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Improving our Understanding of the Klein-Gordon Equation

By P. J. Bussey
University of Glasgow

Abstract- A detailed consideration of the Klein-Gordon equation in relativistic quantum mechanics is presented in order to offer more clarity than many standard approaches. The equation is frequently employed in the research literature, even though problems have often been raised regarding its second-order nature, the status of its negative-energy solutions and the formulation of particle density and flux. Most of these problems can be avoided by dismissing the negative energy solutions. An application of the equation to a broad wave-packet shows that a small amendment to the usual relativistic formalism can be helpful to demonstrate continuity with the non-relativistic case, although difficulties remain when the proposed quantum state has a broad relativistic energy distribution.

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Improving our Understanding of the Klein-Gordon Equation

P. J. Bussey

School of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, U.K.

Abstract- A detailed consideration of the Klein-Gordon equation in relativistic quantum mechanics is presented in order to offer more clarity than many standard approaches. The equation is frequently employed in the research literature, even though problems have often been raised regarding its second-order nature, the status of its negative-energy solutions and the formulation of particle density and flux. Most of these problems can be avoided by dismissing the negative energy solutions. An application of the equation to a broad wave-packet shows that a small amendment to the usual relativistic formalism can be helpful to demonstrate continuity with the non-relativistic case, although difficulties remain when the proposed quantum state has a broad relativistic energy distribution.

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I. Introduction

The simplest approach to a relativistic description of a quantum particle was proposed in 1926 by Klein and by Gordon [1], among others [2]; a historical survey has been given by Kragh [3]. The familiar relativistic equation $E^2 = p^2c^2 + (mc^2)^2$ is quantised by replacing the classical observables E and p^2 by quantum observables $i\hbar\partial/\partial t$ and $-\hbar^2[(\partial/\partial x)^2 + (\partial/\partial y)^2 + (\partial/\partial z)^2]$. Thus, the Klein-Gordon (KG) equation for the wave function $\boldsymbol{\psi}$ is

$$-\hbar^2 \frac{\partial^2 \boldsymbol{\psi}}{\partial t^2} = \left(-\hbar^2 c^2 \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] + m^2 c^4 \right) \psi. \tag{1}$$

Since the energy eigenstate of a free quantum particle is represented by a plane wave of the form $\exp i(\mathbf{k}.\mathbf{x} - \omega t)$, with ω and $\mathbf{k}$ proportional to energy and momentum, the KG equation must hold unavoidably for such states of a spinless relativistic quantum particle. Being linear in $\boldsymbol{\psi}$, it remains valid for linear combinations of these plane-wave eigenstates, just as does the similarly linear (non-relativistic) Schrödinger equation. Although it was first proposed for massive scalar particles, it should apply to other massive particles that are in a definite spin state.

Soon after the equation's proposal, objections were raised that were not fully answered, resulting in uncertainty that is still present about the validity of relativistic quantum mechanics, and of the KG equation in particular. These objections are repeated without resolution in most textbooks on the subject. However, they are ignored in much of the research literature and there has been no shortage of publications, far too many to refer to here, in which the KG equation is accepted, modified, applied in a large variety of contexts, or employed in various interpretations of quantum theory. Particular examples would be the evaluation of CP violation properties of meson states and entanglement in particle systems. The KG equation is certainly in use, and the situation can be puzzling to those encountering the subject.

The purpose of the present paper is to examine to what extent the claimed difficulties with the equation can be overcome, with the aim of clarifying how the equation should be better understood and where it can be confidently applied. We will concentrate on the more basic quantum mechanical issues and, in particular, we will not discuss field theory at any length.

Author: e-mail: peter.bussey@glasgow.ac.uk
Orcid: 0000-0003-0988-7878

II. Traditional Difficulties with the Klein-Gordon Equation

(i) The use of a second-order differential equation, and the negative-energy problem

A problem raised early in the KG equation's history was that a second-order differential equation, such as (1), does not normally allow the future values of its argument to be predicted from a given set of starting values alone. Thus the wave-function ψ at an initial reference time would apparently be insufficient to allow the KG equation to determine the particle's later state, and this was seen as unsatisfactory. This criticism was used to cast doubt on the KG equation and to support a need for a first-order equation, such as that of Dirac, but it can be countered. If $\psi(\mathbf{x})$ is Fourier analysed at an initial time in terms of eigenstates of momentum $\mathbf{k}$, then its future behaviour is well determined from this information alone, using the KG equation for each component, provided that there is no ambiguity in specifying ω for a given $\mathbf{k}$. This requirement becomes the key to understanding many of the issues raised regarding the KG equation, which formally allows solutions with both positive and negative values of ω.

