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Kinematic Relativity of Quantum Mechanics: Free Particle with Different Boundary Conditions

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Abstract

An investigation of origins of the quantum mechanical momentum operator has shown that it corresponds to the nonrelativistic momentum of classical special relativity theory rather than the relativistic one, as has been unconditionally believed in traditional relativistic quantum mechanics until now. Taking this correspondence into account, relativistic momentum and energy operators are defined. Schrödinger equations with relativistic kinematics are introduced and investigated for a free particle and a particle trapped in the deep potential well.

Keywords

Special Relativity, Quantum Mechanics, Relativistic Wave Equations, Solutions of Wave Equations: Bound States

1. Introduction

The known attempts to apply the ideas of special relativity theory (SRT) in quantum mechanics, formulated in the third decade of 20-th century and present in numerous textbooks, are based on using the quantum mechanical momentum operator $\hat{p} = -i\hbar\nabla$ in the nonrelativistic Schrödinger equation for the free particle with the Hamiltonian corresponding to the classical SRT expression for energy:

$$E = \sqrt{m^2c^4 + p^2c^2} = mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots \quad (1)$$

The first term of this expansion mc^2 is constant in an arbitrary reference frame, hence it can be considered as part of the potential, defined with an accuracy up to a constant. The second term in the right hand side looks like the nonrelativistic kinetic energy, hence the third one is the first order correction.

The modified Schrödinger equation with relativistic kinematics becomes

$$i\hbar\frac{\partial}{\partial t}\Psi=\hat{E}\Psi. \tag{2}$$

The accepted treatment of operator present in left hand side $i\hbar\frac{\partial}{\partial t}$ is that it is associated with the total relativistic energy, *i.e.*

$$\hat{E}=i\hbar\frac{\partial}{\partial t}. \tag{3}$$

However, this Schrödinger equation with relativistic kinematics does not correspond to the requirement that the operator of relativistic equation has to be invariant in respect of Lorentz transformations. Two possible solutions of this problem are known. The first one gives the Klein-Gordon equation, following directly from square of total energy of free particle expression applying defined quantum mechanical operators $\hat{p}$ and $\hat{E}$:

$$\left(\Delta-\frac{\partial^2}{\partial(ct)^2}\right)\Psi=\left(\frac{mc}{\hbar}\right)^2\Psi. \tag{4}$$

Right hand side of this equation is invariant in any reference system, so the problem of Lorentz invariance is satisfied and the eigenfunctions of equation transform according to the irreducible representations of the Lorentz group.

The other method is introduced by Dirac. He postulated the possibility of quantum operator $\hat{E}$ linearization, *i.e.* presentation in form

$$\hat{E}=\beta_1\hat{p}_x+\beta_2\hat{p}_y+\beta_3\hat{p}_z+\beta_4, \tag{5}$$

where β_j is fourth order matrices. The conditions for these matrices follow from square of relativistic energy expression, present in operator form:

$$\hat{E}^2=\hat{p}^2c^2+m^2c^4. \tag{6}$$

Finally, the Dirac equation, satisfying invariance in respect of Lorentz transformations, is

$$i\hbar\frac{\partial}{\partial t}\Psi=\left(\beta_1\hat{p}_x+\beta_2\hat{p}_y+\beta_3\hat{p}_z+\beta_4\right)\Psi. \tag{7}$$

In this paper, we show the statements applied for these equations' construction are problematic and an alternative way is necessary. We challenge the existing ideas by defining quantum mechanical momentum and energy operators as corresponding to classical, rather than the relativistic momentum and energy correspondingly. The new definition of operators is then further inspected solving the well-known problems for a free particle and particle trapped in the deep potential well.

2. Main Points of Classical SRT and Quantization

For successful quantization, first the main equations of SRT have to be present in terms of momenta instead of velocities. The Lorentz factor:

$$\gamma = \left(1-\left(v/c\right)^2\right)^{-1/2} = \left(1-\left(p_0/mc\right)^2\right)^{-1/2}, \tag{8}$$

hence the relativistic momentum $p = \gamma m v$, expressed in terms of nonrelativistic one $p_0 = mv$, is

$$p = p_0\left(1-\left(p_0/mc\right)^2\right)^{-1/2}. \tag{9}$$

This expression, essential for relativistic dynamics, defines relativistic momentum, approaching infinity at $p_0 \to mc$ and undefined for larger values of p_0, hence satisfying the condition $p_0 < mc$, following from the usual $v < c$.

