Correspondence between quantum and classical descriptions for free particles

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We define the condition of the quasiclassical state of free particles, which is useful in the approximate treatment of quantum systems. Then we introduce classical pure ensembles. Their states are represented using distribution functions on phase space. We compare distribution functions of classical pure ensembles and Wigner distribution functions of quasiclassical states for free particles and draw two conclusions: (i) A wave function does not describe an individual particle but a classical pure ensemble. (ii) Given a quasiclassical wave function, we can tell which classical pure ensemble is described by it.

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I. INTRODUCTION

The quantum-classical correspondence has been a subject of numerous studies, but it is still a problem that puzzles us. In most textbooks of quantum mechanics, students are still told that quantum mechanics transits to classical mechanics in the small $\hbar$ limit but there are no wave functions for them to test the conclusion. What is the condition of the classical limit? Evidently, the small $\hbar$ limit is not a suitable condition of the classical limit. We cannot merely define $\hbar \to 0$ to be the classical limit. Only when $\hbar$ is negligibly small compared with the relevant dynamical parameters can we use the small $\hbar$ limit [1]. The small $\hbar$ limit is not well-defined mathematically unless some additional conditions are specified [2]. In addition, many works on the subject mainly concentrate on the study of the equation of motion of a state but do not pay much attention to the initial conditions given by a wave function. For example, the Ehrenfest theorem in operator form is beautiful. When the theorem is applied to a wave function, some problems will arise. The theorem always yields the result that zero equals zero for stationary wave functions and for any even or odd wave functions no matter what classical limit is used.

On the other hand, some physicists use the large quantum-number limit and obtain another conclusion. A wave function does not describe an individual particle but an ensemble and the classical limit of quantum mechanics is not classical mechanics but classical statistical mechanics [1,3–9]. Their conclusion can be tested by many wave functions. It is worth noting that the large quantum-number limit is consistent with the necessary condition of the Bohr correspondence principle. In some works, the system described by a wave function is treated as an ensemble [10,11].

Classical mechanics and quantum mechanics both are well known in physics and their formalisms are beautiful in mathematics. To establish the correspondence between them should be easy, if we find the right way. It is convenient to study the correspondence on phase space. Many references can be used in the area [10–16]. The first step is the usage of the condition of quasiclassical states. The choice of distribution functions and classical limit procedures becomes unimportant under this condition. The second step is the introduction of classical pure ensembles. Their probability distribution functions are the general solutions of the classical Liouville equation. It is convenient to compare them with quasiclassical states of quantum mechanics.

In this paper we focus our attention on the simplest system of free particles. Two results are obtained in the correspondence between classical and quantum descriptions of the simple system. (i) A quasiclassical wave function does not describe an individual particle but a classical pure ensemble. (ii) Giving a quasiclassical wave function, we can tell what a classical pure ensemble is described by it. The condition of quasiclassical states and the choice of distribution functions are given in Sec. II. The introduction of classical pure ensembles is done in Sec. III. Exact and approximate solutions of correspondence relations will be given in Secs. IV and V. Some concluding remarks of the paper are summarized in Sec. VI.

II. QUASICLASSICAL STATES AND DISTRIBUTION FUNCTIONS

It is well known that the transition from quantum mechanics to classical mechanics is somewhat similar to the transition from wave optics to geometrical optics. The condition in which quantum mechanics transits to classical mechanics is the limit of zero deBroglie wavelength. We define a critical momentum value $p_c = 2\pi\hbar/a_0$ for convenience of the study, where a_0 is the Bohr radius. We think that wave properties of a free particle with a smaller deBroglie wavelength than a_0 cannot be observed in classical mechanics. Generally, if a state $|\psi\rangle$ satisfies $\langle\psi|\hat{p}^2|\psi\rangle \geqslant p_c^2$, we call it a quasiclassical state.

