Difficulties with the Klein-Gordon Equation

E. Comay
School of Physics and Astronomy
Raymond and Beverly Sackler Faculty of Exact Sciences
Tel Aviv University, Tel Aviv 69978, Israel
Email: elic@tauphy.tau.ac.il

Relying on the variational principle, it is proved that new contradictions emerge from an analysis of the Lagrangian density of the Klein-Gordon field: normalization problems arise and interaction with external electromagnetic fields cannot take place. By contrast, the Dirac equation is free of these problems. Other inconsistencies arise if the Klein-Gordon field is regarded as a classical field.

Keywords: Relativistic Quantum Mechanics, Klein-Gordon Equation

1. Introduction

The Klein-Gordon (KG) equation (called also Schroedinger's relativistic wave equation)

$$(\Box + m^2)\phi = 0 \tag{1}$$

was proposed by several authors in the very early days of quantum mechanics (see [1], bottom of p. 25). Difficulties with this equation were pointed out soon after its publication. In particular, it was claimed that, as a second order equation of the time derivative, solutions of the KG equation cannot represent local probability of a particle (see [2] pp. 7,8). These problems motivated Dirac to construct his relativistic first order differential equation, now regarded as the relativistic form of the Schroedinger equation for a spin-1/2 particle.

The debate surrounding the KG equation has gone on for many decades. Dirac maintained that the KG equation is unacceptable[3] throughout his life. A contradictory point of view argues that problems of the KG equation can be resolved and that Dirac's point of view is incorrect (see [1], second column of p. 24). Today, the KG equation is used as the equation of motion of a massive spinless particle and it can be found in some books discussing classical field theory ([4]-[6]) and in many books on quantum field theory(see e.g. [2], p. 21, [6] and [7]).

This work uses units where $\hbar = c = 1$. In these units, a shorthand notation of dimensions of physical quantities is used. As it turns out, this notation makes the discussion clearer. Thus, mass, energy, momentum, electromagnetic potentials and acceleration have the dimension $[L^{-1}]$. Length and time have the dimension $[L]$ and electric charge, velocity, angular momentum and action are dimensionless. The square brackets used here avoid confusion between the symbol of length and that of the Lagrangian. The Lorentz metric $g_{\mu\nu}$ is diagonal and its entries are (1,-1,-1,-1). 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^μ.

The cornerstone of this work is the variational principle which is used to prove new difficulties with the KG equation. In other words, the work adheres to the variational principle and to results derived from it. Corrections that rely on other physical arguments are beyond the scope of this work. The variational principle is applied here to quantum mechanics and to its classical limit as well. Aspects of quantum field theory are pointed out at the end of this work. Relativistic classical theory, relativistic quantum mechanics and quantum field theory are related in an ascending hierarchical order. A discussion of this kind of relationship between physical theories can be found in [8]. The results of this work provide new arguments supporting Dirac's point of view on the KG equation.

The second section discusses general properties of the KG equation. Problems belonging to the classical limit are discussed in the third section. Concluding remarks are set out in the last section.

2. The Realm of Quantum Mechanics

The Lagrangian density of the KG equation of a free particle is (see [7], p. 26)

$$\mathcal{L} = \frac{1}{2}(\phi_{,\mu}\phi_{,\nu}g^{\mu\nu} - m^2\phi^2). \tag{2}$$

Unless otherwise stated and for the simplicity of the notation, the real KG field is examined (see [7], p. 26). Applying the Euler-Lagrange equation (see, e.g. [7], p. 17)

$$\frac{\partial}{\partial x^\mu}\frac{\partial \mathcal{L}}{\partial \phi_{,\mu}} - \frac{\partial \mathcal{L}}{\partial \phi} = 0. \tag{3}$$

to the Lagrangian density (2), one obtains the KG equation of a free particle (1).

