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Equations of motion for a relativistic wave packet

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Abstract. The time derivative of the position of a relativistic wave packet is evaluated. It is found that it is equal to the mean value of the momentum of the wave packet divided by the mass of the particle. The equation derived represents a relativistic version of the second Ehrenfest theorem.

Keywords. Klein–Gordon equation; classical limit; Ehrenfest theorems.

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1. Introduction

In this article we consider a small relativistic wave packet that moves in external static fields and evaluate the time derivative of its position.

The classical limit of the Klein–Gordon equation can be achieved by assuming that the Planck's constant $\hbar$ converges to zero [1] or by assuming that the coordinate and momentum dispersions of a relativistic wave packet are small [2]. At this point it is necessary to give a brief review of what was achieved in ref. [2]. In ref. [2] substitution

$$\psi = R \exp\left(\frac{i}{\hbar}\theta\right), \tag{1.1}$$

where R and θ are real functions, was applied in the Klein–Gordon formula for the particle probability density, namely

$$\rho = \frac{i\hbar}{2m_0c^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)^2 - \frac{e\phi}{m_0c^2}\psi^*\psi. \tag{1.2}$$

In this way eq. (1.2) was simplified to

$$\rho = \frac{1}{m_0c^2}\left(-\frac{\partial\theta}{\partial t} - e\phi\right)R^2. \tag{1.3}$$

Since for static fields

$$-\frac{\partial\theta}{\partial t} = E, \tag{1.4}$$

eq. (1.3) was further simplified to

$$\rho = \frac{1}{m_0 c^2}\,(E - e\phi)\,R^2. \tag{1.5}$$

Equation (1.5) clearly demonstrates that the Klein–Gordon particle probability density is physically meaningful when the total energy of the particle is larger than the potential function $e\phi$. Obviously, for cases where $E - e\phi > 0$ is not always satisfied, the particle probability density would be physically meaningless. This is why in the standard Klein–Gordon theory it is necessary to use the charge density $\rho_e = e\rho$, which can attain both positive and negative values.

To respect the Klein–Gordon particle probability density function expressed as (1.2), (1.3) and (1.5), densities of other physical quantities in ref. [2] and in this work are defined using the formula

$$\rho_A = \rho\psi^{-1}\hat{A}\psi. \tag{1.6}$$

With respect to (1.6) in ref. [2] and also here the mean values of momentum and energy are defined using relations

$$\langle E\rangle = \int_{-\infty}^{\infty} \psi^{-1}\rho i\hbar\frac{\partial\psi}{\partial t}\mathrm{d}V \tag{1.7}$$

and

$$\langle \underline{p}\rangle = \int_{-\infty}^{\infty} \rho\psi^{-1}(-i\hbar)\underline{\nabla}\psi\mathrm{d}V, \tag{1.8}$$

where integration is over the whole space. In ref. [2] it is shown that substitution equation (1.1) allows that eqs (1.7) and (1.8) can be rewritten as

$$\langle E\rangle = \int_{-\infty}^{\infty} (\langle E\rangle - e\phi)\psi^{*} i\hbar\frac{\partial\psi}{\partial t}\mathrm{d}V \tag{1.9}$$

and

$$\langle \underline{p}\rangle = \int_{-\infty}^{\infty} (\langle E\rangle - e\phi)\psi^{*}(-i\hbar)\underline{\nabla}\psi\mathrm{d}V. \tag{1.10}$$

Further, in ref. [2] it is shown that using substitution equation (1.1) and considering a small wave packet the right-hand sides of eqs (1.9) and (1.10) can be expressed as

$$\langle E\rangle = -\frac{\partial\theta(\langle \underline{r}\rangle)}{\partial t} \tag{1.11}$$

and

$$\langle \underline{p}\rangle = -\nabla_{\langle \underline{r}\rangle}\theta(\langle \underline{r}\rangle), \tag{1.12}$$

where the symbol $\langle \underline{r}\rangle$ denotes the centroid of the wave packet.

