Further Difficulties with the
Klein-Gordon Equation

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Abstract:

The Dirac equation is compared with the Klein-Gordon one. Unlike the Dirac case, it is proved that the Klein-Gordon equation has problems with the Hamiltonian operator of the Schroedinger picture. A special discussion of the Pauli-Weisskopf article and that of Feshbach-Villars proves that their theories of a charged Klein-Gordon particle lack a self consistent expression for this Hamiltonian. Related difficulties are pointed out.
The Klein-Gordon (KG) equation and the Dirac one were published in the very early days of quantum mechanics (see [1], bottom of pp. 25, 34). The KG equation is regarded as the relativistic quantum mechanical equation of a spin-0 massive particle and the Dirac equation describes a spin-1/2 massive particle. The Dirac equation of an electrically charged particle can be found in any textbook on relativistic quantum mechanics and on quantum electrodynamics. This equation is regarded as a correct description of a system belonging to the domain of validity [2] of relativistic quantum mechanics. Thus, for example, the Dirac equation can be used for the hydrogen atom if one is ready to ignore small effects like the Lamb shift.

Unlike the Dirac equation, the KG equation is not free of objections. In particular, Dirac maintained his negative opinion on this equation throughout his life [3]. On the other hand, claims stating that Dirac’s opinion on the KG equation is wrong were published (see [1], second column of p. 24).

New difficulties with the KG equation were published recently [4]. Thus, new arguments proving that the KG wave function cannot describe probability are given; it is proved that a KG particle cannot interact with electromagnetic fields; the classical limit of the Yukawa interaction is inconsistent with special relativity and some other claims.

The 4-current of a particle represents specific properties of its state, namely its density and its 3-current. The KG electromagnetic interaction discussed in [4] relies on the requirement stating that the 4-current of a KG particle (like that of any other particle) should not depend on field variables of external particles. A further discussion of this issue is presented near the end of this work. The present work provides new arguments that do not rely on this requirement. This work examines the structure of the Hamiltonian of the system in relativistic quantum mechanics. The significance of the
corresponding Lagrangian density is pointed out.

Units where \( \hbar = c = 1 \) are used. The Lorentz metric \( g_{\mu\nu} \) is diagonal and its entries are (1,-1,-1,-1). Greek indices run from 0 to 3 and Latin ones run from 1 to 3. The summation convention holds for a pair of upper and lower indices. The lower case symbol \( _\mu \) denotes the partial differentiation with respect to \( x^\mu \). An upper dot denotes the partial differentiation with respect to the time. Thus, \( \dot{\phi} \equiv \phi_{,0} \).

Let us examine the theoretical structure of a Dirac field interacting with an electromagnetic field. This subject is useful not only for its own sake but also for the corresponding analysis of the KG equation which is carried out later. The matter part of the Lagrangian density is (see [5], p. 84)

\[
\mathcal{L} = \bar{\psi}[\gamma^\mu(i\partial_\mu - eA_\mu) - m]\psi,
\]

where \( \gamma^\mu \) denotes a set of four Dirac \( \gamma \) matrices, \( \psi \) is the Dirac wave function, \( \bar{\psi} = \psi^\dagger\gamma^0 \) and \( \psi^\dagger \) is the Hermitian conjugate of \( \psi \). The definition \( \gamma^0 = \beta, \gamma^i = \beta\alpha^i \) relates the Dirac \( \gamma \) matrices and the \( \alpha, \beta \) ones. The components of the 4-potential are the electric potential \( V \) and the vector potential \( A \). Thus, \( A^\mu = (V, A) \).

