Relationship between the Wigner function and the probability density function in quantum phase space representation

Qian Shu Li,[1] Gong Min Wei,[1,2] and Li Qiang Lü[1]
[1]School of Science, Beijing Institute of Technology, Beijing 100081, People's Republic of China
[2]Department of Physics, Capital Normal University, Beijing 100037, People's Republic of China
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This paper discusses the relationship between the Wigner function, along with other related quasiprobability distribution functions, and the probability density distribution function constructed from the wave function of the Schrödinger equation in quantum phase space, as formulated by Torres-Vega and Frederick (TF). At the same time, a general approach in solving the wave function of the Schrödinger equation of TF quantum phase space theory is proposed. The relationship of the wave functions between the TF quantum phase space representation and the coordinate or momentum representation is thus revealed.

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I. INTRODUCTION

Currently the Wigner quasiprobability distribution function [1] enjoys a renaissance in many branches of physics, ranging from quantum optics [2–4], nuclear [5] and solid-state physics to quantum chaos [6,7]. It is anticipated that its application in various related branches of science will become more and more extensive. This renewed interest has triggered a search for a reconstruction of the Wigner function about a completely unknown state [8–12].

As is well known, the Wigner quasiprobability distribution function, which is similar in form to the probability density distribution function in classical Liouville dynamics, is directly constructed using the wave function in the coordinate or momentum representation to the Wigner function, whereby some necessary physical and mathematical conditions are added. The quasiprobability distribution function becomes a principal research line in quantum phase space representation, since the Wigner distribution function was first introduced to deal with the quantum corrections to classical statistical mechanics in 1932. But, one of the drawbacks in the physical interpretation of the Wigner function is that it is not everywhere non-negative. Strictly speaking, the Wigner function is not a *bona fide* probability density in phase space. Certainly, it is not everywhere non-negative for the Wigner function that reflected its quantum behavior and satisfied marginal conditions. Along this line, latter-most works [13–28] on quantum phase space focus on proposing various quantum phase space distribution functions. For example, the Husimi function [14], the purpose of which is to "coarse grain" phase space over cells of volume $\hbar^N$ (N being the number of degrees of freedom), is everywhere non-negative, but it cannot satisfy the marginal conditions. In 1966, Cohen designed a method for forming quasiprobability distributions [15,16]. Now it has been proven that it is impossible to have a quantum phase space distribution being both everywhere non-negative and having the marginal conditions of quantum mechanics satisfied simultaneously [17,18].

Another line of developing quantum phase space theory that is allied to quantum mechanics is to renew directly the definitions of canonical momentum and coordinate operators in the phase space and postulate the existence of the Schrödinger equation and quantum Liouville equation, and then to solve the Schrödinger equation in quantum phase space concretely. For example, Torres-Vega and Frederick's work [29,30] followed such a course. It has been proven by Ban that Torres-Vega and Frederick's quantum phase space theory is equivalent to Harriman's and Ban's theories [31,32]. Torres-Vega and Frederick's theory is similar to the usual quantum mechanics in its coordinate or momentum representation and has the same physical framework. Characteristics of the TF phase space representation include: (1) State vectors of TF quantum phase space retain those mathematical properties of quantum mechanics in coordinate or momentum representation. So, many usual methods and results in coordinate and momentum representation in TF quantum phase space theory can be used. (2) Correspondence between the classical and quantum mechanics may be carried out through the relationship between the classical and quantum Liouville equation. (3) Some results of the TF theory allow easy semiclassical approximation. (4) Phase space contribution function constructed by the square magnitude of this wave function is a *bona fide* probability density distribution function that is everywhere non-negative. But, this probability density is nonunique and does not satisfy marginal conditions. An obvious drawback of Torres-Vega and Frederick's theory is the fact that the number of variables involved in the postulated Schrödinger equation is doubled when compared to cases in coordinate or momentum representation, which causes difficulties in solving the Schrödinger equation in phase space representation. Together with the development of quantum phase space theory, plus the two different lines, the question naturally arises: what kind of relationship exists between them? Deeper understanding of this relationship will benefit in the application of Wigner function and stimulate the application of the TF phase space theory in branches of physics and related subjects. In order to establish this relationship, it is necessary to find a general solution of the Schrödinger equation in phase space representation.