The quantum operator $-i\hbar\nabla$ is without any dependence on speed of light, its eigenvalues are not restricted, hence it demonstrates the correspondence to p_0 rather than to the relativistic momentum p. Moreover, the origin of this operator is nonrelativistic, because it appears in quantum mechanics at least in three different ways, following directly from classical mechanics.

The first one, suggested by Dirac [1], applies Poisson brackets of Lagrangian dynamics for canonical coordinate and momentum, proportional to the imaginary constant. The postulation that corresponding operators of quantum dynamics have to satisfy the analogous condition

$$\left[x_i, \hat{p}_j\right] = i\hbar\delta_{ij} \tag{10}$$

gives

$$\hat{p}_j = -i\hbar\frac{\partial}{\partial x_j}. \tag{11}$$

The second way of introducing this operator follows from de Broglie wave [2] definition

$$\psi_p\left(x,t\right) = \left(2\pi\hbar\right)^{-1/2}\exp\left(-\frac{i}{\hbar}\left(\frac{p^2}{2m}t - px\right)\right). \tag{12}$$

The equation, whose solutions are these waves, is the Schrödinger equation for free nonrelativistic particle. This can be demonstrated by taking the time derivative

$$i\hbar\frac{\partial}{\partial t}\psi_p\left(x,t\right) = \frac{p^2}{2m}\psi_p\left(x,t\right) \tag{13}$$

and two coordinate derivatives

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_p\left(x,t\right) = \frac{p^2}{2m}\psi_p\left(x,t\right). \tag{14}$$

The right hand sides of both equations coincide, hence the de Broglie wave and arbitrary superpositions of these waves are solutions of the Schrödinger equation. Obviously, the conclusion follows that the operator $-i\hbar\partial/\partial x$ corresponds to the nonrelativistic momentum and $i\hbar\partial/\partial t$ is the quantum operator of nonrelativistic kinetic energy $p^2/2m$.

The third method of momentum operator definition follows from translations in the space generator

$$\hat{P}(a) = \exp\left(a\frac{\mathrm{d}}{\mathrm{d}x}\right) \tag{15}$$

definition and momentum conservation law [1]. Action of this operator gives the translation of argument:

$$\hat{P}(a)\psi(x) = \psi(x+a). \tag{16}$$

Intrinsic Hamiltonian of a quantum system is invariant in respect of translations. As a result it gives the center of mass of the system momentum conservation, hence the momentum operator is proportional to the derivative of the corresponding variable. Again, this is the classical momentum.

Therefore, the consideration of origins of the quantum mechanical momentum operator leads to the conclusion that it cannot be associated with relativistic momentum $p = \gamma m v$, having characteristic dependence on speed of light and present in the classical relativity expression $E^2 = c^2 p^2 + m^2 c^4$. The relativistic momentum operator can be expressed in terms of the nonrelativistic one as

$$\begin{aligned}\hat{p} &= \hat{p}_0\left(1-\left(\hat{p}_0/mc\right)^2\right)^{-1/2} \\ &= \hat{p}_0\sum_{k=0}^{\infty}\binom{2k}{k}\left(\frac{\hat{p}_0}{2mc}\right)^{2k},\end{aligned} \tag{17}$$

where $\binom{n}{k} = \frac{n!}{k!(n-k)!}$ is the binomial coefficient.

Now the relativistic momentum operator obtains the necessary dependence on c. Both operators have the same system of eigenfunctions but different corresponding sets of eigenvalues, expressible in the same way, as operators.

