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DERIVATION OF THE KLEIN – GORDON – FOCK EQUATION FROM FIRST PRINCIPLES

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Abstract. In this paper, the Klein − Gordon − Fock equation is derived from the first principles. There is no need to postulate the existence of wave functions or to axiomatically introduce values of equation coefficients within the framework of the applied approach. The equation was derived on an adiabatically variable manifold, locally described by the FRW metric with complete electrodynamics constructed on it. Here the transverse electromagnetic field (TEMF) is quantized due to the adiabatic change in the metric tensor and the Planck constant acts as an adiabatic invariant of the TEMF. Moreover, the wave functions appear in the equations in a natural way, being eigenfunctions of the Sturm − Liouville problem. These are the functions in which the TEMF function is expanded. To summarize, the proposed approach makes obvious the physical meaning both of the equation itself and of quantum mechanics in general.

Keywords: Klein − Gordon − Fock equation, Schrödinger equation, Sturm − Liouville problem, quantization of electromagnetic field

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ВЫВОД УРАВНЕНИЯ КЛЕЙНА – ГОРДОНА – ФОКА ИЗ ПЕРВЫХ ПРИНЦИПОВ

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Аннотация. В работе предложен вывод уравнения Клейна − Гордона − Фока из первых принципов. Предлагаемый подход не требует ни постулирования существования волновых функций, ни аксиоматического введения вида и величин коэффициентов уравнения. Вывод произведен на адиабатически изменяемом многообразии, локально описываемом метрикой Фридмана − Робертсона − Уокера с построенной на нем полной электродинамикой, в которой поперечное электромагнитное поле квантуется вследствие адиабатического изменения тензора метрики. В этом случае

постоянная Планка выступает как адиабатический инвариант поперечного электромагнитного поля, а волновые функции возникают в уравнении естественным образом и являются собственными функциями задачи Штурма – Лиувилля, по которым раскладывается функция поперечного электромагнитного поля. Таким образом, предлагаемый подход делает очевидным физический смысл как самого уравнения, так и квантовой механики в целом.

Ключевые слова: уравнение Клейна – Гордона – Фока, уравнение Шрёдингера, задача Штурма – Лиувилля, квантование электромагнитного поля

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1.Introduction

The Klein – Gordon – Fock (KGF) equation, which depicts the dynamics of massive spinless particles, is the simplest relativistic equation to describe massive fields. Though it is only a model by nature, it is still widely used for an approximate description of various quantum phenomena. One of the main reasons for this is that the KGF equation allows for the calculation of relativistic corrections, such as the description of particle birth in external gauge fields [1], but the KGF equation is also used to reflect the behavior of charge carriers in crystalline systems in the presence of an electromagnetic field [2]. In this case, the KGF equation is used because the electromagnetic field is depicted by the *ab initio* invariant Maxwell equations. By contrast, the Schrödinger equation is not invariant with respect to the Lorentz transformations, that makes it impossible to construct on these grounds a self-consistent and closed theory that adequately describes the behavior of charges in a crystal in the presence of an electromagnetic field.

Unfortunately, the KGF equation has not yet been obtained from the first principles. Usually, it is derived reasoning from the Schrödinger equation which, in turn, was postulated using the following three axioms:

(*i*) Required structure of the equation,

(*ii*) Postulated existence of wave functions,

(*iii*) Introduced the Planck constant as a coefficient.

These have been done to achieve the consensus between the calculated and experimentally measured quantities. Such an axiomatic approach, since the first works of Schrödinger [3], has hidden the physical meaning of quantum phenomena, thus provoking the emergence of many different interpretations of quantum mechanics. This suggests that the axiomatic approach must be revisited in order to understand the physics of quantum processes.

N. G. Chetaev was the first to try to solve the issue, who did this a year after the publication of Schrödinger's work. He tried to remove the first postulate (in the structure of the Schrödinger wave equation), obtaining the structure of the equation from the stable motion conditions, and already published his work in 1931 [4] (see also Refs. [5, 6]). Soon thereafter, Chetaev's result was discussed and extended by many authors (see, for example, Refs. [7, 8] and Refs. therein). Nevertheless, his method has still left room for improvement, because even though he managed to remove the first axiom, the rest are still required to be postulated.

The following section of this paper is dedicated to a few different attempts to derive the Schrödinger equation.

