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CRYPTO-HERMITIAN APPROACH TO THE KLEIN–GORDON EQUATION

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Abstract. We explore the Klein-Gordon equation in the framework of crypto-Hermitian quantum mechanics. Solutions to common problems with probability interpretation and indefinite inner product of the Klein-Gordon equation are proposed.

Keywords: Klein-Gordon equation; probability interpretation; metric operator; crypto-Hermitian operator; quasi-Hermitian operator.

1. Introduction

The urge to unite special theory of relativity with quantum theory emerged shortly after their discovery. The first relativistic wave equation was introduced in 1926 simultaneously by Klein [1], Gordon [2], Kudar [3], Fock [4][5] and de Donder and Van Dungen [6]. Schrödinger himself formulated it earlier in his notes together with the Schrödinger equation [7]. However, with the introduction of the Klein-Gordon equation arose several problems. For given momentum equation allows solutions with both positive and negative energy, it has an extra degree of freedom due to presence of both first and second derivatives and mainly its density function is indefinite and therefore cannot be consistently interpreted as probability density. Also, the predictions based on this equation seemed to disagree with experiments (cf., e.g., the historical remark in [8]). Therefore, few years later all the attention shifted to the Dirac equation.

More than ninety years old problem of proper probability interpretation of the Klein-Gordon equation was first solved in 1934 by Pauli and Weisskopf [9] by reinterpreting the Klein-Gordon equation in the context of quantum field theory. Quantum mechanical approach to the Klein-Gordon equation was forgotten until Ali Mostafazadeh brought it back in 2003 [10]. In his work, he made use of pseudo or quasi-Hermitian approach to quantum mechanics.

Mathematical ideas of quasi-Hermitian theory originate from works of Dieudonné [11] and Dyson [12], though it wasn't until 1992 when the theory was consistently explained and applied in nuclear physics by Scholtz, Geyer and Hahne [13]. This groundbreaking work initiated fast growth of interest popularized in 1998 by Bender and Boettcher [14]. Nowadays the application of the theory is moving away from quantum mechanics to other branches of physics, such as optics.

We would like to return to the problem of proper interpretation of the Klein-Gordon equation in the framework of Quantum mechanics only. Several publications concerning this subject appeared [15–18] or [19–21]. But even these studies did not provide an ultimate answer to all of the open questions. Some of them will be addressed in what follows.

2. Klein-Gordon equation in Schrödinger form

The Klein-Gordon equation for free particle can be written in common form

$$(\Box + \frac{m^2c^2}{\hbar^2})\psi(t,x) = 0 \ , \tag{1}$$

where $\Box = \frac{1}{c^2}\partial_t^2 - \Delta = \partial_\mu \partial^\mu$ is the d'Alembert operator. From now on we will use the natural units $c = \hbar = 1$, furthermore we can denote $K = -\Delta + m^2$ and rewrite (1) as

$$(i\partial_t)^2\psi(t,x) = K\psi(t,x) \ . \tag{2}$$

The fact that the Klein-Gordon equation is differential equation of second order in time gives it an extra degree of freedom. Feshbach and Villars [22] suggested solution to this problem by introducing two-component wave function and therefore making the extra degree of freedom more visible. Following their ideas together with even earlier ideas of Foldy [23], we can replace the Klein-Gordon equation with two differential equation of first order in time. Inspired by convention introduced in [19] we put

$$\Psi^{(1)} = i\partial_t\psi, \quad \Psi^{(2)} = \psi. \tag{3}$$

Now, equation (2) can be decomposed into a pair of partial differential equations

$$i\partial_t\Psi^{(1)} = K\Psi^{(2)}, \tag{4}$$

$$i\partial_t\Psi^{(2)} = \Psi^{(1)}, \tag{5}$$

which, written in the matrix form, become

$$i\partial_t \begin{pmatrix}\Psi^{(1)} \\ \Psi^{(2)}\end{pmatrix} = \begin{pmatrix}0 & K \\ I & 0\end{pmatrix}\begin{pmatrix}\Psi^{(1)} \\ \Psi^{(2)}\end{pmatrix}. \tag{6}$$

Hamiltonian of the quantum system takes form

$$H = \begin{pmatrix} 0 & K \\ 1 & 0 \end{pmatrix}, \tag{7}$$

and enters the Schrödinger equation

$$i\partial_t \Psi(t,x) = H\Psi(t,x), \quad \Psi = \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix}. \tag{8}$$

Two-component vectors $\Psi(t)$ belong to

$$\mathcal{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \tag{9}$$

and the Hamiltonian H may be viewed as acting in $\mathcal{H}$.

