The Wigner representation of quantum mechanics

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Correct use of the Wigner representation of quantum mechanics, which is realized with joint distributions of quasiprobabilities in phase space, requires the use of certain specific rules and attention to a number of properties which distinguish the quasiprobability from a true probability. This paper is mainly concerned with these problems. In the Wigner representation the quantum Liouville equation appears instead of the Schroedinger equation. The solution may have no physical meaning unless it is subjected to a necessary and sufficient condition which selects an allowed class of distributions which describe quantum-mechanical pure states. This condition contains Planck's constant and imposes, besides the uncertainty relations, severe restrictions on the possible form of the Wigner function. When this condition is satisfied, one can reconstruct the wave function from the Wigner function. In the case of an oscillator, the quantization condition for the energies of the stationary states does not follow from the Liouville equation, but from this supplementary condition. Unlike the true probability density, any Wigner function (except Gaussian ones) of a pure state takes on negative values. Another important peculiarity is that the quasiprobability is not concentrated on certain hypersurfaces, but is "smeared out" over the entire phase space. These and other features considered in this paper should be kept in mind when using the Wigner representation in quantum-mechanical problems.

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CONTENTS

1. INTRODUCTION

In 1932 Wigner[1] suggested a representation of quantum mechanics by means of joint distributions of the probabilities (or, more precisely, the quasiprobabilities) for coordinates and momenta in phase space. Until recently this method has not been much used, and even is usually not mentioned in quantum-mechanics textbooks. The Wigner representation is now finding wider application in nonequilibrium quantum statistical mechanics (cf., e.g., Refs. 2–7). Meanwhile, this representation can also be used successfully in purely quantum mechanical problems, so that the number of papers in which it is applied has begun to increase.[8-16] For example, the Wigner representation has turned out to be very convenient for studying quantum systems with Hamiltonians quadratic in the coordinates and momenta.[8,10,11,15] It was used by Korsch and Berry[12] to study the stochastic nature of a quantum dynamical system, and by Korobkin and Sazonov[9] for the approximate solution of a nonlinear Schrödinger equation. As has been emphasized in papers by Shirokov,[13,14,17] the Wigner representation involves only concepts that are common to both quantum and classical mechanics. Therefore it is especially convenient in the consistent derivation of quasiclassical methods, in which, for example, one of the interacting systems is described by quantum mechanics and the other by the classical theory. With the Wigner representation it is easy to obtain quantum corrections to classical results. For example, in Ref. 14 an integral equation is derived whose iteration leads to the successive inclusion of quantum corrections to the classical solution, and an analogous formalism for scattering theory is developed in Ref. 13.

A comparatively detailed exposition of the theory of the Wigner representation is given in a paper by Moyal.[17] Then this theory was considerably extended in a series of papers by Shirokov, which are surveyed in Ref. 17. Their algebraic approach makes possible the construction of a rigorous and consistent mathematical theory. Precisely owing to this, however, it remains relatively unknown to wide circles of physicists, since it requires the use of a special formalism.

Besides papers in which the Wigner representation is used for the solution of specific problems, there are

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many devoted to studying the properties of this representation, which in some ways are very unusual and violate the seemingly intuitive properties of the method. We shall deal with the results of these papers at appropriate points in this review. Here we note that several papers devoted to such generalizations of the Wigner representation will not be discussed. For example, Ref. 20 considers a gauge-invariant Wigner function that arises in the solution of problems involving an electromagnetic field. Reference 19 examines representations of quantum mechanics by means of distributions which are more general than Wigner's. In particular, reflecting distributions allowing the description of spin variables are introduced in that paper. Reference 21 considers a generalization of the quantum Liouville equation, which describes diffusion in phase space, and uses it to discuss the problem of a damped oscillator. Finally, in the cited papers by Shirokov a whole class of representations of quantum mechanics in phase space is considered, which includes the Wigner representation as a special case.

The present paper has two purposes. First, by means of the generally accepted formalism of quantum mechanics we analyze those physical ideas which lead to the Wigner representation. In doing so, we confine ourselves to quantum-mechanical problems only (for simplicity considering only the one-dimensional case), and do not consider problems of quantum statistical mechanics. Second, we consider only methodological questions associated with the correct use of the Wigner representation. Unfortunately, to this day one encounters in the literature the assertion that by means of the Wigner function one cannot find average values of arbitrary quantities; this comes simply from incorrect use of this function. We give special attention to one particular property of the Wigner representation, which is due to the fact that by no means every function $W(p,q)$ that satisfies all the requirements of probability theory can be a "joint density of coordinate and momentum" for a pure quantum state. This is clear from the very fact that a pure state is uniquely described by a function of one variable, $\psi(q)$, whereas the "joint probability density" is a function of two variables. Therefore the admissible quantum densities that correspond to pure states can be described by those functions of two variables that can be uniquely described (in a definite way) in terms of a function of one variable. This imposes on the function $W(p,q)$ an extremely strong condition, which contains Planck's constant. This purely mathematical circumstance leads not only to the well known restriction on $W(p,q)$ which leads to the uncertainty relation, but also to other physically very important conclusions. For example, it turns out that the quantum equation for the evolution in time of the Wigner function in general describes not only the solutions that correspond to quantum mechanics, but also "extraneous" solutions. And only in case the initial condition for the evolution equation satisfies a suitable condition which has just been mentioned can the extraneous solutions be excluded, so that the quantum evolution equation (the quantum Liouville equation) becomes equivalent to the Schrödinger equation, and then the wave function can be reconstructed from the Wigner function up to a phase factor independent of the coordinates. This fact appears most distinctly in the treatment of the quantum oscillator. It is well known (cf., e.g., Sec. 4 of the present paper) that the quantum Liouville equation for the oscillator is identical with the classical equation. Then where does a difference between them arise? It is found that in this case the correct description of the quantum oscillator can be obtained precisely from the general restriction on the possible form of the quantum distribution, and Planck's constant appears in the description only when the correctly stated initial condition is used.

Accordingly, attention to the restrictions imposed on the possible form of quantum distributions is extremely important and eliminates the difficulties pointed out in Ref. 18.

It is also interesting to note that besides the standard uncertainty relation, which in the language of the Wigner function is a relation between its second moments, this function also satisfies another general limitation. It is found (see Sec. 5 of this paper) that its absolute value is bounded by the quantity $(\pi\hbar)^{-1}$, and this is another manifestation of the uncertainty relation.

We now briefly describe the content of this paper. The following part of the Introduction is devoted to an analysis of the formal obstacles to the introduction of a purely probabilistic language in quantum mechanics. In Sec. 2 we examine the connection between the rules for ordering noncommuting operators that are introduced in quantum mechanics, and the possibility of defining an operator for the "joint probability density" of coordinate and momentum. It is shown that the Weyl ordering and the corresponding Wigner function are in a certain sense the most acceptable. In Sec. 3 the properties of the Wigner function are analyzed. We show how by its use one can calculate the quantum averages of any function of the coordinate and momentum. Here it turns out that the rules that assure that the averages so calculated agree with the quantum-mechanical values do not always correspond to the standard rules of probability theory. We then consider the restrictions on the general form of functions $W(p,q)$ that can describe pure quantum states. It will be shown that the uncertainty relation can be derived from this restriction. In Sec. 4 the quantum Liouville equation is derived. It is shown that it can be satisfied by solutions that have no physical meaning, but that the imposition of the previously noted restrictions on the initial distribution automatically "filter out" the extraneous solutions. Then it is proved that the Wigner representation of quantum mechanics is equivalent to the traditional representations. Section 5 gives an analysis of the questions associated with nonpositivity of the quasiprobability. It is shown that the eigenvalues of the quasiprobability operator are equal to $\pm(\pi\hbar)^{-1}$, and the quasiprobability itself is bounded by the condition $|W| \leq (\pi\hbar)^{-1}$. A proof is given that the only nonnegative Wigner function that corresponds to a pure state is a joint Gaussian distribution for the coordinate and momentum which satisfied the limitation that follows from the uncertainty relation.

It is further shown that the function $\bar{W}(p,q)$ averaged with a Gaussian weight over phase space satisfies the condition $0 \leq \bar{W}(p,q) \leq (\pi\hbar)^{-1}$, if the dimensions of the cell over which the average is taken exceed $(\pi\hbar)$. Section 6 is devoted to the formulation of general conclusions.

Let us now consider the statement of the problem in more detail. As is well known, the state vector $|\psi(t)\rangle$ determines the probability density of the coordinate, $W(q,t) = |\langle q|\psi(t)\rangle|^2$ and that of the momentum, $W(p,t) = |\langle p|(t)\rangle|^2$, and also enables us to find the average values of functions that depend on both $\hat{p}$ and $\hat{q}$[1)]

$$\langle f(\hat{p},\hat{q})\rangle = \langle\psi(t)|f(\hat{p},\hat{q})|\psi(t)\rangle.$$

In the case when f depends only on $\hat{q}$, we have

$$\langle\psi(t)|f(\hat{q})|\psi(t)\rangle = \int W(q,t)\,f(q)\,dq.$$

In exactly the same way we have

$$\langle\psi(t)|F(\hat{p})|\psi(t)\rangle = \int W(p,t)\,F(p)\,dp.$$

However, the dynamics of quantum mechanics is determined by the Schrödinger equation for $|\psi(t)\rangle$, and there is no equation that determines directly the time dependence of $W(q,t)$ or $W(p,t)$. At the same time, when $|\psi(t)\rangle$ has been found from the Schrödinger equation we can find mean values of any function $f(\hat{p},\hat{q})$.

The question arises: Is it impossible to get a description of a quantum system directly in terms of probabilities, without resorting to the wave function?

Let us consider the classical problem with the Hamiltonian

$$H = (p^2/2m) + V(q).$$

The classical equations of motion $\dot{q} = p/m, \dot{p} = -V'(q)$ together with the initial conditions $q(0) = q_0, p(0) = p_0$ determine the trajectory $q(t), p(t)$. If, however, for $t = 0$ we are given not the initial conditions $q(0), p(0)$, but only their probability distributions $W_0(q)$, $W_0(p)$, then the dynamics of the system will be described not by the equations $\dot{q} = p/m, \dot{p} = -V'(q)$, but by the equation of evolution for the joint probability density $W(p,q,t)$ or the Liouville equation

$$\frac{\partial W}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial q} + V'(q)\frac{\partial W}{\partial p}, \quad W(p,q,0) = W_0(p,q). \qquad (1.1)$$

We emphasize that Eq. (1.1) describes not a system of many particles, as in statistical mechanics, but the evolution of the probability distribution of the coordinate and momentum of one particle, if its initial state is specified only in a probabilistic way.

We see that in classical mechanics there is no equation describing the evolution of $W(q,t)$ or $W(p,t)$; there is only the Liouville equation for the joint probability density $W(p,q,t)$. Therefore a corresponding quantum equation for $W(q,t)$ or for $W(p,t)$ cannot exist.

However, despite the fact that in quantum mechanics we can find the mean value of any function $f(\hat{p},\hat{q})$, there does not exist any joint probability density $W(p,q,t)$. In fact, if such a function existed, we would have the relation

$$\langle\psi(t)|f(\hat{p},\hat{q})|\psi(t)\rangle = \int\int W(p,q,t)\,f(p,q)\,dp\,dq. \qquad (1.2)$$

However, we have, for example, $\hat{p}\hat{q}^2\hat{p} = \frac{1}{2}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2) + \hbar^2$. At the same time, if Eq. (1.2) were valid, then we would obtain from it the same average value for $f_1 = \hat{p}\hat{q}^2\hat{p}$ and $f_2 = \frac{1}{2}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2)$, whereas these two f's differ by $\hbar$?

Accordingly, it is impossible to construct a joint probability density for coordinate and momentum such that by averaging functions $f(p,q)$ over it we can obtain their quantum mean values $\langle\psi|f(p,q)|\psi\rangle$. The direct cause of this is that if $f_1(\hat{p},\hat{q}) \neq f_2(\hat{p},\hat{q})$, it can still turn out that $f_1(p,q) = f_2(p,q)$.

Nevertheless, it is possible to introduce a function $W(p,q,t)$ such that the use of Eq. (1.2) with suitably ordered functions $\{f(\hat{p},\hat{q})\}$ gives their correct quantum-mechanical mean values, and which satisfies an equation of evolution which is the generalization of Eq. (1.1) to the quantum case. Such a function was first introduced by Wigner[1] for a system of many particles for the purpose of studying quantum corrections to thermodynamic functions. This function is to a large extent analogous to a joint probability density for coordinate and momentum, although it also has a number of peculiarities which do not allow it to be treated as such. We shall call it the quasiprobability, or, more exactly, the quasidensity of the joint distribution of q and p.

2. DEFINITION OF THE JOINT QUASIPROBABILITY OF COORDINATE AND MOMENTUM

As we have found, the formal obstacle to the introduction of a joint probability distribution $W(p,q,t)$ is the lack of an unambiguous correspondence between functions of operators and functions of commuting variables p,q. When operators $\hat{p},\hat{q}$ are replaced by numbers p,q different functions $f_i(\hat{p},\hat{q})$ can go over into the same function $f(p,q)$. This is another aspect of the well known problem of quantization, or the setting up of rules by which to each function $f(p,q)$ of commuting variables p,q one assigns a single function $f(\hat{p},\hat{q})$ of the noncommuting operators.

To remove this ambiguity, we apply certain quantization rules; i.e., we fix a method by which to each function $f(p,q)$ of the numbers p,q there is uniquely assigned a function $f(\hat{p},\hat{q})$ of the noncommuting operators $\hat{p},\hat{q}$. If only functions of this type are used in quantum theory, no ambiguity will arise. Functions of other kinds can always be reduced to the chosen form by using the commutation relations.

[1)] We use the following notations: Operators are indicated with the sign ^: $\hat{q}$ and $\hat{p}$ are coordinate and momentum operators, $[q,p] = i\hbar$, $|q\rangle$ are eigenvectors of the operator $\hat{q}$: $\hat{q}|q\rangle = q|q\rangle$, satisfying the conditions $\langle q'|q''\rangle = \delta(q'-q'')$, $\int|q\rangle dq\langle q| = \hat{1}$, where $\hat{1}$ is the unit operator. $|p\rangle$ are analogous eigenvectors of the operator $\hat{p}$, with $\hat{p}|p\rangle = p|p\rangle$, $\langle p'|p''\rangle = \delta(p'-p'')$, $\int|p\rangle dp\langle p| = \hat{1}$. As is well known, $\langle q|p\rangle = (2\pi\hbar)^{-1/2}\exp(iqp/\hbar)$. Wave functions in the q and p representations will be denoted as $\psi(q,t) = \langle q|\psi(t)\rangle$ and $\psi(p,t) = \langle p|\psi(t)\rangle$.