The Wigner distribution function corresponding to state function $\psi(x,t)$ is

$$\rho_w(x,p,t) = \frac{1}{\hbar\pi}\int dy \exp\left[-\frac{i}{\hbar}2py\right]\psi^*(x-y,t)\psi(x+y,t). \quad (1)$$

The equation of motion of the Wigner distribution function is [12]

$$\frac{\partial\rho_w}{\partial t} + \frac{p}{m}\frac{\partial\rho_w}{\partial x} - \frac{dV(x)}{dx}\frac{\partial\rho_w}{\partial p} = -\frac{1}{3!}\left(\frac{\hbar}{2}\right)^2\frac{d^3V(x)}{dx^3}\frac{\partial^3\rho_w}{\partial p^3} + \cdots. \quad (2)$$

The equation becomes the classical Liouville equation for free particles. Therefore, the Wigner distribution function will be used as a standard one in this study.

Generally, different rules of associating a function of noncommuting operators with the corresponding function of scalar variables yield different distribution functions. For example, the Wigner distribution function can be derived from the Weyl rule of operator ordering [10,15]

$$\exp[i\mu x + i\lambda p] \leftrightarrow \exp[i\mu\hat{x} + i\lambda\hat{p}].$$

Another simple symmetric rule of operator ordering is the Rivier rule [14,15]

$$\exp[i\mu x + i\lambda p] \leftrightarrow \frac{1}{2}\{\exp[i\mu\hat{x}]\exp[i\lambda\hat{p}] + \exp[i\lambda\hat{p}]\exp[i\mu\hat{x}]\}.$$

The distribution function associated to the rule is

$$\rho_R(x,p,t) = \frac{1}{2\sqrt{2\hbar\pi}}[\psi^*(x,t)e^{ipx/\hbar}\phi(p,t) + \text{c.c.}], \tag{3}$$

where $\phi(p,t) = \langle p|\psi(t)\rangle$.

The difference between the two distribution functions exists for the expectation value of the type $\langle (xp)^{2N}\rangle$, where N is an arbitrary positive integer [15]. Consider the difference

$$\begin{aligned}\int dx \int dp x^2p^2\rho_R &= \int dx \int dp x^2 p^2 \rho_w + \int dx \int dp x^2p^2(\rho_R - \rho_w) \\ &= \langle x^2p^2\rangle_w + \hbar^2.\end{aligned} \tag{4}$$

$\hbar^2$ can be neglected compared with $\langle x^2p^2\rangle_w$ for a quasiclassical state. Generally, in the calculation of the expectation value $\langle\psi|\hat{f}|\psi\rangle$ of the physical quantity $f(x,p)$, the difference caused by operator ordering can be neglected in the quasiclassical condition. In other words, the expectation value $\langle\psi|\hat{f}|\psi\rangle$ can be approximately calculated by use of the Wigner distribution function no matter how operators are ordered under the quasiclassical condition.

III. CLASSICAL PURE ENSEMBLES

At the beginning we generally introduce the classical pure ensemble and then reduce it to the system of free particles. Suppose that there are many identical classical particles, with no interaction between them. The motion of each particle is described by functions $x = X(x_0,p_0,t)$ and $p = P(x_0,p_0,t)$ which are solutions of Newton's equation in a time-independent potential $V(x)$. Each particle has its own initial values x_0 and p_0. Giving a probability distribution function $g(x_0,p_0)$ of initial values x_0 and p_0, we obtain a classical ensemble. The state of the ensemble can be expressed by the probability distribution function on phase space:

$$\begin{aligned}\rho_c(x,p,t) = \int dx_0 \int dp_0 \delta(x - X(x_0,p_0,t)) \\ \times \delta(p - P(x_0,p_0,t))g(x_0,p_0).\end{aligned} \tag{5}$$

We call the ensemble a classical pure ensemble.

