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GENERALIZED FOLDY–WOUTHUYSEN TRANSFORMATION AND PSEUDODIFFERENTIAL OPERATORS

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We show that the Foldy–Wouthuysen transformation and its generalizations are simplified if the methods of pseudodifferential operators are used, which also allow estimating the exactness of the transition from the Dirac equation to the reduced equations for electrons and positrons. The methods and techniques used can be useful not only in studying asymptotic solutions of the Dirac equation but also in other problems.

Keywords: Dirac equation, Foldy–Wouthuysen transformation, adiabatic approximation, pseudodifferential operator

1. Diagonalization of the Dirac equation for a free particle

Given the Dirac equation, the Foldy–Wouthuysen transformation [1] allows obtaining nonrelativistic equations of the type of the Pauli equation for the quantum dynamics of electrons and positrons whose kinetic energy is much smaller than mc^2 ($v \ll c$). This transformation is applicable under the assumption that the electric and magnetic fields are small and amounts to a procedure of consecutively applying unitary transformations. There are generalizations of the Foldy–Wouthuysen transformation applicable in a wide range of energies up to relativistic ones (see, e.g., [2]).

To make the subsequent calculations and transformations more transparent, we recall some well-known facts about the Dirac equation [3]. The Dirac equation describes the quantum relativistic motion of electrons and positrons. We assume that the electric and magnetic fields $\boldsymbol{E}$ and $\boldsymbol{H}$ are described by a four-dimensional vector potential $(\mathbf{A}, \Phi)$, $\mathbf{A} = (A_1, A_2, A_3)$. In accordance with the Maxwell equations, the electric and magnetic fields are found from

$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla_x \Phi, \qquad \boldsymbol{H} = \operatorname{rot} \mathbf{A}.$$

The Dirac equation in the coordinate–time space $\mathbb{R}^3_x \times R_t$ has the form

$$i\hbar\frac{\partial \Psi}{\partial t} = \widehat{\mathcal{H}}\Psi, \qquad \widehat{\mathcal{H}} = c\boldsymbol{\alpha}\hat{\boldsymbol{\pi}} + \beta mc^2 + e\Phi, \tag{1.1}$$

where

$$\boldsymbol{\alpha} = \{\alpha_1, \alpha_2, \alpha_3\}, \qquad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix},$$

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$\hat{\boldsymbol{\pi}} = \widehat{\mathbf{p}} - (e/c)\mathbf{A}$, $\widehat{\mathbf{p}} = -i\hbar\nabla_x$, E is the unit 2×2 matrix, $\hbar$, $e < 0$, and m are the Planck constant and the electron charge and mass, and σ_i, $i = 1, 2, 3$, are the standard Pauli matrices satisfying the relations $\sigma_i\sigma_j = \delta_{ij}E + i\varepsilon_{ijk}\sigma_k$, where ε_{ijk} is the totally antisymmetric tensor.

We first assume that the fields $\boldsymbol{E}$ and $\boldsymbol{H}$ are absent, but we keep the potentials in the form of constants $(\mathbf{A}, \Phi)$ in the Dirac equation. We introduce the column vector $\mathbf{p} = (p_1, p_2, p_3)$ consisting of momenta conjugate to the coordinates $\mathbf{x} = (x^1, x^2, x^3)$. Then, using the Fourier transformation with respect to $\mathbf{x}$, we can easily diagonalize the Dirac equation for the Fourier transform $\widetilde{\Psi}(\mathbf{p}, t)$ of the wave function $\Psi(\mathbf{x}, t)$.

The equation for $\widetilde{\Psi}(\mathbf{p}, t)$ has the form

$$i\hbar\frac{\partial\widetilde{\Psi}}{\partial t} = \mathcal{H}\widetilde{\Psi}, \tag{1.2}$$

where $\mathcal{H}(\mathbf{p}, \mathbf{x}) = c\boldsymbol{\alpha}\boldsymbol{\pi} + \beta mc^2 + e\Phi$ and $\boldsymbol{\pi} = \mathbf{p} - (e/c)\mathbf{A}$. The coefficients of the last equation are constants, and diagonalizing it therefore amounts to diagonalizing the self-adjoint matrix $\mathcal{H}$. Its eigenvalues and eigenvectors are well known (see [3]), and we list them, along with the proof, for completeness. We set $\boldsymbol{n} = \boldsymbol{\pi}/|\boldsymbol{\pi}|$, $(\boldsymbol{\sigma}, \boldsymbol{\pi}) = \sigma_1\pi_1 + \sigma_2\pi_2 + \sigma_3\pi_3$, and $(\boldsymbol{\sigma}, \boldsymbol{n}) = \sigma_1 n_1 + \sigma_2 n_2 + \sigma_3 n_3$.

Lemma 1. *Eigenvalues of the matrix $\mathcal{H}$ are smooth functions of the argument $\mathbf{p}$ and are given by*

$$\varepsilon^{\pm}(\boldsymbol{\pi}) = \pm c\sqrt{m^2c^2 + \boldsymbol{\pi}^2} + e\Phi. \tag{1.3}$$

Each of them is doubly degenerate, and the corresponding orthonormalized eigenvectors can be chosen as column vectors of the following 2×4 matrix function that depends smoothly on $\boldsymbol{\pi}$:

$$\chi_0^+ = \xi(\boldsymbol{\pi}) \equiv \begin{pmatrix} C_+E \\ C_-(\boldsymbol{\sigma}, \boldsymbol{n}) \end{pmatrix} \equiv \begin{pmatrix} C_+E \\ \widetilde{C}_-(\boldsymbol{\sigma}, \boldsymbol{\pi})/mc \end{pmatrix}, \qquad \chi_0^- = -i\alpha_2\beta\xi(-\boldsymbol{\pi}), \tag{1.4}$$

where

$$\begin{gathered} C_+(\boldsymbol{\pi}) = \sqrt{\frac{1}{2}\left(1 + \frac{mc}{\sqrt{m^2c^2 + \boldsymbol{\pi}^2}}\right)}, \qquad C_-(\boldsymbol{\pi}) = \sqrt{\frac{1}{2}\left(1 - \frac{mc}{\sqrt{m^2c^2 + \boldsymbol{\pi}^2}}\right)}, \\ \widetilde{C}_-(\boldsymbol{\pi}) = \frac{1}{\sqrt{2}}\sqrt{\frac{m^2c^2}{mc\sqrt{m^2c^2 + \boldsymbol{\pi}^2} + m^2c^2 + \boldsymbol{\pi}^2}} \equiv \frac{mc}{|\boldsymbol{\pi}|}C_-(\boldsymbol{\pi}). \end{gathered} \tag{1.5}$$

The matrices $\chi_0^{\pm}$ satisfy the normalization conditions

$$\chi_0^{\pm *}\chi_0^{\pm} = E, \qquad \chi_0^{\pm *}\chi_0^{\mp} = 0. \tag{1.6}$$

Here and hereafter, the superscript $*$ denotes Hermitian conjugation.

Remark. We give two representations for ξ. Sometimes, it is more convenient to use a formula based on the coefficients C_+ and C_- because ${C_+}^2 + {C_-}^2 = 1$. On the other hand, a formula based on C_+ and $\widetilde{C}_-$ contains objects that depend smoothly on $\boldsymbol{\pi}$ as $\boldsymbol{\pi} \to 0$.

Proof. We represent the eigenvector z of the matrix $\mathcal{H}$ corresponding to an eigenvalue ε as $z = \binom{z_1}{z_2}$, where z_j are two-dimensional vectors. Then the equation $\mathcal{H}z = \lambda z$ can be rewritten as

$$\begin{pmatrix} (mc^2 + e\Phi - \varepsilon)E & c(\boldsymbol{\sigma}, \boldsymbol{\pi}) \\ c(\boldsymbol{\sigma}, \boldsymbol{\pi}) & (-mc^2 + e\Phi - \varepsilon)E \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = 0. \tag{1.7}$$

It follows from the second line in (1.7) that

$$z_2 = \frac{c(\boldsymbol{\sigma}, \boldsymbol{\pi})}{mc^2 - e\Phi + \varepsilon} z_1.$$

We substitute this expression in the first line in (1.7) and take the equality $(\boldsymbol{\sigma}, \boldsymbol{\pi})^2 = \boldsymbol{\pi}^2$ into account to obtain $m^2c^4 + c^2\boldsymbol{\pi}^2 - (\varepsilon - e\Phi)^2 = 0$. This gives the eigenvalues in (1.3) and their double degeneration. To obtain the first matrix in (1.4), we assume that z_1 and z_2 are 2×2 matrices and set $z_1(\boldsymbol{\pi}, \mathbf{x}) = C_+(\boldsymbol{\pi}, \mathbf{x})E$, where $C_+(\boldsymbol{\pi}, \mathbf{x})$ is a normalization constant. From $z^*z = E$, we easily find an equation for $C_+(\boldsymbol{\pi}, \mathbf{x})$,

$$C_+^2\left(1 + \frac{\boldsymbol{\pi}^2}{\left(mc^2 + \sqrt{m^2c^4 + \boldsymbol{\pi}^2}\,\right)^2}\right) = 1.$$

