Inner composition law of pure states as a purification of impure states

V.I. Man’ko a,*, G. Marmo a, E.C.G. Sudarshan b, F. Zaccaria a

a Dipartimento di Scienze Fisiche, Università di Napoli ‘‘Federico II’’ and Istituto Nazionale di Fisica Nucleare, Sezione di Napoli, Mostra d’Oltremare, Pad.20, 80125 Naples, Italy

b Physics Department, Center for Particle Physics, University of Texas, Austin, TX 78712, USA

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Abstract

Quantum interference is described in term of density operators only using a formulated composition law for pure-state density operators. In order to retain the relative phases in quantum mechanics, we use fiducial vectors and fiducial projectors. These aspects are illustrated in terms of quantum tomography and density operators. Entanglement is determined in terms of a phase-dependent multiplication. © 2000 Published by Elsevier Science B.V.

1. Introduction

Quantum mechanics as traditionally formulated [1] involves three principles. Quantum states of the system are normalized vectors \(|\psi\rangle\) in a Hilbert space, (selfadjoint) linear operators correspond to (real) dynamical variables; and the expectation value for any dynamical variable is bilinear (sesquilinear) in the state vectors, these expectation values will be independent of an overall phase of the state vector. The carrier space for physical observations seems to correspond to ‘rays’ in Hilbert space \(|\psi\rangle: e^{i\alpha} |\psi_0\rangle\).

A vector state of a quantum system corresponds to a wave function obeying the linear Schrödinger evolution equation [2]. For the description of mixed states, the notion of density operator, which obeys a linear evolution equation, was introduced by von Neumann [3,4]. A density operator for a vector state is equal to \(|\psi\rangle \langle \psi|\), when the vector state is \(|\psi\rangle\).

The desire to make the description of quantum states more similar to the classical-mechanics description has led to the introduction quasidistributions on the phase space by means of Wigner functions [5]. For the same aim, the Husimi–Kano function [6,7] was also introduced, and this function takes only nonnegative values. In connection with quantum optics, a quasidistribution function with singularities was introduced in [8,9], which is also called a P-distribution function [10].

Recently, in connection with the tomographic procedure of measuring quantum states [11–13] the probability representation of quantum mechanics was suggested [14,15], in which the quantum state is described by a positive probability distribution of the
position. Both the quasidistributions and tomographic probabilities have the common property of being determined by the density operator, and therefore they do not depend on the overall phase factor of the vector state in the Hilbert space of quantum states.

On the other hand, an essential ingredient of quantum mechanics is the superposition principle of vector quantum states [1]. The phase factors of the Hilbert-space vectors play an essential role when one performs the addition of two or more vectors. For example, the relative phase of two vectors is important in superposing them, giving different kinds of Schrödinger cats, either of the type of even and odd coherent states [16] or of the type of cats created in the Kerr medium [17].

The problem we want to discuss in this Letter is how the superposition of vector quantum states is described in the formalism of the density operator.

In particular, this problem will be discussed in connection with the tomographic-probability representation of the quantum state. The tomographic probability is nothing else than the linear integral transform of the density matrix. The superposition of two pure quantum states implies a rule for combining two tomographic probabilities, i.e., a specific composition law of two probabilities. The tomographic-probability description of spin states [17–21] and dynamics of the spin system in the probability representation was studied recently in [22].

The aim of this Letter is to give the definition of composition of density operators for the superposition of vector states. It turns out that we have to use a fiducial vector |ψ₀⟩ to associate with the density operator a vector state in the Hilbert space. We also elucidate the superposition of two tomographic probabilities using their composition rule corresponding to the interference of quantum states. From this viewpoint, we study the relation between two linear equations, namely, the Schrödinger equation for the wave function and the von Neumann equation for the density operator. As we have shown elsewhere [23], the Schrödinger and von Neumann descriptions, respectively, on the Hilbert space and on the space of projector operators are not equivalent. The density operators contain the same physical information as the wave functions only if one formulates a composition law for pure density operators describing the superposition of quantum states. In this sense, an overall phase factor of the wave function is not essential, but the relative phase of two state vectors becomes relevant. Both descriptions become equivalent if a composition law of pure density operators is given.

2. Fiducial vector: a section from projection operators to vector states

In order to formulate a composition law of two projection operators

\[ ρ_1 = |ψ_1⟩⟨ψ_1| \]

and

\[ ρ_2 = |ψ_2⟩⟨ψ_2| \]

which correspond to the superposition of two orthogonal state vectors |ψ₁⟩ and |ψ₂⟩ with complex coefficients \( c_1 \) and \( c_2 \) (\( |c_1|^2 + |c_2|^2 = 1 \)), we use a normalized fiducial vector |ψ₀⟩.

