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Semi-classical limit of relativistic quantum mechanics

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Abstract. It is shown that the semi-classical limit of solutions to the Klein–Gordon equation gives the particle probability density that is in direct proportion to the inverse of the particle velocity. It is also shown that in the case of the Dirac equation a different result is obtained.

Keywords. Quasi-classical limit; Schroedinger equation; Klein–Gordon equation; Dirac equation.

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1. Introduction

The semi-classical limit of the relativistic quantum mechanics can be introduced in the same way as the semi-classical limit of solutions to the Schroedinger equation. The purpose of this report is to consider one-dimensional stationary states and show the properties of the semi-classical limit of solutions to the Klein–Gordon and Dirac equations.

2. Partitioning the Klein–Gordon equation

Substitution

$$\psi = R\exp(i\theta/\hbar), \tag{1}$$

where R and θ are real, is used in the Klein–Gordon equation

$$\left(i\hbar\frac{\partial}{\partial t} - e\phi\right)^2 \psi = c^2\left(-i\hbar\underline{\nabla} - \frac{e}{c}\underline{A}\right)^2 \psi + m_0^2 c^4 \psi. \tag{2}$$

In this way eq. (2) is partitioned into equations

$$c^2\left(\underline{\nabla}\theta - \frac{e}{c}\underline{A}\right)^2 - \left(\frac{\partial\theta}{\partial t} + e\phi\right)^2 + m_0^2c^4 - c^2\hbar^2\frac{1}{R}\Delta R + \hbar^2\frac{1}{R}\frac{\partial^2 R}{\partial t^2} = 0 \tag{3}$$

and

$$c^2R\Delta\theta - R\frac{\partial^2\theta}{\partial t^2} + 2c^2\nabla R\cdot\nabla\theta - 2\frac{\partial R}{\partial t}\frac{\partial\theta}{\partial t} - 2e\phi\frac{\partial R}{\partial t} = 0. \tag{4}$$

Equation (3) is the relativistic Hamilton–Jacobi equation with two additional quantum terms. Equation (4) is a relativistic continuity equation.

For a stationary state substitution (1) can be also written as

$$\psi = R\exp(-iEt/\hbar)\exp(i\theta^*/\hbar), \tag{5}$$

where $\theta = -Et + \theta^*$. In substitution (5) constant E and functions θ^* and R are real and do not depend on time. This allows equation

$$-\partial\theta/\partial t = E. \tag{6}$$

3. Semi-classical limit of the Klein–Gordon equation – Unbound states

Wave function (5) can describe both unbound and bound stationary states. In the case of unbound stationary states the energy of the particle E and the external potential ϕ satisfy condition $E - e\phi > 0$, and R and θ^* are non-sinusoidal functions of x. The fact that R does not depend on time, condition (6), condition $\underline{A} = \underline{0}$ and

$$\hbar \to 0 \tag{7}$$

applied in (3) and (4) written for one dimension give equations

$$-(E - e\phi)^2 + c^2\left(\frac{\partial\theta^*}{\partial x}\right)^2 + m_0^2c^4 = 0 \tag{8}$$

and

$$R\frac{\partial^2\theta^*}{\partial x^2} + 2\frac{\partial R}{\partial x}\frac{\partial\theta^*}{\partial x} = 0. \tag{9}$$

Equation (9) can be rearranged as

$$2\frac{\partial R}{R} = -\frac{\partial(\partial\theta^*/\partial x)}{\partial\theta^*/\partial x} \tag{10}$$

and solved for R. This gives formula

$$R^2 = K^{\mathrm{KG}} \frac{1}{|\partial\theta^*/\partial x|}, \tag{11}$$

where $K^{\mathrm{KG}} > 0$ is a constant. $|\partial\theta^*/\partial x|$ can be expressed using (8)

$$\left|\frac{\partial\theta^*}{\partial x}\right| = \frac{1}{c}\sqrt{(E - e\phi)^2 - m_0^2c^4}, \tag{12}$$

and then applied in (11). This yields equation

$$R^2 = \frac{cK^{\mathrm{KG}}}{\sqrt{(E - e\phi)^2 - m_0^2c^4}}. \tag{13}$$

In the Klein–Gordon theory the charge density is defined as

$$\rho_e^{\mathrm{KG}} = \frac{ie\hbar}{2m_0c^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right) - \frac{e^2\phi}{m_0c^2}\psi^*\psi. \tag{14}$$

Substitution (1) and condition (6) applied in (14) reduce (14) to

$$\rho_e^{\mathrm{KG}} = \frac{e}{m_0c^2}R^2(E - e\phi). \tag{15}$$

Since the expression in the brackets in (15) can acquire both positive and negative values, the particle probability density introduced as

$$\rho^{\mathrm{KG}} = \rho_e^{\mathrm{KG}}/e \tag{16}$$

can be defined only for cases where $E - e\phi > 0$. The fact that the particle probability density defined with (16) is meaningful and useful for cases where $E - e\phi > 0$ has been demonstrated by Marx [1] and by the present author [2]. For one-dimensional unbound, or scattering problems $E - e\phi > 0$. Hence it is possible to use the particle probability density defined by (16).