This gives the formula for $\chi_0^+(\boldsymbol{\pi})$. The formula for $\chi_0^-(\boldsymbol{\pi})$ can be obtained via similar calculations, but it is easier to obtain χ_0^- using the *charge conjugation* principle. We return to this principle below. ■

We now construct the smooth 4×4 matrix-valued function

$$U(\mathbf{p}, \mathbf{A}) = (\chi_0^+, \chi_0^-)$$

and introduce two two-dimensional vector functions $\widetilde{\varphi}^+(\mathbf{p}, t)$ and $\widetilde{\varphi}^-(\mathbf{p}, t)$ and the four-dimensional vector function $\widetilde{\varphi} = \begin{pmatrix} \widetilde{\varphi}^+(\mathbf{p},t) \\ \widetilde{\varphi}^-(\mathbf{p},t) \end{pmatrix}$ by setting

$$\widetilde{\Psi} = U(\mathbf{p}, \mathbf{A})\widetilde{\varphi} = \chi_0^+\widetilde{\varphi}^+ + \chi_0^-\widetilde{\varphi}^-. \tag{1.8}$$

We let $\varphi^\pm(\mathbf{x}, t)$ denote the inverse transforms of the functions $\widetilde{\varphi}^\pm(\mathbf{p}, t)$. Returning to the original variables, instead of (1.8), we obtain

$$\Psi(\mathbf{x}, t) = \widehat{U}\varphi = \widehat{\chi}_0^+\varphi^+(\mathbf{x}, t) + \widehat{\chi}_0^-\varphi^-(\mathbf{x}, t), \tag{1.9}$$

where

$$\widehat{U} = U(-i\hbar\nabla_x, \mathbf{A}), \qquad \widehat{\chi}_0^+ = \chi_0^+\left(-i\hbar\nabla_x - \frac{e}{c}\mathbf{A}\right), \qquad \widehat{\chi}_0^- = \chi_0^-\left(-i\hbar\nabla_x - \frac{e}{c}\mathbf{A}\right). \tag{1.10}$$

Corollary. 1. *Let U be the matrix function in* (1.8) *depending smoothly on* $\mathbf{p}$ *and* $\mathbf{A}$. *It diagonalizes Dirac equation* (1.2)*: the functions $\widetilde{\varphi}^+(\mathbf{p}, t)$ and $\widetilde{\varphi}^-(\mathbf{p}, t)$ satisfy the equations*

$$i\hbar\frac{\partial\widetilde{\varphi}^\pm(\mathbf{p}, t)}{\partial t} = \varepsilon^\pm(\boldsymbol{\pi})\widetilde{\varphi}^\pm(\mathbf{p}, t). \tag{1.11}$$

2. *The operator $\widehat{U} = U(-i\hbar\nabla_x, \mathbf{A})$ is a unitary pseudodifferential operator diagonalizing Dirac equation* (1.1)*: the functions $\varphi^+(\mathbf{x}, t)$ and $\varphi^-(\mathbf{x}, t)$ satisfy the system of pseudodifferential equations*

$$i\hbar\frac{\partial\varphi^\pm(\mathbf{x}, t)}{\partial t} = \hat{L}^\pm\varphi^\pm(\mathbf{x}, t), \tag{1.12}$$

where $\hat{L}^\pm = \varepsilon^\pm\big(-i\hbar\nabla_x - (e/c)\mathbf{A}\big)$.

The vector functions $\varphi^+(\mathbf{x}, t)$ and $\varphi^-(\mathbf{x}, t)$ in (1.9) respectively describe the quantum motion of an electron and a positron. In the nonrelativistic case, $|\boldsymbol{\pi}| \ll mc^2$. Keeping two terms of $\varepsilon^\pm(\boldsymbol{\pi})$ in the expansion in $\boldsymbol{\pi}$, we have

$$i\hbar\frac{\partial\widetilde{\psi}^\pm(\mathbf{p}, t)}{\partial t} = \left(\pm\frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + e\Phi\right)\widetilde{\psi}^\pm(\mathbf{p}, t), \tag{1.13}$$

where

$$\widetilde{\varphi}^{\pm}(\mathbf{p},t)=\exp\biggl(\mp it\frac{mc^2}{\hbar}\biggr)\widetilde{\psi}^{\pm}(\mathbf{p},t).$$

The Fourier transforms $\psi^{\pm}(\mathbf{x},t)$ satisfy the Schrödinger equations

$$i\hbar\frac{\partial\psi^{\pm}(\mathbf{x},t)}{\partial t}=\biggl(\pm\frac{1}{2m}\biggl(-i\hbar\nabla_x-\frac{e}{c}\mathbf{A}\biggr)^2+e\Phi\biggr)\psi^{\pm}(\mathbf{x},t). \tag{1.14}$$

The plus sign corresponds to the electron, and the minus sign corresponds to the positron. It is clear that these last equations follow by quantization of $\boldsymbol{\pi}$.

2. A pseudodifferential ansatz for the generalized Foldy–Wouthuysen transformation

The Foldy–Wouthuysen transformation is an analogue of the above calculations in the presence of weak electric and magnetic fields. We introduce the characteristic parameters: the Compton wavelength $\lambda_{\mathrm{c}}=\hbar/(mc)$ and the energy mc^2. We assume that the electric and magnetic fields $\boldsymbol{E}$ and $\boldsymbol{H}$ satisfy the estimates

$$\biggl|\frac{e\lambda_{\mathrm{c}}\boldsymbol{E}}{mc^2}\biggr|\ll 1,\qquad \biggl|\frac{e\lambda_{\mathrm{c}}\boldsymbol{H}}{mc^2}\biggr|\ll 1.$$

These inequalities mean that the potentials $\mathbf{A}$ and Φ vary slowly in both the time t and the spatial variables $\mathbf{x}$. For greater rigor, we introduce the spatial scale l_0, the characteristic time $T=(l_0/\lambda_{\mathrm{c}})\omega_{\mathrm{c}}^{-1}$, and the small "adiabatic" parameter $\mu=\lambda_{\mathrm{c}}/l_0\ll 1$. We write $\mathbf{A}=\mathbf{A}(\mathbf{x}/l_0,t/T)$ and $\Phi=\Phi(\mathbf{x}/l_0,t/T)$ and assume that $\mathbf{A}(\mathbf{x}',t')$ and $\Phi(\mathbf{x}',t')$ are smooth functions of the arguments $\mathbf{x}'$ and t'. We pass to the dimensionless variables $\mathbf{x}'=\mathbf{x}/L$ and $t'=t/T$ and to the potentials $e'\Phi'=e\Phi/(mc^2)$ and $e'\mathbf{A}'=e\mathbf{A}/(mc^2)$, where $e'=e/|e|=\pm 1$, and divide Eq. (1.1) by mc^2. For simplicity of notation, we omit the prime and finally obtain the Dirac equation in the form

$$i\mu\frac{\partial}{\partial t}\Psi=\mathcal{H}(-i\mu\nabla_x,\mathbf{x})\Psi,\qquad \mathcal{H}=\boldsymbol{\alpha}(-i\mu\nabla_x-e\mathbf{A})+\beta+e\Phi. \tag{2.1}$$

Similar replacements are made in formulas (1.3)–(1.5), which are formally equivalent to setting $m=c=1$ and replacing the operator $-i\hbar\nabla_x$ with the operator $-i\mu\nabla_x$.

Our aim is to construct a unitary transformation (operator) $\widehat{U}$ of Eq. (1.1), bringing this equation to Eqs. (1.12) for the two-dimensional vector functions $\varphi^{+}(\mathbf{x},t)$ and $\varphi^{-}(\mathbf{x},t)$. This cannot be done exactly, as a rule. Foldy and Wouthuysen proposed to represent this procedure as a sequence of unitary transformations that are both approximate in the (small) parameter μ and assume the smallness of the long-momentum operator $\hat{\boldsymbol{\pi}}$. The calculations in [1] and in many other papers (see [2] and the references therein) are quite cumbersome. Here, we intend to show that using pseudodifferential operators and the operator method [4] developed for adiabatic problems [5], [6] allows obtaining more general formulas for the expansion of both the operator $\widehat{U}$ and the operators L without assuming the smallness of $\hat{\boldsymbol{\pi}}$. In the course of these calculations, it is convenient to use the *principle of charge conjugation* (see [3] and the calculations below), which allows investigating only the electron part of the operator $\widehat{U}$, i.e., the operator $\widehat{\chi}^{+}$ and Eq. (1.12) for the function $\varphi^{+}(\mathbf{x},t)$. The second part of $\widehat{U}$ and the function $\varphi^{-}(\mathbf{x},t)$ then follow from calculations for the electron by the replacements $\hat{\boldsymbol{\pi}}\to-\hat{\boldsymbol{\pi}}$ and $e\to -e$ and complex conjugation of some of the functions.