A variation of (1) with respect to \( \bar{\psi} \) yields the Dirac equation (see [5], p. 84)

\[
\gamma^\mu(i\partial_\mu - eA_\mu)\psi = m\psi.
\]

An important quantity is the 4-current of the Dirac particle

\[
j^\mu = \bar{\psi}\gamma^\mu\psi,
\]

which satisfies the conservation law

\[
j^\mu_{,\mu} = 0.
\]
The validity of this relation is independent of the external electromagnetic field (see [6], p. 119). The 0-component of the 4-current (3) represents the density of the Dirac particle

\[ \rho = \bar{\psi} \gamma^0 \psi = \psi^\dagger \psi. \] (5)

The matter part of the Hamiltonian density is derived from the Lagrangian density (1) by the well known relation (see [5], p. 87)

\[ \mathcal{H} = \sum \bar{\psi} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} - \mathcal{L} = \psi^\dagger [\alpha \cdot (-i \nabla - eA) + \beta m + eV] \psi, \] (6)

where the summation runs on \( \dot{\psi} \) and \( \bar{\psi} \). (As a matter of fact, only \( \dot{\psi} \) is found in (1)). Here quantities should be written in terms of coordinates and conjugate momenta. However, this point is not essential for the discussion carried out below. Hence, it is skipped throughout this work.

Using the expression for the density (5), one readily extracts from the Hamiltonian density (6) an expression for the Hamiltonian operator used in the Schroedinger’s picture of relativistic quantum mechanics

\[ H = \alpha \cdot (-i \nabla - eA) + \beta m + eV \] (7)

It is well known that the Hamiltonian operator \( H \) plays a cardinal role in the Schroedinger picture of quantum mechanics, because it defines the time evolution and the energy states of the system (see [5], p. 6)

\[ H \psi = i \frac{\partial \psi}{\partial t}. \] (8)

Now, due to the principle of superposition, quantum mechanics uses equations that are linear in \( \psi \). For this reason, the Hamiltonian operator of (8) should not depend on \( \psi \). This requirement is satisfied by the Dirac Hamiltonian (7).
Substituting the Hamiltonian operator (7) into the quantum mechanical relation (8), one obtains the Hamiltonian form of the Dirac equation

$$ [\alpha \cdot (-i\nabla - eA) + \beta m + eV] \psi = i\frac{\partial \psi}{\partial t}. $$

(9)

The complete agreement between (9) and the Dirac equation (2), derived as the Euler-Lagrange equation of the Lagrangian density (1), indicates the self-consistence of the theory.

It is interesting to note relativistic properties of the Hamiltonian density (6) and of the Hamiltonian operator (7). Examining the first line of (6) and remembering that the Lagrangian density $L$ is a Lorentz scalar, one realizes that (6) is a tensorial component $T^{00}$ of the second rank tensor

$$ T^{\mu\nu} = \sum \psi_{\mu} \frac{\partial L}{\partial \psi_{\nu}} - L g^{\mu\nu}. $$

(10)

This is the required covariance property of energy density. In classical physics, energy density is the $T^{00}$ component of the energy-momentum tensor $T^{\mu\nu}$ (see [7], p. 77). Now, since the probability density $\rho$ of (5) is a 0-component of a 4-vector, one concludes that also the Hamiltonian operator $H$ of (7) is a 0-component of a 4-vector. Evidently, this property is essential for satisfying covariance of the fundamental quantum mechanical relation (8). This discussion shows just one reason for the usefulness of constructing the theory on the basis of a Lagrangian density. This point is used below in the analysis of the Feshbach-Villars (FV) Hamiltonian.

It can be concluded that the following properties hold for the Dirac theory:

1. The conserved 4-current depends on $\psi$ and on the corresponding $\bar{\psi}$ and is independent of the external field $A_\mu$.

2. Since the Dirac Lagrangian density (1) is linear in the time-derivative $\partial \psi/\partial t$, the corresponding Hamiltonian density (6) does not contain
derivatives of $\psi$ with respect to the time. Hence, in the case of a Dirac particle, the fundamental quantum mechanical relation (8) takes the standard form of an explicit first order partial differential equation. Here a derivative with respect to the time is equated to an expression which is free of time derivatives. This property does not hold for Hamiltonians that depend on time derivative operators.

3. The Dirac Hamiltonian operator (7) is free of $\psi$, $\bar{\psi}$ and their derivatives. An examination of (8) proves that this property is consistent with the linearity of quantum mechanics and with the superposition principle as well.

4. The equation (9) obtained from the substitution of the Dirac Hamiltonian operator (7) into the quantum mechanical relation (8), agrees with the Dirac equation (2) obtained as the Euler-Lagrange equation of the Lagrangian density (1).