It is easy to see that the distribution function satisfies the classical Liouville equation. The expectation value of physical quantity $f(x,p)$ in the ensemble is

$$\langle f(t)\rangle_c = \int dx \int dp f(x,p)\rho_c(x,p,t). \tag{6}$$

Let $f(x,p)$ be x and p, respectively, Eqs. (5) and (6) yield

$$\langle x(t)\rangle_c = \int dx_0 \int dp_0 X(x_0,p_0,t)g(x_0,p_0), \tag{7}$$

$$\langle p(t)\rangle_c = \int dx_0 \int dp_0 P(x_0,p_0,t)g(x_0,p_0), \tag{8}$$

$$m\frac{d\langle x(t)\rangle_c}{dt} = \langle p(t)\rangle_c, \tag{9}$$

$$\left\langle \frac{dV(x)}{dx}\right\rangle_c = \int dx_0 \int dp_0 g(x_0 p_0) \left.\frac{dV(x)}{dx}\right|_{x=X(x_0,p_0,t)}. \tag{10}$$

Applying Newton's second law to Eqs. (8) and (10) we get

$$\frac{d\langle p(t)\rangle_c}{dt} = -\left\langle \frac{dV(x)}{dx}\right\rangle_c. \tag{11}$$

Equations (9) and (11) constitute the mathematical formulation of the Ehrenfest theorem in the classical pure ensemble.

Now we return to classical pure ensembles of free particles. When the potential $V(x) = 0$, Eq. (5) becomes

$$\begin{aligned}\rho_c(x,p,t) &= \int dx_0 \int dp_0 \delta\left(x - x_0 - \frac{p_0}{m}t\right)\delta(p - p_0)g(x_0,p_0) \\ &= g\left(x - \frac{p}{m}t, p\right).\end{aligned} \tag{12}$$

When the distribution function of initial values is $g(x_0,p_0) = \delta(x_0 - \zeta)\delta(p_0 - \eta)$, the distribution function is reduced to the state representation of an individual free particle on phase space. For the special ensemble we have from Eqs. (6) and (12)

$$\langle p^2\rangle = \langle p\rangle^2 = (\eta)^2. \tag{13}$$

It is the necessary condition satisfied by the distribution function of an individual free particle.

Giving a quasiclassical wave function, our aim is to find a classical pure ensemble that is in dynamics equivalent to the system described by the wave function. Since the Wigner distribution function $\rho_w(x,p,t)$ of free particles satisfies the classical Liouville equation, it is completely determined by its initial distribution function $\rho_w(x,p)$. It is easy to see the expression of the Wigner distribution function

$$\begin{aligned}\rho_w(x,p,t) &= \int dx_0 \int dp_0 \delta\left(x - x_0 - \frac{p_0}{m}t\right)\delta(p - p_0)\rho_w(x_0,p_0) \\ &= \rho_w\left(x - \frac{p}{m}t, p\right).\end{aligned} \tag{14}$$

Equation (14) is the same form as Eq. (12). We are sure that the system described by a quasiclassical pure state $|\psi(t)\rangle$ must be equivalent to a classical pure ensemble represented by Eq. (12).

IV. EXACT SOLUTIONS

When the initial Wigner distribution function of a quasiclassical wave function is non-negative everywhere, we put $g(x_0,p_0)=\rho_w(x_0,p_0)\geqslant 0$ in Eq. (12) to get the exact solution corresponding to Eq. (14). Because $\rho_c(x,p,t)$ and $\rho_w(x,p,t)$ both satisfy the classical Liouville equation, the choice of $g(x_0,p_0)=\rho_w(x_0,p_0)$ in Eq. (12) guarantees that the two distribution functions are the same and are positive definite in all time as shown by Eqs. (12) and (14). In this section we discuss three categories of important states. They are momentum eigenstates, energy eigenstates, and Gaussian wave packet states of free particles.

A. Momentum eigenstates

Consider the wave function

$$\psi_\eta(x,t) = A\exp\left[\frac{i}{\hbar}\eta x - \frac{i}{2m\hbar}\eta^2 t\right], \quad -\frac{L}{2} < x < \frac{L}{2}, \tag{15}$$

where L is very large.

The Wigner distribution function of the state given by Eq. (1) is

$$\rho_w(x,p,t) = |A|^2\delta(p-\eta), \quad -\frac{L}{2} < x < \frac{L}{2}. \tag{16}$$

When $|A|^2=1/L$, the Wigner distribution function is normalized.