The aim of our investigation below can be formulated as follows: we seek some "electron solution" of Eq. (2.1) in the form [5], [6]

$$\Psi=\widehat{\chi}\varphi^{\pm}(\mathbf{x},t) \tag{2.2}$$

assuming that the function $\varphi^{\pm}(\mathbf{x}, t)$ satisfies Eq. (2.2), which in the dimensionless variables becomes

$$i\mu \frac{\partial \varphi^{\pm}(\mathbf{x}, t)}{\partial t} = \hat{L}^{\pm} \varphi^{\pm}(\mathbf{x}, t). \tag{2.3}$$

Here, $\widehat{\chi}^{\pm}$ and $\hat{L}^{\pm}$ are μ-pseudodifferential operators, i.e., functions of the operators $\widehat{\mathbf{p}} = -i\mu\nabla_x$ and $\mathbf{x}$. The operators $\widehat{\chi}^{\pm}$ can be said to be *intertwining* or *restoring*, and the operators $\hat{L}^{\pm}$ are related to the well-known *Peierls substitution* (see [7]).

We make an important remark. The operators $\widehat{\mathbf{p}} = -i\mu\nabla_x$ and $\mathbf{x}$ do not commute, and the construction of functions of the operators is not unique, being dependent on the chosen ordering of the operators. Two ways of ordering (or "quantization") are used much more frequently than the others. In the first case, which can naturally be called the Feynman–Maslov ordering, we have

$$\widehat{\chi}^{\pm} = \chi^{\pm}\Big(\overset{1}{\widehat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, t, \mu\Big), \qquad \hat{L}^{\pm} = L^{\pm}\Big(\overset{1}{\widehat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, t, \mu\Big), \qquad \widehat{\mathbf{p}} = -i\mu\nabla_x, \tag{2.4}$$

with the smooth symbols $\chi(\mathbf{p}, \mathbf{x}, t, \mu)$ and $L(\mathbf{p}, \mathbf{x}, t, \mu)$ admitting the asymptotic expansions

$$\begin{aligned} &\chi^{\pm}(\mathbf{p}, \mathbf{x}, t, \mu) = \chi_0^{\pm}(\mathbf{p}, \mathbf{x}, t) + \mu\chi_1^{\pm}(\mathbf{p}, \mathbf{x}, t) + \mu^2\chi_2^{\pm}(\mathbf{p}, \mathbf{x}, t) + \dots, \\ &L^{\pm} = L_0^{\pm}(\mathbf{p}, \mathbf{x}, t) + \mu L_1^{\pm}(\mathbf{p}, \mathbf{x}, t) + \mu^2 L_2^{\pm}(\mathbf{p}, \mathbf{x}, t) + \dots. \end{aligned} \tag{2.5}$$

Following Feynman, the numbers over operators denote the order of action of these operators (see [4]). The second case corresponds to the Weyl quantization, and we have

$$\widehat{\chi}^{\pm} = \chi_{\mathrm{W}}^{\pm}\Bigg(\frac{\overset{1}{\widehat{\mathbf{p}}} + \overset{3}{\widehat{\mathbf{p}}}}{2}, \overset{2}{\mathbf{x}}, t, \mu\Bigg), \qquad \hat{L}^{\pm} = L_{\mathrm{W}}^{\pm}\Bigg(\frac{\overset{1}{\widehat{\mathbf{p}}} + \overset{3}{\widehat{\mathbf{p}}}}{2}, \overset{2}{\mathbf{x}}, t, \mu\Bigg), \qquad \widehat{\mathbf{p}} = -i\mu\nabla_x, \tag{2.6}$$

with the Weyl symbols $\chi_{\mathrm{W}}(\mathbf{p}, \mathbf{x}, t, \mu)$ and $L_{\mathrm{W}}(\mathbf{p}, \mathbf{x}, \mu)$, which have asymptotic expansions similar to (2.5). We emphasize that the operators in (2.4) and (2.6) are the same, but their symbols generally differ because of the different ways of ordering (quantizing) the action of $\widehat{\mathbf{p}} = -i\mu\nabla_x$ and $\mathbf{x}$. From the theoretical standpoint, the Weyl quantization is more convenient because it, at least, automatically gives symmetric operators $\hat{L}^{\pm}$ if the equality $L^* = L$ holds. But our experience in solving numerous problems shows that the Feynman–Maslov ordering is much more convenient from the practical standpoint in the sense of obtaining explicit final formulas. It is valid to say that the pragmatic way to act is first to find symbols corresponding to the operators (the coefficients of their asymptotic expansions) based on the Feynman–Maslov ordering and then to pass to pseudodifferential operators based on the Weyl ordering. We give the corresponding recalculation formula based on "self-action inside a pseudodifferential operator."

Specifically, we define the function $b(\mathbf{p}, \mathbf{x}, \mu, \gamma) = a(\mathbf{p} - i\gamma\mu\nabla_x, \mathbf{x}, \mu)$, $\gamma \in \mathbb{R}$, using the formula

$$b(\mathbf{p}, \mathbf{x}, \mu, \gamma) = a\Big(\mathbf{p} - i\gamma\mu\ \mu\overset{2}{\nabla}_x, \overset{1}{\mathbf{x}}, \mu\Big)1.$$

For example, if $a(\mathbf{p}, \mathbf{x}) = \mathbf{p}^2 g(\mathbf{x})$, $x \in \mathbb{R}$, then

$$\left(\mathbf{p} - i\gamma\mu\frac{\partial}{\partial x}\right)^2 g(\mathbf{x}) = \mathbf{p}^2 g - 2i\gamma\mu\frac{\partial g}{\partial x} - \gamma^2\mu^2\frac{\partial^2 g}{\partial x^2}.$$

Let $\hat{L} = L\Big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, \mu\Big)$ be the pseudodifferential operator with the symbol $L(\mathbf{p}, \mathbf{x}, \mu)$. Then the Weyl symbol $L_{\mathrm{W}}(\mathbf{p}, \mathbf{x}, \mu)$ of this operator is related to $L(\mathbf{p}, \mathbf{x}, \mu)$ as [4]

$$L_{\mathrm{W}}(\mathbf{p}, \mathbf{x}, \mu) = L\left(\mathbf{p} + \frac{i\mu}{2}\nabla_x, \mathbf{x}, \mu\right) = \text{(at least, formally)} =$$
$$= \sum_{|\nu|=0}^{\infty} \frac{1}{\nu!}\left(\frac{-i\mu}{2}\right)^{|\nu|} \frac{\partial^{2|\nu|} L}{\partial x^\nu \, \partial p^\nu}(\mathbf{p}, \mathbf{x}, \mu). \tag{2.7}$$

We finally note that all the subsequent reasoning, including the Foldy–Wouthuysen transformation, is within the adiabatic approximation, and we believe that the approach we use here is a very convenient realization of it.

3. Equations for symbols of quantum effective Hamiltonians and intertwining operators

3.1. The basic equations. Substituting (2.2) in (2.1) and taking Peierls substitution (2.3) into account, we obtain the equation

$$\left(\widehat{\mathcal{H}}\widehat{\chi}^{\pm} - \widehat{\chi}^{\pm}\hat{L}^{\pm} - i\mu\frac{\partial\widehat{\chi}^{\pm}}{\partial t}\right)\varphi^{\pm} = 0.$$

Obviously, this equation holds for any function $\varphi^{\pm}$ if the operator equality

$$\widehat{\mathcal{H}}\widehat{\chi}^{\pm} - \widehat{\chi}^{\pm}\hat{L}^{\pm} - i\mu\frac{\partial\widehat{\chi}^{\pm}}{\partial t} = 0 \tag{3.1}$$

holds. We now pass from the operator equation to an equation for symbols of the relevant operators:

$$\mathcal{H}\Big(\mathbf{p} - i\mu \overset{1}{\nabla}_x, \overset{2}{\mathbf{x}}, t\Big)\chi^{\pm}(\mathbf{p}, \mathbf{x}, \mu) = \chi^{\pm}\Big(\mathbf{p} - i\mu \overset{1}{\nabla}_x, \overset{2}{\mathbf{x}}, t, \mu\Big)L^{\pm}(\mathbf{p}, \mathbf{x}, \mu) + i\mu\frac{\partial\chi^{\pm}}{\partial t}(\mathbf{p}, \mathbf{x}, t, \mu). \tag{3.2}$$