The so called Schrödinger form of the Klein-Gordon equation (8) is equivalent to the original Klein-Gordon equation (1). It is in more familiar form, although, new challenge arises with the manifest non-Hermiticity of Hamiltonian (7).

2.1. Eigenvalues

New form of the Klein-Gordon equation (8) has many benefits. One of them is simplification of calculation of its eigenvalues to mere solving the eigenvalue problem for operator K

$$K\psi_n = \epsilon_n \psi_n. \tag{10}$$

The relationship between eigenvalues ϵ_n of the operator K and eigenvalues E_n of the non-Hermitian operator H of the Schrödinger form of the Klein-Gordon equation

$$\begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} = E \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} \tag{11}$$

can be easily seen. Equation (11) is formed from two algebraic equations

$$K\Psi^{(2)} = E\Psi^{(1)}, \quad \Psi^{(1)} = E\Psi^{(2)}. \tag{12}$$

After insertion of the second one to the first one we obtain

$$K\Psi_n^{(2)} = E_n^2 \Psi_n^{(2)}, \tag{13}$$

which compared with equation (10) gives us following relation between eigenvalues

$$\epsilon_n = E_n^2. \tag{14}$$

We can see, that eigenvalues E_n remain real under assumption of $\epsilon_n > 0$.

Relationship between corresponding eigenvectors

$$H\Psi_n^{(\pm)} = E_n^{(\pm)} \Psi_n^{(\pm)}, \quad \Psi_n^{(\pm)} = \begin{pmatrix} \pm\sqrt{\epsilon_n}\psi_n \\ \psi_n \end{pmatrix} \tag{15}$$

is also easy to see.

2.2. Free Klein–Gordon equation

In case of free Klein–Gordon equation operator

$$K = -\Delta + m^2 \tag{16}$$

acting on $\mathcal{H} = L^2(\mathbb{R}^3)$ is positive and Hermitian. It has continuous and degenerate spectrum. As suggested in [10], we identify the space $\mathbb{R}^3$ with the volume of a cube of side l, as l tends to infinity. Than we can treat the continuous spectrum of K as the limit of the discrete spectrum corresponding to the approximation. The eigenvalues are given by

$$\epsilon_{\vec{k}} = k^2 + m^2 \tag{17}$$

and corresponding eigenvectors $\psi_{\vec{k}} = \Psi_{\vec{k}}^{(2)}$ are

$$\psi_{\vec{k}}(\vec{x}) = \langle \vec{x} | \vec{k} \rangle = (2\pi)^{-3/2} e^{i\vec{k}.\vec{x}}, \tag{18}$$

where $\vec{k} \in \mathbb{R}^3$ and $\vec{k}.\vec{k} = k^2$. We can see that $\psi_{\vec{k}} \notin L^2(\mathbb{R}^3)$. They are generalized eigenvectors, i.e. vectors which eventually becomes 0 if $(K - \lambda I)$ is applied to it enough times successively, describing scattering states [10].

Vectors $\psi_{\vec{k}}$ satisfy orthonormality and completeness conditions

$$\langle \vec{k} | \vec{k}' \rangle = \delta(\vec{k} - \vec{k}'), \qquad \int d^3k |\vec{k}\rangle\langle\vec{k}|) = 1 \tag{19}$$

and operator K can be expressed by its spectral resolution as

$$K = \int d^3k (k^2 + m^2) |\vec{k}\rangle\langle\vec{k}|. \tag{20}$$

From the relations (14) and (15) we see that eigenvalues and eigenvectors of H are given by

$$E_{\vec{k}}^{(\pm)} = \pm\sqrt{\vec{k}^2 + m^2}, \quad \Psi_{\vec{k}}^{(\pm)} = \begin{pmatrix} \pm\sqrt{\vec{k}^2 + m^2} \\ 1 \end{pmatrix} \psi_{\vec{k}} \ . \tag{21}$$

The eigenvectors $\Phi_{\vec{k}}^{(\pm)}$ of adjoint operator $H^\dagger$ are

$$\Phi_{\vec{k}}^{(\pm)} = \begin{pmatrix} 1 \\ \pm\sqrt{\vec{k}^2 + m^2} \end{pmatrix} \psi_{\vec{k}}, \tag{22}$$

which form together with $\Psi_{\vec{k}}^{(\pm)}$ complete biorthogonal system

$$\langle \Phi_{\vec{k}'}^{(\nu)} | \Psi_{\vec{k}}^{(\nu')} \rangle = \delta(\vec{k} - \vec{k}') \delta_{\nu\nu'} 2E_{\vec{k}}^{(\nu)}, \tag{23}$$

where $\nu, \nu' = \pm 1$.

