Condition for Any Realistic Theory of Quantum Systems

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In quantum physics, the density operator completely describes the state. Instead, in classical physics the mean value of physical quantities is evaluated by means of a probability distribution. We study the possibility to describe pure quantum states and events with classical probability distributions and conditional probabilities and prove that the distributions have to be nonlinear functions of the density operator. Some examples are considered. Finally, we deal with the exponential complexity problem of quantum physics and introduce the concept of classical dimension for a quantum system.

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A peculiar aspect of the standard quantum formalism is interference; that is, every alternative is not associated with a probability, but with a complex number. This characteristic is at the basis of some famous paradoxes, such as the Schrödinger cat [1], and the ''sign problem'' encountered in quantum Monte Carlo simulations [2], which gives an exponential growth of the numerical complexity. Since the birth of quantum mechanics, many physicists investigated the possibility of its description in terms of classical probabilities. Indeed, a completely equivalent alternative to the Copenhagen interpretation is Bohm mechanics [3,4], recently extended to quantum fields with a variable particle number [5]. These approaches provide a realistic description of quantum systems. Bohm mechanics uses the same mathematical tools of the standard approach as the wave function, so it differs only in the interpretation and does not solve, for example, an important problem such as exponential complexity. The wave function is not defined in the three-dimensional physical space, but in the representation space; thus the number of variables needed to define the Bohmian state grows exponentially with the dimension of the physical system. Since quantum mechanics has a statistical interpretation, there is no *a priori* reason to exclude the possibility to describe the quantum states as statistical ensembles in a smaller space than the Hilbert space. In some cases, the Wigner function provides such a dimensionality reduction [6]. It has some properties of a classical probability distribution in phase space, but in general it can take negative values. When it is positive and only particular measurements are performed, a realistic statistical description in phase space is possible, as in the case of continuous-variable teleportation experiments involving Gaussian states and quadrature measurements [7].

In order to circumvent the sign problem of the Wigner function, some alternative non-negative probability distributions were introduced [8,9], such as the Husimi function. However, also in these cases, a realistic interpretation is not possible in general. Another example of phase-space distribution is the P function, introduced by Glauber [10].

A realistic statistical description of quantum mechanics in a reduced phase space is very important for its possible consequences in Monte Carlo simulations of many-body systems. In the cases where it is possible to interpret the Wigner function as a probability distribution, as in the truncated Wigner approximation, the Monte Carlo approach allows us to efficiently simulate the dynamics of atoms in degenerate bosonic gases [11] and electrons in semiconductors [12]. A general discussion of the method is also reported in Ref. [13].

In this Letter, we analyze the possibility to have a realistic description for experiments involving general states and measurements and prove that a necessary condition has to be fulfilled. Using the nonconflicting hypotheses of the theorem, we finally introduce the concept of classical dimension of a quantum system. In this Letter we use the term ''classical'' as equivalent to ''realistic''; thus, a classical theory is a theory whose variables have definite values and for which it is possible to use the classical rules of the probability theory. In this sense, Bohm mechanics is a classical theory and, consequently, every state is classical, i.e., has a realistic description.

For our purpose, it is sufficient to consider trace-one projectors for events and pure states. We associate the quantum state $|\psi\rangle$ with a distribution of probability $\rho(X|\psi)$ in a suitable classical space, spanned by a set of variables X. This space can be more general than the phase space and with higher dimensionality. No *a priori* hypothesis on it is introduced. We want to give physical meaning to these variables; i.e., we assume that there is an underlying theory of the quantum system described by them. When the system is prepared to a state $|\psi\rangle$, X takes a value with a probability given by ρ. If a von Neumann measurement is performed, the state collapses to a state $|\phi\rangle$ with probability $|\langle\psi|\phi\rangle|^2$. In terms of the realistic theory, we say that the system with coordinates X has a conditional probability $P(\phi|X)$ to give the event ϕ.