To introduce the correspondence between the functions $f(p,q)$ and $f(\hat{p},\hat{q})$ it suffices to define an operator function $\hat{F}(\lambda,\mu)$, which is a generalization of the function $F(\lambda,\mu)=\exp[i(\lambda p+\mu q)]$. In fact, an arbitrary analytic function $f(p,q)$ can be obtained from $F(\lambda,\mu)$ by means of the operation

$$f(p,q)=f\left(\frac{1}{i}\frac{\partial}{\partial\lambda},\ \frac{1}{i}\frac{\partial}{\partial\mu}\right)F(\lambda,\mu)\,|_{\lambda=\mu=0}.$$

Since the operators $\partial/\partial\lambda$ and $\partial/\partial\mu$ commute, there is no ambiguity in writing out $f(\partial/i\partial\lambda,\partial/i\partial\mu)$. Therefore, if we adopt some operator generalization of the function F, for example

$$\hat{F}_1(\lambda,\mu)=e^{i\lambda\hat{p}}e^{i\mu\hat{q}},\quad \hat{F}_2(\lambda,\mu)=e^{i\mu\hat{q}}e^{i\lambda\hat{p}},\quad \hat{F}_3=\frac{1}{2}(\hat{F}_1+\hat{F}_2)$$

and so on, we can define the ordered operator function $\{f(\hat{p},\hat{q})\}$ by means of the formula

$$\{f(\hat{p},\hat{q})\}=f\left(\frac{1}{i}\frac{\partial}{\partial\lambda},\ \frac{1}{i}\frac{\partial}{\partial\mu}\right)\hat{F}(\lambda,\mu)\,|_{\lambda=\mu=0} \tag{2.1a}$$

$$=\frac{1}{4\pi^2}\int\int_{-\infty}^{\infty}\int\int d\lambda\,d\mu\,dp\,dq\,f(p,q)\exp[-i(\lambda p+\mu q)]\hat{F}(\lambda,\mu). \tag{2.1b}$$

Hereafter we shall take $\{f(\hat{p},\hat{q})\}$ to be the ordered function of the operators $\hat{p},\hat{q}$ corresponding to the function $f(p,q)$ according to the operation (2.1). Furthermore, for example, $\{(f_1(p,q)f_2(p,q)\}$ is the function of the operators $\hat{p},\hat{q}$ corresponding to the c-number function $\Phi(p,q)=f_1(p,q)f_2(p,q)$.

For different functions $\hat{F}(\lambda,\mu)$ there will be different operator functions $\{f(\hat{p},\hat{q})\}$ differing in the order of the noncommuting factors $\hat{p},\hat{q}$. If then, using the commutation relations, we bring them to the same order, additional terms will in general appear. Not all functions $\hat{F}$ are equally suitable for our purpose. To choose the most suitable, we turn to the properties of the characteristic function of probability theory.

If p and q are random numbers, the mean value of the function $F(\lambda,\mu)=\exp[i(\lambda p+\mu q)]$ is the characteristic function of the joint probability distribution for p,q:

$$\varphi_{pq}(\lambda,\mu)=\langle F(\lambda,\mu)\rangle=\int\int_{-\infty}^{\infty}\exp[i(\lambda p+\mu q)]W(p,q)\,dp\,dq. \tag{2.2}$$

[Here the angle brackets $\langle\ldots\rangle$ denotes the statistical average over the fluctuations of p,q characterized by the joint probability density $W(p,q)$.] The probability density is expressed in terms of φ_{pq} by the inverse Fourier transformation:

$$W(p,q)=\frac{1}{4\pi^2}\int\int_{-\infty}^{\infty}\varphi_{pq}(\lambda,\mu)\exp[-i(\lambda p+\mu q)]\,d\lambda\,d\mu. \tag{2.3}$$

As is well known, the characteristic function of a probability distribution has the following properties[22]:

a) $\varphi_{pq}(0,0)=1$; b) $\varphi_{pq}(0,\mu)=\langle\exp(i\mu q)\rangle=\varphi_q(\mu)$, $\varphi_{pq}(\lambda,0)=\varphi_p(\lambda)$; c) $\varphi^*_{pq}(\lambda,\mu)=\varphi_{pq}(-\lambda,-\mu)$; d) $|\varphi_{pq}(\lambda,\mu)|\leq 1$; e)* [the (inverse) Fourier transform of] $\varphi_{pq}(\lambda,\mu)$ is a positive definite function; in particular, $W(p,q)\geq 0$ [is $W(p,q)$ is a true probability density].

Translator's note: This last statement has been changed from the original text, which stated that $\varphi_{pq}(\lambda,\mu)$ is itself a positive definite function. Being the mean value of a complex function F, φ_{pq} is, in general, complex. As stated here, property e) is as obvious from the foregoing discussion as the other four properties are.

In the same way as $\langle F(\lambda,\mu)\rangle$ determines the characteristic function, the quantum average $\langle\psi|\hat{F}(\lambda,\mu)\psi\rangle$ can be taken as the definition of the quantum characteristic function in the state $|\psi\rangle$ and the operator $\hat{F}(\lambda,\mu)$ can be taken as the operator of the characteristic function.

As an obvious extension of the properties a), b) we have the conditions

$$\hat{F}(0,\mu)=\exp(i\mu\hat{q}),\quad \hat{F}(\lambda,0)=\exp(i\lambda\hat{p}). \tag{2.4}$$

If the function $\hat{F}$ satisfies these conditions, then in constructing by means of Eq. (2.1) the functions $\{f(\hat{p},\hat{q})\}$, functions of the form $f(\hat{p})$ or $f(\hat{q})$, which depend on only one variable, are obtained from the corresponding functions $f(p),f(q)$ by the simple replacement $p\to\hat{p}$, $q\to\hat{q}$.

The generalization of property c) is the condition

$$\hat{F}^+(\lambda,\mu)=\hat{F}(-\lambda,-\mu). \tag{2.5}$$

It follows from Eq. (2.1b) that when the condition (2.5) is satisfied real functions $f^*(\hat{p},\hat{q})=f(p,q)$ will be converted into Hermitean operators $\{f(p,q)\}^+=\{f(p,q)\}$.

To assure that the condition $|\langle\psi|F(\lambda,\mu)|\psi\rangle|\leq 1$, which generalizes property d), will hold, we require that the operator $\hat{F}$ be unitary:

$$\hat{F}^+(\lambda,\mu)\hat{F}(\lambda,\mu)=\hat{F}(\lambda,\mu)\hat{F}^+(\lambda,\mu)=\hat{1}. \tag{2.6}$$

As for the condition of positive definiteness, it cannot be generalized to the quantum characteristic functions. In a number of cases this leads to violations of the condition that the probability density is positive, as we shall discuss in detail later.

Let us go back to the functions $\hat{F}_1,\hat{F}_2$. It is clear that $\hat{F}_1^+(\lambda,\mu)=\hat{F}_2(-\lambda,-\mu)$; that is, the condition (2.5) does not hold for these operators, because of which real functions $f(p,q)$ will correspond to nonhermitean operators. The function $\hat{F}_3$ satisfies the condition (2.5). However, the unitarity condition (2.6) does not hold for this function. Using the well known formula (cf., e.g., Ref. 23)

$$\exp(\hat{A}+\hat{B})=\exp(\hat{A})\exp(\hat{B})\exp\left(-\frac{1}{2}[\hat{A},\hat{B}]\right), \tag{2.7}$$

which holds provided the commutator $[\hat{A},\hat{B}]$ is a c-number, one can show easily that $\hat{F}_3(\lambda,\mu)\hat{F}_3^+(\lambda,\mu)=\cos^2(\hbar\lambda\mu/2)\cdot\hat{1}\neq\hat{1}$. Therefore, although the operator $\hat{F}_3$ is suitable for the construction of symmetric operator functions, it is not suitable for the operator functions, it is not suitable for the role of the operator characteristic function.

Therefore we shall use the following operator of the characteristic function, which satisfies all the requirements (2.4)–(2.6) which we have formulated:

$$\hat{F}_0(\lambda,\mu)=\exp[i(\lambda\hat{p}+\mu\hat{q})]. \tag{2.8a}$$

The conditions that uniquely require the choice of the operator $\hat{F}$ in the form (2.8a) have been analyzed by Krüger and Poffyn.[24] It turns out that various sets of requirements can be formulated that lead to this same choice.

By means of Eq. (2.7) the operator $\hat{F}_0$ can be put in these forms:

$$\hat{F}_0(\lambda, \mu) = \exp(i\lambda\hat{p}/2)\exp(i\mu\hat{q})\exp(i\lambda\hat{p}/2), \quad (2.8b)$$

$$\hat{F}_0(\lambda, \mu) = \exp(i\mu\hat{q}/2)\exp(i\lambda\hat{p})\exp(i\mu\hat{q}/2), \quad (2.8c)$$

$$\hat{F}_0(\lambda, \mu) = \exp(-i\lambda\mu\hbar/2)\exp(i\lambda\hat{p})\exp(i\mu\hat{q}), \quad (2.8d)$$

$$\hat{F}_0(\lambda, \mu) = \exp(i\lambda\mu\hbar/2)\exp(i\mu\hat{q})\exp(i\lambda\hat{p}). \quad (2.8e)$$

Using the formula[2)]

$$\exp(i\lambda\hat{p})\,|\,q\rangle = |\,q - \lambda\hbar\rangle \quad (2.9)$$

and applying the operator $\hat{F}_0$ taken in the form (2.8d) to the expansion of the unit operator in the basis $|q\rangle$, (see footnote[1)]), we easily get still another useful representation of the operator $\hat{F}_0$:

$$\hat{F}_0(\lambda, \mu) = \int \left|q' - \frac{\lambda\hbar}{2}\right\rangle \exp(i\mu q')\,dq' \left\langle q' + \frac{\lambda\hbar}{2}\right|. \quad (2.8f)$$

The various representations of $\hat{F}_0$ are convenient in various particular cases. For example, if it is necessary to calculate $\partial F_0/\partial\lambda$, it is convenient to use Eq. (2.8b), and to calculate $\partial F_0/\partial\mu$ it is convenient to use Eq. (2.8c).

If we use the function $\hat{F}_0(\lambda, \mu)$ to determine ordered operator functions by means of Eq. (2.1), the results are what is called Weyl symmetric ordering.[25] We note that the use of $\hat{F}_3$ also leads to a symmetric ordering, but it is not identical with the Weyl ordering. For example, for the operator generalizations of the function p^2q^2:

$$\{\hat{p}^2\hat{q}^2\}_3 = \left(\frac{1}{i}\frac{\partial}{\partial\lambda}\right)^2\left(\frac{1}{i}\frac{\partial}{\partial\mu}\right)^2 \hat{F}_3(\lambda, \mu)\,|_{\lambda=\mu=0} = \frac{1}{2}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2),$$

$$\{\hat{p}^2\hat{q}^2\}_0 = \frac{1}{4}(\hat{p}^2\hat{q}^2 + 2\hat{p}\hat{q}^2\hat{p} + \hat{q}^2\hat{p}^2) = \frac{1}{2}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2 + \hbar^2).$$

In the rest of this article we shall understand $\{f(\hat{p}, \hat{q})\}$ to mean the operator obtained from $f(p, q)$ by the formulas (2.1) with the use of the operator characteristic function $\hat{F}_0$ defined by Eqs. (2.8).

An extremely interesting property of operator functions, which follows from their definition, is as follows: If $\hat{A} = \{A(\hat{p}, \hat{q})\}$ and $\hat{B} = \{B(\hat{p}, \hat{q})\}$, then $\hat{C} = \hat{A}\hat{B} \neq \{A(\hat{p}, \hat{q})B(\hat{p}, \hat{q})\}$. Instead of this we have the equation $\hat{A}\hat{B} = \{C(\hat{p}, \hat{q})\}$, where $C(p, q)$ is expressed in terms of $A(p, q)$ and $B(p, q)$ by the following formula,[18] which can be derived easily by using Eqs. (2.1b), (2.7) and (2.8a):

$$C(p, q) = (\pi\hbar)^{-2}\int\int\int\int dp_1 dq_1 dp_2 dq_2\, A(p_1, q_1)\, B(p_2, q_2) \times \exp((2i/\hbar)[q(p_1 - p_2) - p(q_1 - q_2) + q_1p_2 - q_2p_1]). \quad (2.10)$$

In connection with Eq. (2.10) it must be kept in mind that from $\hat{A} \leftarrow A(p, q)$ it does not follow that $\hat{A}^n \leftarrow [A(p, q)]^n$. For example, let

$$H(p, q) = (p^2/2m) + (m\omega^2q^2/2).$$

Then

$$\hat{H} = \{H(\hat{p}, \hat{q})\} = (\hat{p}^2/2m) + (m\omega^2\hat{q}^2/2).$$

But, using the formula $\hat{p}^2\hat{q}^2 = \frac{1}{2}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2 + \hbar^2)$ given a few lines back, we obtain

$$\{H^2(\hat{p}, \hat{q})\} = \left\{\frac{\hat{p}^4}{4m^2} + \frac{m^2\omega^4\hat{q}^4}{4} + \frac{\omega^2\hat{p}^2\hat{q}^2}{2}\right\} = \frac{\hat{p}^4}{4m^2} + \frac{m^2\omega^4\hat{q}^4}{4} + \frac{\omega^2}{4}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2 + \hbar^2) = \{H(\hat{p}, \hat{q})\}^2 + \left(\frac{\hbar\omega}{2}\right)^2. \quad (2.11)$$

[2)] This formula can be derived easily by inserting between $\exp(i\lambda p)$ and $|\,q\rangle$ the expansion of the unit operator in the basis $|\,p\rangle$ and then going back to the basis $|q\rangle$.

