New Relativistic Equation for Statistical Operator

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Abstract In this paper, we derive a covariant quantum equation for the statistical operator $\hat{\varrho}$. This equation is written for a free particle and for a hydrogen atom.

Keywords Lorentz transformation · Momentum and energy of relativistic particle · Statistical operator · Dissipative operators · Relativistic equation

1 Introduction

The Klein—Gordon—Fock equation and the Dirac equation were written shortly after the discovery of the Schrodinger equation

$$i\hbar\,\partial\psi/\partial t \;=\; \widehat{H}\,\psi,$$

where $\psi = \psi(t, \boldsymbol{r})$ is the wave function, $\widehat{H}$ is the Hamiltonian. Relativistic equations were derived for the wave function $\psi = \psi(t, \boldsymbol{r})$.

Then the physicist von Neumann wrote down his equation

$$i\hbar\,\partial\hat{\varrho}/\partial t \;=\; [\widehat{H}\,\hat{\varrho}],$$

in which the statistical operator $\hat{\varrho}$ appeared.

In quantum physics, the main tool is the statistical operator $\hat{\varrho}$. But a covariant quantum equation for this operator has not yet been written, i.e. an equation that does not change under the action of the Lorentz transformation.

Consider two coordinate systems that move at a constant speed $\boldsymbol{V}$ relative to each other [1]. You can always direct the coordinate axes so that they are directed parallel to each other, and the vector $\boldsymbol{V}$ is directed along the x axis. In addition, we will

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assume that the speed of light in these two systems is the same. In this case, the coordinates x, y, z and time t in one coordinate system will be associated with the same values x', y', z' and t' of the other system by the Lorentz transformation [1]

$$\begin{cases} x = \gamma\,(x' + Vt'), \\ y = y', \quad z = z', \\ t = \gamma\,(Vx'/c^2 + t'), \end{cases} \tag{1}$$

where

$$\gamma = (1 - V^2/c^2)^{-1/2}, \tag{2}$$

$V = x/t = \text{const}$ by $x' = 0$.

An equation that has the same form in these coordinate systems is called covariant. In other words, we can say that the covariant equation is invariant with respect to the Lorentz transformation.

Now consider the motion of a single relativistic particle.

The momentum and energy of this particle will be equal

$$\boldsymbol{p}_{\text{relativ}} = \lambda\, m\, v, \ E_{\text{relativ}} = \lambda\, m\, c^2, \tag{3}$$

where

$$\boldsymbol{v} = \mathrm{d}\boldsymbol{r}/\mathrm{d}t \tag{4}$$

is the velocity of the particle, $\boldsymbol{r} = \boldsymbol{r}(t)$ is its radius vector, m is the mass of the particle,

$$\lambda = (1 - v^2/c^2)^{-1/2}. \tag{5}$$

The dynamics of a relativistic particle obeys the equation

$$m\,\mathrm{d}(\lambda\boldsymbol{v})/\mathrm{d}t = \boldsymbol{F}, \tag{6}$$

where $\boldsymbol{F}$ is the force. This equation follows from the equation

$$m\,(\mathrm{d}^2\boldsymbol{r})/(\mathrm{d}\tau^2) = \lambda\boldsymbol{F},$$

where $\mathrm{d}\tau = \mathrm{d}t/\lambda$.

Let's write down another equation

$$m\,c^2 \mathrm{d}\lambda/\mathrm{d}t \;=\; P, \tag{7}$$

where $P = \boldsymbol{F}\,\boldsymbol{v}$ is the power.

Using formula (4) and applying formulas (6) and (7), we obtain a system of two equations for the functions $\boldsymbol{r} = \boldsymbol{r}(t)$ and $\boldsymbol{v} = \boldsymbol{v}(t)$:

$$\begin{cases} \mathrm{d}\boldsymbol{r}/\mathrm{d}t \;=\; \boldsymbol{v}, \\ \lambda(v)\,m\;\mathrm{d}\boldsymbol{v}/\mathrm{d}t \;=\; \boldsymbol{F} \;-\; (\boldsymbol{F}\boldsymbol{v})\;v/c^2\;\boldsymbol{v}. \end{cases} \tag{8}$$

2 The Lindblad Equations

The equation for the statistical operator was derived by the author of this paper from the Lindblad Eq. [2]

$$\mathrm{i}\,\hbar\,\partial\hat{\varrho}/\partial t \;=\; [\widehat{H}\hat{\varrho}] \;+\; \mathrm{i}\,\hbar\,\widehat{D}, \tag{9}$$

where $\hat{\varrho}$ is the statistical operator, $\widehat{H}$ is the Hamiltonian, D is the dissipative operator, which was written by Lindblad and which is equal to

$$\widehat{D} = \sum_{jk} C_{jk}\{2\hat{a}_j\hat{\varrho}\,\hat{a}_k^+ - \hat{a}_k^+\hat{a}_j\hat{\varrho} - \hat{\varrho}\hat{a}_k^+\hat{a}_j\}, \tag{10}$$

where C_{jk} is the unknown coefficients, and $\hat{a}_j$ is the unknown operators that still need to be found.

