Positive-definite states of a Klein-Gordon type particle

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Abstract

A possible way for the consistent probability interpretation of the Klein-Gordon equation is proposed. It is assumed that some states of a scalar charged particle cannot be physically realized. The rest of quantum states are proven to have positive-definite probability distributions.

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1 Introduction

The problem of physical interpretation of the Klein-Gordon equation has a very long history. In the early days of quantum mechanics, Schrödinger [1], Klein [2], Gordon [3], and Fock [4] considered it as a relativistic counterpart
of the Schrödinger wave equation. However, it was impossible to ascribe a consistent probability interpretation to solutions of this equation due to negative values of the corresponding distribution functions, see e.g. [5]. The four-component quantum relativistic wave equation [6], proposed later by Dirac, is free of this problem. This is why the Dirac equation was considered as the unique possible way for the consistent formulation of relativistic quantum mechanics.

Nevertheless, as it has been demonstrated later by Pauli and Weisskopf [7], quantized Klein-Gordon field consistently describes spinless charged particles, $\pi^\pm$ mesons. Probability distributions for the total field energy and the field energy in a space region are positive definite. In the case of free particles this feature is also proper to the probability distribution of momentum. Procedures of measuring these observables are well-defined for Klein-Gordon type particles as well as for Dirac 1/2-spin particles.

At the same time, the measurement of the position is a special problem in the relativistic quantum theory. Indeed, according to the von Neumann reduction postulate [8], a result of the corresponding procedure is that the particle occurs to be in an eigenstate of the position operator. However, as it follows from the Hegerfeldt theorem [9], particles cannot be localized in the finite space region. Consequently, a localized state cannot appear as a result of any measurement procedure. Moreover, such a state would be a superposition of two states with different signs of charge that is prohibited by the fundamental charge superselection rule [10].

From the other hand, the von Neumann measurement is only a special type of the measurement procedures. More general situation occurs when the resulting state differs from the eigenstate of the measured observables. It happens, for example, in the well-studied process of photodetection. In this case, the detection of photons means their absorption. The resulting state consists fewer photons – generally it differs from the Fock numberstate, see e.g. [11]. Similarly one may assume, without referring to any special physical procedure, that in the case of the measurement of the position, resulting states differ from the prohibited eigenstates of the position operator. Consequently, the impossibility of localization does not lead to the impossibility of measuring the position, as it is frequently assumed.

As it was mentioned above, Dirac particles always have positive-definite position probability distribution [12]. In this case there are no conceptual problems for the measurement of the position. However such a problem arises for Klein-Gordon particles – the corresponding probability distribution may have negative values. This problem is addressed in the present contribution.

Newton and Wigner introduced the position operator different from the standard one [13]. Among other, the probability distribution for this ob-
servable has non-negative values even for the case of Klein-Gordon particles. However, this approach meets at least two serious problems – absence of the Lorentz-invariance and difficulties in formulation of the operational procedure for measuring such an observable.

A way for resolving this problem has been proposed by Gerlach, Gromes, and Petzold [14]. It has been shown that the current density of the Klein-Gordon field can be consistently redefined in such a way that the corresponding time component, charge density, is positive definite. Similarly, Mostafazadeh has proposed to redefine the scalar product for the solutions of the Klein-Gordon equation [15]. In the framework of this approach one also gets positive-definite probability distributions for the position.

In this contribution we propose an alternative solution of this old problem that does not require the redefinition of the standard scalar product. Our approach is based on the standard requirement that quantum states of a system can be described only by positive-definite density operator. It will be demonstrated that among the pure states of a Klein-Gordon type particle only eigenstates of the Hamiltonian obey this condition. Hence, all non-stationary positive-definite states are mixed ones.

## 2 Effective density operator

Let us start from the well-known Feshbach-Villars form of the Klein-Gordon equation [16]

\[ i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle, \] (1)

where the Hamiltonian

\[ \hat{H} = (\tau_3 + i\tau_2) \frac{\hat{p}^2}{2m} + \tau_3 mc^2 \] (2)

is \(2 \times 2\) operator-valued matrix and \(\tau_i\) are the Pauli matrices. These matrices describe an internal degree of freedom, so-called charge variable, associated with the sign of frequency that is sign of the charge in the quantum field theory. Utilizing the generalized unitary transformation defined by the operator-valued matrix