This equation can be rewritten as

$$\mathcal{H}(\mathbf{p}, \mathbf{x}, t)\chi^{\pm}(\mathbf{p}, \mathbf{x}, t, \mu) - i\mu\alpha\nabla_x\chi^{\pm}(\mathbf{p}, \mathbf{x}, t, \mu) =$$
$$= \chi^{\pm}\Big(\mathbf{p} - i\mu \overset{1}{\nabla}_x, \overset{2}{\mathbf{x}}, t, \mu\Big)L^{\pm}(\mathbf{p}, \mathbf{x}, t, \mu) + i\mu\frac{\partial\chi^{\pm}}{\partial t}(\mathbf{p}, \mathbf{x}, t, \mu). \tag{3.3}$$

Using the Taylor formula,we can at least formally write

$$\chi^{\pm}\Big(\mathbf{p} - i\mu \overset{1}{\nabla}_x, \overset{2}{\mathbf{x}}, t, \mu\Big) = \chi^{\pm}(\mathbf{p}, \mathbf{x}, t, \mu) + \sum_{|\nu|=1}^{\infty} \frac{1}{\nu!}(-i)^{|\nu|}\mu^{|\nu|}\frac{\partial^{|\nu|}\chi^{\pm}}{\partial p^\nu}(\mathbf{p}, \mathbf{x}, t, \mu)\frac{\partial^{|\nu|}}{\partial x^\nu}, \tag{3.4}$$

where $\nu = (\nu_1, \nu_2, \nu_3)$ is a multi-index and, as usual, $|\nu| = \nu_1 + \nu_2 + \nu_3$, $\nu! = \nu_1!\,\nu_2!\,\nu_3!$, and $\partial^{|\nu|}/\partial\mathbf{x}^\nu = \partial^{|\nu|}/\partial x^{1^{\nu_1}}\partial x^{2^{\nu_2}}\partial x^{1^{\nu_3}}$. Substituting this expression and asymptotic expansions (2.5) in (3.3), after equating the coefficients at the different powers of μ to zero, we obtain a linear system of inhomogeneous algebraic equations for the coefficients $\chi_k^{\pm}(\mathbf{p}, \mathbf{x}, t)$ and $L_k^{\pm}(\mathbf{p}, \mathbf{x}, t)$,

$$\mathcal{H}\chi_0^{\pm} - \chi_0^{\pm}L_0^{\pm} = 0, \tag{3.5}$$

$$\mathcal{H}\chi_k^{\pm} - \chi_k^{\pm}L_0^{\pm} = \chi_0^{\pm}L_k^{\pm} + \mathcal{F}_k^{\pm} + i\frac{\partial\chi_{k-1}^{\pm}}{\partial t}, \quad k = 1, 2, \ldots. \tag{3.6}$$

Here, $\mathcal{H} = \boldsymbol{\alpha}\boldsymbol{\pi} + \beta + e\Phi$, $\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}$, and each function $\mathcal{F}_k^\pm$ is a sum consisting of the products $\partial\chi_j^\pm/\partial x^j$ and $(\partial^\nu\chi_j^\pm/\partial p^\nu)(\partial^\nu L_m^\pm/\partial x^\nu)$ labeled by $j = 1,\dots,k-1$. In what follows, we give formulas for $\mathcal{F}_1^\pm$ and $\mathcal{F}_2^\pm$, but we first note that Eq. (3.5) was investigated in Lemma 1. Hence, we find that the eigenvalues of the matrix function $\mathcal{H}$ are given by

$$L_0^\pm = \varepsilon^\pm(\boldsymbol{\pi}) \tag{3.7}$$

and are doubly degenerate. Therefore, the matrices $\chi_k^\pm$ are composed of two four-dimensional column vectors. In particular, the matrices χ_0^+ depend on $\mathbf{p}$ and $\mathbf{x}, t$ through the long momenta $\boldsymbol{\pi}$. To simplify the notation, as above, we write

$$\chi_0^+ = \xi^+(\boldsymbol{\pi}). \tag{3.8}$$

In what follows, the derivatives $\partial\xi^\pm/\partial x^j$ and $\partial\xi^\pm/\partial p_j$ are understood as the expressions

$$\sum_{k=1}^{3}\frac{\partial\xi^\pm}{\partial\pi_k}\frac{\partial\pi_k}{\partial x^j}, \qquad \sum_{k=1}^{3}\frac{\partial\xi^\pm}{\partial\pi_k}.$$

We say that $L_0^+ = \varepsilon^+(\boldsymbol{\pi})$ and $L_0^- = \varepsilon^-(\boldsymbol{\pi})$ are respectively the *electron* and *positron terms* or *effective Hamiltonians.*

It is clear that the coefficients χ_k^+ can be evaluated independently of the χ_k^-. Moreover, it suffices to find the coefficients $L_k^+(\mathbf{p},\mathbf{x},t)$ and χ_k^+. The $L_k^-(\mathbf{p},\mathbf{x},t)$ and χ_k^- can then be expressed in terms of χ_k^+ using the known procedure of charge conjugation (see, e.g., [3]). We temporarily include the electron charge (parameter) e in the arguments of the functions $L^\pm$ and $\chi^\pm$ and write $L^\pm = L^\pm(\mathbf{p},\mathbf{x},t,\mu,e)$ and $\chi^\pm = \chi^\pm(\mathbf{p},\mathbf{x},t,\mu,e)$.

Lemma 2. *Let $L^+(\mathbf{p},\mathbf{x},t,\mu,e)$, $\chi^+(\mathbf{p},\mathbf{x},t,\mu,e)$ be a solution of Eq.* (3.3) *such that $L^+|_{\mu=0} = L_0^+ = \varepsilon^+(\boldsymbol{\pi})$ and $\chi^+|_{\mu=0} = \xi_0^+(\boldsymbol{\pi})$. Then the functions*

$$\begin{aligned}\chi^-(\mathbf{p},\mathbf{x},t,\mu,e) &= -i\alpha_2\beta\overline{\chi^+}(-\mathbf{p},\mathbf{x},t,\mu,-e),\\ L^-(\mathbf{p},\mathbf{x},t,\mu,e) &= -\overline{L^+}(-\mathbf{p},\mathbf{x},t,\mu,-e)\end{aligned} \tag{3.9}$$

are also solutions of Eq. (3.3), *and*

$$L^-|_{\mu=0} = L_0^- = \varepsilon^-(\boldsymbol{\pi}), \qquad \chi^-|_{\mu=0} = \xi_0^-(\boldsymbol{\pi}). \tag{3.10}$$

We note that $-i\alpha_2\beta$ are real-valued matrices.

Proof. We consider Eq. (3.3) corresponding to the plus sign. We take its complex conjugate and multiply by the matrix $-i\alpha_2\beta$ (the factor $-i$ ensures the realness). This yields

$$\begin{aligned}&-i\alpha_2\beta\big(\overline{\boldsymbol{\alpha}}(\mathbf{p} - e\mathbf{A} + i\mu\nabla_x) + \beta + e\Phi\big)\overline{\chi^+}(\mathbf{p},\mathbf{x},t,e,\mu) =\\ &\qquad = -i\alpha_2\beta\overline{\chi^+}(\mathbf{p} + i\mu\nabla_x,\mathbf{x},t,\mu)\overline{L^+}(\mathbf{p},\mathbf{x},t,e,\mu) - i\mu\frac{\partial}{\partial t}(-i\alpha_2\beta\overline{\chi^+})(\mathbf{p},\mathbf{x},t,e,\mu).\end{aligned} \tag{3.11}$$

Using properties of the Pauli matrices σ_j, we obtain the equalities

$$\begin{aligned}&(i\alpha_2\beta)\alpha_1 = -\alpha_1(i\alpha_2\beta), &&(i\alpha_2\beta)\alpha_2 = \alpha_2(i\alpha_2\beta),\\ &i\alpha_2\beta\alpha_3 = -\alpha_3(i\alpha_2\beta), &&(i\alpha_2\beta)\beta = -\beta(i\alpha_2\beta).\end{aligned}$$

With these equalities and the equality $\overline{\boldsymbol{\alpha}} = \{\alpha_1, -\alpha_2, \alpha_2\}$, we can rewrite (3.11) as

$$\boldsymbol{\alpha}\big((-\mathbf{p} + e\mathbf{A} - i\mu\nabla_x) + \beta - e\Phi\big)(-i\alpha_2\beta)\overline{\chi^+}(\mathbf{p}, \mathbf{x}, t, e, \mu) =$$

$$= -(-i\alpha_2\beta)\overline{\chi^+}(\mathbf{p} + i\mu\nabla_x, \mathbf{x}, t, \mu)\overline{L^+}(\mathbf{p}, \mathbf{x}, t, e, \mu) + i\mu\frac{\partial}{\partial t}\big(-(i\alpha_2\beta)\overline{\chi^+}\big)(\mathbf{p}, \mathbf{x}, t, e, \mu). \qquad (3.12)$$

This equation takes form (3.3) after the replacements $\mathbf{p} \to -\mathbf{p}$ and $e \to -e$. Therefore, formulas (3.9) also give solutions (3.3). Setting $\mu = 0$, we obtain (3.10). ■

Lemma 2 states that it suffices to find the coefficients χ_k^+ and L_k^+ in (2.5), and χ_k^- and L_k^- can then be found using (3.9).