3. Crypto-Hermitian approach

Apparent non-Hermiticity of Hamiltonian (7) can be dealt with by means of the crypto-Hermitian theory (sometimes also called quasi-Hermitian [24] or $\mathcal{PT}$-symmetric [25]).

Hamiltonian is non-Hermitian $H \neq H^\dagger$ only in the false Hilbert space $\mathcal{H}^{(F)} = (V, \langle \cdot|\cdot \rangle)$. The underlying vector space of states is fixed, given by the physical system. However, we have a freedom in the choice of inner product. If we represent our Hamiltonian in different secondary Hilbert space $\mathcal{H}^{(S)} = (V, \langle\langle \cdot|\cdot \rangle)$, with newly defined inner product

$$\langle\langle \cdot|\cdot \rangle = \langle \varphi|\Theta|\psi \rangle, \tag{24}$$

it may become Hermitian. So called metric operator Θ must be positive definite, everywhere-defined, Hermitian and bounded with bounded inverse. Operators for which such inner product exist will be called crypto-Hermitian (c.f. [26]). They satisfy the so called Dieudonée equation

$$H^\dagger \Theta = \Theta H \tag{25}$$

and they are similar to Hermitian operators

$$h = \Omega H \Omega^{-1}, \tag{26}$$

where $\Theta = \Omega^\dagger \Omega$ is invertible and $h = h^\dagger$.

In such scenario, the problem of negative probability interpretation of the Klein-Gordon equation can be reinterpreted as the problem of the wrong choice of metric operator Θ. If we would be able to find more appropriate choice of representation space $\mathcal{H}^{(S)}$, this problem would disappear.

3.1. Computation of the metric

One of the possible ways how to construct metric operator Θ for given crypto-Hermitian Hamiltonian H is by summing the spectral resolution series. It requires the solution of eigenvalue problem for $H^\dagger$. In what follows, we try to construct the metric operator for free Klein-Gordon equation

$$\Theta = \int d^3k \left(\alpha^{(+)} |\Phi_{\vec{k}}^{(+)}\rangle\langle\Phi_{\vec{k}}^{(+)}| + \alpha^{(-)} |\Phi_{\vec{k}}^{(-)}\rangle\langle\Phi_{\vec{k}}^{(-)}| \right), \tag{27}$$

where we insert eigenvectors $\Phi_{\vec{k}}^{(\pm)}$ as computed in (22)

$$\Theta = \int d^3k \begin{pmatrix} \alpha & \beta\sqrt{k^2+m^2} \\ \beta\sqrt{k^2+m^2} & \alpha(k^2+m^2) \end{pmatrix} |\vec{k}\rangle\langle\vec{k}|, \tag{28}$$

where $\alpha = \alpha^{(+)} + \alpha^{(-)}$, $\beta = \alpha^{(+)} - \alpha^{(-)}$. By means of equation (20) we obtain family of metric operators

$$\Theta = \begin{pmatrix} \alpha & \beta K^{1/2} \\ \beta K^{1/2} & \alpha K \end{pmatrix}, \tag{29}$$

where

$$K^{1/2} = \int d^3k \sqrt{k^2+m^2} |\vec{k}\rangle\langle\vec{k}|. \tag{30}$$

With the knowledge of the metric operator (29), we can construct positive definite inner product defining Hilbert space $\mathcal{H}^{(S)}$

$$\begin{aligned} \langle\langle \Psi|\Phi\rangle &= \alpha(\langle\psi|K|\varphi\rangle + \langle\dot{\psi}|\dot{\varphi}\rangle) \\ &\quad + i\beta(\langle\psi|K^{1/2}|\dot{\varphi}\rangle - \langle\dot{\psi}|K^{1/2}|\varphi\rangle), \end{aligned} \tag{31}$$

where $\dot{\varphi}, \dot{\psi}$ denote corresponding time derivatives (In fact, this equation is just an explicit version of equation (24)).