Formula (13) is now used in (15), and that is used in (16) to give

$$\rho^{\mathrm{KG}} = \frac{K^{\mathrm{KG}}(E - e\phi)}{m_0c\sqrt{(E - e\phi)^2 - m_0^2c^4}}. \tag{17}$$

The law of the energy conservation for a relativistic particle in a static potential field can be expressed with equation

$$E = e\phi + \frac{m_0c^2}{\sqrt{1 - v^2/c^2}}, \tag{18}$$

where v is the velocity of the particle. The expression for $1/v$ obtained from (18) is

$$\frac{1}{v} = \frac{1}{c}\frac{(E - e\phi)}{\sqrt{(E - e\phi)^2 - m_0^2c^4}}. \tag{19}$$

Matching (19) with (17) is achieved by putting $K^{\mathrm{KG}} = m_0$.

The derivation of eq. (17) started with eqs (3) and (4). Another way to (17) is to use the Klein–Gordon equation for stationary states

$$(E - e\phi)^2 \psi = -\hbar^2 c^2 \Delta\psi + m_0^2 c^4 \psi. \tag{20}$$

Substitution (5) in (20) partitions (20) into relations

$$(E - e\phi)^2 R = -\hbar^2 c^2 \left(\Delta R - R \left(\frac{1}{\hbar} \nabla\theta^* \right)^2 \right) + m_0^2 c^4 R \tag{21}$$

and

$$2\nabla R \cdot \nabla\theta^* + R\Delta\theta^* = 0. \tag{22}$$

Equations (21) and (22) at condition (7) written for one dimension reduce to (8) and (9). Therefore, eqs (21) and (22) also lead to eqs (13) and (17).

4. Semi-classical limit of the Klein–Gordon equation – Bound states

For bound stationary states we will consider only the region where $E - e\phi > 0$. Outside this region the charge density function reverses its sign. However, this is not a problem because in limit (7) the value of function R^2 outside region $E - e\phi > 0$ and therefore also the charge density (15) rapidly approach zero.

For bound stationary states, R in eq. (5) inside region $E - e\phi > 0$ is a sinusoidal function of x, and θ^* in (5) becomes a constant. Considering this, for one-dimensional bound stationary states we substitute R as

$$R = R_0 \cos\left(\frac{1}{\hbar} \theta_0 \right), \tag{23}$$

where R_0 and θ_0 are real non-sinusoidal functions of x. Substitution (23) is applied in (5). Then (5) and condition $\theta^* =$ const. are applied in (20), which gives equation

$$\begin{aligned}
&(E - e\phi)^2 R_0 \cos\left(\frac{1}{\hbar}\theta_0 \right) \\
&= -\hbar^2 c^2 \left(\frac{\mathrm{d}^2 R_0}{\mathrm{d}x^2} - R_0 \frac{1}{\hbar^2} \left(\frac{\mathrm{d}\theta_0}{\mathrm{d}x} \right)^2 \right) \cos\left(\frac{1}{\hbar}\theta_0 \right) \\
&-\hbar^2 c^2 \left(-2 \frac{\mathrm{d}R_0}{\mathrm{d}x} \frac{1}{\hbar} \frac{\mathrm{d}\theta_0}{\mathrm{d}x} - R_0 \frac{1}{\hbar} \frac{\mathrm{d}^2\theta_0}{\mathrm{d}x^2} \right) \sin\left(\frac{1}{\hbar}\theta_0 \right) + m_0^2 c^4 R_0 \cos\left(\frac{1}{\hbar}\theta_0 \right).
\end{aligned} \tag{24}$$

It is obvious that for the points x where $\cos(\theta_0/\hbar) = 0$, $\sin(\theta_0/\hbar)$ is not zero. Therefore, for those points the expression in (24) that is multiplied by $\sin(\theta_0/\hbar)$ has to be zero. This leads to equation

$$2 \frac{\mathrm{d}R_0}{\mathrm{d}x} \frac{\mathrm{d}\theta_0}{\mathrm{d}x} + R_0 \frac{\mathrm{d}^2\theta_0}{\mathrm{d}x^2} = 0. \tag{25}$$

