On the possibility of constructing relativistic quantum mechanics on the basis of the definition of the functions of differential operators

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Abstract. A new definition of the function of a differential operator that leads to local operators of infinite order is proposed. It allows one to obtain an expression for the square root of the differential operator (the Hamiltonian of a free spinless particle) and to determine the relativistic Schrödinger equation as a close analog of the non-relativistic Schrödinger equation. It is shown that this equation does not lead to difficulties of the Klein-Gordon equation. Boundary conditions that lead to self-adjoint boundary problems similar to Sturm-Liouville problems, periodic boundary value problems, and singular boundary value problems are determined. Some problems of relativistic quantum mechanics are solved.

It is known that the Klein-Gordon equation (KGE) leads to significant difficulties, for example, to solutions corresponding to the states of a free particle with negative energy, complex energy values of a pionic atom with a nuclear charge \(Z > 68\), the paradox of Klein and others. Two-particle KGE is impossible. It is easy to see that the difference between the KGE and the non-relativistic Schrödinger equation (NRSE) is related to the fact that the NRSE is obtained by a formal substitution

\[ \varepsilon \rightarrow i \frac{\partial}{\partial t}, \quad p \rightarrow -i \nabla \]

in the expression of energy through a pulse, and KGE — the same substitution in the expression of the square of the energy via momentum. As a result, KGE is an equation of hyperbolic type, while NRSE is a parabolic type. It can be assumed that the KGE describes a physical field, which, as is well known, does not hold for NRSE, KGE is the basis of quantum field theory, rather than relativistic quantum mechanics (RQM). Apparently, the basis of RQM should be an equation similar to NRSE, that is, it should be determined by standard replacement not in the expression for the square of the energy, but in the expression for the energy:

\[ \varepsilon = \sqrt{m^2 + p^2}. \]

However, this leads to a somewhat unusual equation [1,2]:

\[ \left( i \frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2} \right) \Psi(t, r) = 0. \]
In this equation, there appears an operator having the form of a square root of the differential operator. In an attempt to avoid the need to define this operator mathematically correctly, it is usually [1,2] the equation (2) is declared inadmissible, referring its asymmetry with respect to time and spatial coordinates and non-locality. This gives grounds for abandoning the equation (2), replacing it with the KGE and obtaining all of the above difficulties.

Let’s consider, whether the reasons of refusal of the equation (2) are valid. The asymmetry (2) is related to the real difference between time and space, corresponding to the difference in signs under the squares of the time differentials and spatial coordinates in the expression for the square of the interval: \( ds^2 = dt^2 - dx^2 - dy^2 - dz^2 \). The formula (1) is also not symmetric with respect to the time and space components of the energy-momentum 4-vector. In fact, for the invariance of an equation with respect to certain transformations, it suffices that the set of solutions of this equation is invariant under these transformations [3]. And the statement about the nonlocality of the operator is due to the fact that usually such an operator is defined as pseudo-differential [4], that is, using Fourier or Fourier-Bessel transforms. This definition is used in some works [5,6], which leads to very cumbersome calculations with not always correct results and does not allow to recognize this approach as correct and expedient. It is necessary to clarify the concept of a local operator: it is a linear operator that any function that vanishes on some region of a linear metric space in which it is defined associates a function defined on this region and equal to zero on it [7]. Any self-adjoint differential operator is non-local, regardless of its order, since its definition includes boundary conditions. Obviously, the use of the Fourier transform corresponds to periodic boundary conditions. Therefore, if we define a non-relativistic Hamiltonian as a pseudo-differential operator, its application to other boundary problems would be impossible. In fact, the non-relativistic Schrödinger equation (NRSE) includes a Hamiltonian defined as the local operator \( H = -\nabla^2/(2m) \) on functions \( \psi(\mathbf{r}) \) defined and twice differentiable on some domain \( X \subset \mathbb{R}^3 \), and the boundary conditions are introduced additionally so that they correspond to a given physical problem and that the boundary value problem is self-adjoint. A self-adjoint operator (with its spectrum) appears as a result of solving a self-adjoint boundary problem, they do not operate in the process of solving it. The operator in our equation must be local, so that it can be applied to solving various physical, that is, self-adjoint boundary problems. Obviously, linear differential operators of finite order defined on functions corresponding to the number of times differentiate are local. But we need to define a local operator of infinite order, and it must have the form and properties of the square root of the second-order operator, that is, it can be applied to solving various physical, that is, self-adjoint boundary problems. Obviously, linear differential operators of finite order defined on functions corresponding to the number of times differentiate are local. But we need to define a local operator of infinite order, and it must have the form and properties of the square root of the second-order operator, that is, it must correspond to a particular function of a numerical variable. The definition of the function of a differential operator that leads to a local linear differential operator of infinite order was proposed by one of the co-authors of this paper [8].