In Section 3, we derive the Klein – Gordon – Fock equation from the stability conditions, thus eliminating the need for the first of Schrödinger's three axioms.

In Section 4, we derive the KGF equation without relying on Schrödinger's second and third axioms.

Within the framework of our approach, it has been demonstrated that wave functions naturally arise when the photon function is decomposed by the complete set of the eigenfunctions of a

corresponding Sturm – Liouville problem. It was also shown that the Planck constant appears in the equation as an adiabatic invariant of a transversal electromagnetic (EM) field if changes in metric tensor are considered.

In this paper, Latin indices and Greek indices are $i, j, k, l, m = 1, 2, 3$ and $\alpha, \beta, \gamma, \mu, \nu = 0, 1, 2, 3, 4$ respectively. The signature of the metric is $(1, -1, -1, -1)$.

2. A brief review of a few attempts to derive the Schrödinger equation

The origin of the Schrödinger equation started as far back as de Broglie's wavelength [9], which was an extension of the expression of photon energy discovered by A. Einstein [10]. Intrigued by de Broglie's hypothesis and taking advantage of the well-developed and popular theory of Sturm – Liouville, E. Schrödinger postulated his famous equation [11 – 14] (it should be noted that he first worked on a more generally relativistic case and then moved on to the KGF equation, but this result was not published). However, E. Schrödinger obtained his equation based upon the three axioms mentioned above [3], which cannot be recognized as satisfactory, since it complicates the understanding of the physical foundations of quantum mechanics.

Until recently, there was a big gap between the widespread use of the Schrödinger equation to calculate data describing physical facts and the lack of any extant derivation of the equation from first principles. This made it impossible to understand the physical foundations of quantum physics. For a long time, the approach jokingly named "Shut up and calculate!" (D. Mermin) was dominating, which, in turn, gave rise to many different interpretations of quantum mechanics. This situation inevitably called into question the physical Copenhagen interpretation of the wave functions. The question also arose regarding the nature of the Planck constant. Therefore, it seems appropriate to briefly review a few attempts to derive the Schrödinger equation before going further.

E. Nelson started from Newtonian mechanics, and obtained quantization from gravity, which is akin to the Schrödinger equation [15]. Similar ideas were taken up later, such as by J. Ogborn and E. F. Taylor [16] and by F. Calogero, the latter leading recently to the quantum Painlevé – Calogero Schrödinger wave function [17]. However, on the one hand, the coupling constant of the gravitational interaction is 40 orders of magnitude smaller than that of the electromagnetic one. For this reason, it would be a bit strange to construct quantization on the basis of gravity. On the other hand, interactions in atoms (which are quantized) are significantly electromagnetic. This suggests that the method proposed by E. Nelson and F. Calogero cannot be considered as entirely correct.

K. C. Yung and J. H. Yee tried to derive the equation using a Feynman path integral approach, but this effort led instead to a modified Schrödinger equation [18]. Only at the beginning of the 21st century did papers begin to appear in which attempts were made to take into account the electrodynamic nature of quantum systems. For example, in 2004, J. H. Field decided to put more emphasis towards classical electromagnetism [19] (a paper by D. W. Ward and S. M. Volkmer [20], in which an attempt was made to derive the Schrödinger equation within the framework of Special Relativity by the inclusion of electromagnetic waves, should also be noted here). Then, like K. C. Yung and J. H. Yee [18], J. H. Field tried to derive the Schrödinger equation by not only a Feynman path integral, but also from the Hamilton – Jacobi equation [21].

To end this short history of the derivation of the Schrödinger equation, let us cite among others the work of P. Pelce who derives it by the typical method of considering the density of momentum flux [22] and the work of J. C. Briggs and J. M. Rost who focused more on the origin of the time-dependent equation [23].

Unfortunately, all these attempts did not lead to a clear understanding of the foundations of quantum mechanics, since the nature of the Planck constant remained unclear, and complex wave functions had to be postulated.

Recently, the Schrödinger equation was obtained without the axiomatic introduction of wave functions and of the coefficients of the equation [24]. In that paper it was shown that what are called wave functions are just the eigenfunctions of the Liouville operator that form a complete set of orthogonal functions, in which the EM field of a system can be expanded. In the same paper, the Planck constant was calculated for the first time from the geometry of the universe (see also Refs. [25, 26] for more complete and refined results). This derivation of the Schrödinger equation bypasses the axiomatic approach and opens the door for the derivation of the KGF equation from first principles.