We give explicit formulas for $\mathcal{F}_1^+$ and $\mathcal{F}_2^+$:

$$\mathcal{F}_1^+ = i\sum_{j=1}^{3}\bigg(\frac{\partial\mathcal{H}}{\partial p^j}\frac{\partial\xi^+}{\partial x^j} - \frac{\partial\varepsilon^+}{\partial x^j}\frac{\partial\xi^+}{\partial p^j}\bigg), \qquad (3.13)$$

$$\mathcal{F}_2^+ = i\sum_{j=1}^{3}\bigg(\frac{\partial\mathcal{H}}{\partial p^j}\frac{\partial\chi_1^+}{\partial x^j} - \frac{\partial\varepsilon^+}{\partial x^j}\frac{\partial\chi_1^+}{\partial p^j}\bigg) -$$

$$- i\sum_{j=1}^{3}\frac{\partial\xi^+}{\partial p^j}\frac{\partial L_1^+}{\partial x^j} + \chi_1^+ L_1^+ - \sum_{|\nu|=2}\frac{1}{\nu!}\frac{\partial^2\xi^+}{\partial p^\nu}\frac{\partial^2\varepsilon^+}{\partial x^\nu}. \qquad (3.14)$$

Remark. We already noted that calculations based on the Weyl ordering can be technically much more involved. We illustrate this with the example of an equation for the symbols of the operators $\widehat{\chi}^\pm$ and $\hat{L}^\pm$ based on Weyl ordering (2.6). In this case, passing from the operator equation to the equation for symbols results in

$$\bigg[\boldsymbol{\alpha}\bigg(\mathbf{p} - \frac{i\mu}{2}\nabla_x - e\mathbf{A}\bigg(\mathbf{x} + \frac{i\mu}{2}\nabla_p, t\bigg)\bigg) + \beta + e\Phi\bigg(\mathbf{x} + \frac{i\mu}{2}\nabla_p\bigg)\bigg]\chi_{\mathrm{W}}^\pm(\mathbf{p}, \mathbf{x}, \mu) =$$

$$= \chi_{\mathrm{W}}^\pm\bigg(\mathbf{p} - \frac{i\mu}{2}\nabla_x, \mathbf{x} + \frac{i\mu}{2}\nabla_p, \mu\bigg)L_{\mathrm{W}}^\pm(\mathbf{p}, \mathbf{x}, \mu) + i\mu\frac{\partial\chi_{\mathrm{W}}^\pm}{\partial t}(\mathbf{p}, \mathbf{x}, \mu).$$

To obtain an equation for the coefficients of the decomposition of the symbols $\chi_{\mathrm{W}}^\pm$ and $L_{\mathrm{W}}^\pm$, we must use the Taylor formula with respect to the parameter μ (formally at least) for $\mathbf{A}(\mathbf{x}+(i\mu/2)\nabla_p, t)$, $\Phi(\mathbf{x}+(i\mu/2)\nabla_p, t)$, and $\chi^\pm(\mathbf{p} - (i\mu/2)\nabla_x, \mathbf{x} + (i\mu/2)\nabla_p, t, \mu)$ and then equate the coefficients at the different powers of μ to zero. This again yields a linear system of algebraic inhomogeneous equations for the coefficients of the decompositions of $\chi_k^\pm(\mathbf{p}, \mathbf{x}, \mu)$ and $L_k^\pm(\mathbf{p}, \mathbf{x}, \mu)$ in the parameter μ. The first of the equations in this system is given by (3.5), and the others have structure (3.6) although with much more complicated functions $\mathcal{F}_k^\pm$, because many other derivatives occur along with the $\partial\chi_{\mathrm{W}}^\pm/\partial x^j$ and $(\partial^{|\nu|}\chi_{\mathrm{W}}^\pm/\partial p^\nu)(\partial^{|\nu|}L_{\mathrm{W}}^\pm/\partial x^\nu)$.

3.2. Normalization conditions. The scheme for calculating the coefficients χ_k^+ and L_k^+ using Eq. (3.6) is quite similar to the standard scheme for calculating eigenvectors and eigenvalues in perturbation theory (see, e.g., [8]). Solutions of each equation in (3.6) are not unique, and to reduce the arbitrariness in determining the coefficients χ_k^+ and L_k^+, we can require that the L_2 vector norm of the vector function $\widehat{\chi}^+\varphi^+$ with four components be equal to that of the vector function φ^+ with two components. This gives the equality

$$(\widehat{\chi}^+\varphi^+, \widehat{\chi}^+\varphi^+)_{L_2} = (\varphi^+, \varphi^+)_{L_2}. \qquad (3.15)$$

Using the standard procedure, we "throw over" one of the pseudodifferential operators $\widehat{\chi}^+$ in the scalar product. This gives

$$(\widehat{\chi}^+\varphi^+, \widehat{\chi}^+\varphi^+)_{L_2} = \big(\varphi^+, (\widehat{\chi}^+)^*\widehat{\chi}^+\varphi^+\big)_{L_2},$$

where $(\widehat{\chi}^+)^*$ is the operator conjugate to $\widehat{\chi}^+$. Equation (3.15) then holds if

$$(\widehat{\chi}^+)^*\widehat{\chi}^+ = E, \tag{3.16}$$

where E is the unit 2×2 matrix (or the identity operator in $\mathbb{R}^2$). Based on the properties of pseudodifferential operators, we can write

$$(\widehat{\chi}^+)^* = \chi^*\Big(\overset{2}{\widehat{\mathbf{p}}}, \overset{1}{\mathbf{x}}, t, \mu\Big),$$

where $\chi^*(\mathbf{p}, \mathbf{x}, \mu)$ denotes the Hermitian-conjugate matrix.

We rewrite operator equality (3.16) for the symbol $\chi(\mathbf{p}, \mathbf{x}, \mu)$. In accordance with [9], we obtain

$$\chi^{+*}\Big(\mathbf{p} - i\mu \overset{2}{\nabla}_x, \overset{1}{\mathbf{x}}, \mu\Big)\chi^+(\mathbf{p}, \mathbf{x}, \mu) = E. \tag{3.17}$$

Using the Taylor decomposition, we can, at least formally, rewrite this as

$$\sum_{|\nu|=0}^{\infty} \frac{(-i\mu)^{|\nu|}}{\nu!}\frac{\partial^{|\nu|}}{\partial x^\nu}\bigg\{\frac{\partial^{|\nu|}\chi^{+*}}{\partial p^\nu}(\mathbf{p}, \mathbf{x}, \mu)\chi^+(\mathbf{p}, \mathbf{x}, \mu)\bigg\} = E. \tag{3.18}$$

Substituting expression (2.5) in this equation, equating the coefficients of like powers of μ, and using (3.7) and (3.16), we obtain the recursive system of equations

$$\chi_0^{+*}(\mathbf{p}, \mathbf{x})\chi_0^+(\mathbf{p}, \mathbf{x}) \equiv \xi^{+*}(\boldsymbol{\pi})\xi^+(\boldsymbol{\pi}) = E, \tag{3.19}$$

$$\xi^{+*}(\boldsymbol{\pi})\chi_j^+(\mathbf{p}, \mathbf{x}) + \chi_j^{+*}(\mathbf{p}, \mathbf{x})\xi^+(\boldsymbol{\pi}) = f_j. \tag{3.20}$$

The functions f_j are the products of the functions $\chi_0^+, \dots, \chi_{j-1}^+$ and their derivatives. In particular,

$$f_1 = i\sum_{j=1}^{3}\frac{\partial}{\partial x^j}\bigg(\frac{\partial \xi^{+*}}{\partial p^j}\xi^+\bigg). \tag{3.21}$$

3.3. The scheme for calculating $\boldsymbol{L_j}$ and $\boldsymbol{\xi_j}$. Equation (3.19) is satisfied by virtue of Eqs. (3.7) and (1.6) and the normalization conditions for $\xi^\pm(\boldsymbol{\pi})$.