In Sec. II a general approach to solving the Schrödinger equation in quantum phase space by the Torres-Vega and

Frederick's formulation is proposed, and the relationship between the wave functions in quantum phase space representation and in coordinate or momentum representation is explained. In Sec. III the relationship between the probability density distribution function constructed from the solutions and the Wigner function, and with other related quasiprobability distribution functions, is discussed. A brief summary will be given in Sec. IV.

II. GENERAL SOLUTIONS OF THE SCHRÖDINGER EQUATION IN PHASE SPACE REPRESENTATION

The key point in the Torres-Vega and Frederick's phase space theory [25,26] is the assumption of existence of a Hermitian operator $\hat{\Gamma}$, with the eigenequation $\hat{\Gamma}|\Gamma\rangle = \Gamma|\Gamma\rangle$, where the eigenvalues Γ are not physically observable but might take on any real number, and the eigenvectors $|\Gamma\rangle = |p,q\rangle$ form a complete orthonormal set. In the $|\Gamma\rangle$ eigenvector phase space representation, the canonical momentum and coordinate operators are defined as

$$\hat{P} = \frac{p}{2} - i\hbar\frac{\partial}{\partial q}, \qquad \hat{Q} = \frac{q}{2} + i\hbar\frac{\partial}{\partial p}. \tag{1}$$

The corresponding stationary Schrödinger equation of a system with an arbitrary potential $V(q)$ is postulated to take the following form:

$$\left\{\frac{1}{2\mu}\left(\frac{p}{2} - i\hbar\frac{\partial}{\partial q}\right)^2 + V\left(\frac{q}{2} + i\hbar\frac{\partial}{\partial p}\right)\right\}\psi(\Gamma) = E\psi(\Gamma), \tag{2}$$

where p and q are the classical momentum and coordinate with real values, E is an eigenenergy, and $\psi(\Gamma)$ is the eigenfunction corresponding to the eigenenergy E with

$$\psi(\Gamma) = \langle\Gamma|\psi\rangle. \tag{3}$$

Now, we proceed to solve the Schrödinger Eq. (2). By means of the following relations:

$$e^{ipq/2\hbar}\left(i\hbar\frac{\partial}{\partial p}\right)^n e^{-ipq/2\hbar} = \left(\frac{q}{2} + i\hbar\frac{\partial}{\partial p}\right)^n$$
$$e^{-ipq/2\hbar}\left(-i\hbar\frac{\partial}{\partial q}\right)^n e^{ipq/2\hbar} = \left(\frac{p}{2} - i\hbar\frac{\partial}{\partial q}\right)^n, \tag{4}$$

and by letting $\psi(\Gamma) = e^{-ipq/2\hbar}\phi(p,q)$, Eq. (2) can be transformed into the following form:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2} + V\left(q + i\hbar\frac{\partial}{\partial p}\right)\right\}\phi(p,q) = E\phi(p,q). \tag{5}$$

Further, assume that $V[q + i\hbar(\partial/\partial p)]$ can be expanded as a Taylor's series about $i\hbar(\partial/\partial p)$ for given q, resulting in

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2} + \sum_n V^n(q)\left(i\hbar\frac{\partial}{\partial p}\right)^n\right\}\phi(p,q) = E\phi(p,q), \tag{6}$$

and will have the following property that $\{-(\hbar^2/2\mu)(\partial^2/\partial q^2) + \Sigma_n V^n(q)[i\hbar(\partial/\partial p)]^n\}$ and $i\hbar(\partial/\partial p)$ are commutable. Then, it is possible to expand $\phi(p,q)$ in terms of the eigenfunction $e^{-(i/\hbar)\lambda p}$ of the operator $i\hbar(\partial/\partial p)$ as follows:

$$\phi(p,q) = \int \chi(q,\lambda)e^{-(i/\hbar)\lambda p}d\lambda, \tag{7}$$

where λ is the eigenvalue of the operator $i\hbar(\partial/\partial p)$ corresponding to the eigenfunction $e^{-(i/\hbar)\lambda p}$. Substituting Eq. (7) into Eq. (6), and multiplying both sides of the equation by $e^{(i/\hbar)\lambda' p}$, then integrating both sides of the equation over p, the following equation is obtained:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2} + V(\lambda + q)\right\}\chi(\lambda,q) = E\chi(\lambda,q). \tag{8}$$

In fact, Eq. (8) will become the standard Schrödinger equation in coordinate representation after making a variable replacement, $\xi = \lambda + q$.