In ref. [2] it is demonstrated that application of substitution equation (1.1) in the Klein–Gordon equation for a static external field,

$$\left(i\hbar\frac{\partial}{\partial t} - e\phi\right)^2 \psi = -\hbar^2 c^2 \Delta\psi + m_0^2 c^4 \psi, \tag{1.13}$$

and assuming that the wave packet is small, give equation

$$\left(-\frac{\partial\theta(\langle \underline{r}\rangle)}{\partial t} - e\phi(\langle \underline{r}\rangle)\right)^2 = c^2\left(\underline{\nabla}_{\langle \underline{r}\rangle}\theta(\langle \underline{r}\rangle)\right)^2 + m_0^2 c^4. \tag{1.14}$$

Equation (1.14) is the relativistic Hamilton–Jacobi equation written for the centroid of a wave packet. Equations (1.11) and (1.12) support eq. (1.14) and confirm its clear physical meaning. Besides eqs (1.11), (1.12) and (1.14), ref. [2] presents derivation of equation

$$\langle \underline{p}\rangle = \frac{m_0\langle \underline{v}\rangle}{\sqrt{1-\langle \underline{v}\rangle^2/c^2}}. \tag{1.15}$$

Equation (1.15) is consistent with both the special relativity theory and also with eqs (1.11), (1.12) and (1.14). However, the set of eqs (1.11), (1.12), (1.14) and (1.15) is not complete. The equation that would complement eqs (1.11), (1.12), (1.14) and (1.15) is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \underline{r}\rangle = \frac{1}{m}\langle \underline{p}\rangle. \tag{1.16}$$

Derivation of (1.16) is not given in ref. [2].

In non-relativistic quantum mechanics, eq. (1.16) is known as the second Ehrenfest theorem. The first Ehrenfest theorem relates the time change in momentum of the wave packet and the gradient of the external potential fields

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \underline{p}\rangle = -\langle \underline{\nabla} U\rangle \tag{1.17}$$

(see ref. [3]). The purpose of this work is to derive eq. (1.16) from the Klein–Gordon equation and in this way the classical limit of the Klein–Gordon equation can be given with a complete set of equations, which means with eqs (1.11), (1.12), (1.14), (1.15) and (1.17).

Section 2 gives useful elements of the Klein–Gordon theory for static external fields. Considerations in §2 yield equations that are used in §3 where eq. (1.17) is derived.

2. Equations for static external fields

In this work we assume that wave function ψ has the form of a small wave packet. The external field is assumed to be static and the energy of the particle is always larger than the potential energy.

$$E - e\phi > 0. \tag{2.1}$$

As stated in ref. [4] and also mathematically shown in ref. [2], for external fields where condition (2.1) is satisfied, the Klein–Gordon particle probability density does not vary its sign and hence the Klein–Gordon equation with a single component wave function ψ can be successfully applied to describe physical problems (see eq. (1.5) and the paragraph that follows this equation).

For static fields the wave function, or the wave packet, that satisfies eq. (1.13) can be written as a superposition of wave functions ψ_i'

$$\psi = \sum_i \psi_i' = \sum_i c_i \psi_i \exp\left(-\frac{i}{\hbar} E_i t\right), \tag{2.2}$$

where c_i are constants and functions ψ_i satisfy the Klein–Gordon equation for the stationary states

$$(E_i - e\phi)^2 \, \psi_i = -\hbar^2 c^2 \Delta \psi_i + m_0^2 c^4 \psi_i. \tag{2.3}$$

Obviously, each of the wave function

$$\psi_i' = c_i \psi_i \, \exp\left(-\frac{i}{\hbar} E_i t\right)$$

has to satisfy eq. (1.13). Therefore it is possible to write

$$\left(i\hbar \frac{\partial}{\partial t} - e\phi\right)^2 \psi_i' = -\hbar^2 c^2 \Delta \psi_i' + m_0^2 c^4 \psi_i'. \tag{2.4}$$