We now describe the scheme for calculating the coefficients χ_j^+ and L_j^+. The column vectors of the matrices ξ^+ and ξ^- constitute a basis in the four-dimensional Euclidean space, and we therefore have

$$\chi_j^+ = \xi^+ g_j^+(\mathbf{p}, \mathbf{x}, t) + \xi^- g_j^-(\mathbf{p}, \mathbf{x}, t) \tag{3.22}$$

for all χ_j^+, where $g^\pm(\mathbf{p}, \mathbf{x}, t)$ are smooth 2×2 matrix-valued functions. Substituting (3.22) in (3.6) and (3.20) and using the equalities $\xi^{\pm *}\xi^\pm = E$ and $\xi^{\pm *}\xi^\mp = 0$, we obtain

$$(\varepsilon^- - \varepsilon^+)\xi^- g_j^- = \xi^+ L_j^+ + \mathcal{F}_j^+ + i\frac{\partial \chi_{j-1}^+}{\partial t}, \tag{3.23}$$

$$\xi^{+*}\xi^+ g_j^+ + g_j^{+*}\xi_j^{+*}\xi^+ = f_j \Longleftrightarrow g_j^+ + g_j^{+*} = f_j. \tag{3.24}$$

Equations (3.23) are solvable if and only if their right-hand sides are orthogonal to the column vectors of the matrix xi^+. This immediately gives

$$L_j^+ = -\xi^{+*}\mathcal{F}_j^+ - i\xi^{+*}\frac{\partial \chi_{j-1}^+}{\partial t} \tag{3.25}$$

and

$$g_j^- = -\frac{1}{2\sqrt{1+\boldsymbol{\pi}^2}}\left(\xi^{-*}\mathcal{F}_j^+ + i\xi^{-*}\frac{\partial \chi_{j-1}^+}{\partial t}\right). \tag{3.26}$$

It is clear that Eqs. (3.24) are solvable if and only if $f_j^* = f_j$. For $j = 1$, we have

$$f_1^* = -i\sum_{j=1}^{3}\frac{\partial}{\partial x^j}\left(\xi^{+*}\frac{\partial \xi^+}{\partial p^j}\right) = i\sum_{j=1}^{3}\frac{\partial}{\partial x^j}\left(\frac{\partial \xi^{+*}}{\partial p^j}\xi^+\right) = f_1 \tag{3.27}$$

because

$$\xi^{+*}\frac{\partial \xi^+}{\partial p^j} + \frac{\partial \xi^{+*}}{\partial p^j}\xi^+ = \frac{\partial}{\partial p^j}(\xi^{+*}\xi^+) = 0.$$

For $j \ge 2$, this fact follows from the definition of f_j and Eq. (3.18). We omit the proof.

Solutions of Eq. (3.24) are not unique and can be represented as

$$g_j^+ = \frac{f_j}{2} + v_j,$$

where $v_j(\mathbf{p}, \mathbf{x}, t)$ is a Hermitian smooth antisymmetric 2×2 matrix-valued function, $v_j^* = -v_j$. This nonuniqueness reflects the ambiguity in choosing the operators $\widehat{\chi}^\pm$ and $\hat{L}^\pm$. We can always perform a unitary transformation of the operators $\hat{L}^\pm$. Apart from the simplicity of the final formulas, no mathematical argument for a preferred choice of the v_j exists, in our opinion. At least, we can always set $v_j = 0$ and choose

$$g_j^+ = \frac{f_j}{2}. \tag{3.28}$$

Substituting (3.26) and (3.28) in (3.22), we obtain

$$\begin{aligned}\chi_j^+ &= \frac{1}{2}\xi^+ f_j(\mathbf{p}, \mathbf{x}, t) - \frac{1}{2\sqrt{1+\boldsymbol{\pi}^2}}\xi^-\xi^{-*}\left(\mathcal{F}_j^+ + i\frac{\partial \chi_{j-1}^+}{\partial t}\right)(\mathbf{p}, \mathbf{x}, t) = \\ &= \frac{1}{2}\xi^+ f_j(\mathbf{p}, \mathbf{x}, t) - \frac{1}{2\sqrt{1+\boldsymbol{\pi}^2}}\left(\xi^+ L_k^+ + \mathcal{F}_j^+ + i\frac{\partial \chi_{j-1}^+}{\partial t}\right)(\mathbf{p}, \mathbf{x}, t).\end{aligned} \tag{3.29}$$

Formulas (3.25) and (3.23), together with Lemma 2, give an algorithm for calculating the coefficients (symbols) $L_j^\pm$ and χ_j^+ and the asymptotic decomposition of the operators $\hat{L}^\pm$ and $\widehat{\chi}^\pm$. The problem now is to represent them more explicitly and tractably.

3.4. Arguments regarding the minimal number of terms $L_j^\pm$ and the simplified reduced equations for different solutions. It is not easy to write $L_j^\pm$ in a reasonably simple form in the general case, even for $j = 2$. But it seems that the operators L_j with $j \ge 3$ are typically not very interesting in physical applications. In addition, depending on the behavior of the potentials $\mathbf{A}$ and Φ and additional conditions determining solutions of the reduced equations (and the original Dirac equation), the reduced pseudodifferential equations can themselves be simplified. We illustrate this with the example of a solution of the Cauchy problem for the reduced equation with rapidly oscillating initial data that describes propagation of rapidly oscillating wave packets. Specifically, restricting the electron term and assuming that the potentials $\mathbf{A}$ and Φ are independent of t, we consider the Cauchy problem

$$i\mu\frac{\partial\Phi}{\partial t} = \hat{L}^+\Phi, \qquad \Phi|_{t=0} = a^0(\mathbf{x})e^{iS^0(\mathbf{x})/h} \tag{3.30}$$

in dimensionless variables. Here, the real phase S^0 and the components a_1^0 and a_2^0 of the (complex) vector amplitude a^0 are smooth functions, a^0 has a compact support on which $|\nabla_x S^0|$ is separated from zero, h is a parameter that can take different values μ^κ, and κ is a nonnegative number. For $\kappa > 0$, the original function oscillates but possibly not very strongly, and for $\kappa = 0$, fast oscillations are absent altogether. According to the (multidimensional) WKB method [10], [11], solutions of problem (3.30) are sought in the form

$$\Phi = a(\mathbf{x}, t, h)e^{iS(\mathbf{x},t)/h}, \tag{3.31}$$

where the real phase $S(\mathbf{x}, t)$ and the complex vector amplitude $a(\mathbf{x}, t, h)$ are the new unknown smooth functions and we assume that $a(\mathbf{x}, t)$ is a finitary function with respect to $\mathbf{x}$. Substituting this vector function in Eq. (3.30) and using the formula for commuting a pseudodifferential operator with an exponential [11], we obtain

$$\begin{aligned}\Big(-i\mu\frac{\partial}{\partial t} + \hat{L}^+\Big)\big(a(\mathbf{x}, t)e^{iS(\mathbf{x},t)/h}\big) &= e^{iS(\mathbf{x},t)/h}\bigg[\frac{\mu}{h}S_t a - i\mu\frac{\partial a}{\partial t} + L^+\Big(\frac{\mu}{h}\nabla_x S, \mathbf{x}, t, \mu\Big) - \\ &- i\mu\bigg(\Big\langle\nabla_p L^+\Big(\frac{\mu}{h}\nabla_x S\Big), \nabla_x\Big\rangle a + \frac{1}{2}Q\Big(\frac{\mu}{h}\nabla_x S, \mathbf{x}, t, \mu\Big)\bigg)a + \mu^2\widehat{R}a\bigg].\end{aligned}$$

Here, $\widehat{R} = R\Big((\mu/h)\overset{2}{\nabla}_x S, \overset{2}{\mathbf{x}}, \overset{2}{t}, \overset{1}{\nabla}_x, \mu\Big)$ is the pseudodifferential operator whose action on the function a gives a smooth bounded function if $\mu/h = O(1)$ with $R(\mathbf{p}, \mathbf{x}, t, \xi, \mu)\big|_{\mathbf{p}=0} = 0$, and the components $Q_{jm}(\mathbf{p}, \mathbf{x}, t, \mu)$ of the $2{\times}2$ matrix $Q(\mathbf{p}, \mathbf{x}, t, \mu)$ are defined by

$$Q_{jm} = \operatorname{tr}\bigg(\frac{\partial^2 L_{jm}(\mathbf{p}, \mathbf{x}, t, \mu)}{\partial p^2}\frac{\partial^2 S}{\partial x^2}\bigg).$$