Before entering into details, let us state the restrictions imposed by the variational principle. The action S is a Lorentz scalar and, in units where $\hbar = 1$, it is a pure number. Thus, the relation

$$dS = \mathcal{L}d^3xdt \tag{4}$$

is examined. Since d^3xdt is a Lorentz scalar having the dimensions $[L^4]$, one finds that every term of the Lagrangian density should satisfy the following requirements:

A. It is a Lorentz scalar.

B. Its dimensions are L^{-4}.

First, it is proved that normalization problems of the KG equation still persist. Indeed, in examining (2) and requirement B, one finds that the dimension of the KG field ϕ is $[L^{-1}]$. Thus, ϕ^2 has the dimension $[L^{-2}]$, which means that the corresponding wave function *cannot* represent probability density whose dimension is $[L^{-3}]$. Therefore, the KG field ϕ lacks a fundamental property of a probability function. This result holds for the complex KG field as well.

Another argument leading to this result is that ϕ is a Lorentz scalar and so is $\phi^*\phi$. On the other hand, the probability density is a 0-component of a 4-vector called the 4-current (see [9], pp. 69-71). Hence, the Lorentz scalar $\phi^*\phi$ cannot represent probability density. This discussion provides new arguments supporting the well known claim that the wave function of the KG equation cannot represent probability, which relies on the freedom of defining $\partial\phi/\partial t$ (see [2], pp. 7,8). Hence, the KG wave function cannot be incorporated in the standard formulation of quantum mechanics, where $\psi^*\psi$ represents probability density and $\int \psi^*\hat{O}\psi d^3x$ is the expectation value of any operator $\hat{O}$.

Next, it is proved that a KG particle cannot interact with an external electromagnetic field. Here real and complex KG fields are treated separately. The analysis examines candidates for the interaction term of the Lagrangian density. Each of these candidates should satisfy requirements A and B. Moreover, due to space homogeneity, quantities should not depend explicitly on the spatial coordinates and, due to Lorentz covariance, they should not depend explicitly on the time too. The electromagnetic equations of motion impose further restrictions. Thus, varying the charged particle's coordinates and holding the electromagnetic variables fixed, one should obtain the Lorentz 4-force $F^{\mu\nu}j_\nu$ exerted on a classical charge. Hence, the interaction term of the Lagrangian density should be linear and homogeneous in electromagnetic quantities. By the same token, applying a variation of the electromagnetic field quantities, one should obtain Maxwell equation $F^{\mu\nu}_{,\nu} = -4\pi j^\nu$. Therefore, the interaction part of the Lagrangian density should also be proportional to a quantity representing the 4-current of the investigated charged particle. The electromagnetic fields tensor $F^{\mu\nu}$ is antisymmetric and is unsuitable for this purpose. Indeed, due to requirement A, it must be contracted with a second rank tensor depending on the KG field. Two candidates are $\phi_{,\mu}\phi_{,\nu}$ and $\phi_{,\mu,\nu}$. However, these tensors are symmetric with respect to the indices μ and ν. Hence, their contraction with the antisymmetric tensor $F^{\mu\nu}$ yields a null result.

Thus, the 4-potential of the electromagnetic fields, A_μ, is left as the sole electromagnetic factor of the required interaction term. In order to have a Lorentz scalar it must be contracted with a 4-vector depending on the KG field, which is $\phi_{,\mu}$. The dimension of A^μ is $[L^{-1}]$ and that of $\phi_{,\mu}$ is $[L^{-2}]$. Hence, in order to satisfy the dimensions of requirement B, another factor ϕ should be added. Thus, the candidate for the interaction term is

$$\mathcal{L}_{int} = eA^\mu \phi_{,\mu}\phi \tag{5}$$

where the coefficient e represent the dimensionless elementary electric charge ($e^2 \simeq 1/137$).

Now applying the Euler-Lagrange equation (3) to the candidate for the interaction term (5), one obtains 3 terms

$$e(A^\mu \phi_{,\mu} + A^\mu_{,\mu}\phi - A^\mu \phi_{,\mu}). \tag{6}$$

Here, the first and the last terms cancel each other and the second term vanishes, due to the Lorentz gauge $A^\mu_{,\mu} = 0$. This outcome means that an external electromagnetic field does not affect the motion of a KG particle defined by a real field.