Substituting $g(x_0,p_0)=\rho_w(x_0,p_0)$ into Eq. (12) we get

$$\rho_c(x,p,t) = \rho_w(x,p,t),$$

$$\rho_c(x,p,t) = \frac{1}{L}\int_{-L/2}^{+L/2} dx_0 \int_{-\infty}^{+\infty} dp_0\,\delta\left(x - x_0 - \frac{p_0}{m}t\right) \times \delta(p-p_0)\,\delta(p_0-\eta) = \frac{1}{L}\delta(p-\eta),$$

$$-\frac{L}{2} < x < \frac{L}{2}. \tag{17}$$

Equation (17) means that a momentum eigenstate with eigenvalue η describes a classical pure ensemble in which all particles have the same momentum but their positions distribute uniformly. As to the transition from wave optics to geometrical optics, it is worth noting that a plane wave does not describe a light ray but a light beam no matter how short its wavelength in optics.

Let $x_0=\eta t_0/m$ and $L=\eta T/m$, Eq. (17) can be written as

$$\rho_c(x,p,t) = \frac{1}{T}\int_{-T/2}^{+T/2} dt_0 \int_{-\infty}^{+\infty} dp_0\,\delta\left(x - \frac{\eta}{m}t_0 - \frac{p_0}{m}t\right) \times \delta(p-p_0)\,\delta(p_0-\eta) = \frac{m}{\eta T}\delta(p-\eta),$$

$$-\frac{T}{2} < t < \frac{T}{2}. \tag{18}$$

The equation means that a plane wave describes the averaged motion of a free particle over time. It is consistent with the interpretation on the Bohr correspondence principle given by Ref. [17].

The Wigner distribution function of Eq. (16) does not implicitly depend on $\hbar$; the small $\hbar$ limit can hardly be used in the case. In order to neglect differences caused by operator ordering in distribution functions, the quasiclassical condition of large η^2 is still necessary.

B. Energy eigenstate

Consider the wave function which is an energy eigenfunction with $E=\frac{1}{2m}\eta^2$:

$$\psi_E(x,t) = (C_1 e^{i\eta x/\hbar} + C_2 e^{-i\eta x/\hbar})\exp\left[-\frac{i\eta^2 t}{2m\hbar}\right],$$

$$-\frac{L}{2} < x < \frac{L}{2}, \tag{19}$$

where L is very large. The Wigner distribution function of the state is

$$\rho_w(x,p,t) = [|C_1|^2\delta(p-\eta) + |C_2|^2\delta(p+\eta) + (C_1C_2^* e^{i2\eta x/\hbar} + C_1^* C_2 e^{-i2\eta x/\hbar})\,\delta(p)],$$

$$-\frac{L}{2} < x < \frac{L}{2}. \tag{20}$$

When η is large, the third term is a fast oscillating function of x in the equation. It can be neglected in the distribution function. The normalization condition of the distribution function is $|C_1|^2+|C_2|^2=1/L$.

Substitute $g(x_0,p_0)=\rho_w(x_0,p_0)$ into Eq. (12), and let $x_0=\frac{\eta}{m}t_0$ and $L=\frac{\eta}{m}T$, then we still get

$$\rho_c(x,p,t) = [|C_1|^2\delta(p-\eta) + |C_2|^2\delta(p+\eta)],$$

$$-\frac{T}{2} < t < \frac{T}{2}. \tag{21}$$

Equation (21) is the same as Eq. (20). When $|\eta|$ is large, an energy eigenstate equivalently describes a classical time homogeneous ensemble [4,5].

The energy eigenstate does not satisfy the necessary condition (13) of an individual free particle. Generally, any superposition state of plane waves does not satisfy the necessary condition. It means that there is no wave function that can describe an individual free particle.

C. Gaussian wave packet states

Consider the state of free particles

$$\psi(x,t=0)=\left(\sqrt{\frac{2}{\pi}}\frac{\Delta p}{\hbar}\right)^{1/2}\exp\left[\frac{i}{\hbar}\langle p\rangle x-\frac{(x-x_0)^2}{4(\Delta x)^2}\right], \tag{22}$$

where $4(\Delta x)^2(\Delta p)^2=\hbar^2$ [10]. The initial Wigner distribution function of the state is

$$\rho_w(x,p,t=0)=\frac{1}{\hbar\pi}\exp\left[-\frac{(x-x_0)^2}{2(\Delta x)^2}-\frac{(p-\langle p\rangle)^2}{2(\Delta p)^2}\right]. \tag{23}$$