The relativistic energy of particle, moving in a laboratory reference frame with constant velocity v, equals

$$E = \gamma mc^2 = mc^2\left(1-\frac{2T_0}{mc^2}\right)^{-1/2}. \tag{18}$$

Here again one has the characteristic for SRT energy dependence on velocity. At $T_0 = mv^2/2$ approaching $mc^2/2$, the energy takes infinite value, hence it is defined only for smaller, allowed by SRT, values of nonrelativistic kinetic energy. The corresponding quantum mechanical operator is

$$\hat{E} = mc^2\sum_{k=0}^{\infty}\binom{2k}{k}\left(\frac{\hat{T}_0}{2mc^2}\right)^k, \tag{19}$$

where

$$\hat{T}_0 = -\frac{\hbar^2}{2m}\Delta \tag{20}$$

is the nonrelativistic kinetic energy operator. The above consideration and conclusions concerning the relativistic momentum are valid for the eigenvalues and eigenfunctions of the relativistic energy operator.

The relativistic kinetic energy operator $\hat{T}$ can be expressed in terms of the nonrelativistic one as

$$\hat{T} = \hat{E} - mc^2 = mc^2 \sum_{k=1}^{\infty} \binom{2k}{k} \left(\frac{\hat{T}_0}{2mc^2} \right)^k . \tag{21}$$

In terms of momentum operators, the total relativistic energy operator of a free particle is

$$\hat{E} = mc^2 \sum_{k=0}^{\infty} \binom{2k}{k} \left(\frac{\hat{p}_0}{2mc} \right)^{2k} . \tag{22}$$

Obviously, this expression contains only even degrees of the momentum operator and hence cannot be linearized in terms of $\hat{p}_0$.

Moreover, in the most popular in traditional applications equation

$$\hat{E}^2 = \hat{p}^2 c^2 + m^2 c^4 \tag{23}$$

relativistic energy and momentum operators are present, not the nonrelativistic ones, applied deriving mentioned above Klein-Gordon and Dirac equations. Taking proper operators, this equation appears as identity, because

$$\hat{\gamma}^2 \left(mc^2 \right)^2 - \hat{\gamma}^2 \left(\hat{p}_0 c \right)^2 \equiv \left(mc^2 \right)^2 . \tag{24}$$

Finally, consider the expansion of the relativistic energy operator in terms of the relativistic momentum operator:

$$\hat{E} = \left(\hat{p}^2 c^2 + m^2 c^4 \right)^{1/2} = mc^2 + \frac{\hat{p}^2}{2m} - \frac{\hat{p}^4}{8m^3 c^2} + \cdots \tag{25}$$

If the second term in the right hand side is considered to be the nonrelativistic kinetic energy (as believed in mentioned approaches), we arrive at a strange, not consistent with SRT conclusion that the correction of this is negative, *i.e.* the relativistic kinetic energy of the particle is smaller than the nonrelativistic one. From the definition of the relativistic kinetic energy operator (21) it follows that the expectation value of relativistic kinetic energy, as necessary, is always larger than the nonrelativistic.

3. Relativistic Kinematics

Therefore, the present arguments have shown that the problem of relativistic dynamics application in quantum mechanics needs deeper investigation. The SRT considers free particles, therefore this problem works best for the start of SRT application in quantum mechanics.

From the Schrödinger equation for a free particle and present arguments it follows that two quantum mechanical operators—the first, dependent on time variable $i\hbar \partial / \partial t$, and the second, dependent on radius vector $-\hbar^2 \Delta / 2m$, are associated with the nonrelativistic kinetic energy of particle under consideration. Let us mark them as $\hat{T}_0(t)$ and $\hat{T}_0(\boldsymbol{r})$ correspondingly. Taking this into account opens two different possibilities for the same relativistic kinetic energy operator presentation:

$$\hat{T}(t) = mc^2 \left[\left(1 - \frac{2\hat{T}_0(t)}{mc^2} \right)^{-1/2} - 1 \right] \tag{26}$$

and

$$\hat{T}(\boldsymbol{r}) = mc^2\left[\left(1-\frac{2\hat{T}_0(\boldsymbol{r})}{mc^2}\right)^{-1/2}-1\right]. \quad (27)$$

Due to equivalence of introduced operators one can define the eigenvalues equation as

$$\hat{T}(t)\Psi(\boldsymbol{r},t) = \hat{T}(\boldsymbol{r})\Psi(\boldsymbol{r},t). \quad (28)$$

Let us call this the relativistic Schrödinger equation. The essential part of equation, independent of speed of light, is the Schrödinger equation for free particle:

$$\hat{T}_0(t)\Psi_0(\boldsymbol{r},t) = \hat{T}_0(\boldsymbol{r})\Psi_0(\boldsymbol{r},t). \quad (29)$$