These four points indicate the self consistency of the Dirac theory. It is proved below that difficulties arise if one carries out an analogous analysis of the KG equation.

Let us turn to the Pauli-Weisskopf (PW) theory of a charged KG particle (see Section 3 of [8]). These authors use the Lagrangian density (see eq. (37) therein)

$$L = (\dot{\phi}^* - ieV\phi^*)(\dot{\phi} + ieV\phi) - \sum_{k=1}^{3}(\phi_{k}\phi^* + ieA_k\phi^*)(\phi_{,k} - ieA_k\phi) - m^2\phi^*\phi. \quad (11)$$

Note that minor changes are made in the form of quoted equations. Thus, units where $\hbar = c = 1$ are introduced; $\phi$ denotes the KG wave function and the electromagnetic 4-potential is $A^\mu = (V, A)$. On the other hand, the Lorentz metric of quoted formulas is that of the original articles.
The Hamiltonian density associated with (11) is written next to this equation (see eq. (37a) therein)
\[ \mathcal{H} = (\dot{\phi}^* - ieV\dot{\phi}^*)(\dot{\phi} + ieV\phi) + \sum_{k=1}^{3} (\phi_{k}^* + ieA_k\phi^*)(\phi_{k} - ieA_k\phi) + m^2\phi^*\phi. \] (12)

The Lagrangian density (11) is used in a derivation of the second order equation of motion of a charged KG particle (see eq. (39) therein)
\[ \left(\frac{\partial}{\partial t} - ieV\right)\left(\frac{\partial}{\partial t} - ieV\right)\phi = \sum_{k=1}^{3} \left(\frac{\partial}{\partial x^k} + ieA_k\right)\left(\frac{\partial}{\partial x^k} + ieA_k\right)\phi + m^2\phi. \] (13)

The conserved 4-current of this particle is derived too. The 0-component of this quantity is (see eq. (42) therein)
\[ \rho = i(\phi^*\dot{\phi} - \dot{\phi}^*\phi) - 2eV\phi^*\phi. \] (14)

Unlike the case of a Dirac particle, here the 4-current of a KG particle depends on derivatives of \( \phi \) and on external electromagnetic quantities.

Before proceeding with the analysis, let us write down the canonical Hamiltonian obtained from the application of the first line of (6) to the Lagrangian density (11)
\[ \mathcal{H} = \dot{\phi}^*\dot{\phi} - e^2V^2\phi^*\phi + \sum_{k=1}^{3} (\phi_{k}^* + ieA_k\phi^*)(\phi_{k} - ieA_k\phi) + m^2\phi^*\phi. \] (15)

As mentioned (see [9], p. 68) this expression is not gauge invariant.

Let us examine the issue of the Hamiltonian operator required for the Schroedinger picture of the fundamental quantum mechanical relation (8). It is shown above how easily this task is accomplished for the Dirac Hamiltonian. In this case one just removes the Dirac density factor \( \psi^\dagger\psi \) from the Hamiltonian density (6) and extracts the required expression. This quantity is not given in [8].

The following argument proves that this task can be accomplished neither for the Hamiltonian density (12) nor for that of (15). Let \( \hat{H} \) denote the
required operator. Now, apart from multiplicative factors, the highest order
time derivative of (12) and (15) is $\dot{\phi}^*\dot{\phi}$ and that of the density (14) is $(\dot{\phi}^*\dot{\phi} -
\dot{\phi}^*\phi)$. Hence, $\hat{H}$ cannot contain the operator $\partial/\partial t$, because both $\dot{\phi}^*\dot{\phi}$ and
$(\dot{\phi}^*\dot{\phi} - \dot{\phi}^*\phi)$ have $\dot{\phi}$ as the highest order time derivative of $\phi$. Evidently,
due to the superposition principle and the linearity of quantum mechanics,
$\hat{H}$ should depend neither on $\phi$, $\phi^*$ nor on their derivatives. Hence, under
these restrictions on the structure of $\hat{H}$, it is evident that $\hat{H}$ cannot exist
because $\dot{\phi}^*\dot{\phi}$ is symmetric with respect to $\phi$ and $\phi^*$, whereas $(\dot{\phi}^*\dot{\phi} - \dot{\phi}^*\phi)$ is
antisymmetric with respect to these functions. This proof does not rely on
terms containing the electric charge $e$. Hence, it applies also to the case of
an uncharged KG particle described by a complex field.