Let us associate with the density operators \( ρ_1 \) and \( ρ_2 \) two normalized vectors

\[ |ψ_1⟩ = \frac{ρ_1 |ψ₀⟩}{|⟨ψ₀|ρ_1 |ψ₀⟩|} \]

and

\[ |ψ_2⟩ = \frac{ρ_2 |ψ₀⟩}{|⟨ψ₀|ρ_2 |ψ₀⟩|} \]

If one considers a superposition of two state vectors

\[ |ψ⟩ = c_1 |ψ_1⟩ + c_2 |ψ_2⟩ \]

one obtains a corresponding density operator which reads

\[ ρ = |c_1|^2 |ψ_1⟩⟨ψ_1| + |c_2|^2 |ψ_2⟩⟨ψ_2| + c_1^∗ c_2 |ψ_1⟩⟨ψ_2| + c_2^∗ c_1 |ψ_2⟩⟨ψ_1| \]

Each of the state vectors |ψ₁⟩ and |ψ₂⟩ can be multiplied by constant phase factors \( e^{iθ_1} \) and \( e^{iθ_2} \), respectively. The density operators |ψ₁⟩⟨ψ₁| = \( ρ_1 \) and |ψ₂⟩⟨ψ₂| = \( ρ_2 \) do not depend on these phase factors. But the density operator of superposition (5)
given by (6) depends on the relative phase $\Theta = \Theta_1 - \Theta_2$.

To give the composition law of two density operators $\rho_1$ and $\rho_2$ corresponding to the superposition of the state vectors (5), we define it using the superposition of vectors (3) and (4)

$$\rho = (c_1 | \psi_1 \rangle + c_2 | \psi_2 \rangle)(c_1^* \langle \psi_1 | + c_2^* \langle \psi_2 |). \quad (7)$$

In terms of density operators of pure states $\rho_1$ and $\rho_2$, the density operator (7) reads

$$\rho = |c_1|^2 \rho_1 + |c_2|^2 \rho_2 + [c_1 c_2^* \rho_1 \rho_2 + \text{h.c.}]$$

$$\times \left[ \text{Tr}(\rho_1 P_0) \text{Tr}(\rho_2 P_0) \right]^{-1/2}.$$

(8)

where

$$P_0 = |\psi_0 \rangle \langle \psi_0 |.$$

The first two terms in (8) provide only impure density operator. The rest interference term provides a purification of the impure density operator. (This is an essential departure from classical phase space probabilities in which any nontrivial composition of two extremal states gives exclusively an impure state.)

Let us compare the composition law (8) and the density operator (6). One can see that

$$\rho = \frac{\rho_1 P_0 \rho_2}{\left[ \text{Tr}(\rho_1 P_0) \text{Tr}(\rho_2 P_0) \right]^{1/2}}$$

$$= \left[ \text{Tr}(\rho_1 P_0 \rho_2 P_0) \right]^{-1/2} \rho_1 P_0 \rho_2$$

$$= |\psi_1 \rangle \langle \psi_2 | e^{i\Theta},$$

(9)

where

$$e^{i\Theta} = \frac{\langle \psi_1 | \psi_0 \rangle \langle \psi_0 | \psi_2 \rangle}{\langle \psi_1 | \psi_0 \rangle \langle \psi_0 | \psi_2 \rangle}.$$

(10)

This means that the introduction of a fiducial vector gives us the possibility to describe the relative phase of the state vectors $|\psi_1 \rangle$ and $|\psi_2 \rangle$ in the composition law of the density operators. The role of the fiducial vector $|\psi_0 \rangle$ is to select a vector each within the one-dimensional vector spaces determined, respectively, by the density operators $\rho_1$ and $\rho_2$. The composition law (8) contains three projectors $\rho_1$, $\rho_2$, and $P_0$. One can then see that the effect of the interference phenomenon can be described without using a linear vector-space structure. This means that using the Hilbert space structure to allow for the superposition (addition) of quantum states is redundant. The emerging picture of quantum mechanics is analogous to the picture in the electromagnetic theory where description by means of the vector-potential (analog of the state vector) is a necessary modification of the description by the electromagnetic-field tensor (analog of the density operator) but simultaneously much of the information contained in the vector-potential is redundant as the gauge invariance shows. The composition law (8) provides the ‘pure composition’ rule for projection operators. The conventional sum of two projection operators, say $|c_1|^2 \rho_1 + |c_2|^2 \rho_2$ gives an impure state. To find a pure state (projection operator) incorporating the interference pattern of two pure states $\rho_1$ and $\rho_2$, one needs a purification of the impure state $|c_1|^2 \rho_1 + |c_2|^2 \rho_2$ – this is prescribed by the composition law (8).

