A PRECAUTION NEEDED IN USING THE PHASE-SPACE FORMULATION OF QUANTUM MECHANICS

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We explain the origin of the apparent discrepancy recently reported between results obtained by the phase-space formulation of quantum mechanics and conventional (Schrödinger) quantum mechanics. We show how to arrive at a complete agreement.

1. Introduction

Recently there has been renewed interest in applications of the so-called phase-space formulation of quantum mechanics[1] for both equilibrium[2] and non-equilibrium phenomena[3]. Its basic feature is to provide a framework for the treatment of quantum mechanical problems in terms of classical phase-space language. Following the appearance of the well-known Wigner distribution function[1], many other distribution functions have been considered. For instance, there is anti-normal ordered (smoothed Wigner distribution[4]) and the normal-ordered[5] (P-)distribution functions, the anti-standard-ordered[6]) and the standard-ordered[7]) distribution functions. Each of those distribution functions was created for a particular purpose. In most cases, the Wigner distribution function is the simplest one to use[8-10]). But it can assume negative values. The smoothed Wigner distribution function (SWDF) is obtained by convolution of the Wigner distribution function with a phase-space Gaussian function and is always non-negative.

It has been reported recently[11]) that employment of the SWDF in calculations for nonlinear systems, such as an anharmonic oscillator and the hydrogen atom, causes severe discrepancy with the results obtained by standard (Schrödinger) quantum mechanics. We are able to show that this disagreement may be attributed to an incorrect use of the SWDF. It is the purpose of the present paper to clarify this point and illustrate how to obtain correct results by use of the SWDF.

2. Ensemble averaging via the phase-space representation of quantum mechanics

We shall start from a general point of view of the phase-space representation of quantum mechanics and return later to the case of the SWDF.

Suppose $\hat{\rho}$ is the density operator and $\Omega(u, v)$ is an arbitrary function, a phase-space distribution function[7]) may then be associated with $\hat{\rho}$:

$$P^{(\Omega)}(q, p) = \text{Tr}[\hat{\rho}\hat{\Delta}^{(\Omega)}(q - \hat{q}, p - \hat{p})] \,, \tag{1}$$

where

$$\hat{\Delta}^{(\Omega)}(q - \hat{q}, p - \hat{p}) = (2\pi\hbar)^{-2} \int \int \Omega(u, v)$$

$$\times \exp\left[\frac{-i(u(q - \hat{q}) + v(p - \hat{p}))}{\hbar} \right] du \, dv \,. \tag{2}$$

The ranges of integrations in this paper are always from $-\infty$ to $+\infty$.

The phase-space distribution function defined by eqs. (1) and (2) is normalized:

$$\int \int P^{(\Omega)}(q, p) \, dq \, dp = \text{Tr}(\hat{\rho}) = 1 \,. \tag{3}$$

If one associates an arbitrary operator $\hat{B}$ (other than $\hat{\rho}$) with its phase-space representation by:

$$b^{(\Omega)}(q, p) = 2\pi\hbar \, \text{Tr}[\hat{B}\Delta^{(\tilde{\Omega})}(q - \hat{q}, p - \hat{p})] \,, \tag{4}$$

where

$$\tilde{\Omega}(u, v) = [\Omega(-u, -v)]^{-1} \,, \tag{5}$$

one can calculate the expectation value for $\hat{B}$ through the following "classical" formula:

$$\langle \hat{B} \rangle = \text{Tr}(\hat{\rho}\hat{B})$$

$$= \int \int b^{(\Omega)}(q, p)P^{(\Omega)}(q, p) \, dq \, dp \,. \tag{6}$$

Each phase-space distribution function defined by eqs. (1) and (2) is

characterized by $\Omega(u, v)$, which is often called the filter function. The problem of expressing an operator in an ordered form according to a prescribed rule is equivalent to an operator-phase-space-mapping through an appropriate filter function Ω, whereas $\tilde{\Omega}$ corresponds to the inverse order. Simply for convenience, we call eqs. (1) and (2) the Ω-mapping. Hence if one wishes to use $P^{(\Omega)}(q, p)$, which is obtained from a Ω-mapping, to evaluate the expectation value of $\hat{B}$, one has at the same time to use a $\tilde{\Omega}$-mapping to derive the phase-space function for $\hat{B}$ (apart from a factor $(2\pi\hbar)$ in eq. (4)).