3. The Klein – Gordon – Fock equation derived from the stability conditions

In this section, we show how to remove the first postulate that determines the form of the desired equation. We begin with Chetaev's stability condition first obtained in 1929 [4] (see for details Refs. [5, 6] and discussion in Refs. [7, 8]):

$$\frac{d}{dx^{\mu}}\left(g^{\mu\nu}\frac{d\tilde{S}}{dx^{\nu}}\right)=0, \tag{1}$$

where x^{μ} are coordinates, $\tilde{S}$ is the complete integral of the Hamilton – Jacobi equation for the perturbed Hamiltonian function $\tilde{H}=H+\varepsilon H_1$.

These perturbation conditions correspond to the expansion up to the first terms of the infinitesimal parameter ε.

It is worth noting that the functions S (corresponds to H) and $\tilde{S}$ are not single-valued functions. Therefore, following the Chetaev's method, we define the single-valued functions ψ and φ in the following way:

$$i\frac{S}{S_0}=\ln\left(\frac{\psi}{\psi_0}\right),\quad i\frac{\tilde{S}}{S_0}=\ln\left(\frac{\varphi}{\varphi_0}\right),\quad \text{where}\quad \lim_{\varepsilon\to 0}\varphi=\psi. \tag{2}$$

Constants S_0, ψ_0 and φ_0 were introduced in this equation for convenience. By substituting the definition of $\tilde{S}$ written in Eq. (2) into Eq. (1), we obtain:

$$\left[\frac{1}{\varphi}\frac{\partial}{\partial x^{\mu}}\left(g^{\mu\nu}\frac{\partial\varphi}{\partial x^{\nu}}\right)-\frac{g^{\mu\nu}}{\varphi^2}\left(\frac{\partial\varphi}{\partial x^{\mu}}\right)\left(\frac{\partial\varphi}{\partial x^{\nu}}\right)\right]=0, \tag{3}$$

which, in the limit $\varepsilon\to 0$, gives:

$$\left[\frac{1}{\psi}\frac{\partial}{\partial x^{\mu}}\left(g^{\mu\nu}\frac{\partial\psi}{\partial x^{\nu}}\right)-\sum\frac{1}{\psi^2}\left(\frac{\partial\psi}{\partial x^{\mu}}\right)^2\right]=0. \tag{4}$$

In addition, it also follows from Eq. (2) that:

$$\frac{\partial\psi}{\partial x^{\mu}}=\psi\frac{i}{S_0}\frac{\partial S}{\partial x^{\mu}}=0. \tag{5}$$

For this reason, we can write the following:

$$\left[\frac{1}{\psi}\frac{\partial}{\partial x^{\mu}}\left(g^{\mu\nu}\frac{\partial\psi}{\partial x^{\nu}}\right)+\sum\frac{1}{S_0^2}\left(\frac{\partial S}{\partial x^{\mu}}\right)^2\right]=0. \tag{6}$$

By taking into account the relation $p_{\gamma}p^{\gamma}=m^2c^2$ and redefining the variable $S_0=\hbar$, we obtain the KGF equation:

$$\left(\hbar^2\frac{\partial^2}{\partial x_{\mu}\partial x^{\mu}}+m^2c^2\right)\psi=0. \tag{7}$$

Chetaev's method, which is based on the stability condition, eliminates the first postulate about the equation structure, but the other two postulates about the existence of the wave function and the magnitude of the coefficients in the equation remain unchanged. This drawback of Chetaev's approach arises because:

a) it does not take into account the transverse EM field responsible for all interactions in the quantum system, and

b) because the Universe is assumed to be flat and not expanding (i.e., it was initially postulated that all components of the metric tensor are constant).

However, these initial assumptions contradict observations. Now we will try to bypass these two postulates and derive the equation from the first principles, by considering a complete system. In this case, the main equations of quantum mechanics (the Schrödinger equation and the KGF one) can be derived without using any postulate at all.

4. Derivation of the Klein – Gordon – Fock equation without postulating both wave functions and the Planck constant value

Our aim in this section is to obtain the Klein – Gordon – Fock equation using neither the second nor third axioms (the wave function's existence and postulated value of the Planck constant).