3.2. The discrete case

Unfortunately, the metric operator (29) is unbounded and therefore doesn't satisfy all the requested properties we put upon metric operator. As was emphasized in [27], boundedness of metric operator Θ is very important property, it guarantees that convergence of Cauchy sequences is not affected by introduction of new inner product (24). The possibility of the use of unbounded metrics is treated e.g. in the last chapter of [28].

To overcome the problems with unboundedness of the metric operator (29), we choose to shift our attention to a discrete model. In the discrete approximation the metric operator stays bounded. We make use of equidistant, Runge-Kutta grid-point coordinates

$$x_k = kh, \quad k = 0, \pm 1, \pm 2 \dots, \tag{32}$$

Laplacian can be expressed as

$$-\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}{h^2}, \tag{33}$$

The explicit occurrence of the parameter h will be important for the study of the continuum limit in which the value of h would decrease to zero. Otherwise we may set $h = 1$ in suitable units. Following further ideas from [29], Laplace operator Δ can be discretized into matrix form

$$\Delta^{(n)} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix} \tag{34}$$

Matrix (34) is Hermitian and therefore diagonalizable, i.e. similar to diagonal matrix. Hence for our purposes it is enough to compute with $n \times n$ real diagonal matrix

$$K = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_n \end{pmatrix}. \tag{35}$$

Let A, B, C be real matrices $n \times n$, where $A = A^T$, $B = B^T$. Than we can write the Dieudonné equation (25) by means of block matrices

$$\begin{pmatrix} 0 & I \\ K & 0 \end{pmatrix} \begin{pmatrix} A & C^T \\ C & B \end{pmatrix} = \begin{pmatrix} A & C^T \\ C & B \end{pmatrix} \begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix}. \tag{36}$$

We obtain following conditions

$$C = C^T, \quad KC = C^T K, \quad B = KA = AK. \tag{37}$$

Real symmetric matrix which commutes with diagonal matrix must be diagonal. Thus the form of our metric operator is as follows

$$\Theta = \begin{pmatrix} \alpha_1 & \cdots & 0 & \beta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \alpha_n & 0 & \cdots & \beta_n \\ \beta_1 & \cdots & 0 & a_1\alpha_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \beta_n & 0 & \cdots & a_n\alpha_n \end{pmatrix} . \qquad (38)$$

It depends on $2n$ parameters $\alpha_1 \ldots \alpha_n$, $\beta_1 \ldots \beta_n$. Requirement of positive-definitness of the metric put following conditions on our parameters

$$\alpha_i > 0 \ , \quad a_i\alpha_i^2 > \beta_i^2 \ , \quad i = 1, 2, \ldots, n \ . \qquad (39)$$

We can construct corresponding inner product

$$\begin{aligned} \langle\langle\psi|\varphi\rangle &= \sum_{i=1}^{n} \alpha_i \psi_i^* \varphi_i \\ &+ \sum_{i=1}^{n} \beta_i(\psi_i^*\varphi_{n+i} + \psi_{n+i}^*\varphi_i) \qquad (40) \\ &+ \sum_{i=1}^{n} a_i\alpha_i\psi_{n+i}^*\varphi_{n+i} \ , \end{aligned}$$

where $\psi = (\psi_1, \psi_2, \ldots \psi_{2n})^T$, $\varphi = (\varphi_1, \varphi_2 \ldots, \varphi_{2n})^T$ are complex vectors.

4. Conclusions

In our work, we familiarized the reader with the crypto-Hermitian approach to the Klein-Gordon equation. We computed metric operator in both continuous and discrete cases. Corresponding positive definite inner product for free Klein-Gordon equation was also computed. That is considered a crucial step in proper probability interpretation of the Klein-Gordon equation.

The next step of this process would be construction of appropriate metric operator for the Klein-Gordon equation with nonzero potential V as was done for special cases in [16, 17, 19, 21]. It is also possible to broaden the formalism by adding manifest non-Hermiticity in operator $K \neq K^\dagger$, as was shown in [20].

Related complicated problems with locality, definition of physical observables and attempts to construct conserved four-current can be thoroughly studied in further references [16, 17]. The problems become much simpler if we narrow our attention to real Klein-Gordon fields only. It was shown that in such a case, inner product is uniquely defined [16, 30].

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