For example, if we consider the simplest case where

$$\Omega(u, v) = \tilde{\Omega}(u, v) = 1 , \tag{7}$$

then eqs. (1) and (2) lead to the famous Wigner distribution function P_w, say:

$$P_w(q, p) = \frac{1}{2\pi\hbar} \int \left\langle p - \frac{u}{2} \left| \hat{\rho} \right| p + \frac{u}{2} \right\rangle \exp\left(-\frac{iuq}{\hbar}\right) du . \tag{8}$$

Because of eq. (7), eq. (4) reduces to eq. (8) (without the factor $(2\pi\hbar)^{-1}$), with $\hat{B}$, b_w replaced by $\hat{\rho}$, P_w, respectively. In other words, the distribution function and the phase-space function for any arbitrary $\hat{B}$ are obtained through the same operator-phase-space-mapping, in this and only in this special case. Only the Wigner representation has the following property for arbitrary functions $F_1(x)$ and $F_2(x)$:

$$\text{If} \quad \hat{B} = F_1(\hat{q}) + F_2(\hat{p}), \text{ then } b_w(q, p) = F_1(q) + F_2(p) . \tag{9}$$

Another phase-space distribution function that we are concerned with here is the anti-normal-ordered distribution function[4]), P_a, say, which is obtained by choosing

$$\Omega(u, v) = \exp\left[-\frac{1}{4\hbar} \left(\frac{u^2}{\delta} + \delta v^2 \right) \right] , \tag{10}$$

where $\delta > 0$ is a parameter, $P_a(q, p)$ can also be obtained by convoluting $P_w(q, p)$ with a phase-space Gaussian:

$$P_a(q, p) = \frac{1}{\pi\hbar} \int \int P_w(q', p') \exp[-\delta(q - q')^2/\hbar - (p - p')^2/\delta\hbar] dp' dq' . \tag{11}$$

Hence P_a is also called the smoothed Wigner distribution function (SWDF). It is not difficult to show (see eqs. (1) and (2)) that the relation between two

different phase-space distribution functions is the following[8]):

$$P^{(\Omega_2)}(q, p) = \frac{\Omega_2(i\hbar \, \partial/\partial q, \, i\hbar \, \partial/\partial p)}{\Omega_1(i\hbar \, \partial/\partial q, \, i\hbar \, \partial/\partial p)} \, P^{(\Omega_1)}(q, p) \, . \tag{12}$$

Hence the relation between the Wigner and the SWDF (anti-normal-ordered distribution function) is given by [8,9])

$$P_a(q, p) = \exp\left[\frac{\hbar}{4} \left(\frac{1}{\delta} \frac{\partial^2}{\partial q^2} + \delta \frac{\partial^2}{\partial p^2} \right) \right] P_w(q, p) \, . \tag{13}$$

Also, if one wishes to use the anti-normal-ordered distribution function, one has to use the phase-space function corresponding to normal-ordering for any other operator $\hat{B}$:

$$b_a(q, p) = \exp\left[-\frac{\hbar}{4} \left(\frac{1}{\delta} \frac{\partial^2}{\partial q^2} + \delta \frac{\partial^2}{\partial p^2} \right) \right] b_w(q, p) \, , \tag{14}$$

in order to calculate $\langle \hat{B} \rangle$ through

$$\langle \hat{B} \rangle = \mathrm{Tr}(\hat{\rho} \, \hat{B}) = \int \int P_a(q, p) \, b_a(q, p) \, \mathrm{d}q \, \mathrm{d}p \, . \tag{15}$$

Now we are ready to do an explicit calculation using the SWDF. Let

$$I[B(\hat{q}, \hat{p})] = \int \int B(q, p) P_a(q, p) \, \mathrm{d}q \, \mathrm{d}p \, . \tag{16}$$

We wish to emphasize here that $I[B(\hat{q}, \hat{p})]$ is, in general, not the expectation value of the operator $B(\hat{q}, \hat{p})$. From eq. (14) we conclude that $B(q, p)$ is not equal to $b_a(q, p)$ unless $B(\hat{q}, \hat{p})$ is linear in both $\hat{q}$ and $\hat{p}$; in other words

$$\langle B(\hat{q}, \hat{p}) \rangle \neq I[B(\hat{q}, \hat{p})] \, , \text{ unless } B(\hat{q}, \hat{p}) = C_1\hat{q} + C_2\hat{p} \, . \tag{17}$$

The discrepancy between the phase formulation and the conventional quantum mechanics found in ref. 11 is a result of the neglect of this subtle point. We shall demonstrate below how to obtain the correct answer via SWDF, for the average energy of the system, say.