\[ \hat{S} = \frac{1}{2\sqrt{mc^2 E}} \left[ (\hat{E} + mc^2) + (\hat{E} - mc^2) \tau_1 \right] \] (3)

and the inverted one

\[ \hat{S}^{-1} = \frac{1}{2\sqrt{mc^2 E}} \left[ (\hat{E} + mc^2) - (\hat{E} - mc^2) \tau_1 \right], \] (4)
where
\[ \hat{E} = \sqrt{m^2c^4 + c^2 \hat{p}^2}, \] (5)

the Hamiltonian (2) can be diagonalized to the form
\[ \hat{H}_{\text{FV}} = \hat{S} \hat{H} \hat{S}^{-1} = \tau_3 \hat{E}. \] (6)

The corresponding representation is referred to as the Feshbach-Villars (FV) representation. The same rule,
\[ \hat{A}_{\text{FV}} = \hat{S} \hat{A} \hat{S}^{-1}, \] (7)

is applied for transformation of an arbitrary observable, \( \hat{A} \), in the FV representation.

Consider the observable, \( \hat{A} \), that is a function of the position, \( \hat{q} \), and momentum, \( \hat{p} \); moreover, we suppose that this observable does not depend on the matrices \( \tau_i \),
\[ \hat{A} = f (\hat{p}, \hat{q}). \] (8)

The application of eqs. (3), (4), (7) yields
\[ \hat{A}_{\text{FV}} = (\hat{E} + \tau_1 \chi) \hat{A}. \] (9)

In the last equations \( \mathcal{E} \) and \( \mathcal{X} \) are superoperators, which take the operator \( \hat{A} \) to the operators \( \mathcal{E} \hat{A} \) and \( \mathcal{X} \hat{A} \), respectively, as
\[ \langle p_2 | \mathcal{E} \hat{A} | p_1 \rangle = \varepsilon (p_2, p_1) \langle p_2 | \hat{A} | p_1 \rangle, \] (10)
\[ \langle p_2 | \mathcal{X} \hat{A} | p_1 \rangle = \chi (p_2, p_1) \langle p_2 | \hat{A} | p_1 \rangle, \] (11)

where
\[ \varepsilon (p_2, p_1) = \frac{E(p_2) + E(p_1)}{2\sqrt{E(p_2)E(p_1)}}, \] (12)
\[ \chi (p_2, p_1) = \frac{E(p_2) - E(p_1)}{2\sqrt{E(p_2)E(p_1)}}, \] (13)

and \( |p\rangle \), \( E(p) \) are eigenstates and eigenvalues of the operator (5).

As an example, consider the standard position operator, \( \hat{q} \). In this case,
\[ \mathcal{E} \hat{q} = \hat{\xi}, \] (14)

where \( \hat{\xi} \) is the Newton-Wigner position operator \[13\] in the FV representation,
\[ \hat{\xi} = i\hbar \frac{\partial}{\partial p}, \] (15)
that is the even part of the standard position operator [16]. Similarly,

$$\tau_1 \mathcal{X} \hat{q} = -i \hbar \frac{c^2 \hat{p}}{2E^2(\hat{p})} \tau_1$$

(16)

is the odd part of the position operator. We recall that the even part of an observable is a diagonal matrix in the FV representation and the odd part is an off-diagonal matrix.

Any state of a scalar charged particle satisfies the charge superselection rule [10], i.e. it does not include interference terms between particle and antiparticle. Moreover, without loss of generality one can consider only the positive sign of the charge. This means that the expected value of the observable \( \mathcal{E} \hat{A} \), \((17)\) can be written as

$$\bar{A} = \text{Tr} \left( \hat{\rho} \mathcal{E} \hat{A} \right),$$

(17)

where \( \hat{\rho} \) is the density operator in the FV representation. Specifically, the even part of \( \hat{q}^2 \) is given by

$$\mathcal{E} \hat{q}^2 = \hat{\xi}^2 - \left[ \frac{\hbar c^2 \hat{p}}{2E^2(\hat{p})} \right]^2.$$  

(18)

Hence, the variance of the position,

$$\langle \Delta q^2 \rangle = \langle \Delta \xi^2 \rangle - \left[ \frac{\hbar c^2 \hat{p}}{2E^2(\hat{p})} \right]^2,$$

(19)

may be negative [17] that is a consequence of the fact that the probability distribution is sign indefinite.