Assuming that $h = O(\mu^\kappa)$ and $0 < \kappa \le 1$, we segregate the leading terms with respect to the parameters μ and μ/h in the right-hand side of this equality. Without the oscillating exponential taken into account, they are given by

$$\frac{\mu}{h}S_t a + L_0^+\Big(\frac{\mu}{h}\nabla_x S, \mathbf{x}, t\Big)a + \mu L_1^+(0, \mathbf{x}, t)a.$$

We recall that $L_0^+ = \varepsilon^+(\boldsymbol{\pi})$ is a scalar function. Working within the WKB method, we can equate this expression to zero, which for all fixed $(\mathbf{x}, t)$ gives the problem for eigenvectors a and eigenvalues $-(\mu/h)S_t - \varepsilon^+(\boldsymbol{\pi})$ and eventually the Hamilton–Jacobi equation

$$\frac{\mu}{h}S_t + \varepsilon^+(\boldsymbol{\pi}) + \mu\lambda_\pm(\mathbf{x}, t) = 0,$$

where $\lambda_\pm(\mathbf{x})$ are eigenvalues of $\mu L_1^+|_{\mathbf{p}=0}$. If $h \sim \mu$, then we have the *relativistic* or *short-wave case*, and it is quite reasonable to carry the terms $\mu L_1^+|_{\mathbf{p}=0}$ and $\lambda_\pm(\mathbf{x})$ over to the (transport) equation for the amplitude such that the Hamiltonian in the Hamilton–Jacobi equation becomes $\varepsilon^\pm(\boldsymbol{\pi})$, which precisely specifies classical trajectories determining the phase $S(\mathbf{x}, t)$. In the other critical case $h \sim \sqrt{\mu}$, $\mu/h \sim h$, it must then also be assumed that in dimensionless variables, the electric and vector potentials (more precisely, their “variable constituents”) also have the order h. We then have the nonrelativistic case, but still rapidly oscillating solutions. Very fast oscillations in time can be immediately isolated by setting $S = ct/\mu + S'(\mathbf{x}, \tau)$. Here, $\tau = \mu t/h$ is the “renormalized” time, whose introduction means that the wave packet propagates over (dimensionless) distances of the order of unity in a time τ of the order of unity. Using the Taylor formula, we can then obtain the Hamilton–Jacobi equation for $S'(\mathbf{x}, \tau)$:

$$\frac{\mu}{h} S'_\tau + \frac{(\nabla_x S' - \mathbf{A}')^2}{2m} \Phi' + \lambda_\pm(\mathbf{x}) + O(h) = 0.$$

It is reasonable to move the last term $O(h)$ to the equation for the amplitude a, as is often (though not always) reasonable to do also with the term $\lambda_\pm(\mathbf{x})$, which is responsible for the spin dynamics and which may also be sufficiently small compared with the retained terms. We are then left with the Hamiltonian corresponding to nonrelativistic motion. Hence, the truly small parameter in this nonrelativistic case (still involving oscillating solutions) is $h \approx \sqrt{\mu}$. This case can be called the nonrelativistic “medium-wave” case.

Further analysis based on the WKB method shows that to determine the leading term of the amplitude a in the small parameter $h = \mu^\kappa$ for any $0 < \kappa \leq 1$, it suffices to have an explicit expression for $L_1^+(\mathbf{p}, \mathbf{x}, t)$ along with $L_0^+(\mathbf{p}, \mathbf{x}, t)$; the other terms $L_j^+(\mathbf{p}, \mathbf{x}, t)$, $j \geq 2$, then yield an $O(h)$-correction to the leading asymptotic term.

We now consider the case where the solution of the reduced equation, if it oscillates at all, does so only sufficiently slowly; we assume that the varying parts of the potentials $\mathbf{A}$ and Φ (in dimensionless form) have the order μ^2. Then after the very fast time oscillations in the form of the exponential $e^{itc^2 m}$ are segregated from the solution, the remaining part of the solution is represented as a regular expansion in the parameter μ with the leading term of this expansion determining the nonrelativistic “long-wave” limit. Simple analysis shows that the resulting equation follows from a Taylor expansion of the symbols of the operators $L_0^+ - mc^2$, L_1^+, and L_2^+ in the long momentum $\boldsymbol{\pi} \sim \mu$ and the momentum $\mathbf{p} \sim \mu$ under the assumption that $\boldsymbol{\pi} \sim \mu$ and $\mathbf{p} \sim \mu$ and with order-μ^2 terms retained. This makes it clear that in all cases, first, the terms in the L_j^+ expansion with $j > 2$ give only a correction to the leading term of the asymptotic form of the wave function and, second, it suffices in L_2^+ to keep only its value at $\mathbf{p} = 0$. We therefore give the following definition.

Definition. The symbol $L_0^\pm + \mu L_1^\pm + \mu^2 L_2^\pm|_{\boldsymbol{\pi}=0}$ is called the *essential part* of the (classical) effective Hamiltonian, and the corresponding operator is called the *essential part* of the quantum effective Hamiltonian.

The “medium-wave” and “long-wave” cases pertain to the nonrelativistic case, and the above simplifications result in a Foldy–Wouthuysen transformation; we give the relevant simplifications in Sec. 4.5 below. We emphasize that the WKB method also allows considering the case of small fields but large momenta $\mathbf{p}$; in that case, the semiclassical approximation is similar to the Born approximation.

We also note that the above argument carries over to the case where focal points and caustics occur in the asymptotic solution, as do the effects of multiplicity changes, which can occur when the effective Hamiltonian $\mu L_1^\pm|_{\mathbf{p}=0}$ is included in the higher part: the version of the adiabatic approximation developed here embraces all these cases. This problem is discussed in greater detail in [6].

4. Essential part of the effective Hamiltonian (electron term)

In view of the above, we restrict ourself to calculating L_1^+ and $L_2^+|_{\boldsymbol{\pi}=0}$. With physical applications in mind, we give the final formulas using the original variables and potentials.

4.1. The first correction to the essential part of the effective Hamiltonian. For L_1^+, we have

$$L_1^+ = -\xi^{+*}\left(\mathcal{F}_1^+ + i\frac{\partial\xi^+}{\partial t}\right) = -i\xi^{+*}\left(\sum_{j=1}^{3}\left(\frac{\partial\mathcal{H}}{\partial p^j}\frac{\partial\xi^+}{\partial x^j} - \frac{\partial\varepsilon^+}{\partial x^j}\frac{\partial\xi^+}{\partial p^j}\right) + \frac{\partial\xi^+}{\partial t}\right). \tag{4.1}$$

We note that ξ^+ depends on x and p through the long momenta $\boldsymbol{\pi}$, and therefore

$$\xi^{+*}\left(\sum_{j=1}^{3}(\mathcal{H}_{p^j}\xi^+_{x^j} - \varepsilon^+_{x^j}\xi^+_{p^j}) + \frac{\partial\xi^+}{\partial t}\right) =$$

$$= \sum_{j=1}^{3}\sum_{k=1}^{3}\xi^{+*}\left[\frac{\partial\pi_k}{\partial t} + \frac{\partial\mathcal{H}}{\partial p_j}\frac{\partial\pi_k}{\partial x^j} - \frac{\partial\varepsilon^+}{\partial x^j}\frac{\partial\pi_k}{\partial p_j}\right]\frac{\partial\xi^+}{\partial\pi_k} =$$

$$= \xi^{+*}\sum_{j=1}^{3}\sum_{k=1}^{3}\left[eE_k + e\frac{\pi_j}{\sqrt{m^2c^2+\boldsymbol{\pi}^2}}\frac{\partial A^j}{\partial x^k} - e\alpha^j\frac{\partial A_k}{\partial x^j}\right]\frac{\partial\xi^+}{\partial\pi_k} =$$

$$= \sum_{j=1}^{3}\sum_{k=1}^{3}\left[\left(eE_k + e\frac{\pi_j}{\sqrt{m^2c^2+\boldsymbol{\pi}^2}}\frac{\partial A^j}{\partial x^k}\right)\xi^{+*}\frac{\partial\xi^+}{\partial\pi_k} - e\frac{\partial A_k}{\partial x^j}\xi^{+*}\alpha^j\frac{\partial\xi^+}{\partial\pi_k}\right]. \tag{4.2}$$

Here, $E_k = -\partial A_k/\partial t - \partial\Phi/\partial x^k$ are the electric field components, and we use the equalities

$$\frac{\partial\pi_k}{\partial t} - \frac{\partial\varepsilon^+}{\partial x^j}\frac{\partial\pi_k}{\partial p_j} = eE_k \pm e\frac{\pi_j}{\sqrt{m^2c^2+\boldsymbol{\pi}^2}}\frac{\partial A^j}{\partial x^k}, \qquad \frac{\partial\mathcal{H}}{\partial p_j}\frac{\partial\pi_k}{\partial x^j} = -e\alpha^j\frac{\partial A_k}{\partial x^j}.$$