3 Dissipative Operators

The author of this article wrote the dissipative diffusion and attenuation operators in the form [3, 4]

$$\hat{\boldsymbol{a}} \;=\; \hat{\boldsymbol{p}} \;+\; \mathrm{i}\,\hbar\,\beta\,\widehat{\boldsymbol{F}}/4, \quad \hat{\boldsymbol{b}} \;=\; \hat{\boldsymbol{r}} \;+\; \mathrm{i}\,\hbar\;\;\beta\hat{\boldsymbol{p}}/(4\;\,\mathrm{m}), \tag{11}$$

where $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{p}}$ are the operators of the coordinates and momentum of the particle, $\boldsymbol{F}$ is the operator of the force that acts on it,

$$\beta \;=\; 1/(k_B T).$$

4 New Equation for Statistical Operator

We substitute formulas (11) in the Lindblad Eq. (9). We will have a new equation

$$\begin{aligned} \mathrm{i}\,\hbar\,\partial\widehat{\varrho}/\partial t \; &= \; [\widehat{H}\widehat{\varrho}] \\ &+ \mathrm{i}\; D/\hbar\{[\widehat{\boldsymbol{p}}[\widehat{\boldsymbol{p}}\,\widehat{\varrho}]] + \mathrm{i}\,\hbar\,\beta/2[\widehat{\boldsymbol{p}}[\widehat{\boldsymbol{F}}\widehat{\varrho}]_+]\} \\ &- \mathrm{i}\;\gamma/\hbar\{[\widehat{\boldsymbol{r}}[\widehat{\boldsymbol{r}}\,\widehat{\varrho}]] \; - \mathrm{i}\,\hbar\,\beta/(2\,m)\,[\widehat{\boldsymbol{r}}[\widehat{\boldsymbol{p}}\,\widehat{\varrho}]_+]\}, \end{aligned} \tag{12}$$

here D and γ are the diffusion and attenuation coefficients. In this equation, the terms that will contain β^2 are discarded.

The coefficient β increases to infinity at $T \to 0$. To avoid this absurdity, we add to the energy $k_{\mathrm{B}}T$ another quantum energy $\hbar\omega$, where the frequency ω characterizes the quantum effect of the thermostat on the quantum system in the form of electromagnetic waves and other massless particles:

$$\beta \; = \; 1/(\hbar\,\omega \; + k_B T). \tag{13}$$

5 Non-relativistic Equation for Statistical Operator of Free Particle

For a free particle, the Hamiltonian is equal to the kinetic energy operator

$$\widehat{H} \; = \; \widehat{\boldsymbol{p}}^2/(2\,m), \tag{14}$$

and the diffusion coefficients D are set to zero. So that the non-relativistic equation for the statistical operator of a free particle will have the form

$$\begin{aligned} \mathrm{i}\,\hbar\,\partial\widehat{\varrho}/\partial t \; &= \; [\widehat{\boldsymbol{p}}^2/(2m)\widehat{\varrho}] \\ &- \mathrm{i}\,\gamma/\hbar\{[\widehat{\boldsymbol{r}}[\widehat{\boldsymbol{r}}\,\widehat{\varrho}]] \; + \; \mathrm{i}\,\hbar\,\beta/(2\,m)\;[\widehat{\boldsymbol{r}}\,[\widehat{\boldsymbol{p}}\widehat{\varrho}]_+]\}. \end{aligned} \tag{15}$$

6 Covariant Equation for Free Particle Statistical Operator

We write down the momentum and kinetic energy operators of a relativistic particle

$$\widehat{\boldsymbol{p}}_{\mathrm{relativ}} \; = \; \widehat{\lambda}\,\widehat{\boldsymbol{p}}, \;\; \widehat{E}_{relativ} \; = \; \widehat{\lambda}\,m\,c^2, \tag{16}$$

where

$$\widehat{\boldsymbol{p}} \;=\; \boldsymbol{m}\,\widehat{\boldsymbol{v}}, \quad \widehat{\lambda} \;=\; (1-\widehat{v}^2/c^2)^{-1/2}. \tag{17}$$

