Classical Limit of Relativistic Quantum Mechanical Equations in the Foldy-Wouthuysen Representation

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Abstract

It is shown that, under the Wentzel-Kramers-Brillouin approximation conditions, using the Foldy-Wouthuysen representation allows the problem of finding a classical limit of relativistic quantum mechanical equations to be reduced to the replacement of operators in the Hamiltonian and quantum mechanical equations of motion by the respective classical quantities.

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The Foldy-Wouthuysen (FW) representation [1] possesses unique features that make it special in quantum mechanics. Even for relativistic particles in the external field, the operators in this representation are completely analogous to the respective operators of nonrelativistic quantum mechanics. In particular, the operators of position [2] and momentum are \mathbf{r} and $\mathbf{p} = -i\hbar\nabla$, while that of polarization for half-spin particles is expressed by the Dirac matrix $\mathbf{\Pi}$. In other representations these operators are given by much more awkward formulas (see [1, 3]). The simple and well-defined form of operators corresponding to classical observables is a major advantage of FW representation. Note that in this representation the Hamiltonian and all operators are diagonal in two spinors (block-diagonal). The usage of the FW representation eliminates the chance that ambiguities will occur while solving the problem of finding a classical limit of relativistic quantum mechanics [1, 4].

In the nonrelativistic case, a transition to the quasiclassical approximation is relatively easily done using Wentzel-Kramers-Brillouin method (WKB). It can be applied when a de Broglie wavelength is smaller than the characteristic size of the inhomogeneity region of the external field l:

$$\lambda \ll l. \tag{1}$$

For a one-dimensional problem (motion along x axis only) from (1) it follows that the following inequality holds:

$$\left|\frac{d\lambda}{dx}\right| \ll 1. \tag{2}$$

It is also convenient to use the WKB method in the analysis of relativistic quantum mechanical equations. However, in this case it needs to be modified. Like in nonrelativistic quantum mechanics, a classical limit is reached in the zero-order WKB approximation in \hbar . If the FW representation is used, a transition to the quasiclassical approximation is done in the same way as in nonrelativistic quantum mechanics. In the relativistic case, in order to be able to use the WKB method, conditions (1) and (2) must also be satisfied.

To simplify the analysis, let us consider the case of one-dimensional motion. If no spin effects are taken into account, then the equation for relativistic Hamiltonian in the FW representation can be written as follows:

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi, \quad \mathcal{H} = \sqrt{m^2 c^4 + c^2 \mathbf{p}^2 + \mathcal{V}(x, \mathbf{p})} + U(x).$$
 (3)

This form has, in particular, an equation for scalar particles in the electromagnetic field (see [5]). Since the operators p_y, p_z commute with the Hamiltonian and have definite values, the

operator \mathcal{H} can be represented in the form

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi, \quad \mathcal{H} = \sqrt{m^2 c^4 + c^2 p_x^2 + V(x, p_x)} + U(x).$$
 (4)

For stationary states, a usual form for the wave function can be used (see [6, 7]):

$$\Psi = \exp\left(-\frac{i}{\hbar}Et\right)\Phi(x), \quad \Phi(x) = \exp\left(\frac{i}{\hbar}\mathfrak{S}\right), \tag{5}$$

where E is the total energy of a particle. The function \mathfrak{S} can formally be expanded into a series in powers of the Planck constant:

$$\mathfrak{S} = \mathfrak{S}_0 + \frac{\hbar}{i} \mathfrak{S}_1 + \left(\frac{\hbar}{i}\right)^2 \mathfrak{S}_2 + \dots$$
(6)

When substituting the wave function into the initial equation, we limit ourselves by the terms of zero-order approximation. In the latter approximation, the commutators of x and p_x operators proportional to \hbar can be neglected. Since

$$\boldsymbol{p}^{2}\Psi = (\mathfrak{S}^{\prime 2} - i\hbar\mathfrak{S}^{\prime\prime})\Psi, \qquad (7)$$

ignoring the quantities of the first and higher orders in \hbar , we find

$$\sqrt{m^2 c^4 + c^2 p_x^2 + V(x, p_x)} \Psi = \sqrt{m^2 c^4 + c^2 \mathfrak{S}'^2 + V(x, \mathfrak{S}')} \Psi.$$