Let us turn to the theory described in the FV article[1]. These authors
construct an expression for the Hamiltonian operator of a charged KG parti-

cle that, in the Schroedinger’s picture, takes the standard quantum mechan-

cal form (8). For this purpose they use a 2-component wave function

$$\Psi = \begin{pmatrix} \psi \\ \chi \end{pmatrix}. \quad (16)$$

where $\psi$ and $\chi$ are linear combinations of the KG wave function $\phi$ and of $\dot{\phi}$
(see eqn. (2.11)-(2.17) therein). These authors present the following Hamil-
tonian operator that can be used in the Schroedinger picture of (8) (see (2.18)
therein)

$$H = (\tau_3 + i\tau_2)(1/2m)(\mathbf{p} - e\mathbf{A})^2 + m\tau_3 + eV, \quad (17)$$

where $\tau_2$ and $\tau_3$ are Pauli spin matrices.

The analysis of FV does not rely on a Lagrangian density. Hence, it is
not clear whether or not the Hamiltonian (17) satisfies relativistic covariance.
As a matter of fact, a proof of this essential property is not found in [1]. The
following analysis explains why it is impossible to construct such a proof.
Let us analyze covariance properties of (17). As stated earlier, the fundamental quantum mechanical relation (8) indicates that (17) should be a 0-component of a 4-vector. The last term of (17) is $eV$ where $e$ is a Lorentz scalar denoting the charge of the KG particle and $V$ is the 0-component of the electromagnetic 4-potential $A_\mu$. Hence, the last term of (17) is a 0-component of a 4-vector, as required. The second term of (17) is $m\tau_3$. Here $m$ is a scalar denoting the KG particle’s self mass. Now, the $\tau_3$ Pauli matrix certainly can’t transform like a 0-component of a 4-vector. Therefore, the second term and the last term of (17) have different covariant properties.

Furthermore, the first term of (17) is also inconsistent with the last one, because it is not a 0-component of a 4-vector. Indeed, the following expression shows the tensorial form of this term

$$(p - eA)^2 = (E - eV)^2 - (P_\mu - eA_\mu)(P_\mu - eA_\mu)g^{00}.$$ (18)

Here the first term on the right hand side is a product of two energy quantities. Hence, under a Lorentz transformation, (18) behaves like a tensorial component $W^{00}$. Here, in principle, one may alter the tensorial rank of each term by using the relativistic metric $g_{\mu\nu}$ and the completely antisymmetric unit tensor of the fourth rank $\varepsilon^{\alpha\beta\gamma\delta}$. Evidently, the rank of each of these tensors is an even number. Thus, one cannot put the first term of (17), which is a component of an even rank tensor $W^{00}$ and the last one, which belongs to an odd rank tensor, $A^\mu$, in the same equation, without violating covariance. Obviously, the factor $(\tau_3 + i\tau_2)$ and the Lorentz scalar $1/2m$ cannot settle this contradiction. This discussion proves that (17) violates covariance and therefore it takes an unacceptable form of the Hamiltonian.

The results of this work are described in the following lines. First, the theory derived from the Lagrangian density of a charged Dirac particle is discussed. It is shown that the Hamiltonian density and the Hamiltonian
operator of the Schroedinger picture are derived in a straightforward manner and the results are selfconsistent. In particular, the Euler-Lagrange equation derived from the Lagrangian density agrees with the fundamental quantum mechanical equation $i\partial\psi/\partial t = H\psi$.

It is shown that an analogous structure does not exist for the KG equation. An expression for the Hamiltonian operator of the Schroedinger picture is not given in [8] and it is proved above that this quantity cannot be extracted from the Hamiltonian density (12). Note also that an attempt to construct a Hamiltonian operator for a charged KG particle without relying on a Lagrangian density[1] fails too. In this case it is proved that the suggested Hamiltonian violates relativistic covariance and should be rejected.