A contrast can be made with a scalar classical wave, for example a sound wave. If, at a given time, the amplitude of such a wave is specified as a function of position, this does not differentiate between components travelling in opposite directions, and for a wave of this type a given $\boldsymbol{k}$ can have either sign of ω. For the KG equation, however, this mathematical possibility is to be discounted on the grounds of unphysicality. A relativistic massive particle always has positive energy, which means that for a given $\mathbf{k}$, only a positive value of ω can be assigned. The negative-energy solutions must be rejected, and by doing this we can ensure that the KG wave equation determines the particle's future state unambiguously from its original state, as desired.

Dirac's first-order differential equation for spin-half fermions did not remove the mathematical existence of negative-energy states, but placed them in a new part of the spinor. As is well known, his interpretation of these states was as a "sea" of mostly filled states in which unoccupied states or "holes" behave as antiparticles, whose energy is positive compared to that of an *occupied* negative-energy state. This viewpoint led to the successful expectation that the positron should exist, but it subsequently fell out of favour although it was still supported by Pauli in 1955 [4]. However it will not work at all for bosons, because the entire negative-energy sea could acquire unlimited numbers of bosonic particles, and the vacuum would be unstable. Thus the negative-energy solutions remain problematic.

(ii) The question of "incompleteness"

The apparent incompleteness of a set of solutions that lacks negative-energy contributions has been criticised [5]. But it is clear that the Fourier components in terms of E or ω cannot in any case comprise a formally complete set for a massive real particle, because $|E|$ cannot be less than mc^2; the energy spectrum is obliged to have a cutoff at this value. The set of states in ω is in this sense incomplete, but we may instead rely on the states specified by $\mathbf{k}$, which constitute a complete set of physical states of a positive-mass particle. This seems perfectly satisfactory.

To take a classical example, there is no problem in insisting that Pythagoras' equation shall give only positive solutions for the hypotenuse of a triangle, even though the square root of x^2+y^2 can mathematically take negative values. We state that these solutions are geometrically invalid and ignore them. An analogous approach can be applied to the KG equation. Indeed, it does not seem to disturb us that Einstein's original equation $E^2 = p^2c^2 + (mc^2)^2$ bears negative-energy solutions; these are likewise ignored. It might seem anomalous to retain them in the quantum context.

(iii) Feynman's solution

Feynman's well-known response was to say that negative-energy solutions to (1) (and also to the Dirac equation) correspond to antiparticle states with positive energy, but with the sign of t reversed [6]. The antiparticle states, he supposed, are to be included within the same set of solutions as the particle states. A problem here, however, is that two different treatments of time are then implied within the same equation and its solutions. While this interpretation is generally accepted in connection with Feynman diagrams, it is therefore very untidy with regard to free particles and the KG equation, and it is unclear what to do when a particle is its own antiparticle, as for example the π^0 meson – only one set of states is wanted in this case.

A much clearer and more transparent approach to the KG equation is to treat particles and their antiparticles as solutions to separate but identical equations, with negative-energy solutions for free particles always disallowed. When appropriate, quantum superpositions of particle and antiparticle states may then be constructed for a given system, as is common practice with neutral meson systems. On the other hand, a superposition of positive-charge and negative-charge states is never observed. The issue of combining particle and antiparticle states thus needs to be settled on its own terms in a given physical situation and is not a simple implication of the relativistic quantum formalism.

Feynman's proposal has been applied principally in connection with Feynman diagrams in field theory, in which propagators – that is, virtual particles to which the KG equation does not apply – are employed to indicate the transfer of particle characteristics between different vertices in a scattering process: "streams of influence", we may say. Amongst other things, propagators denote energy flow, which can be positive or negative, since positive energy flowing out of a vertex is the same as negative energy flowing into it. Feynman's picture is therefore in essence dynamical, whereas quantum mechanics (starting from de Broglie's equations) has a foundation in free real-particle states. But an understanding of these is necessary as a basis for Feynman's theory.

As pointed out above, the basic objection to the use of Feynman's idea with the KE equation is that it requires one symbol t to denote two different signs of physical time simultaneously in the same differential equation, and within its one set of solutions. This connotational ambiguity cannot reasonably be accepted.