The Wigner distribution function containing time is given by Eq. (14) [15]

$$\rho_w(x,p,t)=\frac{1}{\hbar\pi}\exp\left[-\frac{\left(x-x_0-\frac{p}{m}t\right)^2}{2(\Delta x)^2}-\frac{(p-\langle p\rangle)^2}{2(\Delta p)^2}\right]. \tag{24}$$

Substituting $g(x_0,p_0)=\rho_w(x_0,p_0,t=0)$ into Eq. (12), we obtain the same distribution function as Eq. (24),

$$\rho_c(x,p,t)=\frac{1}{\hbar\pi}\exp\left[-\frac{\left(x-x_0-\frac{p}{m}t\right)^2}{2(\Delta x)^2}-\frac{(p-\langle p\rangle)^2}{2(\Delta p)^2}\right]. \tag{25}$$

Equations (24) and (25) show us that the wave packet state equivalently describes a classical pure ensemble in large $\langle p\rangle^2$ condition. The probability density function of the classical pure ensemble in position space is

$$\rho_c(x,t)=\frac{1}{\sqrt{\pi\left[2(\Delta x)^2+\left(\frac{1}{m}\Delta pt\right)^2\right]}}\times\exp\left[-\frac{\left(x-x_0-\frac{1}{m}\langle p\rangle t\right)^2}{2(\Delta x)^2+\left(\frac{1}{m}\Delta pt\right)^2}\right]. \tag{26}$$

Because a quasiclassical state including the Gaussian wave packet state of free particles does not describe an individual particle but a classical pure ensemble, the extension of the probability distribution of the system in position space is correct.

There are still some other quasiclassical states having positive definite Wigner distribution functions. Incoherent superposition states from quasiclassical plane waves are such states, but the examples above are the most important for the discussion that a quasiclassical wave function does not describe an individual particle but a classical pure ensemble.

V. APPROXIMATE SOLUTIONS

Generally the Wigner distribution function is not non-negative everywhere. It is a quantum phenomenon and has been observed in many experiments [18,19]. On the one hand, the Wigner distribution function can be used as a standard distribution function since it exactly satisfies the classical Liouville equation. On the other hand, when the Wigner distribution function of a quasiclassical state is not positive definite, we have to find an approximate solution of Eq. (12). The approximate solution should satisfy three conditions. (i) It satisfies the classical Liouville equation of free particles. (ii) It is non-negative everywhere. (iii) It gives results $\langle f(x,p)\rangle_c\approx\langle f(x,p)\rangle_w$ for all usual observables $\{f(x,p)\}$. We discuss the Husimi distribution function ρ_H by use of the following two relations. One is the definition expression of the distribution function [13,15]

$$\rho_H(x,p,t)=\frac{1}{2\pi\hbar}\left|\int_{-\infty}^{+\infty}dx'\,\beta^*_{xp}(x')\psi(x',t)\right|^2, \tag{27a}$$

where $\beta^*_{xp}(x')=(\frac{|\alpha|}{\hbar\pi})^{1/4}\exp[-\frac{|\alpha|}{2\hbar}(x-x')^2+ipx/\hbar]$ represents the wave function for a minimum uncertainty squeezed Gaussian wave packet peaked at (x,p). Evidently the Husimi distribution function is non-negative everywhere on phase space.

The other expression is the relation between $\rho_H(x,p,t)$ and $\rho_w(x,p,t)$ [11,15],

$$\rho_H(x,p,t)=\int dx'\int dp'\,G(x-x',p-p')\rho_w(x',p',t), \tag{27b}$$

where $G(x,p)=\frac{1}{\pi\hbar}\exp[-\frac{|\alpha|}{\hbar}x^2-\frac{1}{\hbar|\alpha|}p^2]$. We discuss some results of relation (27b):

$$\langle p\rangle_H=\int p\rho_H(p,t)dp=\int p\rho_w(p,t)dp=\langle p\rangle_w, \tag{28}$$

$$\langle p^2\rangle_H=\langle p^2\rangle_w+\frac{\hbar|\alpha|}{2}, \tag{29}$$

$$\langle x(t)\rangle_H=\langle x(t)\rangle_w=\frac{1}{m}\langle p\rangle_w t+x_0. \tag{30}$$

In Eq. (30) the Ehrenfest theorem has been used.