The probability of this event, given the state $|\psi\rangle$, is obtained integrating $P(\phi|X)\rho(X|\psi)$ over X as

$$|\langle\phi|\psi\rangle|^2 = \mathrm{Tr}[\hat{P}_\phi \hat{P}_\psi] = \int dX P(\phi|X)\rho(X|\psi), \quad (1)$$

where $\hat{P}_\psi \equiv |\psi\rangle\langle\psi|$. The functions $\rho(X|\psi)$ and $P(\phi|X)$

have to satisfy the conditions

$$\rho(X|\psi) \geq 0, \tag{2}$$

$$\int dX \rho(X|\psi) = 1, \tag{3}$$

$$0 \leq P(\phi|X) \leq 1, \tag{4}$$

for every $|\psi\rangle$ and $|\phi\rangle$.

Note that Eq. (4) is satisfied if $\langle\phi|\phi\rangle$ is equal to 1. Conversely, if $|\phi\rangle$ is not normalizable, the quantity $|\langle\phi|\psi\rangle|^2$, and consequently $P(\phi|X)$, is not a probability but a density of probability. For example, if $|x\rangle$ is a position eigenstate, $|\langle x|\psi\rangle|^2 = |\psi(x)|^2$ corresponds to the probability density of finding a particle at the position x (the position operator has a continuous spectrum). For the theorem proof, it is sufficient to consider measurements with trace-one projectors, as implicitly assumed in Eq. (4). Indeed, the theorem could be proved by merely selecting a two-dimensional subspace for states and measurements. It is clear that, for finite dimensional Hilbert spaces, every vector is normalizable.

A relation as Eq. (1) holds when we evaluate the probability distribution of the position of a particle by means of the Wigner function. The probability to have a particle in the spatial region Ω is

$$\int dq dp P(\Omega|q, p) W(q, p), \tag{5}$$

where

$$P(\Omega|q, p) = \int_\Omega \delta(\bar{q} - q) d\bar{q}, \tag{6}$$

$\delta(\bar{q} - q)$ being the conditional probability density of finding the particle at $\bar{q}$. Since $0 \leq P(\Omega|q, p) \leq 1$, P can be interpreted as a conditional probability. Thus, if the Wigner function is positive and position measurements are involved, a realistic description in phase space is possible [7].

Every probability distribution introduced so far is linear in the density operator, such as the P, the Wigner, and the Q functions [10]. Indeed, the Wigner function was rigorously derived in Ref. [14] using this property and other four assumptions. We will show that linear distributions cannot be interpreted as probability distributions of some realistic theory when general states and measurements are considered. More precisely, by assuming that properties (1)–(4) are fulfilled for *every* ψ and ϕ [15], we prove that the probability distributions associated with pure quantum states are nonlinear functions of the density operator. This is the main result of our work. Note that Bohm mechanics is a perfectly consistent realistic hidden variable theory and that the corresponding probability distributions are nonlinear with respect to the density operator, as we will show.

In general, under the linearity hypothesis a positive probability distribution can be obtained by means of positive operator-valued measurements (POVM) [16]. We consider a pure state $|\psi\rangle$ and define the associated probability distribution with respect to a variable X as

$$\rho(X|\psi) \equiv Tr[\hat{A}(X)\hat{P}_\psi], \tag{7}$$

where $\hat{P}_\psi \equiv |\psi\rangle\langle\psi|$ is a projector and $\hat{A}(X)$ is a generic Hermitian matrix which depends on X. X can be a vector of continuous and/or discrete variables. $\rho(X|\psi)$ must satisfy the properties (2) and (3). The first one is fulfilled if $\hat{A}(X)$ is positive definite, i.e., if its eigenvalues are non-negative. The second one implies that [16]

$$\int dX \hat{A}(X) = \mathbb{1}. \tag{8}$$

After these preliminary remarks, we can prove the theorem. Equations (1)–(4) and (7) are our starting hypotheses. We will show that they are conflicting.