Using the formula $\widehat{\boldsymbol{p}} \;=\; m\,\widehat{\boldsymbol{v}}$, we express the particle velocity operator $\widehat{\boldsymbol{v}}$ in terms of the momentum operator

$$\widehat{\boldsymbol{v}} \;=\; \widehat{\boldsymbol{p}}/m. \tag{18}$$

Thus, we get

$$\widehat{\lambda} = \lambda(\widehat{p}) = \{1 - \widehat{p}^2/(m^2c^2)\}^{(-1/2)}. \tag{19}$$

So we will have the equation [5]

$$\begin{aligned} &\mathrm{i}\hbar\,\partial\widehat{\varrho}/\partial t = mc^2[\lambda(\widehat{p})\widehat{\varrho}] \\ &-\mathrm{i}\,\gamma/\hbar\{\,[\widehat{\boldsymbol{r}}\,[\widehat{\boldsymbol{r}}\;\;\widehat{\varrho}]\,] + \mathrm{i}\;\hbar\,\beta/(2m)\,[\widehat{\boldsymbol{r}}\,[\,\lambda(\widehat{p})\;\widehat{\boldsymbol{p}}\;\;\widehat{\varrho}]_{+}\}. \end{aligned} \tag{20}$$

This equation is a covariant quantum equation for the statistical operator of a free particle.

We simplify the function (19) by applying the notation

$$\xi = \widehat{p}^2/(m^2c^2). \tag{21}$$

In this case, the function takes the form

$$\lambda(\xi) \;=\; (1\;-\;\xi)^{-1/2}. \tag{22}$$

We decompose this function into a Taylor series

$$\lambda(\xi) \;=\; \lambda(0) \;+\; \lambda'(0)\,\xi \;+\; 1/2\,\lambda''\,(0)\xi^2 \;+\;\ldots$$

The derived functions are equal to

$$\begin{aligned} \lambda'(\xi) \;&=\; \mathrm{d}(1-\xi)^{-1/2}/\mathrm{d}\,\xi \\ &= 1/2(1-\xi)^{-3/2}, \end{aligned}$$

$$\begin{aligned} \lambda''(\xi) \;&=\; -1/2d(1-\xi)^{-3/2}/\mathrm{d}\,\xi \\ &= -3/4(1-\xi)^{-5/2},\ldots \end{aligned}$$

Thus we get,

$$\lambda(\xi) \ = \ 1 + \ 1/2\,\xi \ = \ 3/4\xi^2 \ + \ \ldots$$

Substituting the value (21) here leads to the result

$$\lambda(\widehat{p}) = 1 + \widehat{p}^2/(2m^2c^2) - 3\widehat{p}^4/(2m^2c^2)^2 \ + \ \ldots \tag{23}$$

We substitute this operator in Eq. (20). We get

$$\begin{aligned} &\mathrm{i}\,\hbar\,\partial\,\widehat{\varrho}/\partial t \ \cong mc^2[1 + \widehat{p}^2/2m^2c^2) - 3\widehat{p}^4/(2m^2c^2)^2, \widehat{\varrho}] \\ &- \mathrm{i}\,\gamma/\hbar\,\{[\hat{\boldsymbol{r}}\,[\hat{\boldsymbol{r}}\,\widehat{\varrho}]] \ + \ \mathrm{i}\,\hbar\,\beta/(2m)\,[\hat{\boldsymbol{r}}\,[\{1 + \widehat{p}^2/(2\,m^2\,c^2)\}\widehat{\boldsymbol{p}}\,\widehat{\varrho}]_+\,]\,\}. \end{aligned}$$

Transform the first term on the right side of this equation

$$\begin{aligned} &m\,c^2\,[1 + \widehat{p}^2/(2m^2c^2) - 3\widehat{p}^4/(2m^2c^2)^2, \widehat{\varrho}] \\ &= [\widehat{p}^2/(2\,m) \ - \ 3/(4m^3c^2)\ \widehat{p}^4, \ \widehat{\varrho}]. \end{aligned}$$