Equations (2.1) and (2.8) enable us to find the ordered operator $\{f(\hat{p}, \hat{q})\}$ corresponding to a c-number function $f(p, q)$. Another problem frequently arises, that of representing a given operator $\hat{A}$ in Weyl-ordered form. This means that one must find a c-number function $A(p, q)$, called the Weyl symbol of the operator $\hat{A}$, such that $\hat{A} = \{A(\hat{p}, \hat{q})\}$. We shall show that this problem is solved by the following formula (cf., e.g., the supplement to Ref. 25, which presents quite a number of properties of Weyl symbols):

$$A(p, q) = \int \exp(ip\xi/\hbar)\left\langle q - \frac{\xi}{2}\right|\hat{A}\left|q + \frac{\xi}{2}\right\rangle d\xi. \quad (2.12)$$

To do this we find, using Eq. (2.1b), the operator $\{A(\hat{p}, \hat{q})\}$ for which the role of the function $A(p, q)$ is played by the right member of Eq. (2.12):

$$\{A(\hat{p}, \hat{q})\} = \frac{1}{4\pi^2}\int\int\int\int\int d\lambda\, d\mu\, dp\, dq\, d\xi \times \exp\left[-i(\lambda p + \mu q) + \frac{ip\xi}{\hbar}\right]\hat{F}_0(\lambda, \mu)\left\langle q - \frac{\xi}{2}\right|\hat{A}\left|q + \frac{\xi}{2}\right\rangle.$$

We perform the integration over p, which leads to $\delta(\lambda - \xi/\hbar)$, and then that over λ:

$$\{A(\hat{p}, \hat{q})\} = \frac{1}{2\pi}\int\int\int dq\, d\xi\, d\mu \exp(-i\mu q)\hat{F}_0\left(\frac{\xi}{\hbar}, \mu\right)\left\langle q - \frac{\xi}{2}\right|\hat{A}\left|q + \frac{\xi}{2}\right\rangle.$$

Substituting the representation (2.8f) for $\hat{F}_0$ we have

$$\{A(\hat{p}, \hat{q})\} = \frac{1}{2\pi}\int\int\int\int\int dq\, d\xi\, d\mu\, dq'\left|q' - \frac{\hbar}{2}\frac{\xi}{\hbar}\right\rangle \times \exp[i\mu(q - q')]\left\langle q - \frac{\xi}{2}\right|\hat{A}\left|q + \frac{\xi}{2}\right\rangle\left\langle q' + \frac{\hbar}{2}\frac{\xi}{\hbar}\right|.$$

Integration over μ leads to $\delta(q - q')$, and we have

$$\{A(\hat{p}, \hat{q})\} = \int\int dq\, d\xi\left|q - \frac{\xi}{2}\right\rangle\left\langle q - \frac{\xi}{2}\right|\hat{A}\left|q + \frac{\xi}{2}\right\rangle\left\langle q + \frac{\xi}{2}\right|.$$

Introducing new variables $q \pm \xi/2 = q_{1,2}$ and using the formula for the expansion of the unit operator in the basis $|q\rangle$, we have finally

$$\{A(\hat{p}, \hat{q})\} = \int\int |\,q_2\rangle\, dq_2\, \langle q_2|\hat{A}|\,q_1\rangle\, dq_1\, \langle q_1|\,| = \hat{1}\cdot\hat{A}\cdot\hat{1} = \hat{A}. \quad (2.13)$$

Accordingly, by Eq. (2.12) we can find for an operator $\hat{A}$ its Weyl symbol $A(p, q)$ after which Eq. (2.1) can be used to represent the given operator in Weyl-ordered form.

Let us return to the operator $\hat{F}_0(\lambda, \mu)$ of the characteristic function. The quantum characteristic function $\varphi(\lambda, \mu)$ can be expressed in terms of it by the formula

$$\varphi(\lambda, \mu) = \langle\psi|\hat{F}_0(\lambda, \mu)|\,\psi\rangle. \quad (2.14)$$

Consider the mean value of an arbitrary function of the operators $\hat{p}, \hat{q}$; using Eqs. (2.1a) and (2.14) we have

$$\langle\psi|\{f(\hat{p}, \hat{q})\}|\,\psi\rangle = \langle\psi|f\left(\frac{1}{i}\frac{\partial}{\partial\lambda}, \frac{1}{i}\frac{\partial}{\partial\mu}\right)\hat{F}_0(\lambda, \mu)\,|_{\lambda=\mu=0}|\,\psi\rangle = f\left(\frac{1}{i}\frac{\partial}{\partial\lambda}, \frac{1}{i}\frac{\partial}{\partial\mu}\right)\langle\psi|\hat{F}_0(\lambda, \mu)|\,\psi\rangle\,|_{\lambda=\mu=0} = f\left(\frac{1}{i}\frac{\partial}{\partial\lambda}, \frac{1}{i}\frac{\partial}{\partial\mu}\right)\varphi(\lambda, \mu)\,|_{\lambda=\mu=0}.$$

The right member of this equation is of the same form as the corresponding formula of probability theory. Therefore the quantum mean value $\langle\psi|\{f\}|\psi\rangle$ is expressed in terms of the quantum characteristic function φ by the standard formula of the theory of probability.

If we use the definition (2.1b) for $\{\ldots\}$, we obtain

$$\langle\psi|\{(f(\hat{p}, \hat{q})\}|\,\psi\rangle = \int_{-\infty}^{\infty}\int f(p, q)\,W(p, q)\,dp\,dq, \quad (2.15)$$

where

$$W(p, q)=\frac{1}{4\pi^2}\int\int d\lambda\, d\mu\, \exp[-i(\lambda p+\mu q)]\,\langle\psi\,|\,\hat{F}_0(\lambda, \mu)\,|\,\psi\rangle. \quad (2.16)$$

Accordingly, the function $W(p,q)$, which we shall call the quasiprobility density of the joint distribution of coordinate and momentum, or the Wigner function, enables us to calculate quantum-mechanical mean values with Eq. (2.15), which also is of the form standard in probability theory. We note that Eq. (2.16) can be put in the form

$$W(p, q) = \langle\psi\,|\,\hat{W}(p, q)\,|\,\psi\rangle, \quad (2.17)$$

where the quasiprobability density operator, which depends on the c-number arguments p, q is given by

$$\hat{W}(p, q)=\frac{1}{4\pi^2}\int_{-\infty}^{\infty}\int d\lambda\, d\mu\, \exp[-i(\lambda p+\mu q)]\,\hat{F}_0(\lambda, \mu). \quad (2.18)$$

It follows from Eq. (2.1b) that $\hat{W}(p,q)=\{\delta(\hat{p}-p)\delta(\hat{q}-q)\}$.

If we use the representation (2.8f) for $\hat{F}_0(\lambda, \mu)$ and substitute it into Eq. (2.18), then after integration over μ, which leads to $\delta(q-q')$, we obtain the operator $\hat{W}$ in the q representation:

$$\hat{W}(p, q)=\frac{1}{2\pi\hbar}\int\left|q-\frac{\xi}{2}\right\rangle\exp(-ip\xi/\hbar)\,d\xi\left\langle q+\frac{\xi}{\hbar}\right|. \quad (2.19)$$

If we substitute this representation of the operator $\hat{W}$ into Eq. (2.17) we obtain (after replacing the integration variable ξ with $-\xi$)

$$W(p, q)=\frac{1}{2\pi\hbar}\int\exp(ip\xi/\hbar)\,\psi^*\left(q+\frac{\xi}{2}\right)\psi\left(q-\frac{\xi}{2}\right)d\xi. \quad (2.20)$$

Let us consider the density matrix for a pure state, $\rho(q_1, q_2)=\psi(q_1)\psi^*(q_2)$ and introduce new coordinates $q=(q_1+q_2)/2$, $\xi=q_2-q_1$. Then Eq. (2.20) can be written in the form

$$W(p, q)=\frac{1}{2\pi\hbar}\int\rho\left(q-\frac{\xi}{2},\ q+\frac{\xi}{2}\right)\exp(ip\xi/\hbar)\,d\xi. \quad (2.21)$$

Accordingly, the quasiprobability density can be regarded as the Fourier transform of the density with respect to the difference variable.

We point out that if instead of the function $\hat{F}_0(\lambda, \mu)$ we had chosen some different function which goes over into $\exp[i(\lambda p+\mu q)]$ when $\hat{p}\to p, \hat{q}\to q$, then by means of it we could have chosen an ordering of the operators and a quasiprobability W which would lead to correct quantum mean values. For example, if we were to choose for F the function $F_1=\exp(i\lambda p)\exp(i\mu q)$, then we would arrive at an ordering in which operators $\hat{p}$ would always be to the left of operators $\hat{q}$, and the function W would be of the form

$$W_1(p, q) = \langle p\,|\,q\rangle\,\psi^*(p)\,\psi(q), \quad (2.22)$$

where

$$\psi(p) = \langle p\,|\,\psi\rangle,\ \langle p\,|\,q\rangle = (2\pi\hbar)^{-1/2}\exp(-ipq/\hbar).$$

From the point of view of getting correct results of calculations, this function is not inferior to the Wigner function (2.20). However, the properties of the function W_1 are further from those of a probability density (for example, $W_1^*\neq W_1$. In this respect the Wigner function (2.20) is in a certain sense the closest in its properties to a probability density.

3. SOME PROPERTIES OF THE QUASIPROBABILITY

a) Compatibility with the one-dimensional distributions

If we integrate the Wigner function given by Eq. (2.20) over p we obtain

$$\int_{-\infty}^{\infty}W(p, q)\,dp=|\,\psi(q)\,|^2\equiv W(q), \quad (3.1)$$

i.e., the integral of the joint probability density over p leads to the probability density for the coordinate q. We obtain the same result by integrating Eq. (2.16) over p. Here after integrating over p we obtain in the integrand the function $\langle\psi|\hat{F}_0(0, \mu)|\psi\rangle$, and according to the condition (2.4) imposed on $\hat{F}(\lambda, \mu)$ this gives $\langle\psi|\exp(i\mu q)|\psi\rangle$, the characteristic function of the coordinate probability distribution. In just the same way, integrating Eq. (2.16) over q, we obtain in the integrand $\langle\psi|\exp(i\lambda p)|\psi\rangle$, the characteristic function for the momentum. Consequently,

$$\int_{-\infty}^{\infty}W(p, q)\,dq=|\langle p\,|\,\psi\rangle\,|^2\equiv W(p). \quad (3.2)$$

Thus the Wigner quasiprobability distribution, like all other densities constructed so as to satisfy the requirement (2.4), meets the natural demand that the two-dimensional distribution be consistent with the one-dimensional ones. Besides this it is clear from Eq. (3.1) that the double integral of the Wigner function over p and q is equal to unity if the wave function is normalized to unity.

b) Calculation of higher moments

Let us now consider the consequences arising from the relation (2.10). Suppose we have a Hermitean operator $\hat{A}=f(\hat{p}, \hat{q})$ corresponding to an observable A. This operator also need not be in Weyl-ordered form, but by using Eqs. (2.12) and (2.1) or the commutation relation $[\hat{q}, \hat{p}]=i\hbar$ we can always perform identical transformations to write it in the accepted standard form: $\hat{A}=\{A(\hat{p}, \hat{q})\}$.

After this we can find the mean value of the observable A for the state $|\psi\rangle$ by means of Eq. (2.15):

$$\langle A\rangle = \langle\psi\,|\,\hat{A}\,|\,\psi\rangle = \int\int A(p, q)\,W(p, q)\,dp\,dq.$$

We may, however, be interested in the means of certain powers of the observable A. For example, the mean square of the quantum fluctuations of A in the state $|\psi\rangle$ is given, as is well known, by the formula $\langle A^2\rangle-\langle A\rangle^2=\langle\psi|\hat{A}^2|\psi\rangle-\langle\psi|\hat{A}|\psi\rangle^2$, and to find it it is necessary to calculate $\langle\psi|\hat{A}^2|\psi\rangle$. But the operator

$$\hat{A}^2=\{A(\hat{p}, \hat{q})\}^2$$

is not in the necessary ordered form, so that Eq. (2.14) cannot be directly applied to it. If, however, we bring it into this form by means of the commutation relations or find its Weyl symbol from Eq. (2.10), i.e., the function $C(p,q)$ such that

$$\hat{A}^2=\{C(\hat{p}, \hat{q})\},$$

then in general $C(p,q)\neq A^2(p,q)$. Therefore

$$\langle A^2\rangle=\langle\psi\,|\,\hat{A}^2\,|\,\psi\rangle=\int\int C(p, q)\,W\,dp\,dq\neq\int\int A^2W\,dp\,dq. \quad (3.3)$$

Accordingly, despite the fact that for $\langle\psi|\hat{A}|\psi\rangle$ we have the usual representation of probability theory in terms of the integral of AW, no such representation holds for $\langle\psi|\hat{A}^2|\psi\rangle$. In other words the integrals

$$\int\int A^n(p, q)\, W(p, q)\, dp\, dq$$

for $n = 2, 3, \ldots$ are not the mean values of the corresponding powers of the observable A.

This fact, besides the possibility that W takes on negative values, of which we shall speak in detail later, is a manifestation of one of the essential difficulties in interpreting quantum mechanics in purely probabilistic language. The point is that after we have, in the quantization process, set up a correspondence between dynamic variable operators and observables, the possible values of the observables are the eigenvalues of the corresponding operators. Furthermore, if an observable assumes the value A_n, so that $\hat{A}|\psi_n\rangle = A_n|\psi_n\rangle$, then of course $\hat{A}^2|\psi_n\rangle = A_n^2|\psi_n\rangle$, i.e., the operator $\hat{A}^2$ corresponds to the observable A^2. At the same time the law of correspondence between operators and the functions that represent these operators in the phase space (p, q) is different, so that from the correspondence $\hat{A} = \{A(\hat{p}, \hat{q})\} \leftrightarrow A(p, q)$ it does not follow that $\hat{A}^2 \leftrightarrow A^2(p, q)$. For example, if

$$H(p, q) = (p^2/2m) + (m\omega^2 q^2/2), \quad \hat{H} = \{H(\hat{p}, \hat{q})\} = (\hat{p}^2/2m) + (m\omega^2\hat{q}^2/2),$$

then, according to Eq. (2.11),

$$H^2 = \{H(\hat{p}, \hat{q})\}^2 = \left\{H^2(\hat{p}, \hat{q}) - \left(\frac{\hbar\omega}{2}\right)^2\right\}.$$

Therefore, if

$$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \int\int\left[\frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}\right] W(p, q)\, dp\, dq, \tag{3.4a}$$

then

$$\langle E^2\rangle = \langle\psi|\hat{H}^2|\psi\rangle = \int\int\left[\left(\frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}\right)^2 - \left(\frac{\hbar\omega}{2}\right)^2\right] W(p, q)\, dp\, dq. \tag{3.4b}$$

c) Restriction to an allowed class of quantum-mechanical distributions for pure states

It follows from Eq. (2.20) that the function of two variables $W(p, q)$ can be uniquely expressed in terms of a function of one variable $\psi(q)$. This fact decidedly restricts the class of possible functions $W(p, q)$. It is useful to formulate this restriction in terms of the function $W(p, q)$ itself. To do this we take the Fourier transform of Eq. (2.20) with respect to p, and get as the result

$$\int \exp(i\lambda p)\, W(p, q)\, dp = \psi\left(q + \frac{\lambda\hbar}{2}\right)\psi^*\left(q - \frac{\lambda\hbar}{2}\right).$$

Denoting $q \pm (\lambda\hbar/2) = q_{1,2}$, we rewrite this equation in the form

$$\int \exp[ip(q_1 - q_2)/\hbar]\, W\left(p, \frac{q_1 + q_2}{2}\right) dp = \psi(q_1)\,\psi^*(q_2). \tag{3.5}$$

The integral in the left member of Eq. (3.5) must be factorizable in the variables q_1, q_2; it follows that the Wigner function that describes a pure quantum state necessarily satisfies the condition

$$\frac{\partial^2 \ln \rho(q_1, q_2)}{\partial q_1\, \partial q_2} = 0, \tag{3.6}$$

where

$$\rho(q_1, q_2) = \int \exp[ip(q_1 - q_2)/\hbar]\, W\left(p, \frac{q_1 + q_2}{2}\right) dp.$$

In what follows it will be seen that this condition is very important.