Suppose the Hamiltonian is $\hat{H} = \hat{p}/2m + V(\hat{q})$, which is of the same form as eq. (9). Hence the Wigner function for this Hamiltonian is simply

$$H_w(q, p) = q^2/2m + V(q) \, . \tag{18}$$

Substituting eq. (18) into eq. (14) we obtain the corresponding phase-space function when the SWDF is to be used:

$$H_a(q, p) = \left(\frac{p^2}{2m} - \frac{\hbar\delta}{4m}\right) + \sum_{n=0}^{\infty} \left(-\frac{\hbar}{4\delta}\right)^n \frac{1}{n!} V^{(2n)}(q), \tag{19}$$

where $V^{(2n)}(q) = \partial^{2n}V(q)/\partial q^{2n}$. The expectation value of the Hamiltonian can be calculated by using eq. (15). The average potential energy is

$$\langle V(\hat{q})\rangle = \int\int dq\, dp \left[\sum_{n=0}^{\infty} \left(-\frac{\hbar}{4\delta}\right)^n \frac{1}{n!} V^{(2n)}(q)\right] P_a(q, p). \tag{20}$$

Using the relation proved in appendix B:

$$\int\int dq\, dp\, V(q)P_a(q, p) = \sum_{k=0}^{\infty} \left(\frac{\hbar}{4\delta}\right)^k \frac{1}{k!} \langle V^{(2k)}(\hat{q})\rangle_{QM}, \tag{21}$$

where

$$\langle F(\hat{q}, \hat{p})\rangle_{QM} = \langle \psi | F(\hat{q}, \hat{p}) | \psi \rangle_{QM} \tag{22}$$

is the expectation value calculated from conventional quantum mechanics, we obtain

$$\langle V(\hat{q})\rangle = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} (-1)^n \left(\frac{\hbar}{\delta}\right)^{n+k} \frac{1}{n!k!} \langle V^{(2n+2k)}(\hat{q})\rangle_{QM}. \tag{23}$$

If we change summation indices from (n, k) to $(l = n + k, k)$, we get

$$\langle V(\hat{q})\rangle = \sum_{l=0}^{\infty} \left[\sum_{k=0}^{l} (-1)^n \frac{1}{(l-k)!k!}\right]\left(\frac{\hbar}{4\delta}\right)^l \langle V^{(2l)}(\hat{q})\rangle_{QM}. \tag{24}$$

We notice that the quantity in the square-bracket is in fact $(1-1)^l/l!$, which vanishes unless $l = 0$. Hence

$$\langle V(\hat{q})\rangle = \langle V(\hat{q})\rangle_{QM}, \tag{25}$$

in complete agreement with conventional quantum mechanics. Similarly one has

$$\int\int dq\, dp\, p^2 P_a(q, p) = \langle \hat{p}^2\rangle_{QM} + \frac{\hbar\delta}{2}. \tag{26}$$

Thus the average kinetic energy is

$$\int \int \mathrm{d}q \, \mathrm{d}p \left(\frac{p^2}{2m} - \frac{\hbar \delta}{4m} \right) P_{\mathrm{a}}(q, p) = \langle \hat{p}^2 \rangle_{\mathrm{QM}} , \tag{27}$$

again in accord with conventional results.

3. Conclusion

As we have seen, the phase-space method gives the same results as conventional quantum mechanics. This is not surprising, since the phase-space method is just another formulation, historically the fourth, of quantum mechanics.

We shall not discuss the "discrepancy" in the case of hydrogen here. In fact, an exact solution for the hydrogen problem via phase-space method has been recently reported[12]).

In conclusion, we note that although the Wigner distribution function for an harmonic oscillator system has been known[13,14]) for a long time, there have been few attempts to evaluate the corresponding SWDF. A result for pure state is given in ref. 11, but it is in a form of series involving four summations, which is, of course, rather awkward. Since the harmonic oscillator is one of the few exact-soluble systems known, we feel that it is of interest to obtain a better result for its SWDF. After considerable algebra, we were able to derive closed formulae for both pure state and canonical ensemble at temperature T (see appendix A).