In the case of a complex KG field, one can write a conserved 4-current (see [7], p. 40,[10], p. 30)

$$j_\mu = i(\phi^* \phi_{,\mu} - \phi^*_{,\mu}\phi) \tag{7}$$

and the following quantity

$$\mathcal{L}_{int} = -ej^\mu A_\mu. \tag{8}$$

is tested as a candidate for the interaction part of the Lagrangian density. (In (7), the 4-current j^μ pertains to probability. In other cases it represents an electric 4-current.) As required, the dimensions of (7) and of (8) are $[L^{-3}]$ and $[L^{-4}]$, respectively. Moreover, the interaction term (8) is proportional to the electric charge, which is a mandatory property of electrodynamics (see [9], p. 70).

Since (7) is a conserved current, namely $j^{\mu}_{,\mu} = 0$, one expects that Maxwell equations hold for the interaction term (8) (see [9], pp. 73-74). On the other hand, it is proved below that problems exist with the KG equation.

Applying the Euler-Lagrange equation (3) to ϕ^* and $\phi^*_{,\mu}$ of the interaction term of the Lagrangian density (8), one obtains the interaction term of the KG equation for ϕ. Thus, the KG equation becomes

$$(\Box + 2ieA^{\mu}\partial_{\mu} + m^2)\phi = 0 \tag{9}$$

Consider a motionless KG charged particle located inside a uniformly charged spherical shell. Thus, the 4-potential is

$$A_{\mu} = (V, 0, 0, 0). \tag{10}$$

Now, within the realm of quantum mechanics, the (unnormalized) wave function of a motionless KG particle is

$$\phi = e^{-iEt} \tag{11}$$

where the total energy is

$$E = m + U, \tag{12}$$

and the electrostatic energy is $U = eV$. In (11), the omission of the spatial coordinates is an approximation. It is justified if the particle is enclosed in a sufficiently large spherical shell, where the spatial derivatives yield negligible quantities.

Thus, substituting (10)-(12), into (9), one finds

$$[-(m+U)^2 + 2U(m+U) + m^2]\phi = U^2\phi \neq 0. \tag{13}$$

This result shows that the electrostatic interaction of the complex KG field (8) leads to a contradiction.

An attempt to overcome this difficulty can be found in the literature. For this purpose the interaction Lagrangian is (see [11], p. 275, [12], section 3)

$$\mathcal{L}_{int} = ie(\phi^*_{,\mu}\phi - \phi^*\phi_{,\mu})A^\mu - e^2 A_\mu A^\mu \phi^*\phi. \tag{14}$$

Here a second term is added to the previously analyzed interaction (8). However, unlike standard electromagnetic interactions of a charge e with an external potential A_μ, (14) contains 2 terms: one is proportional to the electric charge e and the other is proportional to e^2

One can see explicitly the problem emerging from this point, if the free electromagnetic term of the Lagrangian density

$$\mathcal{L}_{EM-free} = -\frac{1}{16\pi} F^{\mu\nu} F_{\mu\nu} \tag{15}$$

is added to the KG Lagrangian density (14). Varying the electromagnetic potentials and their derivatives, one follows the standard treatment (see [9], section 30) and finds the electromagnetic fields' equation associated with a KG charge. Here, since (14) contains an additional term which is proportional to $e^2 A^\mu A_\mu$, the fields' equation associated with a KG charge is

$$F^{\mu\nu}_{\ \ ,\nu} = -4\pi j^\mu + 8\pi e^2 A^\mu \phi^*\phi, \tag{16}$$

where j^μ is e times the quantity defined in (7).

Eq. (16) is inconsistent with Maxwell equation

$$F^{\mu\nu}_{\ ,\nu} = -4\pi j^\mu. \tag{17}$$

Indeed, unlike Maxwell equation (17), eq. (16) depends explicitly on the potentials. This property means that it is not gauge invariant. Moreover, unlike Maxwellian fields whose inhomogeneous term is proportional to the electric charge e, eq. (16) contains another term which is proportional to e^2.

The foregoing discussion completes the proof that the KG field *cannot* interact with an external electromagnetic field. This result means that a KG particle cannot carry an electric charge.