Now the equation takes the form

$$\begin{aligned} &\mathrm{i}\,\hbar\,\partial\widehat{\varrho}/\partial t \ \cong \ [\widehat{p}^2/(2m) - 3/(4m^3c^2)\widehat{p}^4, \ \widehat{\varrho}] \ - \ \mathrm{i}\,\gamma/\hbar\{[\hat{\boldsymbol{r}}[\hat{\boldsymbol{r}}\widehat{\varrho}]] \\ &+\mathrm{i}\,\hbar\,\beta/(2m)\,[\hat{\boldsymbol{r}}[\{1 + \ \widehat{p}^2/(2m^2c^2)\ \widehat{\boldsymbol{p}}, \ \widehat{\varrho}]_+]\}. \end{aligned} \tag{24}$$

Look closely at this equation. You will see that the operators $\hat{\boldsymbol{r}}$ and $\widehat{p}$ occur here only as products of $\widehat{\boldsymbol{p}}^2$, $\widehat{\boldsymbol{p}}^4$, $\hat{\boldsymbol{r}}^2$, $\hat{\boldsymbol{r}}^2\ \widehat{p}$ *and* $\hat{\boldsymbol{r}}^2\ \widehat{p}^3$. This makes it possible to find the average value of the coordinates $\langle\hat{\boldsymbol{r}}\rangle$ of the particle and its momentum $\langle\widehat{\boldsymbol{p}}\rangle$. And then find the changes in these values over time:

$$\mathrm{d}\langle\hat{\boldsymbol{r}}\rangle/\mathrm{d}t \ = \ \mathrm{Tr}\,(\hat{\boldsymbol{r}}\ \partial\widehat{\varrho}/\partial t), \quad \mathrm{d}\langle\widehat{\boldsymbol{p}}\rangle/\mathrm{d}t \ = \ \mathrm{Tr}\,(\ \widehat{\boldsymbol{p}}\ \partial\widehat{\varrho}/\partial t).$$

As a result, you will have a system

$$\begin{cases} \mathrm{d}\langle\hat{\boldsymbol{r}}\rangle/\mathrm{d}t \ = \ \langle\widehat{\boldsymbol{p}}\rangle/m, \\ \mathrm{d}\langle\widehat{\boldsymbol{p}}\rangle/\mathrm{d}t \ = \ -\alpha/m\langle\widehat{\boldsymbol{p}}\rangle \ + \ \alpha/(m^3c^2)\widehat{p}^2\langle\widehat{\boldsymbol{p}}\rangle, \end{cases} \tag{25}$$

where $\alpha = \beta\,\gamma$. It is natural to assume that $\langle\hat{\boldsymbol{r}}\rangle \ \equiv \ \boldsymbol{r}$ and $\langle\widehat{\boldsymbol{p}}\rangle \ \equiv \ \boldsymbol{p}$. If we also denote the force $\boldsymbol{F} \ = \ -\alpha\boldsymbol{v}$, then after a series of elementary transformations we will teach the system (8).

7 Covariant Quantum Equation for Statistical Operator of Hydrogen Atom

Now we write down a covariant quantum equation for the statistical operator of the hydrogen atom. There are two particles in this atom. This is an electron and a proton, which carry electric charges – e and + e. Therefore, they have potential energy

$$U_{ep}(\boldsymbol{r}_e - \boldsymbol{r}_p) = -e^2/\left|\boldsymbol{r}_e - \boldsymbol{r}_p\right|, \tag{26}$$

where $\boldsymbol{r}_e$ and $\boldsymbol{r}_p$ are the radius vectors of the electron and proton.

The Hamiltonian of the atom will be equal to

$$\widehat{H} = \widehat{\boldsymbol{p}}_e^2/(2m_e) + \widehat{\boldsymbol{p}}_p^2/(2m_p) + U_{ep}(\boldsymbol{r}_e - \boldsymbol{r}_p), \tag{27}$$

where $\widehat{\boldsymbol{p}}_e$ and $\boldsymbol{p}_p$ are the electron and proton pulses, and m_e and m_p are their masses.

We take the dissipative operators to be equal

$$\begin{aligned} \mathrm{i}\,\hbar\,\widehat{D} = &-\mathrm{i}\,\gamma/\hbar\{[\boldsymbol{r}_e - \boldsymbol{r}_p[(\boldsymbol{r}_e - \boldsymbol{r}_p)\,\widehat{\varrho}]]\} \\ &+ \mathrm{i}\,\hbar\,\beta\,(2\,m_e)\,[\boldsymbol{r}_e - \boldsymbol{r}_p[(\widehat{\boldsymbol{p}}_e - \widehat{\boldsymbol{p}}_p)\,\widehat{\varrho}]_+]. \end{aligned} \tag{28}$$