(iv) The probability density question

A third and more serious criticism of the KG equation concerns the particle's spatial probabiity density ρ and current $\boldsymbol{j}$, as discussed in many textbooks; that by Desai [7] has been referenced here. For both the non-relativistic and relativistic cases these quantities should be related by the continuity equation

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \boldsymbol{j}. \tag{2}$$

For a non-relativistic particle, $\rho = \boldsymbol{\psi}^*\boldsymbol{\psi}$, while the current is given by

$$\boldsymbol{j} = \frac{\hbar}{2im}\left[\psi^*(\boldsymbol{\nabla}\psi) - \psi(\boldsymbol{\nabla}\psi^*)\right]. \tag{3}$$

The same equation for $\boldsymbol{j}$ is conventionally taken also in the relativistic case, where m is again the rest mass, but the probability density is now written as

$$\rho = \frac{-\hbar}{2imc^2}\left[\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right]. \tag{4}$$

This equation is counterintuitive, however, although it satisfies (2), and it generates suspicions about the KG equation. For a plane wave, it gives $\rho = (E/mc^2)\psi^*\psi$, which is negative for negative E. Once more, negative energy values are deeply problematic, since a probability density cannot be negative. An alternative suggestion from Pauli and Weisskopf was that we are no longer really discussing particle density but charge density, which can take negative values [8]. This proposal has been taken up by other authors [9], and it evades some of the difficulties, but it does not really address the original task of evaluating particle density and current; the KG equation says nothing about electric charge. Neutral particles remain problematic,[1] and an unsatisfactory discontinuity is introduced between the relativistic and non-relativistic interpretations; after all, a relativistic particle may be just a non-relativistic particle viewed in a different reference frame. In the end, this suggestion would seem to introduce more problems than it solves.

III. The Case of a Broad Wave-Packet

It is instructive to examine the situation in more detail by considering a broad wave-packet moving in one dimension x with mean positive energy $E = \hbar\omega$ and group velocity v_g.[2] To a good approximation its wave function can be represented as

$$\psi = Af(x-\bar{x})e^{i(kx-\omega t)}, \tag{5}$$

where A is a normalisation constant. The function f describes the envelope in x of the wave-packet, whose mean value is $\bar{x} = x_0 + v_g t$ and is x_0 at time $t = 0$. The partial differentials of f with respect to x and t are thus f' and $-f'v_g$ respectively. To avoid the introduction of further momentum components, f is taken to be real. For example, a Gaussian wave-packet with half-width σ has

$$\psi = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{\frac{1}{2}} e^{-(x-\bar{x})^2/4\sigma^2} e^{i(kx-\omega t)}. \tag{6}$$

As usual, v_g equals $\partial\omega/\partial k$ and is given by $\hbar k/m = p/m$ for the Schrödinger equation and $c^2k/\omega = c^2p/E$ for the KG equation. This equals $p/m_{\rm rel}$, where $m_{\rm rel} = \gamma m$ is the relativistic mass and $E = m_{\rm rel}c^2$. (As expected, the relativistic group velocity has an upper bound of c.)

[1] There have been attempts to solve this issue. Greiner [10], following Bjorken and Drell [11] and Feshbach and Villars [12], gives an argument whose conclusion is that a particle such as a π^0 must have a wave-function that is a real mathematical function. But this would have to be a real sinusoidal wave, which cannot be correct, since this is not an eigenstate of the momentum operator $-i\hbar\boldsymbol{\nabla}$!

We consider a sufficiently broad wave-packet such that the values of energy and momentum have narrow widths and the group velocity is well defined. Broadening effects with time are neglected at this level of description.

For a packet given by (5), the non-relativistic case gives

$$\frac{\partial \rho}{\partial t} = \boldsymbol{\psi}^* \frac{\partial \psi}{\partial t} + \boldsymbol{\psi} \frac{\partial \psi^*}{\partial t} = -2v_g |A|^2 f f' \tag{7}$$

and

$$j = \frac{\hbar}{2im}\left[\boldsymbol{\psi}^* \frac{\partial \psi}{\partial x} - \boldsymbol{\psi} \frac{\partial \psi^*}{\partial x}\right] = \frac{\hbar k}{m}|A|^2 f^2. \tag{8}$$

As intuitively expected, j is v_g times the local value of $\boldsymbol{\psi}^*\boldsymbol{\psi}$. Its gradient in x is $j' = 2v_g|A|^2 f f'$, in required agreement with (7) and (2).