Since no acceptable Hamiltonian operator exists for a charged KG particle, one obviously cannot close the logical cycle and prove that the Hamiltonian equation of motion $i\partial\psi/\partial t = H\psi$ is consistent with the Euler-Lagrange equation obtained from the KG Lagrangian density (11). This is certainly not an easy task, because the KG equation has a second order derivative with respect to the time whereas the Hamiltonian density and the fundamental quantum mechanical equation $i\partial\psi/\partial t = H\psi$ contain only first order derivatives.

The following discussion compares the structure of the Lagrangian density of the Dirac equation with that of the KG one and provides a possible explanation of the origin of the difficulties of the latter. The unit system where $\hbar = c = 1$ facilitates this task. Here dimensions of every physical quantity is written in terms of one unit, which is taken here to be that of length $[L]$. Thus, energy and momentum have the dimension of $[L^{-1}]$.

The action $S$ is dimensionless. Thus, the relation

$$dS = (\int \mathcal{L}d^3x)dt$$

(19)
proves that the dimension of the Lagrangian density is $[L^{-4}]$. The first line of (6) proves that this is also the dimension of the Hamiltonian density $\mathcal{H}$. Now, in the case of the Dirac equation, terms take the first power of energy, momentum and mass (henceforth called energy-like quantities). By contrast, it is shown above that this relation holds for the Dirac equation where (2) is equivalent to (9). Hence, the dimension of the product $\bar{\psi}\psi$ is $[L^{-3}]$. Thus, in the case of the Dirac equation terms representing energy-like quantities play a general role and take the same form for all states of the Dirac particle. On the other hand $\psi$ and $\bar{\psi}$ represent specific information concerning the particle’s state. This is the underlying reason for the straightforward extraction of the Dirac Hamiltonian operator (7).

The structure of the KG Lagrangian density (11) (and that of the associated Hamiltonians (12) and (15)) differs from that of the Dirac case. Here energy terms take the second power. Hence, the dimension of the product $\phi^*\phi$ is $[L^{-2}]$. Now, since the dimension of density is $[L^{-3}]$, one finds that in the case of a complex field of an uncharged particle, the expression for the density is $i(\phi^*\dot{\phi} - \dot{\phi}^*\phi)$. A complication arises in the case of a charged particle (14), where the density of the KG particle depends on electromagnetic quantities too.

Now, in the KG equation of motion (13), energy-like quantities do not represent specific properties of the KG field but have a general meaning and take the same form for all states of the KG particle. On the other hand, the expression for the density (14) describes a specific property of the field. Thus, energy-momentum operators $(i\partial/\partial t, -i\nabla)$ play two different roles in the structure of the KG theory: in the KG equation of motion they represent energy-momentum and contain no specific property of the field whereas in the expression for the density (14) - which is a specific property of the solution
- one energy operator changes its role and is used for this purpose.

The situation becomes even more unexpected in the case where electric charge and electromagnetic fields are a part of the system. Here the substitution \( P^\mu \rightarrow P^\mu - eA^\mu \) (see [5], p. 84 and [8], eq. (36)) is performed. Thus, \( eA^\mu \), which is a companion of energy-momentum, is carried together with the latter and plays a part in the description of the density of the KG particle.

This discussion explains how the KG theory uses energy-momentum operators for two distinct roles: as energy-momentum operators representing energy balance in the KG equation, and as a part of the expression representing a specific property of the solution, namely its 4-current in general and its density in particular. This ambiguity is probable the underlying reason for the inability to extract the KG Hamiltonian operator from the Hamiltonian density (12).

The following difficulties of the KG equation are discussed above:

1. The theory lacks the Hamiltonian operator required for the Schroedinger picture.

2. Assuming that this Hamiltonian is constructed, it is not clear that the second order KG equation is equivalent to the fundamental quantum mechanical equation \( i\partial\psi/\partial t = H\psi \).

3. No justification is given to the dependence of the 4-current of the KG particle on the external electromagnetic 4-potential.

4. No justification is given to the different meaning of energy-momentum operators: as energy-momentum operators in the KG equation and as an element in the description of the 4-current, which is a property of a specific solution.
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