When $\langle x^2\rangle$ is finite, we have from Eq. (27b)

$$\langle x^2(t)\rangle_H=\langle x^2(t)\rangle_w+\frac{\hbar}{2|\alpha|}. \tag{31}$$

Noticing the result

$$\langle(x-\langle x\rangle_w)^2\rangle_w\geqslant 0,\quad \langle x^2\rangle_w\geqslant\left(\frac{1}{m}\langle p\rangle_w t+x_0\right)^2,$$

we can freely choose parameter $|\alpha|$ so that each last term can be neglected in Eqs. (29) and (31) for quasiclassical states.

Differentiating $\rho_H(x,p,t)$ with respect to t we get from Eqs. (14) and (27b)

$$\begin{aligned}\frac{\partial}{\partial t}\rho_H(x,p,t)\\ &= -\int dx' \int dp' G(x-x',p-p')\frac{p'}{m}\frac{\partial}{\partial x'}\rho_w\left(x'-\frac{p'}{m}t,p'\right)\\ &= \frac{p}{m}\int dx' \int dp' \rho_w(x',p',t)\frac{\partial}{\partial x'}G(x-x',p-p')\\ &= -\frac{p}{m}\frac{\partial}{\partial x}\rho_H(x,p,t).\end{aligned} \tag{32}$$

The Husimi distribution function of a state of free particles satisfies the Liouville equation also.

The Fourier transform of $G(x,p)$ in Eq. (27b) is

$$F_G(\omega,\omega') = \mathcal{F}[G(x,p)] = \exp\left[-\frac{\hbar}{4|\alpha|}\omega^2 - \frac{\hbar|\alpha|}{4}(\omega')^2\right]. \tag{33}$$

Let $F_w(\omega,\omega',t)=\mathcal{F}[\rho_w(x,p,t)]$, $F_H(\omega,\omega',t)=\mathcal{F}[\rho_H(x,p,t)]$, the convolution theorem for Eq. (27b) yields [20]

$$F_H(\omega,\omega',t) = \exp\left[-\frac{\hbar}{4|\alpha|}\omega^2 - \frac{\hbar|\alpha|}{4}(\omega')^2\right]F_w(\omega,\omega',t). \tag{34}$$

$F_H(\omega,\omega',t)$ decreases with the increase of ω and ω'. The equation means that the effect of $G(x,p)$ in Eq. (27b) is equivalent to the role of a "low-pass filter."

Similarly, we have for Fourier transforms of marginal distribution functions $\rho_H(x,t)$ and $\rho_w(x,t)$

$$F_H(\omega,t) = \exp\left[-\frac{\hbar}{4|\alpha|}\omega^2\right]F_w(\omega,t), \tag{35}$$

where $\rho_H(x,t)=\int_{-\infty}^{+\infty}dp\rho_H(x,p,t)$ and $\rho_w(x,t)=\int_{-\infty}^{+\infty}dp\rho_w(x,p,t)$.

In the following calculation the approximate expression on the real unity step function $u(x)$ will be used [20]:

$$\begin{aligned}u\left(x+\frac{\Delta}{2}\right)-u\left(x-\frac{\Delta}{2}\right) &= \int_{-\infty}^{+\infty} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\exp[i\omega x]\\ &= \int_{-\infty}^{+\infty} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\exp[-i\omega x]\\ &\approx \int_{-\omega_m}^{+\omega_m} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\exp[-i\omega x],\end{aligned} \tag{36}$$

where $\omega_m=2\pi/\Delta$. Since the integrated function is a decay oscillating function of ω, the approximation is good.