It is possible to write formula (8) in a more predicative way. Namely,

$$\rho = \sum_{i,j=1}^2 c_i c_j^* \frac{\rho_i P_0 \rho_j}{\text{Tr}(\rho_i P_0 \rho_j P_0)^{1/2}}.$$

(11)

Now we may incorporate the factor $P_0$ by using a $K$-deformed associative product on the space of operators by setting

$$A \cdot_K B := AKB; \quad K = P_0,$$

as considered in [24]. In this more compact form, the extension to many projection operators can be easily written down and, for composition of $n$ density operators, it reads

$$\rho = \sum_{i,j=1}^n c_i c_j^* \frac{\rho_i \cdot_K \rho_j}{\text{Tr}(\rho_i \cdot_K \rho_j \cdot_K P_0)^{1/2}}.$$

(12)

While writing (11) and (12) we used the relations:

$$P_0^2 = P_0,$$

$$\rho_i = \frac{\rho_i P_0 \rho_i}{\text{Tr}(\rho_i P_0 \rho_i P_0)},$$

$$\text{Tr}(\rho_i P_0) \text{Tr}(\rho_i P_0) = \text{Tr}(\rho_i P_0 \rho_j P_0) .$$

(13)

The relative phases of the pure quantum states can be included into relative phases by complex numbers $c_i, c_j^*$. 
3. Tomographic probability of pure states

In the probability representation of quantum states, the full set of tomographic probability densities (marginal distribution) determines the density operator. Given the normalized wave function $\psi(x) = \langle x | \psi \rangle$ the marginal distribution reads [25]

$$w_{\psi}(X, \mu, \nu) = \frac{1}{2\pi|\nu|} \left| \int \psi(y) \exp\left( \frac{i\mu}{\nu} y^2 - \frac{iXy}{\nu} \right) dy \right|^2.$$  

(14)

This dependence scales according to

$$w(\xi X, \xi \mu, \xi \nu) = \frac{1}{|\xi|} w(X, \mu, \nu).$$  

(15)

Since in (14) there is no dependence on constant phase of $\psi(y)$ the marginal distribution is determined by the density matrix. The marginal distribution is a positive normalized function, i.e.,

$$w(X, \mu, \nu) \geq 0, \quad \int w(X, \mu, \nu) dX = 1.$$  

(16)

The inverse transform for (14) determines the density matrix in the coordinate representation

$$\psi(x) \psi^*(x') = \frac{1}{2\pi} \int w(Y, \mu, x-x') \times \exp \left[ i \left( Y - \mu \frac{x+x'}{2} \right) \right] dY d\mu.$$  

(17)

Relation (17) can be represented in the ‘basis-independent’ form [14,15]

$$\rho = \frac{1}{4\pi|\nu|} \left| \int w(Y, \mu, \nu) \exp \left[ \left( X - \frac{\mu\nu}{2} \right) \right] \right|$$  

$$\times e^{i\nu^2} e^{-i\nu^2} dX d\mu d\nu.$$  

(18)

The physical meaning of the marginal distribution function is that it is equal to the probability density of position $X$ measured in an ensemble of reference frames in phase space. The ensemble is described by two parameters $\mu$ and $\nu$. The parameters $\mu$ and $\nu$ read

$$\mu = \cos \varphi e^{i\lambda}, \quad \nu = \sin \varphi e^{-i\lambda},$$

where $\varphi$ is the rotation angle of the reference frame and $\lambda$ is scaling parameter of the reference frame. The composition law for the density operators $\rho_1, \rho_2$ can be transcribed into composition law of the tomographic probabilities. The idea of doing this is as follows:

The marginal distribution can be considered as the symbol of the density operator [26] (analogously to the Weyl symbol which is the Wigner function [5] of the quantum state). In this representation, product of the operators is translated into star-product Moyal product of the marginal distributions. Using this procedure for Eq. (8) one get the composition law of tomographic probabilities

$$w(X, \mu, \nu) = \left| c_1 \right|^2 w_1(X, \mu, \nu) + \left| c_2 \right|^2 w_2(X, \mu, \nu) + 2 \Re \{ c_1 c_2^* e^{i\alpha} w_{12}(X, \mu, \nu) \},$$  