Thus, the terms of zeroth order in the Planck constant satisfy the following equation:

$$E = \sqrt{m^2 c^4 + c^2 \mathfrak{S}'^2 + V(x, \mathfrak{S}')} + U(x),$$
(8)

which defines an implicit function \mathfrak{S}' of x. It is clear that the quantity \mathfrak{S}' is a classical generalized momentum of a particle $\mathcal{P}(x)$. Therefore,

$$\mathfrak{S} = \int \mathcal{P}(x) dx. \tag{9}$$

Thus, \mathfrak{S} is a time-independent part of the action, while, according to the initial equation (4), the total action of a particle is found to be

$$S = -Et + \mathfrak{S} = -Et + \int \mathcal{P}(x)dx.$$
⁽¹⁰⁾

Formula (10) is completely consistent with the classical theory and coincides with the analogous one deduced for the WKB approximation in nonrelativistic quantum mechanics [6,

7]. Thus, while using the FW representation in relativistic quantum mechanics, a transition to the classical limit corresponds to the zero-order WKB approximation in \hbar . As follows from (4),(8)–(10), this can be done by replacing the operators in the Hamiltonian by the respective classical quantities.

It is easy to show that such a replacement can be carried out in equations of motion as well. Any quantum mechanical Hamiltonian is an operator function of generalized momenta p_i and corresponding coordinates x^i . By neglecting the terms proportional to \hbar , we may not take into account the noncommutativity of operators of dynamical variables and write a total time derivative of the Hamiltonian in the form

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial t} + \frac{\partial\mathcal{H}}{\partial p_i}\frac{dp_i}{dt} + \frac{\partial\mathcal{H}}{\partial x^i}\frac{dx^i}{dt}.$$

Since

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial t},$$

then, in zero-order approximation in \hbar , the operator equations of motion can be represented in a form similar to classical Hamilton equations:

$$\frac{dx^i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x^i}.$$
(11)

The possibility of replacing the operators in the Hamiltonian by respective classical quantities according to (11) leads to that of the same replacement in the operator equations of motion.

There are some peculiarities in applying the WKB method in gravitation theory [8]. However, when using the Hamiltonian approach (see [9–12]), the problem of transiting to the classical limit is simplified and reduced to that considered above. The general form of the classical Hamiltonian of a spinless particle in arbitrary electromagnetic and gravitation fields is determined by Eq. (2.5) given in [13]. It was shown in [12] that, according to the results obtained in [14] and in order to describe particles with spin, it should be complemented by the term $\mathbf{s} \cdot \mathbf{\Omega}$ proportional to the angular velocity of spin rotation $\mathbf{\Omega}$.

The same term is added to the spinless part of the Hamiltonian also to describe spin effects in electromagnetic and weak interactions. Since the Hamiltonian is given in the FW representation, only the upper spinor can be used. In this case the operator s is expressed through the spin matrices for particles with respective spin. For particles with spin s > 1/2, the operator \mathcal{H} may include the products of spin matrices. After carrying out a transition to the classical limit described above, the Hamiltonian of particles with spin contains generalized momenta corresponding coordinates and spin matrices (including their products). In this case, to find spin dynamics, it is very convenient to use the method based on the equation for the matrix Hamiltonian, often called the method of spin amplitudes (see [15] and references therein). A transition to the classical limit is reduced to averaging the spin matrices and their products over amplitude spin functions. Such averaging leads to the introduction of polarization vector \mathbf{P} and tensor P_{ij} , given by the equations (see [15, 16])

$$P_i = \frac{\langle s_i \rangle}{S}, \quad P_{ij} = \frac{3 \langle s_i s_j + s_j s_i \rangle - 2S(S+1)\delta_{ij}}{2S(2S-1)}, \quad i, j = x, y, z.$$
(12)

Here s_i indicates spin matrices and S is a spin quantum number.

It should be taken into account that, in relativistic quantum mechanics, like in nonrelativistic quantum mechanics (see [7]), there are some limitations to the use of this WKB method. The smallness of the discarded term in (7), that contains a higher derivative not always guarantees the smallness of its contribution to the solution for $\mathfrak{S}(x)$. This situation can occur when the field extends to distances greater than the characteristic length l, at which it experiences a noticeable change. A quasiclassical approximation turns then out to be inapplicable in tracing the behavior of the wave function at large distances [7].

Thus, when the conditions of the WKB approximation are satisfied, the usage of the FW representation in most cases allows one to reduce the problem of finding a classical limit of relativistic quantum mechanical equations to the replacement of operators in the Hamiltonian and quantum mechanical equations of motion by the respective classical quantities.

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