Consider a laboratory on the Earth, i.e., the closest location to us, which is a very small region of the Universe. In this case, the metric of the laboratory is locally similar to the Friedman – Robertson – Walker metric. Considering that, due to the expansion of the Universe, the metric tensor adiabatically and slowly changes over time, it becomes obvious that the energy and momentum of the transverse electromagnetic field occupying the volume of λ^3 are no longer conserved – the energy and momentum are no longer integrals of movement. In this case, an approximately conserved value is the adiabatic invariant of the transverse EM field known as the Planck constant $h = 6.6 \cdot 10^{-27}$ erg·s (see Refs. [24 – 26] for more details).

On the one hand, we want to get an equation describing the movement of microparticles (for example, electrons), for which the characteristic dimensions are about 10^{-13} cm, while the wavelength of the transverse EM field (responsible for all interactions) for the optical range is about $5 \cdot 10^{-5}$ cm. For this reason, the difference in the occupied volume of 24 orders of magnitude allows us to assume that even in a hypothetical case of possible influence of changes in the metric on the characteristics of the particles themselves (we speak mainly about the rest energy), the classical law of conservation of the 4-vector of energy-momentum of the particle under consideration, can be applied for our goal with good accuracy.

On the other hand, we are looking specifically for the KGF differential equation, which has a structure reminiscent of the corresponding equation of classical physics. In other words, we are not looking for the equations of movement obtained in Ref. [26], but instead the KGF equation. For these reasons, we can consider a relativistic particle characterized by a mass m and begin with the relativistic equation for 4-momentum:

$$p_\mu p^\mu - m^2 c^2 = 0. \tag{8}$$

Our final aim (the KGF equation) is obviously a differential equation. So, to obtain it, we should apply the inverse Fourier transform to Eq. (8). However, the only harmonic function we may use for this transform is the function that describes the transverse EM field. We emphasize that the EM field is the only carrier of interaction in cases of interest, so it makes no sense to consider any other functions.

The fact that the transverse EM field is quantized itself, regardless of the presence or absence of charges nearby, was shown by A. Einstein and P. Debye at the beginning of the 20th century. However, recently it has been shown how the transverse EM field is quantized (see Refs. [24 – 26]). The indicated works showed that the transverse EM field is described by the following harmonic functions:

$$\varphi = \exp(-ik_\alpha x^\alpha), \tag{9}$$

where k_α, x^α are 4-vectors, $k_\alpha = p_\alpha/\hbar$.

Here the reduced Planck constant $\hbar$ appears as an adiabatic invariant of the transverse EM field (see Refs. [24 –26]) and is completely determined by geometry (metric of space), therefore its axiomatic postulation into the equations is no longer required.

Let us apply to Eq. (8) the inverse Fourier x-coordinate transformation by using the harmonic function of the transverse EM field (9):

$$\int \left(p_\mu p^\mu - m^2 c^2 \right) \varphi\left(k_\alpha x^\alpha \right) d\Omega = 0, \tag{10}$$

where $d\Omega$ is a 4-volume element and the integration is carried out over the photon's volume.

In more detail one can write:

$$\int p_\mu p^\mu \exp\left\{ -\frac{i}{\hbar} p_\alpha x^\alpha \right\} d\Omega - m^2 c^2 \int \exp\left\{ -\frac{i}{\hbar} p_\alpha x^\alpha \right\} d\Omega = 0, \tag{11}$$

where do we get:

$$\int \hbar^2 \frac{\partial}{\partial x_\alpha}\frac{\partial}{\partial x^\alpha}\exp\left\{-\frac{i}{\hbar}p_\alpha x^\alpha\right\}d\Omega + m^2c^2\int \exp\left\{-\frac{i}{\hbar}p_\alpha x^\alpha\right\}d\Omega = 0, \tag{12}$$

or

$$\int\left(\hbar^2\frac{\partial}{\partial x_\alpha}\frac{\partial}{\partial x^\alpha}+m^2c^2\right)\varphi\left(p_\alpha x^\alpha\right)d\Omega = 0, \tag{13}$$

where, under the integration, one can see the Liouville operator that has a complete set of orthogonal eigenfunctions in which any function can be expanded.

