightarrow\quad & x + f'(x) = \sqrt{2}\alpha, \\
\Leftrightarrow\quad & \frac{d}{dx}f(x) = \sqrt{2}\alpha - x, \\
\Leftrightarrow\quad & df(x) = (\sqrt{2}\alpha - x)dx, \\
\Rightarrow\quad & f(x) = -\frac{1}{2}(x - \sqrt{2}\alpha)^2.
\end{aligned}$$

Therefore $\varphi_\alpha(x) = C_\alpha e^{-\frac{1}{2}(x-\sqrt{2}\alpha)^2} = C_\alpha e^{-\frac{1}{2}(x-x_0-ip_0)^2}$.
Constant C_α is determined as usual from the normalization condition:

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} dx\, |\varphi_\alpha(x)|^2 = |C_\alpha|^2 \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}(x-\sqrt{2}\alpha)^2} e^{-\frac{1}{2}(x-\sqrt{2}\alpha^*)^2} \\
&= |C_\alpha|^2 \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}(x-x_0-ip_0)^2} e^{-\frac{1}{2}(x-x_0+ip_0)^2} \\
&= |C_\alpha|^2 \int_{-\infty}^{\infty} dx e^{-(x-x_0)^2+p_0^2} = |C_\alpha|^2 e^{p_0^2} \int_{-\infty}^{\infty} dx e^{-(x-x_0)^2} = |C_\alpha|^2 e^{p_0^2}\sqrt{\pi},
\end{aligned}$$

which gives

$$C_\alpha = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{1}{2}p_0^2} e^{ip_0x_0},$$

where we have chosen the global phase $\exp(ip_0x_0)$ in order to recover the expression obtained by Schrödinger in 1930:

$$\varphi_\alpha(x) = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{1}{2}p_0^2} e^{ip_0x_0} e^{-\frac{1}{2}(x-x_0-ip_0)^2} = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{1}{2}(x-x_0)^2+ip_0x}.$$

d) Find the Wigner function of the coherent state. What is the shape of this function in the phase space?

Solution: The results of our calculations in question 2 a) cannot be used straightforwardly because coherent states have complex wave functions.
For $\hbar = 1$ using the intermediate expression in the last equation we have

$$\begin{aligned} W_\alpha(x,p) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ipy}\varphi_\alpha(x-y/2)\varphi_\alpha^*(x+y/2)\,dy \\ &= \frac{1}{2\pi}\frac{1}{\sqrt{\pi}}e^{-p_0^2}\int_{-\infty}^{\infty} e^{ipy}e^{-\frac{1}{2}(x-x_0-ip_0-y/2)^2}e^{-\frac{1}{2}(x-x_0+ip_0+y/2)^2}\,dy \\ &= \frac{1}{2\pi\sqrt{\pi}}e^{-p_0^2}\int_{-\infty}^{\infty} e^{-((x-x_0)^2+(ip_0+y/2)^2-ipy)}\,dy \\ &= \frac{1}{2\pi\sqrt{\pi}}e^{-p_0^2}e^{-(x-x_0)^2}\int_{-\infty}^{\infty} e^{-(y'^2-2ip(y'-ip_0)+(ip)^2-(ip)^2)}\,2dy', \quad y' = ip_0 + y/2 \\ &= \frac{1}{\pi\sqrt{\pi}}e^{-p_0^2}e^{-(x-x_0)^2}\int_{-\infty}^{\infty} e^{-(y'-ip)^2-p^2+2pp_0}\,dy' \\ &= \frac{1}{\pi\sqrt{\pi}}e^{-(x-x_0)^2}e^{-p^2+2pp_0-p_0^2}\sqrt{\pi} = \frac{1}{\pi}e^{-(x-x_0)^2-(p-p_0)^2}. \end{aligned}$$

The Wigner function has a Gaussian centered at (x_0, p_0) and

$$\langle\hat{x}\rangle_\alpha = x_0, \quad \langle\hat{p}\rangle_\alpha = p_0.$$

Using the Wigner function one can also verify that coherent states saturate the Heisenberg uncertainty relation (for $\hbar = 1$)

$$\Delta x\Delta p \geq \frac{1}{2}\hbar,$$

where

$$\Delta x = \sqrt{\langle(\hat{x}-\langle\hat{x}\rangle_\alpha)^2\rangle_\alpha}\,, \quad \Delta p = \sqrt{\langle(\hat{p}-\langle\hat{p}\rangle_\alpha)^2\rangle_\alpha}.$$