First let us show that the restriction (3.6) on the form of the function W, together with the condition $W^* = W$ is not only a necessary but also a sufficient condition for W to describe a pure state. Indeed, regarding Eq. (3.6) as an equation for $\rho(q_1, q_2)$, we find that its general solution is of the form $\rho(q_1, q_2) = f(q_1)\varphi(q_2)$. Then, from the representation of $\rho(q_1, q_2)$ in terms of W and the condition $W^* = W$ it follows that $\rho^*(q_1, q_2) = \rho(q_2, q_1)$. From this we see that $f^*(q_1)\varphi^*(q_2) = f(q_2)\varphi(q_1)$, and consequently $\varphi^*(q_2)/f(q_2) = \varphi(q_1)/f^*(q_1) = \text{const} = A = A^*$. Then $\varphi(q) = Af^*(q)$, and if we introduce the notation $F(q) = A^{1/2}f(q)$ we get for the function $\rho(q_1, q_2)$, which satisfies the condition (3.6), the representation

$$\rho(q_1, q_2) = \int W\left(p, \frac{q_1 + q_2}{2}\right)\exp[ip(q_1 - q_2)/\hbar]\, dp = F(q_1)\, F^*(q_2). \tag{3.5a}$$

Accordingly, if the function W satisfies the condition (3.6), then it describes the pure state that corresponds to the wave function $F(q)$.

Writing Eq. (3.5a) in the variables $q = (q_1 + q_2)/2, \lambda = (q_1 - q_2)/\hbar$, we have

$$\int \exp(i\lambda p)\, W(p, q)\, dp = F\left(q + \frac{\lambda\hbar}{2}\right) F^*\left(q - \frac{\lambda\hbar}{2}\right).$$

The right member of this equation contains the Planck constant $\hbar$, and in the left member it can be contained only in W. Consequently, if the function W satisfies the condition (3.6), it necessarily contains Planck's constant.[3)]

In Eq. (3.5a) let us set $q_2 = q_0$ and $q_1 = q$. Then

$$F(q) = [F^*(q_0)]^{-1}\int W\left(p, \frac{q + q_0}{2}\right)\exp[ip(q - q_0)/\hbar]\, dp.$$

Setting $q_1 = q_2 = q_0$, we have

$$|F(q_0)|^2 = \int W(p, q_0)\, dp, \quad F^*(q_0) = \sqrt{\int W(p, q_0)\, dp}\,\exp(-i\varphi).$$

A value of q_0 can always be chosen such that $F^*(q_0) \neq 0$. Substituting this expression in the formula for $F(q)$, we get the relation

$$F(q) = \int W\left(p, \frac{q + q_0}{2}\right)\exp[ip(q - q_0)/\hbar]\, dp\left[\int W(p, q_0)\, dp\right]^{-1/2}\exp(i\varphi), \tag{3.7}$$

which allows us to reconstruct the wave function $F(q)$, up to a phase factor, from the Wigner function. It is easy to verify that if the function W is given by Eq. (2.20), and consequently satisfies the condition (3.6), then substitution of this function in Eq. (3.7) leads to the relation $F(q) = \psi(q)\exp(i\alpha)$, $\alpha^* = \alpha$.

Accordingly, Eq. (3.6) is a necessary and sufficient condition for the function W to describe a pure quantum state, and if it is satisfied the wave function can be reconstructed, up to a constant phase factor, from the Wigner function.

[3)] The writer is very grateful to V. I. Ritus, who called attention in his critique of this article to the possibility of proving in this manner that Planck's constant appears in the Wigner function.

If we apply the inversion formula (3.7) to a function W which does not satisfy the condition (3.6), we also can obtain some function $F(q)$. However, if we substitute this function into Eq. (2.20) instead of $\psi(q)$, the reconstricted function $W(p,q)$ will not be the same as the original one. This agreement or disagreement can be used also as a necessary and sufficient criterion for whether or not the state described by a function W is a pure state.

Since the condition (3.6) indicates that it is possible to reconstruct the wave function, quasidensities that satisfy this condition automatically satisfy the uncertainty relation. First let us illustrate this with an example. Consider a joint Gaussian distribution for p and q. The general form of this is:

$$W(p,q)=[2\pi\sigma_p\sigma_q\sqrt{1-r^2}]^{-1} \times\exp\left(-\frac{1}{2(1-r^2)}\left[\frac{(p-\bar p)^2}{\sigma_p^2}-\frac{2r(p-\bar p)(q-\bar q)}{\sigma_p\sigma_q}+\frac{(q-\bar q)^2}{\sigma_q^2}\right]\right); \quad (3.8)$$

here $\bar q,\bar p$ are the mean values, σ_q,σ_p the root-mean-square deviations, and r is the correlation coefficient of the coordinate and momentum. It follows from Eq. (3.6) that the parameters of the distribution must be connected by the relation

$$\sigma_p^2\sigma_q^2(1-r^2)=\hbar^2/4. \quad (3.9)$$

Since $0\leqslant r^2\leqslant 1$, it follows from Eq. (3.8) that $\sigma_p\sigma_q\geqslant\hbar/2$. Accordingly, an arbitrary Gaussian distribution cannot correspond to a pure quantum-mechanical state. Only if its parameters are connected by the relation (3.9) will will it describe a pure state of a quantum-mechanical system.

We shall make several remarks in connection with the distribution (3.8),(3.9). First, as has been shown in Ref. 28, a Gaussian distribution with its parameters related by Eq. (3.9) is the only positive Wigner distribution for a pure state (see Sec. 5); all other Wigner functions that describe pure states necessarily take on negative values for some values of p,q. The Gaussian distribution (3.8),(3.9) corresponds to the correlated coherent states introduced in Ref. 29. For these states the sign of equality is attained in the general uncertainty relation which holds for a given value of the correlation coefficient r:

$$\sigma_A^2\sigma_B^2(1-r^2)\geqslant\frac{1}{4}|\langle[\hat A,\hat B]\rangle|^2. \quad (3.10)$$

The uncertainty condition in this form was first established in Refs. 30 and 31 for Hermitean operators in pure states, and was extended in Ref. 29 to the case of nonhermitian operators in mixed states.

We note that from the condition (3.9) one can also derive relations for higher statistical moments. Since for the Gaussian probability distribution the higher moments can be expressed in terms of the second-order moments, we have the relation

$$[\langle(p-\bar p)^{2n}\rangle\langle(q-\bar q)^{2n}\rangle]^{1/2n}=\frac{[(2n-1)!!]^{1/n}}{\sqrt{1-r^2}}\frac{\hbar}{2}.$$

For larger values of n there is roughly a linear increase of the right member of this equation with n.

The relation (3.6) can be used to test whether an arbitrarily chosen function $W(p,q)$ can represent a pure quantum state. For example, it is easily verified that a function $W(p,q)$ which is constant inside a rectangular region in the (p,q) plane and zero outside this region cannot describe a pure quantum state.

The formal proof that a quasidensity $W(p,q)$ that satisfies the restriction (3.6) agrees with the uncertainty relation is very simple. Indeed, we have to show that

$$\left[\int\int(p-\bar p)^2W(p,q)\,dp\,dq\right]\left[\int\int(q-\bar q)^2W(p,q)\,dp\,dq\right]\geqslant\hbar^2/4 \quad (3.11)$$

where

$$\bar p=\int\int pW(p,q)\,dp\,dq,\quad \bar q=\int\int qW(p,q)\,dp\,dq.$$

But it follows from Eq. (3.7) that from a function $W(p,q)$ that satisfies the condition (3.6) we can reconstruct $\psi(q)$ up to a constant phase factor. Also it has already been shown that the average values $\langle\psi|\hat p|\psi\rangle,\langle\psi|\hat p^2|\psi\rangle,\langle\psi|\hat q|\psi\rangle,\langle\psi|\hat q^2|\psi\rangle$ are equal to the corresponding averages found by using W, if this function is constructed from the given $\psi(q)$. Since when the condition (3.6) is satisfied the correspondence between $\psi(q)$ and $W(p,q)$ is reciprocally unique, the mean values in question are identical and the relation (3.11) holds, since it has been proved for mean values calculated as $\langle\psi|\ldots|\psi\rangle$.

We point out a further property of the function $W(p,q)$ which holds for pure states. Starting from Eq. (2.20), it is easy to show that

$$\int\int W^2(p,q)\,dp\,dq=(2\pi\hbar)^{-1}.$$

This property distinguishes the Wigner function of a pure state from those of mixed states. In the general case the relation is

$$\int\int W^2(p,q)\,dp\,dq\leqslant(2\pi\hbar)^{-1}, \quad (3.12)$$

with the sign of equality only for a pure state.

Before deriving the relation (3.12) we give a useful formula which expresses the transition probability from state $|\psi_i\rangle$ to state $|\psi_k\rangle$ in terms of the Wigner functions $W_j(p,q)=\langle\psi_j|W(p,q)|\psi_j\rangle$

$$2\pi\hbar\int\int W_i(p,q)\,W_k(p,q)\,dp\,dq=|\langle\psi_i|\psi_k\rangle|^2. \quad (3.13)$$

This formula is easily proved by direct calculation of the integral involved, if one uses the representation (2.20) for the Wigner functions.

Let us consider mutually orthogonal states $|\psi_1\rangle,|\psi_2\rangle,\ldots,(\langle\psi_i|\psi_k\rangle=\delta_{ik})$ with the corresponding Wigner functions $W_i(p,q)$, and form from them the mixed state described by the function

$$W(p,q)=\sum\alpha_iW_i(p,q).$$

Obviously the probabilities α_i must satisfy the conditions

$$0\leqslant\alpha_i\leqslant1,\ \sum\alpha_i=1. \quad (3.14)$$

Consider the expression

$$\int\int W^2(p,q)\,dp\,dq=\sum\sum\alpha_i\alpha_k\int\int W_iW_k\,dp\,dq.$$

Since in our case $\langle\psi_i|\psi_k\rangle=\delta_{ik}$, it follows from Eq. (3.13)

that

$$\int\int W^2(p, q)\,dp\,dq = (2\pi\hbar)^{-1}\sum \alpha_i^2.$$

But by Eq. (3.14) $\sum \alpha_i^2 \leqslant 1$, so that the relation (3.12) holds. The equality $\sum \alpha_i^2 = 1$ is possible only in the case when one of the coefficients α_k is equal to unity and the rest are equal to zero, i.e., in a pure state. Owing to this Eq. (3.12) is sometimes used as a criterion for testing whether a state is a pure state. Here, however, it must be kept in mind that the equality sign in Eq. (3.12) is a necessary, but by no means a sufficient, condition for a pure state. It can be so used only if it is already established that W is a linear combination of Wigner functions of pure states with coefficients satisfying the conditions (3.14). But if we are considering some actual Wigner function W, concerning which we know only that it satisfies the normalization condition and gives the equality sign in Eq. (3.12), we are not justified in assering that it is the Wigner function of some pure state. Moreover, in general it can fail to be a Wigner function at all, since it may lead to negative mean values of operators known to be positive. As an example, consider the function

$$\widetilde{W}(p, q) = (3\pi\hbar)^{-1}(8\mathscr{E} - 2\mathscr{E}^2 - 1)\exp(-\mathscr{E}), \qquad (3.15)$$

where

$$\mathscr{E} = \frac{2}{\hbar\omega}[(p^2/2m) + (m\omega^2 q^2/2)].$$

It can be verified easily that this function satisfies the normalization condition and makes Eq. (3.12) an equality. But the condition (3.6) is not satisfied for it, and the function (3.15) is not the Wigner function of a pure state. In this case it is easy to explain the apparent contradiction. The point is that the function (3.15) can be represented in the form

$$\widetilde{W}(p, q) = \frac{2}{3}W_0(p, q) + \frac{2}{3}W_1(p, q) - \frac{1}{3}W_2(p, q),$$

where $W_i(p, q)$ are Wigner functions corresponding to stationary states of the harmonic oscillator [see Eq. (5.43)]. The coefficients are chosen here so that $\sum \alpha_k = \sum \alpha_k^2 = 1$, and therefore the sign of equality holds in Eq. (3.12). The contradiction is due to the fact that the conditions (3.14) are violated and one of the "probabilities" is negative.

When the conditions (3.14) are violated the Wigner function of the mixed state is not positive definite, and this can manifest itself in that when it is used to calculate the mean value of a clearly positive quantity the result may turn out negative. This contradiction, however, cannot appear for every positive operator. For example, if one of the coefficients (say α_3) is negative but the positive operator A being averaged satisfies the condition $\hat{A}|\psi_3\rangle = 0$, the mean value obtained can be nonnegative. Therefore for mixed states a check that the Wigner function is positive definite (that the coefficients α_k are positive) must precede the use of the criterion (3.12). Such a check, however, is a very complicated problem.

At the same time, the criterion (3.6) is both a necessary and a sufficient condition for the "purity" of a state, and its use gives rise to no difficulties.

4. THE EQUATION OF EVOLUTION OF THE QUASIPROBABILITY (THE QUANTUM LIOUVILLE EQUATION) AND SOME OF ITS CONSEQUENCES

a) Derivation of the equation of evolution

Since the dynamics of a quantum system is determined by the Schrödinger equation

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = [(\hat{p}^2/2m) + V(\hat{q})]\,|\psi\rangle, \quad |\psi(t_0)\rangle = |\psi_0\rangle, \qquad (4.1)$$

the Wigner function $W(p, q)$ constructed from a solution of Eq. (4.1) will also depend on the time. Let us find the equation of evolution for this function.