It is interesting to note that the Dirac field is free of the 2 discrepancies derived above for the KG field. Indeed, the Lagrangian density of a free Dirac particle is (see [7], p. 54, [4], p. 102 and [6], p. 126)

$$\mathcal{L}_{Dirac} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi. \tag{18}$$

Here the dimension of ψ is $[L^{-3/2}]$ and that of $\bar{\psi}\psi$ is $[L^{-3}]$, as required for a function representing probability density. The electromagnetic interaction term of the Dirac field is the well known quantity(see [7], p. 84, [4], p. 102 and [6], p. 135)

$$\mathcal{L}_{int} = \bar{\psi}(-e\gamma^\mu A_\mu)\psi. \tag{19}$$

Indeed, $\bar{\psi}e\gamma^\mu\psi$ is the Dirac conserved 4-current (see [10], p. 46, [12], pp. 23-24) and it is independent of electromagnetic field quantities. Hence, (19) is linear in A_μ, as required (see [9], section 30).

3. The Classical Limit

In the rest of this work it is shown that further problems arise if one regards the KG field as a classical field (see [4]-[6]). The first problem is examined for the simple case of a free KG particle. Here the (yet unnormalized) wave function is assumed to take the form

$$\phi = e^{i(\mathbf{p}\cdot\mathbf{x}-Et)}. \tag{20}$$

The action of a free classical particle and that of a free KG particle are compared. It is proved that problems exist even for this simple noninteracting solution of the KG equation. Since for the KG particle we have a Lagrangian density, there is a need for a definite expression for the probability density. Here the 0-component of the 4-current (7) is used as the probability density ρ. Thus, for the free wave (20), one finds that

$$\rho = 2E\phi^*\phi \tag{21}$$

From now on, it is assumed that the normalization of ϕ of (20) satisfies

$$\int 2E\phi^*\phi d^3x = 1. \tag{22}$$

Let us examine the action of an ordinary classical particle. Here, one may use the Lagrangian (see [9], p. 25)

$$L = -m(1 - v^2)^{1/2}. \tag{23}$$

Thus, the particle's action is

$$dS = -m(1 - v^2)^{1/2}dt. \tag{24}$$

On the other hand, the Lagrangian density of a complex KG field is (see [7], p. 38)

$$\mathcal{L} = \phi^*_{,\mu}\phi_{,\nu}g^{\mu\nu} - m^2\phi^*\phi. \tag{25}$$

Substituting (20) into (25) and using the probability density (21), one finds for the KG action

$$dS = [\int \frac{E^2 - p^2 - m^2}{2E}(2E\phi^*\phi)\, d^3x]dt = 0. \tag{26}$$

Hence, the action of the classical complex KG field (26) is inconsistent with that of the standard classical action (24).

Another contradiction arises if one examines the real KG field and Einstein's equations for the gravitational field (see [9], p. 276)

$$R^{\mu\nu} - \frac{1}{2}Rg^{\mu\nu} = 8\pi kT^{\mu\nu}. \tag{27}$$

Here $T^{\mu\nu}$ is the energy-momentum tensor of matter and of the electromagnetic fields and k is the gravitational constant.

The energy-momentum tensor can be derived from the Lagrangian density in more than one way (see [9], pp. 77-80, 270-273). Thus, for the real KG field ϕ, the components of the energy-momentum tensor are

$$T^{\mu\nu} = \frac{\partial\mathcal{L}}{\partial\phi_{,\mu}}\phi^{,\nu} - \mathcal{L}g^{\mu\nu}, \tag{28}$$

Substituting the Lagrangian density (2) into this expression, one finds

$$T_{\mu\nu} = \phi_{,\mu}\phi_{,\nu} - \frac{1}{2}[(\phi_{,\alpha}\phi_{,\beta}g^{\alpha\beta} - m^2\phi^2)]g_{\mu\nu} \tag{29}$$

(See [12], eq. (6) for the complex KG analog of this expression.)