From Eqs. (1) and (7), we have

$$\mathrm{Tr}\left\{\left[\int dX P(\phi|X)\hat{A}(X) - \hat{P}_\phi\right]\hat{P}_\psi\right\} = 0,$$

for every $|\psi\rangle$ and $|\phi\rangle$. Thus,

$$\hat{P}_\phi = \int dX P(\phi|X)\hat{A}(X). \tag{9}$$

Since $\hat{A}(X)$ is positive definite and $P(\phi|X) \geq 0$, it is evident that

$$P(\phi|X) \neq 0 \Rightarrow \hat{A}(X) \propto \hat{P}_\phi. \tag{10}$$

Thus, if $P(\phi|X) \neq 0$ and $P(\phi'|X) \neq 0$, then $\phi = \phi'$. We can define the following one-valued function:

$$\chi: X \to \chi(X) \quad \text{such that} \quad P(\chi(X)|X) \neq 0. \tag{11}$$

The function $\chi(X)$ spans the entire Hilbert space, but it is not necessarily invertible. It is possible to introduce an auxiliary set $Y(X)$ of variables in order to have the bijective mapping $X \leftrightarrow (\chi, Y)$. Y can be continuous and/or discrete. We suppose that it is continuous without loss of generality. Condition (10) implies that

$$P(\phi|\chi, Y) = 0 \quad \text{if} \quad \phi \neq \chi, \tag{12}$$

$$\hat{A}(\chi, Y) \equiv \alpha(\chi, Y)\hat{P}_\chi, \tag{13}$$

where $\alpha(\chi, Y) \geq 0$. Equations (9), (12), and (13) give

$$\int \mathcal{D}\chi dY P(\phi|\chi, Y)\alpha(\phi, Y) = 1, \tag{14}$$

for every ϕ. Since $P(\phi|\chi, Y)$ is different from zero in a set with zero measure of the χ space [Eq. (12)] and it is smaller or equal to 1, $\int dY \alpha(\phi, Y)$ must be infinite for every ϕ, but this is impossible because of the normalization condition (8) and Eq. (13). □

Since the properties (2)–(4) are the minimal necessary conditions for a realistic theory, we have to discard the linear assumption, i.e., Eq. (7). This is sufficient to remove the contradiction, as shown below, when we will explicitly write the probability density and conditional probability for the Bohm theory.

Now, we consider some examples to illustrate our result. The P, the Wigner, and the Q functions can be defined for systems described by boson creation and annihilation operators, $\hat{a}^\dagger$ and $\hat{a}$, respectively [10]. It is well known that the P and the Wigner functions cannot be probability distributions. The first one is highly singular for particular states, as squeezed states or superposition of coherent states. The second one is well defined for every state, but can assume negative values; i.e., Eq. (2) is not satisfied. The Q function requires a more detailed discussion. It is smooth, positive, and normalized; thus our theorem says that Eq. (4) cannot be satisfied. Consider a one-mode system and denote the Q function corresponding to a state $|\psi\rangle$ by $Q(\alpha|\psi)$, where α is a complex number. The expectation value of an observable $M(\hat{a}^\dagger, \hat{a})$ in antinormal form is given by the average of the function $M(\alpha^*, \alpha)$ with respect to $Q(\alpha|\psi)$, The expectation value of the number of particles is $\langle\hat{a}^\dagger\hat{a}\rangle = \langle\hat{a}\hat{a}^\dagger\rangle - 1 = \int d^2\alpha(|\alpha|^2 - 1)Q(\alpha|\psi)$; thus we have that $\sum_{n=0}^{\infty} nP(n|\alpha) = |\alpha|^2 - 1$, where $P(n|\alpha)$ is the conditional probability of measuring n particles for the phase-space state α. This equation implies that the conditional probability has to be negative for some values of n and $|\alpha|^2 < 1$, in agreement with our theorem.