Eq. (17) can be considered as a scalar product of two elements, \( \hat{\rho} \) and \( \mathcal{E} \hat{A} \), in the operator space. The action of the Hermitian-conjugated superoperator \( \mathcal{E} \) can be transferred from \( \hat{A} \) to \( \hat{\rho} \) in eq. (17), i.e. \( \text{Tr} \left( \hat{\rho} \mathcal{E} \hat{A} \right) = \text{Tr} \left( \mathcal{E} \hat{\rho} \hat{A} \right) \). This fact can be simply proved by using Eqs. (12), (13). Further introducing the operator

$$\hat{\rho}_\mathcal{E} = \mathcal{E} \hat{\rho},$$

(20)

which we refer to as the effective density operator, eq. (17) is rewritten,

$$\bar{A} = \text{Tr} \left( \hat{\rho}_\mathcal{E} \hat{A} \right).$$

(21)

Similarly, the probability distribution to get the value \( A \) is

$$P \left( A \right) = \text{Tr} \left( \hat{\rho}_\mathcal{E} |A\rangle \langle A| \right),$$

(22)
where $A$ and $|A\rangle$ are eigenvalues and eigenstates, respectively, of the operator $\hat{A}$.

As it follows from eq. (20), the superoperator $\mathcal{E}$ takes each density operator, $\hat{\rho}$, to the effective density operator, $\hat{\rho}_E$. Since

$$\varepsilon(p_2, p_1) = \varepsilon(p_1, p_2) > 1 \quad \text{for} \quad p_2 \neq p_1,$$

$$\varepsilon(p, p) = 1,$$

there exist sign-indefinite effective density operators, $\hat{\rho}_E$, assigned to the positive-definite density operators, $\hat{\rho}$. Consequently, the probability distribution (22) may have negative values even for some positive-definite density operators, $\hat{\rho}$. This is the reason of problems in consistent probability interpretation of the Klein-Gordon equation.

The above consideration enables us to formulate the following assumption. Let us suppose that the states of a Klein-Gordon type particle are described by the positive-definite effective density operators, $\hat{\rho}_E$. Inverting the map (20), we get the following condition for the density operators:

$$\hat{\rho} = \mathcal{E}^{-1} \hat{\rho}_E,$$

where $\hat{\rho}_E$ is a positive-definite operator for which $\text{Tr}(\hat{\rho}_E) = 1$, $\mathcal{E}^{-1}$ is the superoperator inverted to $\mathcal{E}$ and defined by the rule

$$\langle p_2 | \mathcal{E}^{-1} \hat{\rho}_E | p_1 \rangle = \varepsilon^{-1}(p_2, p_1) \langle p_2 | \hat{\rho}_E | p_1 \rangle.$$  

Taking into account that

$$\varepsilon^{-1}(p_2, p_1) = \varepsilon^{-1}(p_1, p_2) < 1 \quad \text{for} \quad p_2 \neq p_1,$$

$$\varepsilon^{-1}(p, p) = 1,$$

we conclude that under the above assumption the states of a Klein-Gordon type particle are mostly mixed. Only eigenstates of the Hamiltonian are pure and obey the condition (25).

### 3 Observables

The above consideration deals with the observables that are arbitrary functions of position and momentum. However, some observables do not belong to this class. For example, the Hamiltonian (2) is a function of position, momentum, and charge variable. At the same time, the expected value of the Hamiltonian is determined only by diagonal matrix elements of the density operator. As it follows from eqs. (24), (28),

$$\langle p | \hat{\rho}_E | p \rangle = \langle p | \hat{\rho} | p \rangle.$$
Hence, the expected value of the Hamiltonian is given by

$$\bar{H} = \text{Tr} \left( \hat{\varrho}_x \hat{E} \right),$$

(30)

where $\hat{E}$ is defined by eq. (5). This result adopts the rule (8) for the evaluation of the expected value of the Hamiltonian.