Here the Yukawa field is examined (see [5], p. 21,[13])

$$\phi = g\frac{e^{-mr}}{4\pi r}. \tag{30}$$

This expression is real and time independent. Now, the energy density is the T^{00} component of (29). Hence, one finds for the Yukawa field (30)

$$\begin{aligned} T^{00} &= \frac{1}{2}[(\frac{g}{4\pi}\frac{\partial(e^{-mr}/r)}{\partial r})^2 + m^2\phi^2] \\ &= (\frac{1}{2r^2} + \frac{m}{r} + m^2)\phi^2. \end{aligned} \tag{31}$$

This result proves that the mass of a real KG particle does not behave like an ordinary mass. Indeed, the energy momentum tensor of an ordinary massive particle is (see [9], p. 82)

$$T^{\mu\nu} = \frac{\mu}{\gamma}v^\mu v^\nu, \tag{32}$$

where the coefficient μ denotes mass density (to be distinguished from the index μ) and $\gamma = (1 - v^2)^{-1/2}$ is the relativistic factor. Thus, the energy momentum tensor of ordinary matter is proportional to the mass whereas in the KG cases of (29) and (31), it is a quadratic function of the mass. This result proves that the mass of a real KG field is not an ordinary mass.

Another point belonging to classical physics is the 4-force exerted on a particle and the associated 4-acceleration. These notions are valid in the validity domain of the classical limit and the 4-force is parallel to the 4-acceleration. In the case of the Yukawa field, the potential is the Lorentz scalar KG field (30). Hence, the 4-force, which is a 4-vector, is proportional to $\phi_{,\mu}$. Now, in the rest frame of the source, the Yukawa field is time independent and, in spherical coordinates, it depends only on the radial coordinate r. Hence, ϕ of (30) yields $\partial\phi/\partial t = \partial\phi/\partial\theta = \partial\phi/\partial\varphi = 0$. These results prove that, at a given field point $\mathbf{r}$, the Yukawa 4-force takes the form

$$f^{\mu} = (0, \lambda\mathbf{r}), \tag{33}$$

where λ is an appropriate coefficient.

On the other hand, the relation

$$v^{\mu}v_{\mu} = 1 \rightarrow v^{\mu}a_{\mu} = 0 \tag{34}$$

means that, in Minkowski space, the 4-acceleration (and the 4-force) must be orthogonal to the 4-velocity. The Yukawa 4-force does not satisfy this requirement. For example, take a particle moving towards the origin of the Yukawa potential (30). Hence, the 4-velocity of the particle takes the form

$$v^{\mu} = \gamma(1, -v\mathbf{r}/r). \tag{35}$$

Evidently, the scalar product of (33) and (35) does not vanish. This result proves that the classical limit of the Yukawa potential is inconsistent with special relativity.

By contrast, in the case of electrodynamics, the Lorentz force density is

$$f^{\mu} = F^{\mu\nu}j_{\nu}, \tag{36}$$

where $F^{\mu\nu}$ is the antisymmetric tensor of the fields. Since the 4-current j_{ν} is parallel to the 4-velocity (see [9], pp. 70), one realizes that the orthogonality requirement is satisfied.

4. Concluding Remarks

Several conclusions can be derived from the results obtained above. The following remarks probably do not exhaust this issue.

In electrodynamics there are two kinds of entities: massive particles carrying charge and massless electromagnetic fields that mediate interaction between charged particles. The KG particle may be regarded as an entity that plays two roles. However, as explained here, these roles are divided between the complex and the real KG fields. Thus, the free complex KG field has a conserved 4-current (7) whereas the real KG field lacks this property. Hence, the real KG field cannot describe a free massive particle. On the other hand, the Yukawa interaction term of the Lagrangian takes the form (see [6], p. 135)

$$\mathcal{L}_{int} = g\bar{\psi}\psi\phi. \tag{37}$$

Now, like any other Hamiltonian, the associated Hamiltonian of (37) is a Hermitian operator and ϕ of this expression must be real. Hence, the complex KG field cannot be used as an interaction mediator.

This discussion shows that the real and the complex KG fields pertain to two distinct physical tasks. The problems and contradictions of these fields, which are derived above, are relevant to these tasks.

As explained, the results hold for quantum mechanics and for its classical limit. However, quantum field theory is a covering theory of relativistic quantum mechanics and of its nonrelativistic version[8]. It is well known that there is a close connection between the Dirac field of quantum field theory and the Dirac's equation in relativistic quantum mechanics and of its nonrelativistic approximation as well. This work shows that, in the case of a KG particle, problems exists within the realm of classical and quantum mechanics. Hence, in the case of a KG particle, it is necessary to explain the transition from quantum field theory to quantum mechanics.