Appendix A

SWDF for pure state of a harmonic oscillator and an canonical ensemble of harmonic oscillators at temperature T

The Wigner distribution function given by eq. (8) can be rewritten as

follows:

$$P_w(q, p) = \frac{1}{2\pi} \int e^{-i\tau p} \psi^*(q - \tfrac{1}{2}\tau\hbar)\psi(q + \tfrac{1}{2}\tau\hbar) \, d\tau \,, \tag{A.1}$$

where $\psi(q)$ is the wavefunction of the system considered.

Cartwright[15]) introduced a more general form for the SWDF:

$$P_a^{\alpha\beta}(q, p) = \int \int dq' \, dp' \, P_w(q, p) G^{\alpha\beta}(q - q', p - p') \,, \tag{A.2}$$

with a two parameter phase-space Gaussian

$$G^{\alpha\beta}(q, p) = \frac{(\alpha\beta)_{1/2}}{\pi\hbar} \exp\left[-\frac{1}{\hbar}(\alpha q^2 + \beta p^2) \right]. \tag{A.3}$$

After some manipulation Cartwright[15]) proved an interesting formula for the SWDF:

$$P_a^{\alpha\beta}(q, p) = \frac{(\pi\hbar\alpha)^{1/2}}{2\pi^2\hbar^2} \exp\left(-\frac{\alpha q^2}{\hbar}\right) \sum_{n=0}^{\infty} \frac{\gamma^n}{n!} \left| \int fx^n \, dx \right|^2. \tag{A.4}$$

Here

$$\gamma = \frac{1}{2\hbar}\left(\frac{1}{\beta} - \alpha\right) \tag{A.5}$$

and

$$f(x, q, p) = \psi^*(x) \exp\left[-\left(\alpha + \frac{1}{\beta}\right)\frac{x^2}{4\hbar} + (\alpha q + ip)\frac{x}{\hbar} \right]. \tag{A.6}$$

In our case, $\alpha = \delta = 1/\beta$, $\gamma = 0$, eqs. (A.4) and (A.5) reduce to their simplest form:

$$P_a(q, p) = \frac{(\pi\hbar\delta)^{1/2}}{2\pi^2\hbar^2} \exp\left(-\frac{\delta q^2}{\hbar}\right) \left| \int f \, dx \right|^2 \tag{A.7}$$

and

$$f(x, q, p) = \psi^*(x) \exp\left[-\frac{\delta x^2}{2\hbar} + (\delta q + ip)\frac{x}{\hbar} \right]. \tag{A.8}$$

Now we consider the explicit form of the wavefunction for the nth level of a harmonic oscillator:

$$\psi_n(x) = N_n \, e^{-\lambda^2 x^2/2} H_n(\lambda x) \,, \tag{A.9}$$

where H_n is the nth Hermite polynomial and

$$\lambda = \left(\frac{M\omega}{\hbar}\right)^{1/2}, \quad N_n = \left(\frac{\lambda^2}{\pi}\right)^{1/4}\left(\frac{1}{2^n n!}\right)^{1/2}. \tag{A.10}$$

In order to carry out the integration in eq. (A.7), we use the generating function for the Hermite polynomial

$$G(Z, t) = e^{-t^2 + 2tZ} = \sum_{n=0}^{\infty} \frac{H_n(Z)}{n!} t^n \tag{A.11}$$

to rewrite the integral as follows:

$$\int f \, dx = N_n \int dx \, H_n(\lambda x) \exp\left[-\left(\frac{\delta}{2\hbar} + \frac{\lambda^2}{2}\right)x^2 + (\delta q - ip)\frac{x}{\hbar}\right]$$

$$= N_n \frac{\partial^n}{\partial t^n}\bigg|_{t=0} \int G(\lambda x, \pi) \exp\left[\left(\frac{\delta}{\hbar} + \frac{\lambda^2}{2}\right)x^2 + (\delta q + ip)\frac{x}{\hbar}\right] dx$$

$$= N_n \frac{\partial^n}{\partial t^n}\bigg|_{t=0} \left(\frac{\pi}{D}\right)^{1/2} \exp\left[-\left(1 - \frac{\lambda^2}{D}\right)t^2 + \frac{\lambda a}{D} t + \frac{a^2}{4D}\right], \tag{A.12}$$

where $D = \delta/2\hbar + \lambda^2/2$ and $a = (\delta q + ip)/\hbar$.