Now, we consider the case of a two-dimensional Hilbert space. It is possible to construct a probability distribution $\rho(n|\psi)$ with the following three matrices [17]: $\hat{A}_1 = \frac{1}{3} \times (1 + \hat{\sigma}_3)$, $\hat{A}_2 = \frac{1}{3}1 - \frac{1}{6}\hat{\sigma}_3 + \frac{\sqrt{3}}{6}\hat{\sigma}_1$, and $\hat{A}_3 = \frac{1}{3}1 - \frac{1}{6}\hat{\sigma}_3 - \frac{\sqrt{3}}{6}\hat{\sigma}_1$, where $\hat{\sigma}_i$ are the Pauli matrices. The distribution has three values and is positive and normalized. Also in this case, the conditional probability $P(\phi|n)$ cannot satisfy Eq. (4). For example, when $\phi = (1, 0)$, Eq. (1) is fulfilled if and only if $P(\phi|1) = 3/2$ and $P(\phi|2) = P(\phi|3) = 0$.

We can define another probability distribution as $\rho(\theta, \phi|\psi) = \frac{1}{2\pi}\mathrm{Tr}[|\theta, \phi\rangle\langle\theta, \phi|\hat{\rho}]$, where $|\theta, \phi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$ and $|0\rangle, |1\rangle$ are two orthonormal vectors. θ and ϕ are the polar coordinate of a point of the Bloch sphere. In the integrals with respect to these coordinates, we use the measure $\sin\theta d\theta d\phi$. The distribution is positive and normalized. For $|\psi\rangle = |0\rangle$, we have $\rho(\theta, \phi|0) = [\cos(\theta/2)]^2/2\pi$. The probability of obtaining the state $|0\rangle$ is equal to 1; thus

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta P(0|\theta, \phi)\rho(\theta, \phi|0) = 1. \qquad (15)$$

We assume *ab absurdo* that $0 \leq P(0|\theta, \phi) \leq 1$. Then the equality is satisfied only if $P(0|\theta, \phi) = 1$, for $\theta \neq \pi$. But this implies that the probability to obtain $|0\rangle$ when the system is in the state $|1\rangle$ is different from zero, since the corresponding probability distribution $\rho(\theta, \phi|1) = [\sin(\theta/2)]^2/2\pi$ is zero only for $\theta = 0$. This is absurd because $|0\rangle$ and $|1\rangle$ are orthogonal. All the previous examples show that at least one property required by the theorem is not satisfied.

Discarding the linear hypothesis, we investigate how to construct a probability distribution associated with every density operator which satisfies the conditions (1)–(4). The Bohm mechanics provides a simple example of true probability. For the sake of simplicity, here we consider only the case of a fixed number of particles [3,4]. Recently, the theory has been extended to quantum fields and accounts for creation and annihilation of a particle [5]. The dynamical variables are a multiparticle wave function χ and the coordinates $\vec{x}$ in the configuration space. If the quantum system is in a pure state ψ, the variable χ is merely equal to ψ and the distribution of the coordinates $\vec{x}$ is $|\psi(\vec{x})|^2$; thus

$$\rho(\vec{x}, \chi|\psi) \equiv |\psi(\vec{x})|^2\delta(\chi - \psi), \qquad (16)$$

where ψ is the state in the Hilbert space of the quantum system. This function is obviously nonlinear in ψ because of the Dirac delta. In Bohm mechanics, the position measurement gives the variables $\vec{x}$ as result. Thus, the conditional probability of finding the system in a volume Ω in the representation space is

$$P(\Omega|\vec{x}, \chi) = \int_\Omega d\vec{x}_0\delta(\vec{x}_0 - \vec{x}). \qquad (17)$$

Measurements of other observables, such as momentum, can be performed by a suitable unitary evolution and a subsequent measurement of position. During the evolution, the coordinates $\vec{x}$ go to a new value which is a function of x and ψ. This enables one to obtain a positive conditional probability for every measurement from Eq. (17).