Assume that a special solution for Eq. (8) exists with the following form:

$$\chi(q,\lambda) = g(\lambda)\varphi(q + \lambda), \tag{9}$$

in which $g(\lambda)$ is chosen as an arbitrary nonzero function, and $\varphi(q+\lambda)$ is the eigenfunction of the Schrödinger equation in coordinate representation corresponding to the eigenvalue E. Substituting Eq. (9) into Eq. (7), Eq. (7) becomes

$$\phi(p,q) = \int g(\lambda)\varphi(q + \lambda)e^{-(i/\hbar)\lambda p}d\lambda. \tag{10}$$

Finally, the general solution of the Schrödinger equation (2) can be obtained,

$$\psi(\Gamma) = e^{-ipq/2\hbar}\int g(\lambda)\varphi(q + \lambda)e^{(-i/\hbar)\lambda p}d\lambda. \tag{11}$$

It is obvious that once the Schrödinger Eq. (8) in coordinate representation is solved, solution of the corresponding Schrödinger Eq. (2) in phase space representation can be obtained via Eq. (11). To some extent, efforts in an attempt to solve the Schrödinger equation directly in phase space are reduced. Similar procedures can be applied to the discussion from momentum representation to phase space representation.

As is well known, Fourier transform of wave functions between coordinate and momentum representation is unique, while the transform of wave functions from phase space representation to coordinate or momentum representation is a simple Fourier project transform [26], but not unique. We substitute the solution (11) into the Fourier project transform formula and obtain

$$\langle q|\psi\rangle = A\int_{-\infty}^{\infty} dp\langle\Gamma|\psi\rangle\exp\left(\frac{ipq}{2\hbar}\right)$$
$$= A\int_{-\infty}^{\infty} dp\left[\int_{-\infty}^{\infty} g(\lambda)\varphi(q+\lambda)e^{-i\lambda p/\hbar}d\lambda \times\exp\left(-\frac{ipq}{2\hbar}\right)\exp\left(-\frac{ipq}{2\hbar}\right)\right] = A\varphi(q), \quad (12)$$

and

$$\langle p|\psi\rangle = B\int_{-\infty}^{\infty} dq\langle\Gamma|\psi\rangle\exp\left(-\frac{ipq}{2\hbar}\right) = BC(p). \quad (13)$$

As an example, we turn to the harmonic oscillator system. We could make use of the solution in coordinate representation

$$\varphi_n(q) = N_n e^{-(\mu\omega/2\hbar)q^2}H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}q\right), \quad (14)$$

and obtain the following solution in T-F phase space representation from Eq. (11):

$$\psi(\Gamma) = e^{-ipq/2\hbar}\int g(\lambda)N_n e^{-(\mu\omega/2\hbar)(q+\lambda)^2} \times H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}(q+\lambda)\right)e^{-(i/\hbar)\lambda p}d\lambda. \quad (15)$$

If the arbitrary nonzero function $g(\lambda)$ is chosen as

$$g(\lambda) = \sqrt{\frac{\mu\omega}{2\pi\hbar}}e^{-(\mu\omega/2\hbar)\lambda^2}, \quad (16)$$

and using

$$H_n(\lambda) = (-1)^n e^{\lambda^2}\frac{d^n}{d\lambda^n}e^{-\lambda^2}, \quad (17)$$

we have

$$\psi(\Gamma) = \frac{1}{\sqrt{2\pi\hbar n!}}\left(\sqrt{\frac{\mu\omega}{2\hbar}}q - i\frac{p}{\sqrt{2\hbar\mu\omega}}\right)^n \times\exp\left\{-\frac{1}{2\hbar\omega}\left(\frac{p^2}{2\mu}+\frac{1}{2}\mu\omega^2q^2\right)\right\}. \quad (18)$$

The set of solutions, Eq. (18), is exactly the solutions obtained by making use of the ladder operators [26] of T-F.