Let $\Psi_k(x)$ be a complete set of eigenfunctions of the Liouville operator. Then we can expand Eq. (9):

$$\varphi(p,x) = \sum_l a_l(p)\psi_l(x), \tag{14}$$

and the previous equation becomes:

$$\int d\Omega\sum_l a_l(p)\left(\hbar^2\frac{\partial}{\partial x_\alpha}\frac{\partial}{\partial x^\alpha}+m^2c^2\right)\psi_l\left(x\right) = 0. \tag{15}$$

However, as already mentioned above, neither the Schrödinger equation nor the KGF one contains the transverse EM field. If we assume that this field is not equal to zero (i.e., the decomposition coefficients $a_l(p)$ are not equal to zero) and that the eigenfunctions of the Liouville operator are orthogonal, which is the case, meaning that the expression in brackets in Eq. (15) is zero. "Removing" the EM field and equating the constants with one (we let $\hbar = 1$ and $c = 1$) we obtain the usual form of the equation:

$$\left(\partial^\mu\partial_\mu - m^2\right)\psi_l\left(x\right) = 0. \tag{16}$$

This is the Klein – Gordon – Fock equation.

As can be seen in this case, there is no need to postulate the values of the coefficients in the equation, such as the value of the reduced Planck constant, nor to postulate the wave function. The wave functions appear naturally as eigenfunctions of the Sturm – Liouville problem, and these functions are the ones that we use to expand the transverse EM field of the system under consideration. It is in this way that the transverse EM field is included in the model and appears in the complete Eq. (15).

Furthermore, it is precisely this cancelation of the EM field when moving from Eq. (15) to Eq. (16) that leads to the problem of what is called the collapse of wave functions (EPR paradox). In fact, in expression Eq. (15), the EM field (described by decomposition coefficients $a_l(p)$) is present. Moreover, in Eq. (15) the integration over the entire volume λ^3 of the EM field is carried out, which causes the complete Eq. (15) to be non-local. In turn, Eq. (16) is local; it does not contain any transversal EM field of the system, which provokes the emergence of the problem of the collapse of wave functions.

5. Conclusion

As mentioned above, until now, postulates have always been used to derive the Schrödinger equation and the KGF one. So, in these equations, the coefficients were postulated, or (which is the same postulate) the value of the Planck constant was taken so that the result of the calculation would coincide with the experimental data. However, this value of the Planck constant can be calculated from the first principles. In fact, considering that the universe is expanding, i. e., the metric of space adiabatically and slowly changes over time, it becomes obvious that the energy and momentum of the transversal EM field are no longer conserved (see cosmological redshift). In other words, the system, which includes the transverse EM field, can no longer be considered as closed. It is not isolated. In this case, the only approximately conserved value will be the adiabatic invariant of the EM field. For mechanical systems, the theory of adiabatic invariance is well developed and has long been known (see, for example, the first volume of Landau and Lifshitz textbooks, where there is a section dedicated specifically to the adiabatic invariance of mechanical systems). However, for the transverse EM field, such a task has first been investigated

relatively recently (see Ref. [24] and a more detailed version in Refs. [25, 26]). As it was shown in the mentioned papers, in the case when the metric of space is slowly changing, the EM field adiabatic invariant is the Planck constant. In this case, the value of the Planck constant arises from the geometry, and it coincides with a laboratory-measured value to the second significant digit, which is consistent with the experimental errors in the measurements of cosmological parameters (the Hubble constant and cosmological one), which, in turn, characterize the dynamics of the metric of the local universe.

Given the obtained results, on the one hand, the axiomatic postulation of the coefficients in the Schrödinger's or KGF's equation is no longer required, since these coefficients naturally appear when considering the EM field (always existing in any system and, moreover, responsible for quantization and the evolution of the quantum system). On the other hand, the role of the transverse EM field becomes clear; it is not so in the equations of Schrödinger and KGF precisely, because these equations were postulated and not derived from the first principles.

We have derived the KGF equation from first principles without using any axiom. The wave functions are the eigenfunctions of the Sturm – Liouville problem, and these functions are the ones that we use to expand the transverse EM field of the described system. The complete Eq. (15) contains an EM field through which all interactions in the system occur (we note here that the KGF equation does not contain a transverse EM field and therefore is incomplete). Moreover, Eq. (15) is not local, because it includes integration over the photon's volume. For this reason, it will not undergo a collapse of the wave function. It should therefore be used for the description of particle birth in external gauge fields [1] and for the description of the behavior of charge carriers in crystalline systems in the presence of an EM field [2].

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