It is easy to see from Eq. (36),

$$\begin{aligned}\int_{-\Delta/2}^{+\Delta/2} dx\rho_H(x,t)\\ &= \int_{-\infty}^{+\infty} dx\left[u\left(x+\frac{\Delta}{2}\right)-u\left(x-\frac{\Delta}{2}\right)\right]\rho_H(x,t)\\ &= \int_{-\infty}^{+\infty} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\int_{-\infty}^{+\infty} dx\rho_H(x,t)\exp[-i\omega x]\\ &= \int_{-\infty}^{+\infty} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)F_H(\omega,t).\end{aligned} \tag{37}$$

The equation can be written as from Eqs. (35)–(37),

$$\begin{aligned}\int_{-\Delta/2}^{+\Delta/2} dx\rho_H(x,t)\\ &= \int_{-\infty}^{+\infty} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\exp\left[-\frac{\hbar}{4|\alpha|}\omega^2\right]F_w(\omega,t)\\ &\approx \int_{-\omega_m}^{+\omega_m} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\exp\left[-\frac{\hbar}{4|\alpha|}\omega^2\right]\\ &\quad\times\int_{-\infty}^{+\infty} dx\rho_w(x,t)\exp[-i\omega x].\end{aligned} \tag{38}$$

Choosing Δ so that $\frac{\hbar}{4|\alpha|}\omega_m^2=\frac{\hbar}{4|\alpha|}(\frac{2\pi}{\Delta})^2=0.1$, we approximately get from Eqs. (36) and (38),

$$\begin{aligned}\int_{-\Delta/2}^{+\Delta/2} dx\rho_H(x,t)\\ &\approx \int_{-\infty}^{+\infty} dx\rho_w(x,t)\int_{-\omega_m}^{+\omega_m} d\omega\frac{1}{\omega\pi}\sin\left(\frac{\omega\Delta}{2}\right)\exp[-i\omega x]\\ &= \int_{-\infty}^{+\infty} dx\left[u\left(x+\frac{\Delta}{2}\right)-u\left(x-\frac{\Delta}{2}\right)\right]\rho_w(x,t)\\ &= \int_{-\Delta/2}^{+\Delta/2} dx\rho_w(x,t),\end{aligned} \tag{39}$$

where $\Delta=\pi\sqrt{\frac{10\hbar}{|\alpha|}}$.

Applying the shift theorem of the Fourier transform to $u(x'-x)$, we generally have

$$\int_{x-\Delta/2}^{x+\Delta/2} dx'\rho_H(x',t) \approx \int_{x-\Delta/2}^{x+\Delta/2} dx'\rho_w(x',t). \tag{40}$$

Though $\rho_H(x,t)$ does not equal $\rho_w(x,t)$, Eq. (40) holds approximately.

Similarly for marginal distribution functions $\rho_H(p,t)$ and $\rho_w(p,t)$ we have

$$\int_{p-\Delta'/2}^{p+\Delta'/2} dp'\rho_H(p',t) \approx \int_{p-\Delta'/2}^{p+\Delta'/2} dp'\rho_w(p',t), \tag{41}$$

where $\Delta'=\pi\sqrt{10|\alpha|\hbar}$.

Applying the same approximate procedure to distribution function $\rho_H(x,p,t)$ we get

$$\int_{x-\Delta/2}^{x+\Delta/2} dx' \int_{p-\Delta'/2}^{p+\Delta'/2} dp' \rho_H(x',p',t) \approx \int_{x-\Delta/2}^{x+\Delta/2} dx' \int_{p-\Delta'/2}^{p+\Delta'/2} dp' \rho_w(x',p',t) \geqslant 0, \quad (42)$$

where Δ and Δ' are the same as the above values and $\Delta\Delta' = 10\pi^2\hbar$.

Generally we can tell the probability of a particle in an area that is larger than the $\Delta\Delta'$ on phase space in spite of the uncertainty relation. In macroscopic classical mechanics where $\Delta\Delta' = 10\pi^2\hbar$ is small, Eq. (42) means that $[\rho_w(x,p,t) - \rho_H(x,p,t)]$ is a fast oscillating function of x and p on phase space.