Let the analytic function \( f(z) \) (symbol) be holomorphic in some neighborhood of zero, has branch points, each of which is connected by a cut with an infinitely distant point, and the extensions of the cuts beyond the branch points intersect at the origin, \( x \in Q \subset \mathbb{R}^k \) \( D \) is a linear local differential operator (ordinary or partial derivatives), and \( u(x) \) is a function such that all its images are defined on the domain \( Q \) \( (D^n u)(x), n = 0, 1, 2, \ldots \), and the set of limit points of the sequence

\[
\{ \gamma_n(x_0) \} = \left\{ \frac{1}{|D^n u(x_0)|^{1/n}} \exp \left( \frac{i \varphi_n}{n} \right) \right\},
\]

where \( \varphi_n = \arg(|D^n u(x_0)|) \), is bounded and does not intersect the set of cut points of \( f(z) \) for all \( x_0 \in Q \). Then the function is defined on \( Q \) by an analytic continuation of the function

\[
(f(\alpha D)u)(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \alpha^n (D^n u)(x), \quad \forall x \in Q
\]
by the real parameter $\alpha$ from $\alpha = 0$ to $\alpha = 1$:

$$
(f(D)u)(x) = \sum_{i=0}^{\infty} \frac{(1 - \alpha p)^i}{i!} \sum_{k=0}^{\infty} \frac{(\alpha p - \alpha p^{-1})^k}{k!} \cdots \sum_{l=0}^{\infty} \frac{\alpha^l f^{i+k+\ldots+l}(0)}{l!} (D^{i+k+\ldots+l}u)(x). \tag{3}
$$

We set $f(z) = \sqrt{m^2 + z^2}$, where $m > 0$ (rest mass of the particle). We choose a holomorphic branch in the following way: $f(0) = m$, cut the cuts along the imaginary axis from $z = i$ to $z = i\infty$ and from $z = -i$ to $z = -i\infty$. $D = -i\nabla$. The corresponding equation has the form (2).

Let $u(r) = \exp(ipr)$, $\forall r \in Q \subset \mathbb{R}^3$, $(Q$ — open set), $p \in \mathbb{C}^3$. Then, if $p \in \mathbb{R}^3$,

$$
H(-i\nabla)u(r) = f(-i\nabla)u(r) = \sqrt{m^2 - \nabla^2} \exp(ipr) = \sqrt{m^2 + \nabla^2} \exp(ipr), \quad \forall r \in Q.
$$

Note that if $f(-i\nabla)$ was defined as a pseudo-differential operator, then $Q = \mathbb{R}^3$ would be necessary for such a result. The absence of this necessity shows the localness of our definition.

If $u(r) = \exp(\lambda r)$, $\forall r \in Q \subset \mathbb{R}^3$, then if $|\lambda| < m$,

$$
H(-i\nabla)u(r) = \sqrt{m^2 - \nabla^2} \exp(\lambda r) = \sqrt{m^2 - \lambda^2} \exp(\lambda r), \quad \forall r \in Q,
$$

and if $|\lambda| \geq m$, then the function $u(r) = \exp(\lambda r)$ is not included in the domain of the operator $H(-i\nabla)$.

It is interesting that in contrast to operators of finite order the operator $H(-i\nabla)$ has an inverse, since the function $f^{-1}(z)$ also decomposes into a Taylor series and its holomorphic branch can be defined with those same cuts. For example, for $p \in \mathbb{R}$

$$
H^{-1}(-i\nabla)u(r) = (m^2 - \nabla^2)^{-1/2} \exp(pr) = (m^2 + p^2)^{-1/2} \exp(ipr), \quad \forall r \in Q,
$$

It was shown in [8] that the equation (2) is relativistically invariant, that is, the set of its solutions is invariant under Lorentz transformations. It should be called the relativistic Schrödinger equation (RSE). From this follows the continuity equation:

$$
\frac{\partial}{\partial t} \rho(t, r) = -\nabla \cdot j(t, r),
$$

where

$$
\rho(t, r) = |\Psi(t, r)|^2 + m^2 |H^{-1}(-i\nabla)\Psi(t, r)|^2 + |V(-i\nabla)\Psi(t, r)|^2,
$$

$$
 j(t, r) = \Psi(t, r) V(-i\nabla) \Psi(t, r) + \Psi(t, r) V^*(-i\nabla) \Psi^*(t, r).
$$

These expressions include the velocity operator

$$
V(-i\nabla) = -i\nabla(m^2 - \nabla^2)^{-1/2} = i \left( \sqrt{m^2 - \nabla^2} r - r \sqrt{m^2 - \nabla^2} \right)
$$

in complete agreement with the principles of quantum mechanics and the mechanics of the theory of relativity. Let us consider in more detail the one-dimensional stationary RSE:

$$
(\varepsilon - \sqrt{m^2 - \nabla_x^2}) \psi(x) = 0, \quad \forall x \in Q \subset \mathbb{R}. \tag{4}
$$

where $\nabla_x = d/dx, A, B \in \mathbb{C}$. It has solutions of the kind

$$
\psi(x) = \exp \left( i \sqrt{\varepsilon^2 - m^2} x \right), \quad \forall x \in Q.
If $\varepsilon \in (0, m)$, then $p$ — is purely real, if $\varepsilon \in (0, m)$, then $p$ — is purely imaginary, if $\varepsilon \leq 0$, then such a value $p$ does not exist, therefore, the problem of negative energies of a free particle do not exist. Thus, a free stationary RSE, a linear differential equation of infinite order, has either two linearly independent solutions, or none. It is not difficult to verify that if $\psi_1(x)$ and $\psi_2(x)$ are solutions of the equation (2) on $Q \subset \mathbb{R}$, then $Q$ is constant function