It is simplest to start from the equation for $\rho(q_1, q_2, t) = \psi(q_1, t)\psi^*(q_2, t)$:

$$\frac{\partial\rho}{\partial t} = \left[\frac{i\hbar}{2m}\left(\frac{\partial^2}{\partial q_1^2} - \frac{\partial^2}{\partial q_2^2}\right) + \frac{1}{i\hbar}(V(q_1) - V(q_2))\right]\rho(q_1, q_2, t).$$

In accordance with Eq. (2.21), which connects ρ and W, we set $q_{1,2} = q \mp (\xi/2)$. Then in the new variables we obtain the equation

$$\frac{\partial\rho}{\partial t} = \left[-\frac{i\hbar}{m}\frac{\partial^2}{\partial q\,\partial\xi} + \frac{1}{i\hbar}\left(V\left(q - \frac{\xi}{2}\right) - V\left(q + \frac{\xi}{2}\right)\right)\right]\rho\left(q - \frac{\xi}{2}, q + \frac{\xi}{2}\right). \qquad (4.2)$$

We now differentiate Eq. (2.21) with respect to t and substitute Eq. (4.2):

$$\frac{\partial W(p, q, t)}{\partial t} = \frac{1}{2\pi\hbar}\int d\xi \exp(ip\xi/\hbar) \times\left[-\frac{i\hbar}{m}\frac{\partial^2\rho}{\partial q\,\partial\xi} + \frac{1}{i\hbar}\left(V\left(q - \frac{\xi}{2}\right) - V\left(q + \frac{\xi}{2}\right)\right)\rho\right]. \qquad (4.3)$$

We transform the first term, bringing $\partial/\partial q$ outside the integral sign and integrating by parts over ξ:

$$\frac{1}{2\pi\hbar}\int -\frac{i\hbar}{m}e^{ip\xi/\hbar}\frac{\partial^2\rho}{\partial q\,\partial\xi}\,d\xi = \frac{i\hbar}{m}\frac{\partial}{\partial q}\frac{1}{2\pi\hbar}\int \rho\frac{\partial}{\partial\xi}e^{ip\xi/\hbar}\,d\xi = \frac{i\hbar}{m}\frac{ip}{\hbar}\frac{\partial W}{\partial q}.$$

We transform the second term, noting the formula

$$\xi^n\exp(ip\xi/\hbar) = \left(\frac{\hbar}{i}\frac{\partial}{\partial p}\right)^n\exp(ip\xi/\hbar),$$

from which it follows that for functions V analytic at the point q

$$V\left(q \pm \frac{\xi}{2}\right)\exp(ip\xi/\hbar) = V\left(q \pm \frac{\hbar}{2i}\frac{\partial}{\partial p}\right)\exp(ip\xi/\hbar).$$

Then we have

$$\frac{1}{i\hbar}\frac{1}{2\pi\hbar}\int d\xi\,\rho\left[V\left(q - \frac{\xi}{2}\right) - V\left(q + \frac{\xi}{2}\right)\right]\exp(ip\xi/\hbar)$$
$$= \frac{i1}{i\hbar}\frac{1}{2\pi\hbar}\int d\xi\,\rho\left[V\left(q + \frac{i\hbar}{2}\frac{\partial}{\partial p}\right) - V\left(q - \frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right]\exp(ip\xi/\hbar)$$
$$= \frac{1}{i\hbar}\left[V\left(q + \frac{i\hbar}{2}\frac{\partial}{\partial p}\right) - V\left(q - \frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right]W(p, q, t)$$

As the result we get the equation of evolution for the function W, written in operator form:

$$\frac{\partial W}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial q} + \frac{1}{i\hbar}\left[V\left(q + \frac{i\hbar}{2}\frac{\partial}{\partial p}\right) - V\left(q - \frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right]W. \qquad (4.4a)$$

This same equation can also be written in a different form:

$$\frac{\partial W}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial q} + \frac{2}{\pi\hbar^2}\int W(p - p', q)\,dp'\int V(q - q')\sin\frac{2p'q'}{\hbar}\,dq'. \qquad (4.4b)$$

This is obtained if in the right member of Eq. (4.3) we substitute the inversion of Eq. (2.21):

$$\rho\left(q - \frac{\xi}{2}, q + \frac{\xi}{2}\right) = \int W(p', q)\exp(-ip'\xi/\hbar)\,dp'.$$

Equation (4.4) is the quantum generalization of the classical Liouville equation (1.1). It was derived in

Wigner's paper.[1] We shall call it the quantum Liouville equation.

We now discuss some properties of Eq. (4.4).

b) The classical limit

If we expand the potential V in series at the point q, Eq. (4.4a) can be written in the form of the following expansion:

$$\frac{\partial W}{\partial t}+\frac{p}{m}\frac{\partial W}{\partial q}-V'(q)\frac{\partial W}{\partial p}=-\frac{\hbar^2}{24}V'''(q)\frac{\partial^3 W}{\partial p^3}+\dots \tag{4.5}$$

Accordingly, when we neglect quantities of the order $\hbar^2$ the quantum Liouville equation goes over into the classical equation.

The transition to the classical limit can be examined in more detail. To do so we represent Eq. (4.4a) in the form

$$\frac{\partial W}{\partial t}+\frac{p}{m}\frac{\partial W}{\partial q}-V'(q)\frac{\partial W}{\partial p}=\left[\frac{1}{i\hbar}\left(V\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)-V\left(q-\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right)-V'(q)\frac{\partial}{\partial p}\right]W. \tag{4.6}$$

We introduce the notation

$$\Phi(p,q,t)=\left[\frac{1}{i\hbar}\left(V\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)-V\left(q-\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right)-V'(q)\frac{\partial}{\partial p}\right]W \tag{4.7}$$

and write Eq. (4.6) in the form of an inhomogeneous classical Liouville equation,

$$\frac{\partial W}{\partial t}+\frac{p}{m}\frac{\partial W}{\partial q}-V'(q)\frac{\partial W}{\partial p}=\Phi(p,q,t). \tag{4.8}$$

The solution of Eq. (4.8) with the initial condition $W(p,q,0)=W_0(p,q)$ can be written in the form

$$W(p,q,t)=\iint G(p,q,t;p_0,q_0,0)W_0(p_0,q_0)\,dp_0\,dq_0+\int_0^t dt_0\iint G(p,q,t;p_0,q_0,t_0)\Phi(p_0,q_0,t_0)\,dp_0\,dq_0; \tag{4.9}$$

here G is the Green's function of the classical Liouville equation, which is of the form

$$G(p,q,t;p_0,q_0,t_0)=\delta(p-\bar p(t;t_0,p_0,q_0))\,\delta(q-\bar q(t;t_0,p_0,q_0)), \tag{4.10}$$

where p,q are the solutions of the classical equations of motion

$$\frac{d\bar q}{dt}=\bar p/m,\quad \frac{d\bar p}{dt}=-V'(\bar q)$$

with the initial conditions

$$\bar p(t_0;t_0,p_0,q_0)=p_0,\quad \bar q(t_0;t_0,p_0,q_0)=q_0.$$

We now substitute Eq. (4.7) into the right member of Eq. (4.9).

The result is the equation

$$W(p,q,t)=W^{(0)}(p,q,t)+\int_0^t dt_0\iint dp_0\,dq_0 G(p,q,t;p_0,q_0,t_0)\times\left[\frac{1}{i\hbar}\left(V\left(q_0+\frac{i\hbar}{2}\frac{\partial}{\partial p_0}\right)-V\left(q_0-\frac{i\hbar}{2}\frac{\partial}{\partial p_0}\right)\right)-V'(q_0)\frac{\partial}{\partial p_0}\right]W(p_0,q_0,t_0). \tag{4.11a}$$

Here we have introduced the notation

$$W^{(0)}(p,q,t)=\iint G(p,q,t;p_0,q_0,0)\,W_0(p_0,q_0)\,dp_0dq_0. \tag{4.12}$$

If we use the Fourier transform of the function $W(p_0,q_0,t_0)$ with respect to p_0 in the right member of Eq. (4.11a) and perform the action of the operator $\partial/\partial p_0$, the equation can be put in the form of a pure integral equation

$$W(p,q,t)=W^{(0)}(p,q,t)+\frac{1}{2\pi}\int_0^t dt'\iint dp'\,dq'\left\{\iint d\lambda\,dp_0\lambda G(p,q,t;p_0,q',t')\sin[\lambda(p_0-p')]\times\left[V'(q')-\frac{1}{\lambda\hbar}\left(V\left(q'+\frac{\lambda\hbar}{2}\right)-V\left(q'-\frac{\lambda\hbar}{2}\right)\right)\right]\right\}W(p',q',t'). \tag{4.11b}$$

Equation (4.11) was derived by Shirokov.[14] We shall explain its meaning. The function $W^{(0)}(p,q,t)$ defined by Eq. (4.12) is formally the solution of the classical Liouville equation corresponding to the initial distribution $W_0(p,q)$. Therefore, if we consider the solution of Eq. (11b) in the form of an iterative series, its next terms will bring in quantum corrections to the classical solution. It must be remembered, however, that in our treatment of pure quantum-mechanical states by means of the Shirokov equation the function $W_0(p_0,q_0)$ in Eq. (4.12), and consequently also the function $W^{(0)}(p,q,t)$ will already contain the Planck constant [owing to the restriction (3.6)]. Therefore it would be more correct to call $W^{(0)}(p,q,t)$ not the classical solution, but an initial classical distribution developing according to the laws of quantum mechanics.

c) Existence of extraneous solutions and their removal

If the potential $V(q)$ is of the form $V_0+V_1q+V_2q^2$, then $\frac{1}{i\hbar}\left[V\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)-V\left(q-\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right]=V'(q)\frac{\partial}{\partial p}$.

Accordingly, for the oscillator problem the classical and quantum Liouville equations are identical, and the right side of Eq. (4.5) vanishes identically. However, as is well known, the solution of the problem of the quantum oscillator is decidedly different from the classical solution. Therefore *in the Wigner representation the difference between classical and quantum mechanics does not reduce merely to a difference between the quantum and classical Liouville equations.* With this example we shall demonstrate that *Eq* (4.4) *is satisfied not only by the solutions that correspond to quantum mechanics, but also by some "extra" solutions.* Indeed, for the oscillator problem the quantum Liouville equation is satisfied by any solution of the classical equation.

Because the quantum Liouville equation is liner, the "extra" solutions can describe the evolution of linear combinations of Wigner functions corresponding to different pure states. Furthermore, if the coefficients of this linear combination satisfy the conditions (3.14), then we have to do with the evolution of a mixed state, whereas if these conditions are not satisfied [as in the example (3.15)], the "extra" solutions have no physical meaning at all.

For quantum-mechanical problems the initial condition for Eq. (4.4) must satisfy the relation (3.6), i.e.,

$$\frac{\partial^2}{\partial q_1\partial q_2}\ln\left[\int W_0\left(p,\frac{q_1+q_2}{2}\right)\exp[ip(q_1-q_2)/\hbar]\,dp\right]=0. \tag{4.13}$$

At the same time, the initial condition for the classical Liouville equation can be an arbitrary positive function. As has already been pointed out, owing to the condition (4.12) *Planck's constant is involved not only in the*

quantum Liouville equation, but also in the initial condition for it. Therefore the quantum features of the problem can also be due to specifically quantum initial conditions. For example, in the case of the quantum oscillator this is precisely the case.

We shall show that if the condition (4.13) is satisfied for the initial distribution, then it will also be satisfied at all later times. In fact, when this condition holds we can reconstruct from $W(p,q,0)$ the wave function of the initial state. Since by Schrödinger's equation a pure initial state remains pure throughout time, the Wigner function also, calculated from the solution of the Schrödinger equation for $t>0$ will describe a pure state, and consequently will satisfy the condition (3.6).

Accordingly, if the initial distribution of the quasiprobability belongs to the class of admissible quantum distributions, it will remain admissible over the course of time.

d) Equivalence of the Wigner and Schröedinger representations of quantum mechanics

We have so far been studying the Wigner representation of quantum mechanics by starting from the Schrödinger representation. We shall now show that if we take as foundation the Wigner representation, then from it we can obtain the Schrödinger representation. It is clear that, along with the quantum Liouville equation, we must include in the formulation of the Wigner representation the condition (4.13), since otherwise, as we have already seen, this equation can be satisfied by solutions that have no bearing on quantum mechanics, and are even devoid of physical meaning.

Accordingly, let the function $W(p,q,t)$ satisfy Eq. (4.4), and let the initial distribution $W(p,q,0)=W_0(p,q)$ satisfy the condition (4.13). We shall show that in this case the wave function reconstructed from $W(p,q,t)$ by means of Eq. (3.7) will satisfy the Schrödinger equation and the required initial condition for it. Thus we shall show that there is a reciprocally unique correspondence between the two representations.

As was shown earlier, if the condition (4.13) is satisfied at the initial time, then it is satisfied at all later times. But in this case, as has been shown, the Wigner function can be represented in the form

$$W(p,q,t)=\frac{1}{2\pi\hbar}\int e^{ip\xi/\hbar}F^*\left(q+\frac{\xi}{2},t\right)F\left(q-\frac{\xi}{2},t\right)d\xi. \qquad (4.14)$$

Substituting Eq. (4.14) into Eq. (4.4a), after obvious transformations we can write the latter equation in the form

$$\int d\xi \exp\left(\frac{ip\xi}{\hbar}\right)\frac{\partial}{\partial t}\left[F^*\left(q+\frac{\xi}{2},t\right)F\left(q-\frac{\xi}{2},t\right)\right]$$
$$+\int d\xi\left[\frac{\hbar}{im}\frac{\partial}{\partial\xi}\exp\left(\frac{ip\xi}{\hbar}\right)\right]\frac{\partial}{\partial q}\left[F^*\left(q+\frac{\xi}{2}\right)F\left(q-\frac{\xi}{2}\right)\right]$$
$$+\frac{1}{i\hbar}\int d\xi F^*\left(q+\frac{\xi}{2}\right)F\left(q-\frac{\xi}{2}\right)\left[V\left(q-\frac{i\hbar}{2}\frac{i\xi}{\hbar}\right)-V\left(q+\frac{i\hbar}{2}\frac{i\xi}{\hbar}\right)\right]\exp\left(\frac{ip\xi}{\hbar}\right)=0.$$

Integrating the second term by parts, and using the fact that the total integral is equal to zero for arbitrary p, we equate its integrand to zero:

$$\frac{\partial}{\partial t}\left[F^*\left(q+\frac{\xi}{2}\right)F\left(q-\frac{\xi}{2}\right)\right]-\frac{\hbar}{im}\frac{\partial^2}{\partial q\,\partial\xi}\left[F^*\left(q+\frac{\xi}{2}\right)F\left(q-\frac{\xi}{2}\right)\right]$$
$$+\frac{1}{i\hbar}\left[V\left(q+\frac{\xi}{2}\right)-V\left(q-\frac{\xi}{2}\right)\right]F^*\left(q+\frac{\xi}{2}\right)F\left(q-\frac{\xi}{2}\right)=0.$$

After changing to the variables $q\pm(\xi/2)=q_{1,2}$, noting $2(\partial^2/\partial q\,\partial\xi)=(\partial^2/\partial q_1^2)-(\partial^2/\partial q_2^2)$ we obtain

$$i\hbar\frac{\partial}{\partial t}[F^*(q_1)F(q_2)]-\frac{\hbar^2}{2m}\left[F(q_2)\frac{\partial^2F^*(q_1)}{\partial q_1^2}-F^*(q_1)\frac{\partial^2F(q_2)}{\partial q_2^2}\right]$$
$$+[V(q_1)-V(q_2)]F^*(q_1)F(q_2)=0.$$

Dividing this equation by $F^*(q_1)F(q_2)$, we write it in the form

$$\frac{1}{F(q_2)}\left[i\hbar\frac{\partial F(q_2)}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2F(q_2)}{\partial q_2^2}-V(q_2)F(q_2)\right]$$
$$=\frac{1}{F^*(q_1)}\left[-i\hbar\frac{\partial F^*(q_1)}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2F^*(q_1)}{\partial q_1^2}-V(q_1)F^*(q_1)\right]=\Phi(t)=\Phi^*(t),$$

here $\Phi(t)$ is an arbitrary function of the time, independent of the coordinates.