III. QUANTUM PHASE SPACE QUASIPROBABILITY DISTRIBUTION FUNCTIONS

To make sense, the wave function $\psi(\Gamma)$ in phase space representation is required to satisfy the normalization condition, i.e.,

$$\int \psi(\Gamma)\psi(\Gamma)^* d\Gamma = \int |\psi(\Gamma)|^2 d\Gamma = 1, \quad (19)$$

and hence $P(\Gamma)=|\psi(\Gamma)|^2$ can be viewed as a probability density function in $|\Gamma\rangle$ representation quantum phase space. It is important to point out that $d\Gamma$ is not the usual volume element $dp\,dq$ defined in the classical phase space, while all the quasiprobability distribution functions $f^Q(p,q)$ such as the Wigner function and Husimi function are normalized in classical phase space, i.e.,

$$\int f^Q(p,q)dp\,dq = 1. \quad (20)$$

Then, the relationship between $d\Gamma$ and $dp\,dq$ can be defined

$$d\Gamma = |J|dp\,dq, \quad (21)$$

where $|J|$ is the Jacobi's transformation determinant which can be determined through the following procedures. Using results from the Torres-Vega and Frederick's theory [26]

$$\langle\Gamma|q'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\{-ip[q'-(q/2)]/\hbar\}, \quad (22)$$

and normalization condition

$$\delta(q'-q'') = \langle q'|q''\rangle = \int \langle q'|\Gamma\rangle\langle\Gamma|q''\rangle d\Gamma = \int \langle q'|\Gamma\rangle\langle\Gamma|q''\rangle|J|dp\,dq, \quad (23)$$

$|J|$ could be chosen as a delta function, $\delta(q'-q)$. Certainly, this is only a simple selection and implies that the variables p and q are still under the control of the uncertainty principle.

From Eq. (19), we can get

$$\int\int\int \langle\psi|q'\rangle\langle q'|\Gamma\rangle\langle\Gamma|q''\rangle\langle q''|\psi''\rangle d\Gamma dq' dq'' = 1, \quad (24)$$

and use the relations [26]

$$\langle q'|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dp\,\langle\Gamma|\psi\rangle|_{q=q'}e^{ipq'/2\hbar}, \quad (25)$$

$$\langle\psi|q'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dp\,\langle\psi|\Gamma\rangle|_{q=q'}e^{-ipq'/2\hbar}, \quad (26)$$

and from Eq. (24)

$$\int |\psi(\Gamma)|^2 d\Gamma = \frac{1}{2\pi\hbar}\int\int\left(\int \langle\psi|\Gamma\rangle|_{q=q'}\,\langle\Gamma|\psi\rangle|_{p=p'}^{q=q'}dp\right)dp'\,dq' = 1. \quad (27)$$

Comparing Eq. (27) with Eq. (20), we can introduce the quasiprobability distribution functions in the classical phase space

$$f^Q(p',q') = \frac{1}{2\pi\hbar}\int (\langle\psi|\Gamma\rangle|_{q=q'}\langle\Gamma|\psi\rangle|_{\substack{q=q'\\p=p'}})dp. \quad (28)$$

By means of Eq. (11), we can obtain

$$f^Q(p,q) = \frac{1}{2\pi\hbar}\int \phi^*(p,q)\phi(p',q)dp'. \quad (29)$$

Furthermore, letting $g(\lambda)=1$ in Eq. (11), a more detailed expression of Eq. (29) can be given as

$$f^Q(p,q) = \frac{1}{2\pi\hbar}\int\int\int \varphi^*(q+\lambda')\varphi(q+\lambda)e^{-[i(\lambda p-\lambda' p')]/\hbar}dp'\,d\lambda'\,d\lambda. \quad (30)$$