It is proved in Section 2 that the dimension of a KG field $\phi^*\phi$ is $[L^{-2}]$ and that it is unsuitable for representing density of a KG massive particle. The same conclusion is obtained from the fact that $\phi^*\phi$ is a Lorentz scalar. The density j_0 of the conserved 4-current of the complex KG field (7) is a sum of terms that take the form $\phi^*_{,\mu}\phi$. This form differs from the ordinary quantum mechanical expression of probability, which is the square of the absolute value of a wave function.

The 0^- π mesons cannot be regarded as KG particles. Indeed, charged π mesons are found in a free state, very far away from the interaction region and quantum mechanics as well as its classical limit hold in this case. Thus, since it is proved in Section 2 that a KG particle cannot carry electric charge, one concludes that the $\pi^\pm$ mesons are not KG particles. Isospin symmetry extends this conclusion to the π^0 meson.

This conclusion is supported by the following general argument. It is now known that a π meson is not an elementary structureless particle but a composite system that contains a quark and an antiquark. Hence, a field function $\phi(x^\mu)$ which depends on a *single* set of 4 coordinates x^μ may be relevant to the center of mass coordinates of the system but it *cannot* describe its internal degrees of freedom.

Further problems arise if the KG field is regarded as a classical field. Here, as shown in Section 3, the action of a complex

KG field, the mass parameter of the real KG Lagrangian density and the Yukawa force disagree with the corresponding classical quantities.

On the other hand, it should be stated that this work does not deny the usage of the KG equation as a *phenomenological equation.* Indeed, by definition, a phenomenological equation is evaluated mainly (or only) by its usefulness in describing a specific set of data. This kind of evaluation is of a practical nature and is immune to theoretical counter-arguments. The case of the π mesons illustrates this issue. Thus, in low energy experiments, where excitations of the 0^- quark-antiquark ground state can be ignored, a π meson may be regarded as an elementary object and the KG equation may be used phenomenologically. This approach pertains also to bound states of a proton and a π^- meson.

This work provides an example of the strength of the variational principle. Thus, if one adheres to it then restrictions on the validity of physical theories may arise. Here it is shown that if this approach is applied then the KG equation encounters contradictions in the standard relations between wave function and probability, in electromagnetic interactions and in classical aspects of the problem.

Acknowledgment: I thank Prof. L. Horwitz for carefully reading the manuscript and making useful remarks.

References:

[1] Feshbach H and Villars F 1958 Elementary Relativistic Wave Mechanics of Spin 0 and Spin 1/2 Particles *Rev. Mod. Phys.* **30**, 24-45

[2] Weinberg S 1995 The Quantum Theory of Fields (Cambridge: University Press). Vol. 1.

[3] Dirac P A M 1978 Mathematical Foundations of Quantum Theory Ed Marlow A R (New York: Academic). (See pp. 3,4).

[4] Barut A O 1965 Electrodynamics and Classical Theory of Fields and Particles (New York: MacMillan). See pp. 102, 211.

[5] Mandl F 1965 Introduction to Quantum Field Theory (New York: Interscience). P. 13.

[6] Sterman G 1993 An Introduction to Quantum Field Theory (Cambridge: University Press). P. 7.

[7] Bjorken J D and Drell S D 1965 Relativistic Quantum Fields (New York: McGraw).(See chapter 12.)

[8] Rohrlich F 1965 Classical Charged Particles (Reading Mass: Addison-wesley). pp. 3-6.

[9] Landau L D and Lifshitz E M 1975 The Classical Theory of Fields (Oxford: Pergamon)

[10] Ryder L H 1985 Quantum Field Theory (Cambridge University Press: Cambridge)

[11] Schweber S S 1964 An Introduction to Relativistic Quantum Field Theory (New York: Harper).

[12] Pauli W and Weisskopf V 1934 The Quantization of the Scalar Relativistic Wave Equation *Helv. Phys. Acta* **7** 709-731. English translation: Miller A I 1994 Early Quantum Electrodynamics (Cambridge: University Press). pp. 188-205.

[13] Bjorken J D and Drell S D 1964 Relativistic Quantum Mechanics (New York: McGraw).(See p. 211.)