Accordingly, the equation for $F(q)$ can be written in the form

$$i\hbar\frac{\partial F}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2F}{\partial q^2}-[V(q)+\Phi(t)]F(q,t)=0. \qquad (4.15a)$$

If we introduce the function

$$\psi(q,t)=F(q,t)\exp\left[\frac{i}{\hbar}\int_0^t\Phi(t')\,dt'\right],$$

which differs from F only by a phase factor independent of the coordinates, then it satisfies the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2}+V(q)\psi. \qquad (4.15b)$$

It is also obvious that for $t=0$ the wave function satisfies an initial condition which corresponds to the initial distribution of the quasiprobability.

Accordingly, we have shown that from a quantum Liouville equation with an initial condition satisfying the restriction (4.13) on the allowable form of pure quantum distributions, there follows the Schrödinger equation. In particular, if the initial distribution satisfies, besides the condition (4.13), the condition for it to be a stationary distribution

$$-\frac{p}{m}\frac{\partial W_0}{\partial q}+\frac{1}{i\hbar}\left[V\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)-V\left(q-\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right]W_0=0, \qquad (4.16)$$

then in Eq. (4.15a) the term $i\hbar\partial F/\partial t$ will be absent, and the function $\Phi=-E$ will not depend on the time. In this case Eq. (4.15a) takes on the form of the eigenvalue equation for the energy

$$-\frac{\hbar^2}{2m}\frac{\partial^2F}{\partial q^2}+V(q)F=EF. \qquad (4.15c)$$

Another way to describe stationary states, based on subjecting the function W to a second equation of the same type as the Liouville equation, is described in Ref. 15. In that paper, as also in Ref. 34, there is also an investigation of the eigenfunctions of the quantum Liouville equation.

We shall illustrate the role of the condition (4.13) with the example of the oscillator. If $V(q)=m\omega^2q^2/2$, the solution of Eq. (4.16) is of the form

$$W_0(p,q)=f\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right),$$

i.e., an arbitrary function of the Hamiltonian is a stationary solution of the Liouville equation. But an arbitrary solution of this form does not satisfy the condition (4.13), which selects the admissible quantum distributions. Let us suppose for simplicity that $f(H)$ is of the form

$$W_0(p, q)=N\exp\left[-\alpha\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right] \tag{4.17}$$

with an unknown coefficient α. Substituting Eq. (4.17) into Eq. (4.13) and calculating the integral, we easily verify that it can be factored with respect to the variables q_1, q_2 only if

$$\alpha = 2/\hbar\omega, \tag{4.18}$$

i.e., the stationary probability distribution for the oscillator can be of the form

$$W_0(p, q)=\frac{1}{\pi\hbar}\exp\left[-\frac{2}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right]. \tag{4.19}$$

The mean value of the oscillator energy in this state is given by

$$\langle E\rangle=\frac{1}{\pi\hbar}\iint\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\exp\left[-\frac{2}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right]dp\,dq=\frac{\hbar\omega}{2}.$$

However, in order to find $\langle E^2\rangle$ we must average over *the distribution* $W_0(p, q)$ *not the function* $H^2(p, q)$, *but the* function $H^2(p, q)-(\hbar\omega/2)^2$, which, according to Eq. (3.4b), corresponds to the operator H^2 in the Wigner representation. It is not hard to verify that

$$\langle E^2\rangle=\frac{1}{\pi\hbar}\iint\left[\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)^2-\left(\frac{\hbar\omega}{2}\right)^2\right]\times\exp\left[-\frac{2}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right]dp\,dq=\left(\frac{\hbar\omega}{2}\right)^2. \tag{4.20}$$

We here encounter an important peculiarity of the Wigner representation. On one hand, we see that $\langle E^n\rangle = (\hbar\omega/2)^n$ for $n=1, 2, \ldots$ If we were dealing with an ordinary probability density, in this case it would have to be

$$W_{\rm cl}(p, q)=\frac{\omega}{2\pi}\delta\left(H(p, q)-\frac{\hbar\omega}{2}\right),$$

i.e., it would have to be concentrated on lines of equal energy. We see, however, that the quasiprobability density corresponding to a fixed energy value $E=\hbar\omega/2$ is nevertheless "smeared out" over the entire phase plane and is different from zero where $H(p, q)\neq\hbar\omega/2$.

A second important circumstance to which we wish to call attention is that we have obtained the quantization condition on the oscillator energy not from the equation of motion for $W(p, q)$ (the quantum Liouville equation), but from the supplementary condition which distinguishes those Wigner distributions that correspond to pure quantum states. From this example it can be seen quite clearly that in the Wigner representation Planck's constant can enter the theory not only from the equation of evolution (which is a consequence of the Schrödinger equation), but also from the initial condition, which in the quantum problem has to satisfy the supplementary equation (4.13), which assures, in particular, that the uncertainty relation is satisfied in the initial state.

5. CONDITIONS FOR NONNEGATIVITY OF THE QUASIPROBABILITY AND THE SMOOTHED QUASIPROBABILITY

We have already mentioned that the Wigner quasiprobability $W(p, q)$ does not satisfy the condition that it be positive definite. Here we shall examine this question in more detail. For this purpose we find the eigenvalues and eigenvectors of the operator $\hat{W}(p, q)$. Using Eq. (2.19), we write it in the form

$$\hat{W}(p, q)=\frac{1}{\pi\hbar}\hat{J}(p, q), \tag{5.1}$$

where

$$\hat{J}(p, q)=\frac{1}{2}\int\left|q-\frac{\xi}{2}\right\rangle\exp(-ip\xi/\hbar)\,d\xi\left\langle q+\frac{\xi}{2}\right|. \tag{5.2}$$

Let us consider the operator $\hat{J}^2(p, q)$:

$$\hat{J}^2(p, q)=\frac{1}{4}\int\int\left|q-\frac{\xi_1}{2}\right\rangle e^{-ip\xi_1/\hbar}\,d\xi_1\left\langle q+\frac{\xi_1}{2}\right|q-\frac{\xi_2}{2}\Big\rangle e^{-ip\xi_2/\hbar}\,d\xi_2\left\langle q+\frac{\xi_2}{2}\right|.$$

Since

$$\left\langle q+\frac{\xi_1}{2}\right|q-\frac{\xi_2}{2}\Big\rangle=\delta\left(\frac{\xi_1+\xi_2}{2}\right)=2\delta(\xi_1+\xi_2),$$

we have

$$\hat{J}^2(p, q)=\frac{1}{2}\int\left|q-\frac{\xi}{2}\right\rangle d\xi\left\langle q-\frac{\xi}{2}\right|=\int|q'\rangle\,dq'\,\langle q'|=\hat{1}.$$

Accordingly, the square of the operator $\hat{J}$ is equal to $\hat{1}$:

$$\hat{J}^2(p, q)=\hat{1}. \tag{5.3}$$

Consequently, the eigenvalues of the operator $\hat{J}$ can be ±1, and the eigenvalues of the operator W, connected with J by Eq. (5.1) are $\pm(\pi\hbar)^{-1}$.

Let us consider the action of $\hat{J}$ on some vector $|\psi\rangle$:

$$|\tilde{\psi}_{pq}\rangle=\hat{J}(p, q)\,|\psi\rangle. \tag{5.4}$$

Multiplying this equation on the left by $\langle q'|$ and denoting $\langle q'|\tilde{\psi}_{pq}\rangle=\tilde{\psi}_{pq}(q')$, we write the transformation (5.4) in the coordinate representation:

$$\tilde{\psi}_{pq}(q')=\frac{1}{2}\int\delta\left(q'-q+\frac{\xi}{2}\right)\exp(-ip\xi/\hbar)\,\psi\left(q+\frac{\xi}{2}\right)d\xi=\psi(2q-q')\exp\left[-\frac{2ip}{\hbar}(q-q')\right].$$

As we have already explained, the eigenvalues of the operator $\hat{J}$ are ±1. Therefore, in order to find the eigenfunctions of this operator we must find the solutions of the equation $\tilde{\psi}_{pq}(q')=\pm\psi(q')$, or, if we use the expression we have obtained for $\tilde{\psi}_{pq}$,

$$\psi(q')=\pm\exp\left[\frac{-2ip(q-q')}{\hbar}\right]\psi(2q-q'). \tag{5.5}$$

Let us introduce instead of $\psi(q')$ a new unknown function $\alpha(q')$ in accordance with the equation

$$\psi(q')=\exp(ipq'/\hbar)\,\alpha(q'-q),\quad\alpha(q')=\exp\left[-\frac{ip}{\hbar}(q'+q)\right]\psi(q'+q). \tag{5.6}$$

Then, expressing ψ in Eq. (5.5) in terms of α, we obtain the equation

$$\alpha(q'-q)=\pm\alpha(q-q'). \tag{5.7}$$

A solution of Eq. (5.7) corresponding to the eigenvalue $+1$ of the operator J is an arbitrary even function $\alpha(q')$, and to the eigenvalue—1 corresponds an arbitrary odd function $\alpha(q')$. Accordingly, the operator $\hat{J}$ can be called[25] a parity operator.[4)] Its properties are described in more detail in Refs. 25, 32, and 33.

An arbitrary even (odd) function $\alpha(q')$ can be written in the form

$$\alpha^{\pm}(q')=\int_0^\infty\Phi^{\pm}(\varkappa;\ p, q)^{\cos}_{\sin}(\varkappa q')\,d\varkappa. \tag{5.8}$$

[4)] It is easy to show that the operator $\hat{J}$ satsifies the equations[32,33]

$$\hat{J}(p, q)(\hat{q}-q)\hat{J}(p, q)=-(\hat{q}-q),\quad\hat{J}(p, q)(\hat{p}-p)\hat{J}(p, q)=-(\hat{p}-p).$$

Here the functions $\Phi^{\pm}$ can depend on p, q as parameters, since the operator $\hat{J}(p,q)$ depends on them. Substituting the resulting values $\alpha^{\pm}(q')$ in Eq. (5.6), we find that

$$\psi^{\pm}(q') \equiv \langle q' | p, q, \pm \rangle = \exp(ipq'/\hbar) \int_0^{\infty} \Phi^{\pm}(\varkappa; p, q) \begin{matrix}\cos\\ \sin\end{matrix} (\varkappa(q'-q))\, d\varkappa.$$

Then for the eigenvectors $|p, q, \pm\rangle$ we easily obtain

$$|p, q, \pm\rangle = \int |q'\rangle\, dq'\, \langle q' | p, q, \pm\rangle = \int_0^{\infty} \Phi^{\pm}(\varkappa; p, q)\, d\varkappa \int |q'\rangle \exp(ipq'/\hbar) \begin{matrix}\cos\\ \sin\end{matrix} (\varkappa(q'-q))\, dq'. \quad (5.9)$$

We see that an arbitrary eigenvector of the operator $\hat{J}$ can be expanded in terms of the vectors

$$|p, q; \pm, \varkappa\rangle = \frac{1}{\sqrt{\pi}} \int |q'\rangle \exp(ipq'/\hbar) \begin{matrix}\cos\\ \sin\end{matrix} (\varkappa(q'-q))\, dq'. \quad (5.10a)$$

The normalizing factor $\pi^{-1/2}$ is here chosen so that for $\varkappa, \varkappa' \geq 0$ the normalization conditions

$$\langle p, q; \pm, \varkappa | p, q; \pm, \varkappa' \rangle = \delta(\varkappa - \varkappa'), \langle p, q; \pm, \varkappa | p, q; \mp, \varkappa' \rangle = 0 \quad (5.11)$$

are satisfied. (Here we take simultaneously either the two upper or the two lower signs.) Using the formula

$$|p'\rangle = (2\pi\hbar)^{-1/2} \int |q'\rangle \exp(ipq'/\hbar)\, dq',$$

which related the basis vectors of the coordinate and momentum representations, we can perform the integration in Eq. (5.10a), writing the sine and cosine as combinations of exponentials. We then arrive at the formulas

$$|p, q; +, \varkappa\rangle = \sqrt{\hbar/2}\, [\exp(-i\varkappa q) |p + \hbar\varkappa\rangle + \exp(i\varkappa q) |p - \hbar\varkappa\rangle],$$
$$|p, q; -, \varkappa\rangle = \frac{\sqrt{\hbar/2}}{i} [\exp(-i\varkappa q) |p + \hbar\varkappa\rangle - \exp(i\varkappa q) |p - \hbar\varkappa\rangle]. \quad (5.10b)$$

Using these formulas we can easily verify that the eigenfunctions so found form a complete system:

$$\int_0^{\infty} [|p, q; +, \varkappa\rangle \langle p, q; +, \varkappa| + |p, q; -, \varkappa\rangle \langle p, q; -, \varkappa|]\, d\varkappa = \int_{-\infty}^{\infty} |p'\rangle\, dp'\, \langle p'| = \hat{1}. \quad (5.12)$$

According to Eq. (5.1) we have the relations

$$\hat{W}(p, q) |p, q; \pm, \varkappa\rangle = \pm (\pi\hbar)^{-1} |p, q; \pm, \varkappa\rangle. \quad (5.13)$$

An arbitrary state vector $|\psi\rangle$ can be expanded in terms of the eigenvectors of the operator W. Using Eq. (5.12), we get the expansions

$$|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle,$$
$$|\psi_{\pm}\rangle = \int_0^{\infty} |p, q; \pm, \varkappa\rangle\, d\varkappa \langle p, q; \pm, \varkappa | \psi\rangle. \quad (5.14)$$

$|\psi_+(p,q)\rangle$ and $|\psi_-(p,q)\rangle$ can be interpreted as the projections of the state vector onto subspaces of states making positive and negative contributions to the quasiprobability at the point (p, q). It must be kept in mind that these expansions are different for different values of p, q. It follows from Eq. (5.11) that $\langle \psi_+ | \psi_- \rangle = 0$, and from both (5.13) and (5.14) that

$$\hat{W}(p, q) |\psi_{\pm}\rangle = \pm (\pi\hbar)^{-1} |\psi_{\pm}\rangle. \quad (5.15)$$

Using the expansion (5.14), Eq. (5.15), and the orthogonality relation $\langle \psi_+ | \psi_- \rangle = 0$, we can write the Wigner function $W = \langle \psi | \hat{W} | \psi \rangle$ in the form[32]

$$W(p, q) = (\pi\hbar)^{-1} [\langle \psi_+ | \psi_+ \rangle - \langle \psi_- | \psi_- \rangle]. \quad (5.16)$$

Accordingly, $W(p, q)$ can be represented as the difference of two nonnegative quantities, and the sign of W depends on their ratio.