Taking into account the expansions for these operators like given in Equation (21), one can present Equation (28) as

$$\sum_{k=1}^{\infty}\binom{2k}{k}\left(\frac{1}{2mc^2}\right)^k\left[\hat{T}_0^k(t)-\hat{T}_0^k(\boldsymbol{r})\right]\Psi(\boldsymbol{r},t) = 0. \quad (30)$$

After some transformation of commuting, due to dependence on different variables, the kinetic energy operators the equation takes the simplified form

$$\left[\sum_{k=1}^{\infty}\binom{2k}{k}\left(\frac{1}{2mc^2}\right)^k\sum_{j=1}^{k-1}\hat{T}_0^j(t)\hat{T}_0^{k-1-j}(\boldsymbol{r})\right]\left[\hat{T}_0(t)-\hat{T}_0(\boldsymbol{r})\right]\Psi(\boldsymbol{r},t) = 0, \quad (31)$$

leading to the conclusion that the eigenfunctions of the relativistic equation are the same as the corresponding eigenfunctions of the nonrelativistic equation, *i.e.*:

$$\Psi(\boldsymbol{r},t) = \Psi_0(\boldsymbol{r},t). \quad (32)$$

Due to separability of operators of both nonrelativistic and relativistic equations, the eigenfunctions are presentable as products of functions, dependent on time and spatial variables:

$$\Psi(\boldsymbol{r},t) = \Psi_{\mathcal{E}}(\boldsymbol{r})\Psi_{\mathcal{E}}(t). \quad (33)$$

As usual these functions are defined as eigenfunctions of corresponding stationary equations

$$\hat{T}(\boldsymbol{r})\Psi_{\mathcal{E}}(\boldsymbol{r}) = \mathcal{E}\Psi_{\mathcal{E}}(\boldsymbol{r}) \quad (34)$$

and

$$\hat{T}(t)\Psi_{\mathcal{E}}(t) = \mathcal{E}\Psi_{\mathcal{E}}(t). \quad (35)$$

The eigenfunctions of these operators are identical to the eigenfunctions of corresponding stationary nonrelativistic equations, but their eigenvalues are different. If we define the eigenvalue of the nonrelativistic equation as E, the eigenvalue of the relativistic equation, corresponding to the same eigenfunction, is

$$\frac{\mathcal{E}}{mc^2} = \left(1-\frac{2E}{mc^2}\right)^{-1/2}-1. \quad (36)$$

Due to the upper bound for nonrelativistic kinetic energy $E < mc^2/2$, this equation implies that the set of eigenvalues of the relativistic stationary equation is restricted in comparison to the nonrelativistic set. This fact corresponds very well with the spirit of SRT.

To investigate the discrete spectrum, consider the problem of a free particle, trapped in the spherical well with impenetrable walls. The nonrelativistic stationary Schrödinger equation is

$$\hat{T}_0(r\theta\varphi)\psi_{nl\mu}(r\theta\varphi)=E_{nl}^{(0)}\psi_{nl\mu}(r\theta\varphi), \tag{37}$$

where

$$\hat{T}_0(r\theta\varphi)=-\frac{(\hbar c)^2}{2mc^2}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{\hat{L}^2(\theta\varphi)}{r^2}\right]. \tag{38}$$

Here and further, for the sake of simplicity, the conversion factor $\hbar c=197.3269788(12)$ MeVfm, as defined in [3], and rest energy of particle expressed in electronvolts, are used. For wave functions, written in spherical harmonics

$$\psi_{nl\mu}(r\theta\varphi)=u_{nl}(r)Y_{l\mu}(\theta\varphi), \tag{39}$$

the boundary condition is:

$$u_{nl}(r)=0 \text{ if } r=R, \tag{40}$$

where R is the radius of the spherical well. The solutions of this equation are the spherical Bessel functions. Boundary conditions define the spectrum of the nonrelativistic Schrödinger equation.

The Schrödinger equation with the relativistic kinetic energy operator has the same eigenfunctions but different corresponding eigenenergies:

$$\frac{\mathcal{E}_{nl}}{mc^2}=\left(1-\frac{2E_{nl}}{mc^2}\right)^{-1/2}-1. \tag{41}$$

Obviously, in the nonrelativistic approximation $\left(E_{nl}\ll mc^2/2\right)$, as necessary, $\mathcal{E}_{nl}\to E_{nl}$.