In the relativistic case, we start from the representation for ρ given by (4). The wave-packet (5) now gives

$$\rho = \frac{\hbar}{mc^2} A^* A f^2 \omega = \frac{E}{mc^2} \boldsymbol{\psi}^* \boldsymbol{\psi} = \gamma \psi^* \psi, \tag{9}$$

since the terms in $f f'$ cancel; γ is the usual relativistic factor for the particle and ρ is clearly positive. We obtain

$$\frac{\partial \rho}{\partial t} = -2\frac{\hbar \omega}{mc^2}|A|^2 f f' v_g = -2\gamma v_g |A|^2 f f'. \tag{10}$$

Taking the expressions for j unchanged from (3) and (8), we obtain the required result

$$j' = 2\frac{\hbar k}{m}|A|^2 f f' = 2\gamma v_g |A|^2 f f' = -\partial \rho / \partial t. \tag{11}$$

The KG equation thus gives a well-defined account of a relativistic particle whose wave function has the form of a broad wave-packet, but the conventionally adopted expressions for probability density and current gradient now give results that contain a factor of γ. Since (4) and (3) are purely conventional, and the probability density must be normalised to unity anyway, it would be convenient to redefine them to remove this factor. In this way, equations (4) and (3) may be written as

$$\rho_{\text{rel}} = \gamma^{-1} \frac{-\hbar}{2imc^2}\left[\boldsymbol{\psi}^* \frac{\partial \psi}{\partial t} - \boldsymbol{\psi} \frac{\partial \psi^*}{\partial t}\right], \text{ which reduces to } \boldsymbol{\psi}^*\boldsymbol{\psi}, \tag{12}$$

[2]This topic has been treated by Mosley [13] with a different mathematical perspective from that offered here.

and
$$\boldsymbol{j}_{\rm rel} \;=\; \gamma^{-1}\frac{\hbar}{2im}\left[\psi^*(\boldsymbol{\nabla}\psi)-\psi(\boldsymbol{\nabla}\psi^*)\right]. \tag{13}$$

These amended equations are valid provided that the wave packet has an acceptably well-defined value of γ. They represent the probability density and current for a relativistic wave-packet more naturally than (4) and (3), since the quantity $\psi^*\psi$ is non-negative and may now be given its usual interpretation, while (2) continues to hold. The rest mass m in (4) and (3) is to be replaced by the relativistic mass $m_{\rm rel} = m\gamma$, which clearly expresses the continuity between the non-relativistic and relativistic accounts.

IV. A More General Case

The example of the previous section does not give a complete answer to the probability density problem. To investigate further, we examine the case of a wave function that is the sum of components with different energy. Let

$$\psi = \sum_j \psi_j, \text{ where } \psi_j = a_j e^{i(\mathbf{k_j}.\mathbf{x}-\omega_j t)}. \tag{14}$$

Thus $\partial\psi_j/\partial t = -i\omega_j\psi_j$. The terms in the sum may have arbitrary positive energies $\hbar\omega_j$ and arbitrary amplitudes a_j, subject to unitarity. Then (4) gives

$$\begin{aligned}\rho \;&=\; \frac{\hbar}{2m}\sum_j \omega_j \sum_k (\psi_k^*\psi_j + \psi_k\psi_j^*)\\ &=\; \frac{\hbar}{m}\sum_j \omega_j\,(|a_j|^2 + \sum_{k\neq j}|a_j a_k|\cos\phi_{jk}),\end{aligned} \tag{15}$$

where ϕ_{jk} is the phase difference between ψ_j and ψ_k at a given spacetime point $(\mathbf{x}, t)$. Even with the ω_j positive, ρ is not necessarily positive in this situation. This is easily seen by considering the case of just two terms, which gives

$$\rho = \frac{\hbar}{m}\left[\omega_1\left(|a_1|^2 + |a_1a_2|\cos\phi_{12}\right) + \omega_2\left(|a_2|^2 + |a_1a_2|\cos\phi_{12}\right)\right]. \tag{16}$$

If the two amplitudes are equal in magnitude, then both terms are non-negative. Otherwise, the term with smaller amplitude can become negative and does not have to be cancelled everywhere by the other term if $\omega_1 \neq \omega_2$. Thus ρ can become negative, and this may be expected to be true in general for more than two components and for the case of a broad continuous distribution in ω.