Let us find the quantities $\langle \psi_{\pm} | \psi_{\pm} \rangle$. If we use the notation

$$\psi(p, q; \pm, \varkappa) = \langle p, q; \pm, \varkappa | \psi \rangle,$$

then on the basis of Eq. (5.14) we have

$$\langle \psi_{\pm} | \psi_{\pm} \rangle = \int_0^{\infty} |\psi(p, q; \pm, \varkappa)|^2\, d\varkappa, \quad (5.17)$$

and from Eq. (5.10a)

$$\psi(p, q; \pm; \varkappa) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp[-ipq'/\hbar] \begin{matrix}\cos\\ \sin\end{matrix} (\varkappa(q-q'))\, \psi(q')\, dq'. \quad (5.18)$$

Substituting Eq. (5.18) in Eq. (5.17) and performing the integration over $\varkappa$, we easily obtain the formulas

$$\langle \psi_+(p, q) | \psi_+(p, q) \rangle = 2^{-1} [1 + \pi\hbar W(p, q)]. \quad (5.19a)$$
$$\langle \psi_-(p, q) | \psi_-(p, q) \rangle = 2^{-1} [1 - \pi\hbar W(p, q)]. \quad (5.19b)$$

Since $\langle \psi_{\pm} | \psi_{\pm} \rangle \geq 0$, from these equations follows the restriction[32]

$$|W(p, q)| \leq (\pi\hbar)^{-1}. \quad (5.20)$$

The bound on $|W|$ can be interpreted as another manifestation of the uncertainty relation, applying here not to the second moments of the function W, but to its form as a whole. It follows from Eq. (5.19) that since $W(p, q) \to 0$ for $|p| \to \infty$, $|q| \to \infty$, then here too

$$\langle \psi_+ | \psi_+ \rangle \approx \langle \psi_- | \psi_- \rangle \approx 2^{-1}.$$

Accordingly, even if the Wigner function is positive, the contribution to it from states with negative probability is always different from zero.

It is easy to ascertain when does the Wigner function takes on values $\pm(\pi\hbar)^{-1}$. To do so we resolve the wave function into the sum of even and odd parts, $\psi(q) = \psi_{even}(q) + \psi_{odd}(q)$, $\psi_{even}(-q) = \psi_{even}(q)$, $\psi_{odd}(-q) = -\psi_{odd}(q)$. Then, using Eq. (2.20), we obtain

$$\pi\hbar W(0, 0) = \int \psi^*(q)\, \psi(-q)\, dq = \int [|\psi_{even}(q)|^2 - |\psi_{odd}(q)|^2]\, dq.$$

Forming the sum and difference of this equation and the normalization integral

$$1 = \int [|\psi_{even}(q)|^2 + |\psi_{odd}(q)|^2]\, dq,$$

we have

$$1 + \pi\hbar W(0, 0) = 2\int |\psi_{even}|^2\, dq, \quad 1 - \pi\hbar W(0, 0) = 2\int |\psi_{odd}|^2\, dq. \quad (5.21)$$

From this it follows that if $\psi_{even, odd} = 0$, then $W(0, 0) = \mp(\pi\hbar)^{-1}$, and conversely, of $W(0, 0) = \pm(\pi\hbar)^{-1}$, then $\psi_{even, odd}(q) = 0$ almost everywhere.

Now, following Ref. 28, we shall show that *a necessary and sufficient condition for the Wigner function of a pure state to be nonnegative is that it be described by a wave function of the form*

$$\psi_{a, b}(q) = \exp\left[-\frac{1}{2}(aq^2 + 2bq + c)\right], \quad \mathrm{Re}\, a > 0. \quad (5.22)$$

The proof that the condition is sufficient is trivial: Calculating from Eq. (2.20) the function $W_{a,b}(p,q)$ corresponding to the state $\psi_{a,b}(q)$ and writing $\mathrm{Re}a=a_1$, $\mathrm{Im}a=a_2$, $\mathrm{Re}b=b_1$, $\mathrm{Im}b=b_2$, we easily find that $W_{a,b}(p,q)$ *is the joint Gaussian distribution of coordinate and momentum of the form* (3.8) *with parameters*

$$\bar{q}=-\frac{b_1}{a_1},\quad \bar{p}=\frac{\hbar}{a_1}(a_2b_1-a_1b_2),$$
$$\sigma_q^2=(2a_1)^{-1},\quad \sigma_p^2=\frac{\hbar^2(a_1^2+a_2^2)}{2a_1},\quad r=-a_2/\sqrt{a_1^2+a_2^2}, \tag{5.23}$$

which, of course, satisfy Eq. (3.9). The resulting function satisfies $W_{a,b}>0$ for arbitrary a,b,p,q.

We shall now prove that the condition (5.22) is necessary. Suppose the function $W(p,q)$ corresponding to some normalized wave function $\psi(q)$ satisfies the condition $W(p,q)\geqslant 0$. Along with this function we consider the Wigner function that corresponds to a wave function of the form (5.22), in which $a_2=0$ and $b=z$ is an arbitrary complex number. This function is of the form (3.8) and everywhere strictly positive. Let us now consider the integral of the product of these functions and use Eq. (3.19):

$$2\pi\hbar\int\int W(p,q)\,W_{a_1,z}(p,q)\,dp\,dq=|\langle\psi|\psi_{a_1,z}\rangle|^2. \tag{5.24}$$

Since the function of Gaussian form $W_{a_1,z}>0$ (strictly positive) and $W(p,q)\geqslant 0$, for arbitrary z the integrand here is nonnegative and there can always be found a region (perhaps multiply connected) in which it is strictly positive (since W cannot be identically zero owing to the normalization condition). Therefore the integral on the left side of Eq. (5.24) is strictly positive and does not vanish for any value of the complex variable z. It follows from this that the function

$$F(z)=\exp\left(\frac{c}{2}\right)\langle\psi|\psi_{a_1,z}\rangle=\int\psi^*(q)\exp\left[-\frac{1}{2}a_1q^2-zq\right]dq. \tag{5.25}$$

is an entire analytic function of the complex variable z, with no zeros. Let us estimate $|F(z)|^2$, applying the Schwartz inequality:

$$|F(z)|^2\leqslant\int|\psi(q)|^2\,dq\int\exp\left[-a_1q^2-(z+z^*)q\right]dq=\sqrt{\frac{\pi}{a_1}}\exp\left[\frac{(\mathrm{Re}z)^2}{a_1}\right].$$

From this inequality it follows that the order of increase[5)] of the function $F(z)$ does not exceed 2. Accordingly, $F(z)$ is an entire analytic function having no zeros and with order of increase not larger than 2. Then, according to a well known theorem of Hadamard (cf. e.g., Ref. 35) $F(z)$ is of the form

$$F(z)=\exp(\alpha z^2+\beta z+\gamma).$$

Substituting this expression in Eq. (5.25) and setting $z=i\varkappa$, we have

$$\int_{-\infty}^{\infty}\exp(-i\varkappa q)\,\psi^*(q)\exp(-a_1q^2/2)\,dq=\exp(-\alpha\varkappa^2+i\beta\gamma+\gamma).$$

Accordingly, the Fourier transform of the obviously integrable function $\psi^*(q)\exp(-a_1q^2/2)$ is a function of Gaussian form. It follows that the function $\psi^*(q)\exp(-a_1q^2/2)$ is itself Gaussian, and consequently the function $\psi(q)$ itself is of the form (5.22).

[5)] The order of increase of a function $F(z)$ is defined as the limit $\rho=\overline{\lim}_{z\to\infty}[\ln\ln M(|z|)/\ln|z|]$, where $M(|z|)=\max_{\varphi}|F(|z|e^{i\varphi})|$, $\varphi^*=\varphi$.

We note that for $a^*=a$ (i.e., $a_2=0$) the wave function (5.22) describes a coherent state $|z\rangle$, which is an eigenfunction of the annihilation operator $a=q/2l+(il/\hbar)p$, where $l=(2a_1)^{-1/2}$. In the general case, when $a_2\neq 0$ the state described by the wave function (5.22) is not a coherent one. However, as is shown in Ref. 29, one can introduce creation and annihilation operators

$$\hat{a}=\frac{e^{-i\varphi}}{2l}\hat{q}+\frac{il}{\hbar\cos\varphi}\hat{p},\quad \hat{a}^+=\frac{e^{i\varphi}}{2l}\hat{q}-\frac{il}{\hbar\cos\varphi}\hat{p},\quad |\varphi|<\frac{\pi}{2}, \tag{5.26}$$

satisfying the usual condition $[a,a^+]=1$, but such that the eigenfunctions of the operator $\hat{a}$ (called by the writers correlated coherent states)

$$\hat{a}\,|\,z,\ \varphi\rangle=z\,|\,z,\ \varphi\rangle \tag{5.27}$$

are described by wave functions of the general form (5.22) with $a_2\neq 0$. The Wigner function constructed by means of correlated coherent states is Gaussian and has the parameters

$$\sigma_q^2=l^2/\cos^2\varphi,\quad \sigma_p^2=\hbar^2/4l^2,\quad r=\sin\varphi,$$
$$\bar{q}=-\frac{2l}{\cos\varphi}\,\mathrm{Re}\,z,\quad \bar{p}=\frac{\hbar}{l}\,\mathrm{Im}\,(ze^{i\varphi}). \tag{5.28}$$

Furthermore the coordinate and momentum are correlated (with correlation coefficient r), and the sign of equality is attained in the uncertainty relation (3.10).

In the general case, *if the initial state of a quantum system is described by a wave function* (5.22), *so that* $W(p,q,t=0)>0$, *then in the course of time the function* $W(p,q,t)$ *does not remain Gaussian, and consequently begins to take on negative values.* An exception is the case when the Hamiltonian of the system is quadratic. In this case the property of nonnegativity of the Wigner function is preserved in time.[33]

We shall now show that with some coarsening of the description one can always achieve positivity of the quasiprobability. For this purpose we must consider not the density $W(p,q)$, but the "probability" that the phase point will be in a finite region $\Delta p\Delta q$ of the phase plane; i.e., we must consider the quantity

$$P_{\Delta p\Delta q}(p,q)=\int\int_{\Delta p\Delta q}W(p+p_1,\,q+q_1)\,dp_1\,dq_1, \tag{5.29a}$$

where the integration extends over the region $(p,q)\in\Delta p\Delta q$. For simplicity we consider instead of the region $\Delta p\Delta q$ with a sharp boundary a region with a somewhat "smeared" boundary, and introduce the quantity

$$P_{\Delta p\Delta q}(p,q)=\int_{-\infty}^{\infty}\int\exp\left(-\frac{p_1^2}{2\Delta_p^2}-\frac{q_1^2}{2\Delta_q^2}\right)W(p+p_1,\,q+q_1)\,dp_1\,dq_1. \tag{5.29b}$$

The equivalent cell area on the phase plane is

$$(\Delta p\Delta q)_{eq}=\int_{-\infty}^{\infty}\int\exp\left(-\frac{p_1^2}{2\Delta_p^2}-\frac{q_1^2}{2\Delta_q^2}\right)dp_1\,dq_1=2\pi\Delta_p\Delta_q. \tag{5.30}$$

Following Ref. 36, we substitute in Eq. (5.30) the representation (2.20) of the Wigner function. Doing the integration over p, we obtain

$$P_{\Delta p\Delta q}=\frac{\Delta p}{\sqrt{2\pi}\,\hbar}\int\int dq'\,d\xi\,\psi^*\left(q+q'+\frac{\xi}{2}\right)\psi\left(q+q'-\frac{\xi}{2}\right)$$
$$\times\exp\left(-\frac{\Delta_p^2\xi^2}{2\hbar^2}-\frac{q'^2}{2\Delta_q^2}+\frac{ip\xi}{\hbar}\right).$$

If we introduce here new variables of integration $q+q'\pm(\xi/2)=q_{1,2}$, after simple transformations we obtain the

result

$$P_{\Delta p\Delta q}=\frac{\Delta p}{\sqrt{2\pi}\,\hbar}\exp(-q^2/2\Delta_q^2)\int\int f^*(q_1)f(q_2)\exp(\gamma q_1 q_2)\,dq_1\,dq_2,$$

where we have introduced the following notations:

$$\gamma=\frac{4\Delta_p^2\Delta_q^2-\hbar^2}{4\hbar^2\Delta_q^2},\quad f(q_2)=\psi(q_2)\exp\left(-\frac{4\Delta_p^2\Delta_q^2+\hbar^2}{8\hbar^2\Delta_q^2}q_2^2+\frac{qq_2}{2\Delta_q^2}-\frac{ipq_2}{\hbar}\right).$$