Introducing a new variable by $t' = St$ and $S = (1 - \lambda^2/d)^{1/2} = ((\delta - \hbar\lambda^2)/(\delta + \hbar\lambda^2))^{1/2}$, we can cast eq. (A.12) into another Hermite polynomial:

$$\int f \, dx = N_n\left(\frac{\pi}{D}\right)^{1/2} S^n \exp\left(\frac{a^2}{4D}\right) \frac{\partial^n}{\partial t'^n}\bigg|_{t'=0} \exp\left[-t'^2 + \frac{\lambda a}{DS} t'\right]$$

$$= N_n\left(\frac{\pi}{D}\right)^{1/2} S^n \exp\left(\frac{a^2}{4D}\right) H_n\left(\frac{\lambda a}{2DS}\right). \tag{A.13}$$

Combination of eqs. (A.7) and (A.13) gives the SWDF for the nth eigenstate of a harmonic oscillator:

$$P_a(q, p; n) = \frac{\lambda}{2^n n! \pi} \left(\frac{\delta}{\hbar}\right)^{1/2} \frac{|\delta - \hbar\lambda^2|^n}{(\delta + \hbar\lambda^2)^{n+1}}$$

$$\times \exp(-a_1 q^2 - a_2 p^2) H_n(b_1 q + ib_2 p) H_n(b_1 q - ib_2 p), \tag{A.14}$$

where

$$a_1 = \frac{\lambda^2}{1 + \hbar\lambda^2/\delta} , \qquad a_2 = \frac{1}{\hbar\delta(1 + \hbar\lambda^2/\delta)} ,$$

$$b_1 = \frac{\lambda}{(1 - \hbar^2\lambda^4/\delta^2)^{1/2}} , \qquad b_2 = \frac{\lambda}{\delta(1 - \hbar^2\lambda^4/\delta^2)^{1/2}} . \tag{A.15}$$

Next we turn to a consideration of a canonical ensemble of harmonic oscillators at temperature T. The corresponding Wigner distribution function is[14]):

$$P_{\mathrm{w}}(q, p) = \frac{1}{\pi\hbar} \tanh\left(\frac{\hbar\omega\beta}{2}\right) \exp\left[-\frac{2}{\hbar\omega} \tanh\left(\frac{\hbar\omega\beta}{2}\right) H(q, p)\right] . \tag{A.16}$$

The SWDF can be easily obtained by combining eqs. (A.16) and (11). The result is

$$P_{\mathrm{a}}(q, p) = \frac{1}{\pi\hbar(g_1 g_2)^{1/2}} \tanh\left(\frac{\hbar\omega\beta}{2}\right)$$

$$\times \exp\left[-\tanh\left(\frac{\hbar\omega\beta}{2}\right)\left(\frac{m\omega\delta}{g_1\hbar} q^2 - \frac{1}{g_2\hbar\delta m\omega} p^2\right)\right] , \tag{A.17}$$

where

$$g_1 = m\omega \tanh\left(\frac{\hbar\omega\beta}{2}\right) + \delta , \tag{A.18}$$

and

$$g_2 = \frac{1}{m\omega} \tanh\left(\frac{\hbar\omega\beta}{2}\right) + \frac{1}{\delta} . \tag{A.19}$$

Appendix B

Proof of eq. (21)

Substituting eqs. (A.1) and (11) into eq. (16) with $B(\hat{q}, \hat{p}) = V(\hat{q})$, where $V(\hat{q})$ is an arbitrary potential, and performing the p'-, p- and τ-integrations, we get

$$I[V(\hat{q})] = \left(\frac{\delta}{\pi\hbar}\right)^{1/2} \int \mathrm{d}q' \, \psi(q')\psi^*(q') \int \mathrm{d}q \, V(q) \, \mathrm{e}^{-\delta(q-q')^2/\hbar} . \tag{B.1}$$

The q-integration can be carried out by a Taylor expansion of the potential

around q':

$$V(q) = \sum_{n=0}^{\infty} \frac{V^{(n)}(q')}{n!} (q - q')^{n} . \tag{B.2}$$

Only the terms with even n contribute, so that eq. (B.1) can be rewritten as following:

$$I[V(\hat{q})] = \sum_{k=0}^{\infty} \left(\frac{\hbar}{2\delta} \right)^{k} \frac{(2k-1)!!}{(2k)!} \langle V^{(2k)}(\hat{q}) \rangle_{\text{OM}} , \tag{B.3}$$

where we define $(-1)!! = 1$. Hence we have proved eq. (21) by observing that $(2k - 1)!!/(2k)! = 1/2^{n}k!$.

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