Bohm mechanics is a dispersion-free theory; i.e., the hidden variables fix exactly the results of measurements. It corresponds to have conditional probabilities equal to 0 or 1. This characteristic is not necessarily required by a realistic theory [18]. Indeed, the minimal requirements are Eqs. (1)–(4). Discarding the dispersion-free hypothesis, the simplest probability distribution for a pure state ψ is

$$\rho(\chi|\psi) = \delta(\chi - \psi), \qquad (18)$$

where χ is the variable of the classical system. The corresponding conditional probability for the event ϕ is $P(\phi|\chi) = |\langle\phi|\chi\rangle|^2$.

Although these two examples sound trivial, they show that properties (1)–(4) are not conflicting. At this point, we raise a question regarding the exponential complexity of quantum mechanics. In the case of Eq. (18), the dimension of the phase space spanned by the variables χ is obviously the dimension of the Hilbert space of ψ. It is well known that the dimension of the Hilbert space grows exponentially with the physical dimension of the system. For example, it is 2^N for N spins 1/2. Thus, also the number of variables χ of the classical theory has exponential growth. Every known hidden variable theory has this feature. However, if we discard some required property, such as positivity, the dimension of the X space can be considerably reduced. For example, the Hilbert space dimension of one boson mode is infinite, since the number of particles goes from zero to infinity, but the corresponding Wigner functions have only two variables, although we cannot regard these variables as describing a classical system because of the negativity of the Wigner function. In general, for a Hilbert space with dimension D_{quant}, it is possible to find quasiprobability distributions where X can assume only $D_{\mathrm{quant}} \times D_{\mathrm{quant}}$ values; that is, if the Hilbert space dimension is finite, we can have a space of X with dimension equal to zero. So, on one hand, we have an example of true probability distribution on a space with the same dimension of the Hilbert space, while on the other one, we can have quasiprobability distributions on a space with a considerably lower dimension. We define D_{class} as the lowest dimension of the sample space X among all the theories that satisfy the conditions (1)–(4) and raise the following question: Is it possible to have $D_{\mathrm{class}} \ll D_{\mathrm{quant}}$? Equation (18) says that $D_{\mathrm{class}} \le D_{\mathrm{quant}}$. The introduction of a probability distribution $\rho(X|\psi)$ and a conditional probability $P(\phi|X)$ for each event allows one to place the question of the exponential complexity nature of quantum mechanics onto a clear and well-defined ground, and the proof that $D_{\mathrm{class}} = D_{\mathrm{quant}}$ or that $D_{\mathrm{class}} \ll D_{\mathrm{quant}}$ would cast new light upon this question. The evaluation of D_{class} is not a trivial problem, and there is no evident reason for assuming it equal to D_{quant}. We have demonstrated that the solution of the problem requires one to discard probability distributions linear in the density operator. Note that we have not dealt with dynamical considerations, but only with the problem of a classical representation of quantum states.

In conclusion, we have studied the possibility of a classical description of quantum states and events by means of probability distributions and conditional probabilities that must satisfy the properties (1)–(4). We have demonstrated that the probability distribution has to be a nonlinear function of the density operator. We have illustrated the proof with some examples, such as the P, the Wigner, and the Q functions, and two cases of POVM for a two-state system. We have shown that for Bohm mechanics the distributions of probability are nonlinear functions of the density operator, as required by our theorem to any realistic theory. Finally, the concept of classical dimension D_{class} of a quantum system has been introduced. Every known hidden variable theory does not have a phase-space dimension smaller than the Hilbert space dimension D_{quant}. We conclude with a nontrivial question. Does a classical theory exist whose phase-space dimension is much smaller than D_{quant}? That is, is $D_{\mathrm{class}} \ll D_{\mathrm{quant}}$? Bohm mechanics could be considered as a pure interpretation curiosity, since it uses essentially the same tools of quantum mechanics, whereas a theory with much lower dimensionality would have important implications. We have put this problem onto a well-defined ground, and its solution could clarify the nature of the exponential complexity of quantum mechanics.

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