V. Discussion

We have identified the most major source of difficulty with the KG equation as associated with solutions with negative energy; once these are dismissed, many of the claimed problems disappear. In practice, many applications of the theory ignore such states implicitly, but it is interesting to observe just how troublesome they turn out to be.[3]

The question of apparently negative probability densities is more complex. Most practical applications (including field treatments) concern particles in plane-wave states, although a more realistic approach requires a wave-packet model. Within the KG equation, such states do not give a probability problem. (A plane wave has $f = 1$ in eq. (5).) The state should have a well-defined central positive energy and a narrow energy width. A non-relativistic particle wave function is also well described in this way when viewed in a boosted reference frame, because its spread in γ remains small. This does not imply that the Schrödinger equation and its dynamics can be similarly transformed. A proposal for a more relativistic adaptation of the Schrödinger equation has been given by Grave de Peralta et al. [15].

Baym, unusually among textbook authors, says that the KG equation is “quite useful”, while repeating the problems that we have already discussed [18]. He shows that particle wave-packets that are narrowly confined in space are problematic. This is no doubt true, and such particles also have a broad energy spectrum. However the states discussed in section 4.4 do not necessarily have narrow spatial wave-packets, and so the difficulty appears to be more general than Baym indicates.

A particle state with a substantial spread of relativistic energy possesses no proper rest frame and thus no non-relativistic counterpart. In the absence of well defined energy, the redefinitions (12) and (13) cannot be applied. In this case (4) can give probability densities that are not always positive, although the case of two contributing amplitudes of equal magnitude remains well behaved. Here, therefore, there apppear to be unresolved issues regarding the interpretation of relativistic quantum theory; the main problem is found with the probability density and current rather than with the KG equation itself. A similar problem might also arise with regard to a single-particle excited state of a quantum field, if it had poorly defined relativistic energy. Such states are not commonly discussed, and this is a topic that invites further examination.

One simple suggestion would be that while the probability density seems clearly measurable, corresponding to the position of a particle, its current may not always be a valid measurable variable. Its interpretation, we have seen, is plausible in the case of a broad wave packet. In general, however, it does not correspond to a Hermitian quantum variable and so is not a property of a particle that is measurable in the normal quantum scheme. Perhaps, then, it should not be considered as fundamentally important.

A limitation to any first-quantised relativistic theory is that dynamical problems can be treated only approximately. It is perfectly possible to solve the KG equation with a potential energy term included, for example to evaluate a pionic atom [16, 17]. Here however, as with the Dirac equation, a major issue is well known, namely that the use of a simple potential does not give precise results in a relativistic context. Field theories are set up to avoid negative energies of real particles, and in the end provide a more comprehensive physical account, but we may still wish to explore the limits of the more basic quantum method.

[3] Removing such states is also a feature of the Foldy-Wouthuysen treatment of the Dirac equation [10]. Some aspects of the present discussion can also be applied to the Dirac equation, but we do not pursue this in detail here. Another approach, with doubtful success, is to modify the KG equation so as to produce only positive-energy solutions [14].

VI. Conclusions

Special relativity relies in an essential way on the use of well-defined frames of reference. A quantum particle with a broad energy spread lacks a proper frame of reference, and so it may be no surprise if such states present interpretational difficulties. However if a free particle is in a state with positive energy that is sufficiently well-defined to provide a usable proper reference frame, the Klein-Gordon equation gives an acceptable account of its basic quantum features, and the most frequent criticisms are overcome. With a minor amendment to the standard notation, the relativistic mass can now be used in the probability current equation, giving a natural continuity between the non-relativistic and relativistic treatments. Despite the objections of many distinguished practitioners of the subject, the negative-energy solutions to the equation are not physically usable in describing single particles; real antiparticles should be treated separately and in a parallel way to the particles. For many neutral meson systems, the two classes of state can then be combined in an extended quantum formulation.

In the end, a relativistic equation of the Klein-Gordon type cannot be avoided for the description of free spinless quantum particles and those with fixed-spin states. However, its application may be restricted to states in which the particle has a proper relativistic rest frame. With due allowance for this constraint, the Klein-Gordon equation is able to retain an important role in quantum mechanics. Its place is assured, provided that limitations such as discussed above are kept in mind.

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