Quantum Mechanics II

Exercise 4: 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:

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

which are "diagonal elements" of the density matrix of $\hat{\rho}$ in x - representation. The diagonal elements are interpreted as a probability distribution. We can also verify that $\langle x|\hat{\rho}|x\rangle \geq 0$ due to hermiticity of $\hat{\rho}$ and

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

which verify the requirements to a probability distribution.

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

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

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.

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

where C_1 is the square of the normalization constant of $\phi_1(x)$ and C_{int} is the value of the integral over y, which does not depend on both x and p variables. We can observe that the Wigner function has Gaussian shape.

Observing the calculations of $W_1(x,p)$ we can easy conclude that $W_2(x,p)$ 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

$$W_{1+2} = \frac{CC_{\text{int}}}{2}\left(e^{-\frac{1}{2}(4(x-5)^2+p^2)} + e^{-\frac{1}{2}(4(x+5)^2+p^2)}\right).$$

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

<u>Solution</u>: 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

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

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

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

Note that here $C_{\rm int}$ is the same as in question 2 a) because the integrands are given by the functions which differ only by the shift of the argument.

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 as is the final result up to the complex conjugation. Summing up all four terms we obtain

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

c) Compare 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:

$$W_{12}(x,p) = W_{1+2}(x,p) + CC_{\text{int}}e^{-\frac{1}{2}(4x^2+p^2)}\cos 10p$$

This term makes a crucial difference. Whereas W_{1+2} is always positive being a convex combination of two positive Gaussian functions, the cross term may have negative values. The constants C and C_{int} are the same for all three terms in $W_{12}(x,p)$. The exponential functions in these terms are almost the same with the only difference in the shift of the argument 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_{1+2} may then take negative values. This illustrates non-classical correlations which exist in the superposition of two "classical" Gaussian states and which are absent in the 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 $\hbar = 1$.

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

Accordingly, 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 eigenbasis of the number operator. What is the representation in this basis coherent state for $\alpha = 0$? Solution: The representation of the coherent state in the eigenbasis of the number operator is formally written as

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

where vectors $|n\rangle$ are solutions of the eigenvalue equation $\hat{N}|n\rangle = n|n\rangle$ and we know that they can be obtained as

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

The overlap of the coherent state with the number state is

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

The overlap in the right hand side can be found using normalization of the coherent state.

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

which leads to

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

The choice of the phase of the square root corresponds to the choice of the global phase of $|\alpha\rangle$.

Finally, we have

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

and therefore, $|\alpha = 0\rangle = |0\rangle$ is the vacuum state. It is consistent with the fact that it contains zero excitation/particles (see 3 a)).

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

$$\hat{x} = \int_{-\infty}^{\infty} x|x\rangle\langle x|\,dx$$

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

<u>Solution:</u>

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

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

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

where we dropped index α in function $\varphi(x)$. Let us look for solution in the form $\varphi(x) = Ce^{f(x)}$, where C is normalization constant. Then we have

$$\begin{aligned}
& xCe^{f(x)} + f'(x)Ce^{f(x)} = \sqrt{2}\alpha Ce^{f(x)} \\
\Rightarrow\ & x + f'(x) = \sqrt{2}\alpha \\
\Leftrightarrow\ & \frac{d}{dx}f(x) = \sqrt{2}\alpha - x \\
\Leftrightarrow\ & df(x) = (\sqrt{2}\alpha - x)dx \\
\Rightarrow\ & f(x) = -\frac{1}{2}(x - \sqrt{2}\alpha)^2
\end{aligned}$$

Therefore $\varphi(x) = Ce^{-\frac{1}{2}(x-\sqrt{2}\alpha)^2}$.

d) What is the shape of the Wigner function of the coherent state 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

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

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

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