For angular momentum $l=0$ the solutions can be presented in analytical form:

$$E_{n0}=\frac{1}{2mc^2}\left(\frac{\pi\hbar c}{2R}\right)^2 n^2, n=1,2,3,\cdots, \tag{42}$$

and

$$\frac{\mathcal{E}_{n0}}{mc^2}=\left(1-\left(\frac{\pi\hbar c}{2Rmc^2}\right)^2 n^2\right)^{-1/2}-1. \tag{43}$$

This expression demonstrates that in a spherical well with impenetrable walls, the only allowed states are those corresponding to the quantum number

$$n<\frac{2Rmc^2}{\pi\hbar c}. \tag{44}$$

This does not exclude a case where there are no allowed states at all in such a well. It happens when $Rmc^2<\pi\hbar c/2$. Taking the given above value of conversion factor, the right hand side of condition equals approximately 310 MeVfm Radius of well multiplied by mass of particle has to be larger than this value for at least one bound state to exist. On the other hand, in a corresponding nonrelativistic well there is an infinite number of bound states at any radius of well and mass of particle.

4. Conclusions

The operator of the introduced Schrödinger equation with relativistic kinematics is not invariant in respect of Lorentz transformations and from our consideration, it follows that construction of such operators, if possible, is immensely difficult. However, the Lorentz invariant theory is necessary for the description of ultrarelativistic processes and problems, like high energy phenomena obtainable in universe or the reactions in colliders. At high relativistic velocities, and hence high kinetic energies, the most interesting interactions among particles, responsible for surrounding us world structure and development, cannot play a remarkable role.

Therefore, the most actual applications of low energies quantum mechanics are obtained by solving the stationary Schrödinger equation, giving qualified description of bound states and excitation spectra of different quantum systems in huge energy intervals. Now, when experimental equipment is able to analyze different structures and phenomena with very high precision, the role played by relativistic effects stays remarkable and has to be investigated in a proper way. The first step in this direction is investigation of the stationary Schrödinger equation with the relativistic kinetic energy operator instead of the nonrelativistic one, present in the original equation. The obtained slight enough modifications of corresponding results of the original Schrödinger equation in low energies limit demonstrate high quality of nonrelativistic approach. In the larger energies region, the introduced innovation produces significant spectrum modifications and opens new possibilities for old problems of relativistic quantum mechanics solution.

The consideration of relativistic momentum operator, present in the known SRT equation $E^2 = m^2c^4 + p^2c^2$, as classical momentum leads to the conclusion that the first order correction of the nonrelativistic kinetic energy has the negative sign (Equation (1)), which means the expectation value of relativistic kinetic energy is smaller than the nonrelativistic one. This result, until now existing in applications for relativistic effects evaluation in atomic [3] and nuclear theory [4], creates "softer" than necessary kinetic energy and allows strange decisions concerning relativistic corrections of binding energies and excitations spectra of these quantum systems.

Our definition of the relativistic momentum operator classifies Klein-Gordon and Dirac equations as not completely relativistic. They are both invariant in respect of Lorentz transformations, but apply the definition of the nonrelativistic momentum operator instead of the relativistic one. This approach eliminates from equations basic for SRT dependence of relativistic energy and relativistic momentum on velocity, defined by Lorentz factor. Moreover, the Dirac equation does not contain any input information about the electron, hence predicts the spin, equal $\hbar/2$, for all particles without any exemptions. The equation for free particle (7) in the nonrelativistic limit has to be consistent with corresponding Schrödinger equation, however, this cannot be established. The operator in front of the eigenfunction of right-hand side of this equation, seen as the relativistic free particle Hamiltonian, predicts the velocity of particle, equal to the speed of light c [2]. Finally, the Dirac equation is undefined for two- and more-particles system.

Therefore, new ideas of SRT application in quantum mechanics are necessary. As will be shown in following publications, our approach is applicable for the many-particle system and in the low kinetic energies approximation, reproduces the results of the corresponding nonrelativistic Schrödinger equation.

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