Since the external fields are static, eq. (2.4) can also be rewritten as

$$\left(i\hbar \frac{\partial}{\partial t} - e\phi\right) (E_i - e\phi) \, \psi_i' = -\hbar^2 c^2 \Delta \psi_i' + m_0^2 c^4 \psi_i'. \tag{2.5}$$

For a narrow wave packet the energies E_i are close to each other. For this reason, each E_i can be approximated as $\langle E \rangle$, where $\langle E \rangle$ is the mean value of all energies E_i, i,e.,

$$\langle E \rangle = \sum_i c_i^2 E_i. \tag{2.6}$$

Equation (2.6) assumes that functions ψ_i are normalized and factors c_i satisfy the condition

$$\sum_i c_i^2 = 1.$$

So we can write the approximation

$$E_i = \langle E \rangle \, . \tag{2.7}$$

Approximation (2.7) is used in eq. (2.5), and then this equation can be turned into

$$i\hbar \frac{\partial}{\partial t} \psi_i' = (\langle E \rangle - e\phi)^{-1} (-\hbar^2 c^2) \Delta \psi_i' + (\langle E \rangle - e\phi)^{-1} m_0^2 c^4 \psi_i' + e\phi \psi_i'. \tag{2.8}$$

Equation (2.8) is now summed and then eq. (2.2) is considered. This gives equation

$$i\hbar \frac{\partial}{\partial t} \psi = (\langle E \rangle - e\phi)^{-1} \, (-\hbar^2 c^2) \Delta \psi + (\langle E \rangle - e\phi)^{-1} \, m_0^2 c^4 \psi + e\phi \psi. \tag{2.9}$$

Equation (2.9) and its conjugate, namely

$$-i\hbar\frac{\partial}{\partial t}\psi^* = (\langle E\rangle - e\phi)^{-1}(-\hbar^2c^2)\Delta\psi^* + (\langle E\rangle - e\phi)^{-1} m_0^2c^4\psi^* + e\phi\psi^* \tag{2.10}$$

will be used for deriving eq. (1.5).

3. Time derivative of the position of wave packet

In this section we turn to one-dimensional formulae because integration per parts will be used. With respect to eq. (1.6) the mean value of a physical quantity A is defined using the formula

$$\langle A\rangle = -\int_{-\infty}^{\infty}\psi^{-1}\rho\hat{A}\psi\,\mathrm{d}x. \tag{3.1}$$

Equation (3.1) was suggested and used in ref. [2] to derive eqs (1.1)–(1.4). In ref. [2] it is shown that (3.1) can also be written as

$$\langle A\rangle = -\int_{-\infty}^{\infty}(\langle E\rangle - e\phi)\,\psi^*\hat{A}\psi\,\mathrm{d}x, \tag{3.2}$$

(see eqs (1.7) and (1.8) for three dimensions). Considering (3.2) the mean value of the wave packet coordinate can be changed as

$$\langle x\rangle = \int_{-\infty}^{\infty}(\langle E\rangle - e\phi)\,\psi^* x\psi\,\mathrm{d}x. \tag{3.3}$$

The time derivative of eq. (3.3) is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}(\langle E\rangle - e\phi)\psi^* x\psi\,\mathrm{d}x\\ &= \int_{-\infty}^{\infty}(\langle E\rangle - e\phi)\left(\frac{\partial\psi^*}{\partial t}x\psi + \psi^* x\frac{\partial\psi}{\partial t}\right)\mathrm{d}x.\end{aligned} \tag{3.4}$$

When eqs (2.9) and (2.10) are applied in eq. (3.4), eq. (3.4) changes to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \int_{-\infty}^{\infty} i\hbar c^2\left(\psi^* x\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi^*}{\partial x^2}x\psi\right)\mathrm{d}x. \tag{3.5}$$