For the points x in (24) where $\sin(\theta_0/\hbar) = 0$, $\cos(\theta_0/\hbar)$ is not zero, and for those points we get

$$(E - e\phi)^2 R_0 = -c^2 \left(\hbar^2 \frac{\mathrm{d}^2 R_0}{\mathrm{d}x^2} - R_0 \left(\frac{\mathrm{d}\theta_0}{\mathrm{d}x} \right)^2 \right) + m_0^2 c^4 R_0. \tag{26}$$

In limit (7) the number of points where the values of $\cos(\theta_0/\hbar)$ and $\sin(\theta_0/\hbar)$ are zero, increases without restriction and the distance between any two such adjacent points becomes infinitely small. Therefore, in limit (7) functions R_0 and θ_0 have to satisfy both (25) and (26) where the quantum term is neglected. However, eqs (25) and (26) are the same as eqs (9) and (8). Hence (25) and (26) give (13) and (17). Equations (13) and (17) are thus valid for both bound and unbound one-dimensional problems.

5. Semi-classical limit of the Dirac equation

The Dirac equation is a differential equation for a four-component column matrix function $\underline{\psi}$

$$i\hbar \frac{\partial \underline{\psi}}{\partial t} = \left(c\underline{\underline{\alpha}} \cdot \left(-i\hbar \underline{\nabla} - \frac{e}{c} \underline{A} \right) + m_0 c^2 \underline{\underline{\beta}} + e\phi \right) \underline{\psi}. \tag{27}$$

The charge density that follows from (27) is given with expression

$$\rho_e^{\mathrm{Dir}} = e \sum_\mu \psi_\mu^+ \psi_\mu, \tag{28}$$

where $\mu = 1, ..., 4$. The integral of charge density (28) is always of the same sign as e, and for bound stationary problems it is equal to e.

Let us write the coordinate dependent parts of functions ψ_μ as

$$\psi_\mu = R_\mu \exp\left(-\frac{i}{\hbar} Et \right) \exp\left(\frac{i}{\hbar} \theta_\mu^* \right) \tag{29}$$

for one-dimensional scattering problems, or, as

$$\psi_\mu = R_{0\mu} \cos\left(\frac{1}{\hbar} \theta_{0\mu} \right) \exp\left(-\frac{i}{\hbar} Et \right) \exp\left(\frac{i}{\hbar} \theta_\mu^* \right) \tag{30}$$

for one-dimensional bound stationary problems. (Note that functions θ_μ^* in (29) are not constants, but the same functions in (30) are assumed to be constants. Compare this with assumptions about functions in eqs (5) and (23).) Since each function ψ_μ has to satisfy the Klein–Gordon equation, the semi-classical limit of each of the four terms in the right side of (28) will behave as the right side of eq. (13). In this way (28) divided by e gives expression

$$\rho^{\mathrm{Dir}} = \frac{\rho_e^{\mathrm{Dir}}}{e} = \frac{c \sum_\mu K_\mu^{\mathrm{KG}}}{\sqrt{(E - e\phi)^2 - m_0^2 c^4}}. \tag{31}$$

If the dimensions of the physical quantities balance in (17), they cannot balance in (31). Hence (31) has to be corrected. To achieve this, (31) is rewritten as

$$\rho^{\rm Dir} = \frac{\rho_e^{\rm Dir}}{e} = \frac{Dc\sum_\mu K_\mu^{\rm KG}}{\sqrt{(E-e\phi)^2 - m_0^2c^4}}, \tag{32}$$

where the value of D is 1 but its dimensions allow to balance (32).

The right side of eq. (32) does not comply with the right sides of eqs (17) and (19). Therefore, the Dirac particle probability density of one-dimensional stationary problems at condition (7) is not directly proportional to the inverse of the particle velocity.

6. Non-relativistic limit

For velocities smaller than the velocity of light, eqs (17) and (19) should reduce to the corresponding formulae of non-relativistic mechanics.

Classical equivalents of eqs (17) and (19) are equations

$$\rho_{\rm Schr} = R_{\rm Schr}^2 = \frac{K_{\rm Schr}}{\sqrt{2(E_{\rm Class} - U)}} \tag{33}$$

and

$$\frac{1}{v} = \sqrt{\frac{m_0}{2(E_{\rm Class} - U)}}, \tag{34}$$

where the subscript 'Schr' and 'Class' stand for the words 'Schroedinger' and 'classical'. Equation (33) is obtainable from the Schroedinger equation. Equation (34) comes from the law of the energy conservation in classical mechanics

$$E_{\rm Class} - U = \frac{1}{2} m_0 v^2.$$

Equations (17) and (19) reduce into eqs (33) and (34) if we put $U = e\phi$ and $E = m_0c^2 + E_{\rm Class}$ and then neglect both U and $E_{\rm Class}$ with respect to E and m_0c^2.

References

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