(19)

where

$$w_{12}(X, \mu, \nu) = \frac{1}{4\pi|\nu|} \left| \int w_1(Y_1, \mu_1, 0) w_2(Y_2, \mu_2, 0) \right|$$  

$$\times e^{i(Y_1-Y_2)} d\mu_1 d\mu_2 dY_1 dY_2 \left[ e^{\frac{\mu_1}{2\nu}(q_1^2-q_2^2) - \frac{X}{\nu}(q_1-q_2)} \right]$$  

$$\times w_1(Y_1, \mu_1, q_1) w_2(Y_2, \mu_2, q_2) d\mu_1 d\mu_2 dY_1 dY_2 dq_1 dq_2,$$  

(20)

with the factor $e^{i\alpha}$ being related to the fiducial vector by Eq. (10).

4. Entanglement and purification of the product of density matrices

In this section, we provide only a sketch of the application of our purification procedure to entangle-
The density operator of a composite system $AB$ with subsystems $A$ and $B$ may be chosen to be pure or impure. For a pure density operator $\rho_{AB}$, one can get the density operator $\rho_A$ and $\rho_B$ by partial trace operation:

$$\rho_A = \text{Tr}_B (\rho_{AB}), \quad \rho_B = \text{Tr}_A (\rho_{AB}) .$$

It is not necessary that $A$ and $B$ have the same dimensionality. Unless $\rho_{AB}$ is a direct product of pure states of $A$ and $B$, a pure $\rho_{AB}$ yields impure $\rho_A$ and $\rho_B$. But they will have the same rank $n$ and the same nonnegative eigenvalues that sum up to unity.

The density operator

$$\rho'_{AB} = \rho_A \otimes \rho_B \neq \rho_{AB}$$

is impure. Thus, the whole is greater than the sum of two parts: there is additional information in $\rho_{AB}$. These are the ‘entanglement’ terms [2].

We purify the product $\rho'_{AB}$ in the same way that we used before for the mixture of two density operators $\rho_1$ and $\rho_2$. Here we have $n$ such mutually orthogonal pure states mixed together and need $(n - 1)$ phase angles $\phi_1 = 0, \phi_2, \ldots, \phi_n$. The diagonal form of $\rho'_{AB}$ has only $n$ nonzero diagonal elements $\lambda_j, j = 1,2,\ldots,n$. We need to introduce the off-diagonal elements $\sqrt{\lambda_j \lambda_k} \, e^{i(\phi_j - \phi_k)}$ in the $(j,k)$ location. Note that while we have $n(n - 1)/2$ off-diagonal terms, there are only $(n - 1)$ phases $\phi_j$.

We call the purification of the density matrix $\rho'_{AB}$ the phase-dependent multiplication law of the density matrices $\rho_A$ and $\rho_B$.

While purification is dependent on the phase angle, the form of the entanglement is constructed by supplementing additional information like the one contained in the fiducial vector $|\psi_0\rangle$.

5. Conclusions

Quantum mechanics can be formulated using either the notion of state vectors in Hilbert spaces or density operators and different types of quasidistributions.

A special type of representation uses tomographic probabilities. The superposition of states and of mixture of states are two different types of ‘addition of solutions’ of the density matrices of pure states. As is shown in this work, to describe the pure-state superposition within the framework of the density-matrix formalism (in terms of tomographic probabilities), a composition law of states can be formulated. Employing this composition law, one can work within the framework of density operators only and still take into account all the quantum interference effects.

The main result of our Letter is the formulation of the composition law for density operators of pure quantum states, which yields the rule of purification of the impure mixture of quantum states. This composition law is compatible with the evolution described by the Schrödinger or the von Neumann descriptions of pure quantum states and provides a rule to associate a pure state out of two pure states.

The basic idea of our Letter can also be used for a formulation of the purification rule for the product of two density matrices that describes the phenomenon of entanglement.

In this Letter, we have not discussed the purification of mixture of two impure states. Our basic idea can be made to work also in this situation. This can be done in two steps. We first extract a projection operator (a pure state) out of a mixture. This is going to be defined on the space of projection operators associated with $\mathcal{H} \otimes \mathcal{H}$. The actual subspace in the second factor will be the span of $A \ket{\psi_0}, A^2 \ket{\psi_0}, \ldots, A^k \ket{\psi_0}$, where $k$ is the rank of the mixture represented by $A$. Once we have got projection operators we may proceed as in the case we have already considered. Further details shall appear in a forthcoming Letter.

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