$$W(x) = \psi_1(x)V\psi_2(x) - \psi_2(x)V\psi_1(x),$$

where

$$V = -i(m^2 - \nabla_x^2)^{-1/2}\nabla_x.$$  

Apparently, the function $W(x)$ is the relativistic analogue of the non-relativistic Wronskian. Its form makes it possible to find the boundary conditions that lead to self-adjoint boundary problems for the equation (4). If $Q = (a, b)$, then the corresponding Hilbert space is defined by the scalar product:

$$(\psi_1, \psi_2)_a^b = \int_a^b [\psi_1^*(x)\psi_2(x) + m^2(H^{-1}\psi_1^*)(x)(H^{-1}\psi_2)(x) + (V^*\psi_1^*)(x)(V\psi_2(x)) dx].$$  \hspace{1cm} (5)

It is easy to show that a regular self-adjoint problem can be given by boundary conditions that take the function $W(x)$ to zero at the end points:

$$\psi(a) \cos \alpha + i(V\psi)(a) \sin \alpha = 0, \quad \psi(b) \cos \beta + i(V\psi)(b) \sin \beta = 0,$$

where $\alpha, \beta \in \mathbb{R}$ (similar to the Sturm-Liouville problem [10]) or periodic boundary conditions that ensure the equality $W(a) = W(b)$. These problems were solved in [9]. The spectrum of these problems is purely point-wise, bounded from below, each value of the spectrum is a single-valued function, the eigenfunctions form a complete system of functions that is orthogonal in the sense of the scalar product (5). A singular boundary value on $Q = [0, \infty)$ is given by conditions of the form

$$\psi(0) \cos \alpha + i(V\psi)(0) \sin \alpha = 0,$$

where $\alpha \in \mathbb{R}$, and the condition that the solution tends to zero as $x \to \infty$.

This problem has both a continuous and a point spectrum, the latter is either empty or consists of a single value. All values of the spectrum are single-valued, all solutions of the continuous spectrum are orthogonal to the solution of the point spectrum in the sense (5) with $a = 0, b = \infty$ and orthogonal to each other in the sense that

$$\int_0^\infty (\psi_1, \psi_2) dx = \delta(\varepsilon_1 - \varepsilon_2),$$

$\psi_1(x)$ — solution corresponding to the value $\varepsilon_i$ of the continuous spectrum. The boundary problem on $Q = \mathbb{R}$ is given, just as for NSE, without boundary conditions, only by the condition of boundedness. The spectrum is also bounded from below, purely continuous, each its value is twofold.

The proposed formalism makes it possible to obtain solutions to problems, the application of which to KGE is either impossible or leads to paradoxical results. As an example, we give a solution of the problem of the S-states of the point spectrum of the negative $\pi$-meson in Coulomb field of atomic nucleus with charge $Ze$. For a radial wave function, we have a stationary equation:

$$\left[\varepsilon + Ze^2 r^{-1} - \sqrt{m^2 - \nabla^2_z} \right] \chi(r) = 0, \quad \forall r > 0.$$

4
As shown in work [9], the spectrum of S-states has the form
\[ \varepsilon_n = m(n^2 + Z^2 \alpha^2)^{-1/2}. \]

The spectrum is real, pointwise, bounded below, for small \( Z \), it is approximately described by the non-relativistic Balmer formula.

Consider the two-particle one-dimensional RSE [11]:
\[ \left( i \frac{\partial}{\partial t} - \sqrt{m_1^2 - \frac{\partial^2}{\partial x_1^2}} - \sqrt{m_2^2 - \frac{\partial^2}{\partial x_2^2}} \right) \Psi(t, x_1, x_2), \quad \forall t, x_1, x_2 \in \mathbb{R}. \]

Note that the time variable is one. The problem of reflection of a particle from an ideal mirror of finite mass is given by the condition that the solution vanishes for all \( t \) if \( x_1 \geq x_2 \) and the continuity condition of the solution. As shown in work [10], From this equation and boundary condition follow the laws of conservation of energy and momentum of this physical system and the value of the transmitted pulse
\[ k = 2\varepsilon(p_1\varepsilon_2 - p_2\varepsilon_1)[\varepsilon^2 - (p_1 + p_2)^2]^{-1}. \]

We have obtained the same result as in classical relativistic mechanics. In this case, the laws of conservation of energy and momentum are satisfied.

In [9-12], solutions of some physical problems were obtained, the application of which KGE leads to paradoxical results, or is impossible. All solutions are exact, without divergences.

So, apparently, the use of the local definition of the function of the differential operator proposed in [9] allows us to formulate the basis for a new version of relativistic quantum mechanics free from the difficulties of the generally accepted theory based on KGE. We can assume that RSE is the basis of mathematically correct and physically plausible relativistic quantum mechanics of spinless particles [13].

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