Expanding $\exp(\gamma q_1 q_2)$ in Taylor series, we obtain

$$P_{\Delta p\Delta q}=\frac{\Delta p}{\sqrt{2\pi}\,\hbar}\exp(-q^2/2\Delta_q^2)\sum_{n=0}^{\infty}\frac{\gamma^n}{n!}|C_n|^2, \tag{5.31}$$

with the notation

$$C_n=\int q_1^n f(q_1)\,dq_1.$$

It can be seen from Eq. (5.31) that for $\gamma\geqslant 0$ all the terms of the series are nonnegative, and consequently $P_{\Delta p\Delta q}\geqslant 0$ for

$$\Delta_p\Delta_q\geqslant\frac{\hbar}{2},\quad(\Delta p\Delta q)_{eq}\geqslant\pi\hbar. \tag{5.32}$$

The simplest case is $\gamma=0$, i.e., $\Delta_p\Delta_q=\hbar/2$. Then in Eq. (5.31) there is left only the term with $n=0$, and we obtain (writing P_0 for $P_{\Delta p\Delta q|\gamma=0}$)

$$P_0(p,q)=\frac{1}{2\sqrt{2\pi}\,\Delta_q}\left|\int\psi(q_1)\exp\left[-\frac{ipq_1}{\hbar}-\frac{(q-q_1)^2}{4\Delta_q^2}\right]dq_1\right|^2. \tag{5.33}$$

The same result can be derived by examining the trace of the operator

$$\hat{P}_{\Delta p\Delta q}=\int_{-\infty}^{\infty}\exp\left[-\frac{p_1^2}{2\Delta_p^2}-\frac{q_1^2}{2\Delta_q^2}\right]\hat{W}(p+p_1,q+q_1)\,dp_1\,dq_1, \tag{5.34}$$

i.e., considering the eigenvalue problem

$$\hat{P}_{\Delta p\Delta q}(p,q)|p,q\rangle=\mathcal{P}|p,q\rangle. \tag{5.35}$$

Then, if we look for the eigenvectors in the form of an expansion in terms of $|q'\rangle$, the equation for $\langle q'|p,q\rangle$ is reduced by the substitution

$$\langle q'|p,q\rangle=\exp\left[\frac{i(q'-q)p}{\hbar}-\frac{\Delta p(q'-q)^2}{2\hbar\Delta_q}\right]\Phi(q'-q)$$

to the integral equation

$$\int_{-\infty}^{\infty}\Phi(q'')\exp\left[-\frac{1}{2}\left(\frac{\Delta p}{\hbar}+\frac{1}{2\Delta_q}\right)^2(q''-\alpha q')^2\right]dq''=Q\Phi(q'). \tag{5.36}$$

Here we have used the notation

$$\alpha=\frac{\Delta p\Delta q-(\hbar/2)}{\Delta p\Delta q+(\hbar/2)},\quad Q=\frac{\sqrt{2\pi}\,\hbar}{\Delta p}\mathcal{P}. \tag{5.37}$$

Using the well known formula for the Hermite polynomials[37]

$$\int_{-\infty}^{\infty}H_n(\nu x)\exp[-(x-y)^2]\,dx=\sqrt{\pi}\,(1-\nu^2)^{n/2}H_n\left(\frac{\nu y}{\sqrt{1-\nu^2}}\right),$$

we obtain the solution of Eq. (5.36) in the form

$$\Phi_n(q')=H_n(q'\sqrt{\Delta p/\hbar\Delta_q}),\quad Q_n=Q_0\alpha^n,\quad Q_0=\frac{\sqrt{2\pi}\,\hbar\Delta_q}{\Delta p\Delta_q+(\hbar/2)},$$

with $n=0,1,2,\ldots$ Using Eq. (5.37), we obtain for the eigenvalues of the operator $\hat{P}_{\Delta p\Delta q}$:

$$\mathcal{P}_n=\mathcal{P}_0\alpha^n,\quad\mathcal{P}_0=\frac{\Delta p\Delta q}{\Delta p\Delta q+(\hbar/2)},\quad n=0,1,2,\ldots \tag{5.38}$$

For $\alpha\geqslant 0$ all the eigenvalues are nonnegative. From Eq. (5.37) we see that the condition $\alpha\geqslant 0$ is identical with Eq. (5.32). For $\alpha=0$ there is left in the expansion of the operator $P_{\Delta p\Delta q}$ in terms of its eigenvectors the single term with $n=0$, and this leads to the same formula (5.33) as obtained by another method.

Reference 16 considers smoothed Wigner functions and analyzes several examples, including the case of the hydrogen atom. Reference 38 gives quite a number of weight functions $G(p,q)$ for which

$$\int\int G(p,q)\,W(p,q)\,dp\,dq\geqslant 0$$

(it must be noted that here no displacement of the arguments p',q' is made; that is the positive nature of the smoothed function is established only for the point $p=0$, $q=0$).

After the averaging the restriction (5.20) on $W(p,q)$ takes the following form [we use Eqs. (5.29b), (5.30), and (5.32)]:

$$\begin{aligned}P_0(p,q)&=|P_0(p,q)|\\&\leqslant\left|\int\int\exp[-(q_1^2/2\Delta_q^2)-(p_1^2/2\Delta_p^2)]\,W(p+p_1,q+q_1)\,dp_1\,dq_1\right|\\&\leqslant\int_{-\infty}^{\infty}\int\exp[-(q_1^2/2\Delta_q^2)-(p_1^2/2\Delta_p^2)]\,(\pi\hbar)^{-1}\,dp_1\,dq_1=1,\end{aligned}$$

that is,

$$0\leqslant P_0(p,q)\leqslant 1. \tag{5.39}$$

Consequently, it is permissible for all the "probability" to be concentrated in one cell of phase space. We note that the normalized quantity $P_0(p,q)/\pi\hbar$ can be treated as a smoothed density of quasiprobability:

$$\overline{W}(p,q)=[(2\pi)^{3/2}\hbar\Delta_q]^{-1}\left|\int\psi(q')\exp\left[-\frac{ipq'}{\hbar}-\frac{(q-q')^2}{4\Delta_q^2}\right]dq'\right|^2. \tag{5.40}$$

It follows from Eq. (5.39) that the smoothed density $\overline{W}$ is restricted by the condition $\overline{W}\leqslant(\pi\hbar)^{-1}$. Moreover, since $\overline{W}\geqslant 0$, we have

$$0\leqslant\overline{W}(p,q)\leqslant(\pi\hbar)^{-1}. \tag{5.41}$$

It must be pointed out that despite the fact that the averaged quasidensity $\overline{W}$ cannot assume negative values, it can still not be regarded as an ordinary probability density, which could lead to genuine quantum averages. This is due, first, to the fact that exact quantum averages can be obtained only by using the quasidensity W, which can also take on negative values. Calculations with the smoothed density $\overline{W}$ in general lead to errors. Second, the rules of correspondence remain in force between operators and the functions that represent them in phase space, which lead to relations contradicting the usual rules of probability for the calculations of higher moments [cf. Eq. (3.3) and text following it]. Therefore, even after averaging, the positive Wigner quasidensity still has properties very different from those of the usual probability.

As an example we consider the Wigner functions for the oscillator. The wave function for the nth stationary state is

$$\psi_n(q)=(2^n n!)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega q^2}{2\hbar}\right)H_n(q\sqrt{m\omega/\hbar}). \tag{5.42}$$

The corresponding quasiprobability density can be calculated exactly and is given by

$$W_n(p,q)=\frac{(-1)^n}{\pi\hbar}\exp\left[-\frac{2}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right]L_n\left(\frac{4}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right); \tag{5.43}$$

here $L_n(x)$ are the Laguerre polynomials ($L_0=1, L_1=1-x, L_2=1-2x+(x^2/2), \ldots$). For $n=0$ we have a joint Gaussian distribution, in which coordinate and momentum are statistically independent. It is identical with the distribution (4.19), which we derived earlier from other considerations. For $n=1$ we have

$$W_1(p,q)=\frac{1}{\pi\hbar}\exp\left[-\frac{2}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right]\cdot\left[\frac{4}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)-1\right].$$

Here we encounter a case of negative quasiprobability density, since $W_1(p,q)<0$ for

$$\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}<\frac{\hbar\omega}{4}.$$

With increasing level number n the first zeros of the Laguerre polynomial decrease in absolute value, as a result of which the regions where $W_n(p,q)<0$ become narrower and narrower elliptical strips in the (p,q) plane.

Let us now examine the smoothed quasiprobability (5.40). The calculation with this formula leads to the expression

$$\overline{W}_n(p,q)=(2\pi\hbar n!)^{-1}\left[\frac{1}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right]^n\exp\left[-\frac{1}{\hbar\omega}\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)\right] \tag{5.44}$$

(this relatively simple expression for $\overline{W}_n$ is obtained only in the case when the averaging parameter Δ_q^2 in Eq. (5.40) is taken equal to $\hbar/2m\omega$; in all other cases the averaged quasidensity is not a function of the oscillator energy only). The maximum of the function $\overline{W}_n$ is located at $(p^2/2m)+(m\omega^2q^2/2)=n\hbar\omega$. For large n this value of the argument is in the region where the averaged Wigner function varies most smoothly.

If we calculate the mean values of various powers of the energy in the nth state, using the unaveraged Wigner function and converting the various powers of the energy operator to the Weyl ordered form, then we naturally obtain the exact values $\langle\langle(E_n)^m\rangle=[(n+\frac{1}{2})\hbar\omega]^m$.

If, on the other hand, we use the smoothed quasidensity for the calculation, the mean values of the energy found with it are $\overline{E}_n=(n+1)\hbar\omega$; i.e., they exceed the true means by $\hbar\omega/2$. Meanwhile the spacing of the energy levels is correct. Let us also find the quantity $\overline{E}_n^2$. If we use the formula

$$\overline{E}_n^2=\int\int\overline{W}_n(p,q)\left[\left(\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}\right)^2-\left(\frac{\hbar\omega}{2}\right)^2\right]dp\,dq,$$

we obtain $\overline{E}_n^2=(\hbar\omega)^2(n^2+3n+7/4)$. For the mean square "fluctuation" of the energy we then find

$$\overline{E}_n^2-(\overline{E}_n)^2=(\hbar\omega)^2\left(n+\frac{3}{4}\right),$$

and for the fractional "fluctuation"

$$[\overline{E}_n^2-(\overline{E}_n)^2]/(\overline{E}_n)^2=\frac{n+\frac{3}{4}}{(n+1)^2}.$$

For $n\to\infty$ the fractional "fluctuation" approaches zero, so that the smoothed probability distribution for the quantity (E/n) in the nth stationary state approaches a δ function for $n\to\infty$.

Of course, the true values are $\langle E_n^2\rangle-\langle E_n\rangle^2\equiv 0$, so that the difference of this quantity from zero characterizes only the error incurred by replacing W_n with $\overline{W}_n$.

In this example it can be seen how the transition to the classical limit occurs in the Wigner representation. For $n\to\infty$ the quasidensity $W_n(p,q)$ itself does not approach the limit $\delta[H(p,q)-(n+\frac{1}{2})\hbar\omega]$, but becomes a more and more rapidly oscillating function. At the same time the smoothed quasiprobability $\overline{W}_n$ strongly distorts the results of the calculations for small n, but becomes asymptotically exact (if we neglect the shift of all levels by $\hbar\omega/2$) for $n\to\infty$.

6. BASIC CONCLUSIONS

The Wigner representation of quantum mechanics is equivalent to the traditional interpretation, but for its proper use requires that certain specific rules be followed and attention paid to a number of properties that distinguish the Wigner quasidensity from a true probability density.

Instead of the Schrödinger equation we have in the Wigner representation the quantum Liouville equation for Wigner's joint quasiprobability density of coordinate and momentum. Solutions of this equation can also fail to correspond to quantum-mechanical problems unless the initial conditions for the equation are subjected to a supplementary restriction, which selects the admissible class of quantum conditions that describe pure states. When this condition is satisfied one can reconstruct the wave function from the Wigner function. This supplementary condition contains Planck's constant and, besides the uncertainty relation, brings with it very severe limitations of the possible form of the Wigner quasidensity; by no means every distribution that agrees with the uncertainty relation can correspond to some quantum problem. If the Wigner quasidensity does not depend on the time and satisfies the indicated restriction, it leads to an orginary stationary state in quantum mechanics. For the quantum oscillator the quantum Liouville equation is identical with the classical one and the condition for quantization of the energies of stationary states arises precisely from the restriction of the admissible form of pure-state quantum distributions.

The Wigner quasidensity $W(p,q)$ itself, together with the rules by which the calculation of average values is conducted, has a number of specific properties which distinguish it from a true probability density. First of all, it can take both positive and also negative values. Its absolute value is limited by the condition $|W(p,q)|\leq(\pi\hbar)^{-1}$. The second essential difference between the quasiprobability and ordinary probability is due to the fact that the integrals of various powers of a function $A(p,q)$, multiplied by $W(p,q)$ are not the quantum mean values of the corresponding powers of the operator A; these last must be calculated by more complicated formulas. From this follows, for example, the peculiar property of the quasidensity that for stationary states with fixed energies it is not concentrated on the lines of equal energy in the (p,q) plane. Accordingly, the "blurring" of the quasidensity does not indicate a corresponding spread of "random variables" described by this density, since the rules for calculating mean values with W are not the same as the rules of probability

when one deals with statistical moments of higher degrees.

When smoothed with a Gaussian weight, the quasidensity (its smoothed value $\bar{W}$) becomes nonnegative, provided the equivalent averaging area is large enough, $(\Delta p \Delta q)_{eq} \geq \pi\hbar$. Also it then satisfies the condition $0 \leq \bar{W} \leq (\pi\hbar)^{-1}$. However, the smoothing of the density leads to errors in the calculations of mean values, as compared with exact quantum-mechanical means.

The smoothed density $\bar{W}$ takes on more importance in the transition to the classical limit. As can be seen from the example of the quantum oscillator, for high excited states the Wigner quasidensity W_n becomes a remarkable finely etched function, taking on positive and negative values in closely spaced regions in the (p, q) plane. At the same time, as n increases, the smoothed quasidensity $\bar{W}_n$ becomes concentrated around the line $H(p, q) = E_n$ and takes on a δ-like form so that the fractional error in the calculation of mean values by its use approaches zero. Accordingly, in the passage to the classical limit it is $\bar{W}$, not W, that becomes more important.

Drawing a final conclusion, we can say that, if correctly used, the Wigner representation can be a convenient instrument in quite a number of quantum-mechanical problems. By means of the Wigner function one can calculate mean values of any physical quantities that may be of interest. In itself, however, the Wigner function is without physical meaning, and the intuitive value of the Wigner representation is in a large degree illusory. In any case, a too literal treatment of the quasiprobability as a true probability can lead to incorrect conclusions even when the quasiprobability is indeed nonnegative.

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