The right-hand side of eq. (3.5) can be rearranged as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \int_{-\infty}^{\infty} i\hbar c^2\left(\psi^*\frac{\partial^2(x\psi)}{\partial x^2} - \frac{\partial^2\psi^*}{\partial x^2}x\psi\right)\mathrm{d}x - \int_{-\infty}^{\infty} i\hbar c^2\psi^*\frac{\partial\psi}{\partial x}\mathrm{d}x. \tag{3.6}$$

To continue with eq. (3.6) we use the identity

$$\psi^*\frac{\partial^2(x\psi)}{\partial x^2} - \frac{\partial^2\psi^*}{\partial x^2}(x\psi) = \frac{\partial}{\partial x}\left[\psi^*\frac{\partial(x\psi)}{\partial x} - \frac{\partial\psi^*}{\partial x}(x\psi)\right]. \tag{3.7}$$

When eq. (3.7) is used in the first integral in eq. (3.6), this integral becomes zero. Hence eq. (3.6) reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \int_{-\infty}^{\infty} c^2\psi^*(-i\hbar)\frac{\partial\psi}{\partial x}\mathrm{d}x. \tag{3.8}$$

The integrand in (3.8) can be amended and then written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \int_{-\infty}^{\infty} (\langle E\rangle - e\phi(\langle x\rangle))\frac{c^2}{(\langle E\rangle - e\phi(\langle x\rangle))}\psi^*(-i\hbar)\frac{\partial\psi}{\partial x}\mathrm{d}x. \tag{3.9}$$

It is useful that the first fraction in the right-hand side of (3.9) is taken to the front of the integral sign

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{c^2}{(\langle E\rangle - e\phi\,(\langle x\rangle))}\int_{-\infty}^{\infty} (\langle E\rangle - e\phi\,(\langle x\rangle))\,\psi^*(-i\hbar)\frac{\partial\psi}{\partial x}\mathrm{d}x. \tag{3.10}$$

Assuming that the wave packet is small allows that within the wave packet x coordinate can be approximated as $\langle x\rangle$. This also means that in the integral in (3.10) the wave packet centroid $\langle x\rangle$ can be approximated as x. Looking now at eq. (1.10) we see that the integral in the right-hand side of eq. (3.10) stands for the mean value of momentum. Therefore for one dimension we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{c^2}{(\langle E\rangle - e\phi\,(\langle x\rangle))}\langle p_x\rangle\,, \tag{3.11}$$

where $\langle p_x\rangle$ denotes the momentum of the wave packet along the x coordinate. To go on with (3.11) we apply eqs (1.11) and (1.12) in eq. (1.14). Then eqs (1.14) and (1.15) give the relation

$$E - e\phi\,(\langle x\rangle) = \frac{m_0c^2}{\sqrt{1-(\langle v_x\rangle c)^2}}, \tag{3.12}$$

where $\langle v_x\rangle$ denotes the velocity of the wave packet along the x coordinate. With respect to the special relativity theory, we can introduce the mass of the wave packet using the formula

$$m = \frac{m_0}{\sqrt{1-(\langle v_x\rangle c)^2}} \tag{3.13}$$

Equations (3.12) and (3.13) applied in (3.11) give the relation

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{1}{m}\langle p_x\rangle\,, \tag{3.14}$$

which is the second Ehrenfest theorem that was now derived from the Klein–Gordon equation. Equation (3.14) generalized to three dimensions becomes eq. (1.16).

4. Conclusions

The difference between eqs (3.14) and (1.16) is that eq. (1.16) was derived from the Schroedinger equation without neglecting anything, but eq. (3.14) was derived by assuming a small relativistic wave packet that is moving in static external fields. It is quite possible that the Klein–Gordon equation can yield the mean value theorems (1.11), (1.12), (1.14), (1.15) and (3.14) for a general case. However, such an achievement would require techniques that allow transition from the second partial time derivatives to the first partial time derivative of the wave function. Such an approach has not yet been found.

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