We use the Husimi distribution function of a quasiclassical state as the approximate solution of the classical distribution function corresponding to the state. Now expression (12) of the distribution function becomes

$$\rho_c(x,p,t) = \int dx_0 \int dp_0 \delta\left(x - x_0 - \frac{p_0}{m}t\right)\delta(p - p_0)\rho_H(x_0,p_0) = \rho_H\left(x - \frac{p}{m}t, p\right). \quad (43)$$

Consider expectation values of two physical quantities x^2p^2 and xp^2. When $\langle x^2p^2\rangle_w$ is finite, the expectation value can be written as

$$\langle x^2p^2\rangle_w = \langle x^2p^2\rangle_H + \int dx \int dp x^2p^2[\rho_w(x,p,t) - \rho_H(x,p,t)]. \quad (44)$$

Because x^2p^2 slowly varies and $(\rho_w - \rho_H)$ oscillates fast on phase space, the last term can be neglected compared with other terms.

Another expectation value $\langle xp^2\rangle_w$ can be written as

$$\langle xp^2\rangle_w = \left\{\int_{-\infty}^{0} dx \int dp xp^2\rho_H(x,p,t) + \int_{-\infty}^{0} dx \int dp xp^2[\rho_w(x,p,t) - \rho_H(x,p,t)]\right\} + \left\{\int_{0}^{+\infty} dx \int dp xp^2\rho_H(x,p,t) + \int_{0}^{+\infty} dx \int dp xp^2[\rho_w(x,p,t) - \rho_H(x,p,t)]\right\}. \quad (45)$$

In each bracket the last term can be neglected compared with the other terms.

The positive definite distribution function $\rho_H(x,p,t)$ satisfies the classical Liouville equation and gives results $\langle f(x,p)\rangle_H \approx \langle f(x,p)\rangle_w$ for all the usual observables $\{f(x,p)\}$. It can be seen from Eqs. (28)–(31) and the calculation above that the approximation is quite good for quasiclassical states. Therefore, when the Wigner distribution function of a quasiclassical state is not non-negative everywhere, the Husimi distribution function of the state is the approximate solution of the classical distribution function corresponding to the state.

VI. CONCLUDING REMARKS

The Bohr correspondence principle tells us that a state with large quantum numbers is a quasiclassical state. Generally, superposition states have no quantum numbers. In order to study the correspondence generally, we should give a condition of quasiclassical states for them. The condition of quasiclassical states for free particle systems is given in the first paragraph of Sec. II.

The Wigner distribution function for a state of free particles exactly satisfies the classical Liouville equation. Therefore, classical pure ensembles are defined. Their probability distribution functions satisfy the classical Liouville equation also. The probability distribution functions can be written from classical solutions of free particles. They are general solutions of the classical Liouville equation. Especially, the distribution function of an individual free particle is included in general solutions.

A solution of the classical Liouville equation is completely determined by the initial function of the solution. It is convenient for us to establish the correspondence between quantum and classical descriptions of a system. If the initial Wigner distribution function $\rho_w(x,p,t=0)$ of a quasiclassical state is non-negative everywhere on phase space, the classical distribution function corresponding to the state can be written from general solutions by putting $\rho_c(x,p,t=0) = \rho_w(x,p,t=0)$. Some important states belong to the case and give correspondence results directly. A quasiclassical momentum eigenstate equivalently describes a classical position homogeneous ensemble. A quasiclassical energy eigenstate describes a classical time homogeneous ensemble. There is no quasiclassical state that can describe an individual free particle. A quasiclassical Gaussian wave packet state corresponds to a classical pure ensemble whose initial distribution function is a Gaussian function of x and p on phase space. The extension of the wave packet state in position space can be understood well by use of the classical ensemble corresponding to the state.

If the initial Wigner distribution function $\rho_w(x,p,t=0)$ of a quasiclassical state is not positive definite on phase space, the Husimi distribution function $\rho_H(x,p,t)$ of the state can be used as the approximate solution of the classical distribution function corresponding to the state. The Husimi distribution function satisfies the classical Liouville equation and is positive definite on phase space. Furthermore, the Husimi distribution function of a quasiclassical state gives results $\langle f(x,p)\rangle_H \approx \langle f(x,p)\rangle_w$ for all usual observables $\{f(x,p)\}$. Generally, the system of free particles described by a quasiclassical state is equivalent to a classical pure ensemble of free particles in dynamics.

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