Choosing $q'=q-\lambda/2$ and integrating over the variables p' and λ' in Eq. (30), the famous Wigner quasiprobability density distribution function will be given as

$$f^W(p,q) = \frac{1}{2\pi\hbar}\int \varphi^*\left(q-\frac{\lambda}{2}\right)\varphi\left(q+\frac{\lambda}{2}\right)e^{-i\lambda p/\hbar}d\lambda. \quad (31)$$

Integrating the variables p' and λ' directly in Eq. (30) will give rise to the standard ordering distribution function

$$f^S(p,q) = \frac{1}{2\pi\hbar}\int \varphi^*(q)\varphi(q+\lambda)e^{-i\lambda p/\hbar}d\lambda, \quad (32)$$

and the antistandard ordering distribution function

$$f^{AS}(p,q) = [f^S(p,q)]^* = \frac{1}{2\pi\hbar}\int \varphi^*(q-\lambda)\varphi(q)e^{-i\lambda p/\hbar}d\lambda, \quad (33)$$

as were proposed by Kirkwood [13].

It is important to note that the relationship Eq. (21) plays a key role in association with the quasiprobability density distribution functions from the probability density $|\langle\Gamma|\psi\rangle|^2$ on $|\Gamma\rangle$ representation. In fact, the Jacobi's determinant $|J|$ naturally exhibits the uncertainty principle. It might help us in understanding why the quasiprobability density distribution functions [e.g., in Eqs.(31)–(33)] are not everywhere non-negative in classical phase space and hence, strictly speaking, cannot represent a *bona fide* probability in phase space, and on the other hand, why the quantum probability density distribution functions are non-negative everywhere, yet do not satisfy the marginal conditions $|\langle\Gamma|\psi\rangle|^2$ describing only a probability density on $|\Gamma\rangle$ representation.

IV. CONCLUSION

The Wigner function in classical phase space, as defined by Eq. (31) for a pure state, is a quasiprobability distribution function constructed from the wave function in the coordinate or momentum representation, while the $|\langle\Gamma|\psi\rangle|^2$ on $|\Gamma\rangle$ representation is a *bona fide* probability density function constructed directly from the wave function of the Schrödinger equation in T-F phase space representation. From Eq. (27) to Eq. (33), we observe that the probability density function $|\langle\Gamma|\psi\rangle|^2$ on $|\Gamma\rangle$ representation is equivalent to various known quasiprobability distribution functions in physics. Here, the Jacobi's determinant $|J|$-associated $d\Gamma$ with $dp\,dq$ plays a prominent and crucial role in the transformation from $|\langle\Gamma|\psi\rangle|^2$ to various known quasi probability distribution functions revealing characteristics of the Wigner function and $|\langle\Gamma|\psi\rangle|^2$ function. In fact, due to the characteristics of the Jacobi's determinant $|J|$, the Wigner function is not everywhere non-negative in classical phase space and $|\langle\Gamma|\psi\rangle|^2$ cannot satisfy the marginal conditions in classical phase space because its normalization condition holds only for $d\Gamma=|J|dp\,dq$ but not for $dp\,dq$.

At the same time, the general form of the solution (wave function) about the stationary Schrödinger equation in T-F quantum phase space with an arbitrary potential $V(q)$ is obtained, and the relationship between this and the corresponding wave function in the coordinate or momentum representation has also been discussed. In other words, the method of general solution of the Schrödinger equation in T-F phase space representation from the solutions in the coordinate or momentum representation has been proposed, and the structure of the general solution in T-F quantum phase space is revealed. That is to say, the general form of solution in Eq. (11) exists, just as related functions between the arbitrary function $g(q)$ [as shown in Eq. (11)] with a phase factor $e^{-ipq/2\hbar}$ as against a wave function $\varphi(q)$ connected also to a phase factor $e^{-ipq/2\hbar}$ exist. Usually, if the arbitrary function $g(q)$ is taken as a Gaussian-type function, the function $g(q)$ seems to play the role of a localizing wave function $\varphi(q)$ in the coordinate representation. It further reveals the finite local characteristics of the general solution of the Schrödinger equation in the T-F quantum phase space.

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