Another example is the velocity operator,

$$\hat{v} = \frac{1}{i\hbar} \left( \hat{q} \hat{H} - \hat{H} \hat{q} \right),$$

(31)

which is a function of the position, $\hat{q}$, and the Hamiltonian, $\hat{H}$. More generally, let us consider arbitrary functions of position, momentum, and energy, i.e.

$$\hat{B} = F \left( \hat{p}, \hat{q}, \hat{H} \right).$$

(32)

In the FV representation this observable has the form

$$\hat{B}^{\text{FV}} = (\mathcal{E} - \tau_1 \mathcal{X}) F \left( \hat{p}, \hat{\xi}, \tau_3 \hat{E} \right),$$

(33)

where $\hat{\xi}$ is the Newton-Wigner position operator, eq. (15). It now follows that the expected value of this observable is given by

$$\bar{B} = \text{Tr} \left[ \hat{\varrho}_x \mathcal{E} F \left( \hat{p}, \hat{\xi}, \hat{E} \right) \right],$$

(34)

where we suppose the positive sign of the charge. In terms of the effective density operator it is rewritten as

$$\bar{B} = \text{Tr} \left[ \hat{\varrho}_x F \left( \hat{p}, \hat{\xi}, \hat{E} \right) \right].$$

(35)

Arguing as above, we conclude that for the observable (32) one can also apply the effective density operator (20) and require its positivity.

4 Relativistic phase-space representation

An example of the positive-definite states is a natural generalization of the coherent state $|\alpha\rangle$

$$\hat{\varrho}_\alpha = \mathcal{E}^{-1} |\alpha\rangle \langle \alpha|,$$

(36)

where $|\alpha\rangle$ is an eigenstate of the operator

$$\hat{a} = \frac{1}{\sqrt{2}} \left( \hat{\xi} + i \frac{\lambda}{\hbar} \hat{p} \right),$$

(37)
\( \hat{\xi} \) is the Newton-Wigner position operator [15], \( \lambda \) is a scaling length. Contrary to the non-relativistic case, for a review see e.g. [18], the coherent state (36) is not pure. However, it manifests the properties essential for the usual coherent states. Particularly, the coherent states (36) minimize the Heisenberg uncertainty relation,

\[
\langle \Delta q^2 \rangle \langle \Delta p^2 \rangle = \frac{\hbar^2}{4}.
\] (38)

At the same time, the pure relativistic coherent states of a scalar charged particle, see e.g. [17], [19], [20], [21] and references therein, are not positive definite and do not obey the condition (25).

Similarly to [22], we present the \( s \)-parameterized phase-space distribution of a scalar charged particle as

\[
P(\alpha; s) = \frac{1}{\pi^2} \int d^2 \beta \text{Tr} \left[ \hat{\rho}_\varepsilon e^{(\hat{a}^\dagger - \alpha^*)\beta - (\hat{a} - \alpha)\beta^* + s|\beta|^2} \right].
\] (39)

For \( s = 0 \) eq. (39) defines the relativistic Wigner function considered in [25], for \( s = 1 \) – the relativistic Glauber-Sudarshan distribution, for \( s = -1 \) – the relativistic Husimi-Kano distribution. The density operator \( \hat{\rho} \) can be expressed in terms of the Glauber-Sudarshan distribution [23],

\[
\hat{\rho} = \int d^2 \alpha P(\alpha; 1) \hat{\rho}_\alpha,
\] (40)

where \( \hat{\rho}_\alpha \) is given by eq. (36). Likewise, the Husimi-Kano distribution [24], can be expressed in terms of the density operator \( \hat{\rho} \),

\[
P(\alpha; -1) = \frac{1}{\pi} \text{Tr} (\hat{\rho} \hat{\rho}_\alpha).
\] (41)

The phase-space distribution (39) includes the complete information about the density operator and can be used for the characterization of the quantum states of a Klein-Gordon type particle.

5 Conclusions

We have demonstrated that the reason of problems in consistent probability interpretation of the Klein-Gordon equation is that a lot of quantum states are described by sign-indefinite density operators. Particularly, the most of
pure states are sign indefinite. From the other hand, there exist the states of a Klein-Gordon type particle that are characterized by positive-definite density operators. We suppose that only such states have physical realization. This assumption is in a good accordance with the basic principles of quantum physics.

The eigenstates of the Hamiltonian are positive definite. Since such states are stationary, the unitary evolution does not result in the appearance of negative-definite states. The positive-definite non-stationary states of a Klein-Gordon type particle are mixed. The unitary evolution cannot be characterized by decreasing the entropy, i.e., it cannot purify the states. In this reason such states are positive-definite for any moment of time.

In the outlook we address the following problems. First of all, the question about the Lorentz invariance of the proposed approach is still open. In other words, the question is whether the state, which is positive definite in a given reference frame, is positive definite in other reference frames? Another problem is in the generalization of the proposed approach to the case of quantized Klein-Gordon field. We believe that resolving these problems results in the progress of the scalar charged particles theory.

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