Now we write down the non-relativistic equation

$$\mathrm{i}\,\hbar\,\partial\,\widehat{\varrho}/\partial\;t = [\widehat{H}\,\widehat{\varrho}] + \mathrm{i}\,\hbar\,\widehat{D}.$$

In relativistic physics, the formulas are known

$$\widehat{\boldsymbol{p}}^{(e)}_{\text{relativ}} = \widehat{\lambda}_e\,\widehat{\boldsymbol{p}}_e,\;\ldots\widehat{E}^{(e)}_{\text{relativ}}\,\widehat{\lambda}_e\,m^e\,c^2, \tag{29}$$

where

$$\widehat{\lambda}_e = \lambda(\widehat{\boldsymbol{p}}_e/m_e) = \{1 - \widehat{\boldsymbol{p}}_e^2/(m_e^2\,c^2)\}^{-1/2} \tag{30}$$

for the electron;

$$\widehat{\boldsymbol{p}}^{(\boldsymbol{p})}_{\text{relativ}} = \widehat{\lambda}_{\boldsymbol{p}}\widehat{\boldsymbol{p}}_{\boldsymbol{p}},\ldots\;\widehat{E}^{(\boldsymbol{p})}_{\text{relativ}} = \widehat{\lambda}_{\boldsymbol{p}}m_{\boldsymbol{p}}\,c^2, \tag{31}$$

where

$$\widehat{\lambda}_{\boldsymbol{p}} = \lambda(\widehat{\boldsymbol{p}}_{\boldsymbol{p}}/m_{\boldsymbol{p}}) = \{1 - \widehat{\boldsymbol{p}}_{\boldsymbol{p}}^2/m_{\boldsymbol{p}}^2)\}^{-1/2} \tag{32}$$

for the proton.

Now we write down a covariant quantum equation for the statistical operator of the hydrogen atom

$$\begin{gathered} \mathrm{i}\,\hbar\,\partial\,\widehat{\varrho}/\partial t \\ = [\lambda\widehat{\boldsymbol{p}}_e/m_e]m_e\,c^2 + \lambda(\widehat{\boldsymbol{p}}_{\boldsymbol{p}}/m_{\boldsymbol{p}})m_{\boldsymbol{p}}\,c^2 \\ + U_{ep}(\boldsymbol{r}_e - \boldsymbol{r}_p),\ \widehat{\varrho}] \\ -\mathrm{i}\,\gamma/\hbar\{[(\boldsymbol{r}_e - \boldsymbol{r}_p)[(\boldsymbol{r}_e - \boldsymbol{r}_p)\,\widehat{\varrho}\,]]\} \\ +\mathrm{i}\,\hbar\,\beta/(2m_e)[(\boldsymbol{r}_e - \boldsymbol{r}_p) \\ [\lambda(\widehat{\boldsymbol{p}}_e/m_e)\widehat{\boldsymbol{p}}_e - \lambda(\widehat{\boldsymbol{p}}_p/m_p)\widehat{\boldsymbol{p}}_p,\ \widehat{\varrho}]_+]. \end{gathered} \tag{33}$$

8 Conclusion

We have not forgotten that almost all microscopic particles have spins. Since the statistical operator $\widehat{\varrho}$ is the main characteristic of particles in quantum theory, it must also take into account spins.

Consider the operator $\widehat{\varrho}$ of a single particle. Like any other particle, its state is described by four operators, one of which is the spin operator $\widehat{\sigma}$. For example, in the coordinate representation, the operator $\widehat{\varrho}$ depends on three coordinates $\widehat{x},\ \widehat{y},\ \widehat{z}$ and the spin operator $\widehat{\sigma}$:

$$\widehat{\varrho} = \widehat{\varrho}(\widehat{x},\ \widehat{y},\ \widehat{z},\ \widehat{\sigma}).$$

Spin manifests itself only when a term that describes the effect of spin appears in the equation for the operator $\widehat{\varrho}$. Otherwise, the spin is not visible. Here is the simplest example.

An electron in a magnetic field has energy

$$E_{\text{магнит}} = -\mu_{\mathrm{B}}\,\sigma\,\mathcal{H}\,,$$

where $\mu_B = e\,\hbar/(2\,m)$—Bora magneton, $\sigma = \pm\,1/2$ – electron spin,

$$\mathcal{H} = \mathcal{H}(t, \boldsymbol{r})$$

is a modulus of the magnetic field strength. Now in the equation for the operator $\widehat{\varrho}$ we can write the term

$$- \mu_{\mathrm{B}} \left[\hat{\sigma} \hat{\mathcal{H}} \hat{\varrho} \right].$$

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