We evaluate the matrices $\xi^{+*}\partial\xi^+/\partial\pi_k$ and $\xi^{+*}\alpha^j\partial\xi^+/\partial\pi_k$. After some calculations, we have

$$C_+^2 + C_-^2 = 1, \qquad (\boldsymbol{\sigma},\boldsymbol{n})\frac{\partial}{\partial\pi_k}(\boldsymbol{\sigma},\boldsymbol{n}) = -\frac{i[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_k}{|\boldsymbol{\pi}|^2}, \tag{4.3}$$

$$C_+C_- = \frac{|\boldsymbol{\pi}|}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}}, \qquad \frac{C_-}{C_+} = \frac{|\boldsymbol{\pi}|}{\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc}. \tag{4.4}$$

From (4.3), we obtain

$$\xi^{+*}\frac{\partial\xi^+}{\partial\pi_k} = \frac{1}{2}\frac{\partial}{\partial\pi_k}(C_+^2 + C_-^2) + C_-^2(\boldsymbol{\sigma},\boldsymbol{n})\frac{\partial}{\partial\pi_k}(\boldsymbol{\sigma},\boldsymbol{n}) =$$

$$= -\frac{i[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_k}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big(\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc\big)}, \tag{4.5}$$

where $[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_k$ denotes the kth component of the vector product. From (4.4), we similarly find

$$(\chi_0^+)^*\alpha^j\frac{\partial\chi_0^+}{\partial\pi_k} = C_+\frac{\partial\big(C_-\sigma_j(\boldsymbol{\sigma},\boldsymbol{n})\big)}{\partial\pi_k} + C_-(\boldsymbol{\sigma},\boldsymbol{n})\sigma_j\frac{\partial C_+}{\partial\pi_k} =$$

$$= \frac{\partial(C_+C_-n_j)}{\partial\pi_k} + iC_+^2\frac{\partial\big(C_+^{-1}C_-[\boldsymbol{n}\times\boldsymbol{\sigma}]_j\big)}{\partial\pi_k} =$$

$$= \frac{\partial}{\partial\pi_k}\left(\frac{\pi_j}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}}\right) + iC_+^2\frac{\partial}{\partial\pi_k}\left(\frac{[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_j}{\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc}\right) =$$

$$= \frac{1}{2}\frac{\partial^2\varepsilon^+}{\partial\pi_k\,\partial\pi_j} + \frac{i\varepsilon_{jkl}\sigma_l}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}} - \frac{i[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_j\pi_k}{2\big(m+\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big)(m^2c^2+\boldsymbol{\pi}^2)}. \tag{4.6}$$

Combining (4.2), (4.5), and (4.6), we finally obtain

$$\begin{aligned}
L_1^+ =& -i\hbar\sum_{j=1}^3\sum_{k=1}^3\Bigg[\Bigg(eE_k + e\frac{\pi_j}{\sqrt{m^2c^2+\boldsymbol{\pi}^2}}\frac{\partial A^j}{\partial x^k}\Bigg)\frac{i[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_k}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big(m+\sqrt{m^2c^2+\boldsymbol{\pi}^2}\,\big)} + \\
&+ ie\hbar\frac{\partial A_k}{\partial x^j}\Bigg(\frac{1}{2}\frac{\partial^2\varepsilon_+}{\partial\pi_k\,\partial\pi_j} + \frac{i\varepsilon_{jkl}\sigma_l}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}} - \frac{i[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_j\pi_k}{2\big(mc+\sqrt{m^2c^2+\boldsymbol{\pi}^2}\,\big)(m^2c^2+\boldsymbol{\pi}^2)}\Bigg)\Bigg] = \\
=& -\frac{i}{2}\sum_{j=1}^3\varepsilon^+_{p^jx^j} - \frac{e\hbar(\boldsymbol{\sigma},\boldsymbol{H})}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}} - \frac{e\hbar\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big(\sqrt{m^2+\boldsymbol{\pi}^2}+mc\big)}.
\end{aligned}\tag{4.7}$$

4.2. The second correction to the essential part of the effective Hamiltonian. We find the correction $L_2|_{\boldsymbol{\pi}=0}$. We have

$$\begin{aligned}
L_2 =& -i\chi_0^*\Bigg[\sum_{j=1}^3\Bigg(\frac{\partial\mathcal{H}}{\partial p^j}\frac{\partial\chi_1^+}{\partial x^j} - \frac{\partial\varepsilon^+}{\partial x^j}\frac{\partial\chi_1^+}{\partial p^j}\Bigg) + i\frac{\partial\chi_1^+}{\partial t}\Bigg] + \\
&+ i\sum_{j=1}^3\chi_0^*\frac{\partial\xi^+}{\partial p^j}\frac{\partial L_1^+}{\partial x^j} - \frac{1}{2}f_1L_1^+ + i\sum_{|\nu|=2}\frac{1}{\nu!}\chi_0^*\frac{\partial^2\xi^+}{\partial p^\nu}\frac{\partial^2\varepsilon^+}{\partial x^\nu},
\end{aligned}\tag{4.8}$$

$$f_1 = -i\sum_{j=1}^3\frac{\partial}{\partial x^j}\Bigg(\xi^{+*}\frac{\partial\xi^+}{\partial p^j}\Bigg) = -\sum_{j=1}^3\frac{\partial}{\partial x^j}\Bigg(\frac{[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_j}{4\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big(\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc\big)}\Bigg).$$

Using explicit formulas for $C_\pm$, $\xi^\pm$, and other relevant functions, we obtain the equalities for small $\boldsymbol{\pi}$:

$$\begin{aligned}
&C_+ = 1-\frac{\boldsymbol{\pi}^2}{8m^2}+O(|\boldsymbol{\pi}|^4), \qquad C_- = -\frac{|\boldsymbol{\pi}|}{2m}\Bigg(1-\frac{3\boldsymbol{\pi}^2}{8m^2}+O(|\boldsymbol{\pi}|^4)\Bigg), \\
&\xi^+ = \begin{pmatrix} 1-\dfrac{\boldsymbol{\pi}^2}{8m^2c^2}+O(|\boldsymbol{\pi}|^4) & \\ & \dfrac{(\boldsymbol{\sigma},\boldsymbol{\pi})}{2mc}+O(|\boldsymbol{\pi}|^3)\end{pmatrix}, \\
&f_1 = \frac{e\hbar}{8m^2c^2}(\boldsymbol{\sigma},\boldsymbol{H})+O(|\boldsymbol{\pi}|^2), \qquad \chi_0^*\frac{\partial\chi_0}{\partial p_j} = -\frac{i[\boldsymbol{\pi}\times\boldsymbol{\sigma}]_j}{4m^2c^2}+O(|\boldsymbol{\pi}|^3), \\
&L_1^+ = \frac{ie}{2mc}(\nabla_x,\mathbf{A}) - \frac{e\hbar(\boldsymbol{\sigma},\boldsymbol{H})}{2mc} - \frac{e\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{4m^2c^2}+O(|\boldsymbol{\pi}|^2), \\
&\frac{\partial^2\varepsilon}{\partial x^i\,\partial x^j} = \frac{e^2}{mc}\frac{\partial A_k}{\partial x^i}\frac{\partial A^k}{\partial x^j}+e\frac{\partial^2\Phi}{\partial x^i\partial x^j}+O(|\boldsymbol{\pi}|^2), \\
&\mathcal{F}_1^+ = \frac{ie}{2mc}\begin{pmatrix}-\dfrac{(\boldsymbol{E},\boldsymbol{\pi})}{2m}\\ (\boldsymbol{E},\boldsymbol{\sigma})\end{pmatrix} + \frac{ie}{2m}\begin{pmatrix}-(\nabla_x,\mathbf{A})-i(\boldsymbol{\sigma},\boldsymbol{H})\\ \dfrac{3\sigma^j\pi_kA^k_{,j}}{2m}\end{pmatrix}+O(|\boldsymbol{\pi}^2|).
\end{aligned}\tag{4.9}$$

Using these expressions, with the same accuracy, we obtain

$$\chi_1^+ = -\frac{\mathcal{F}_1^+}{2mc}+\xi^+\Bigg(f_1-\frac{L_1^+}{2mc}\Bigg)+O(\boldsymbol{\pi}^2) = \frac{e}{4m^2c^2}\begin{pmatrix}\dfrac{i(\boldsymbol{E},\boldsymbol{\pi})}{2m}+\dfrac{\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2m}\\ -i(\boldsymbol{E},\boldsymbol{\sigma})\end{pmatrix} +$$

$$
+\frac{e}{4m^2}\left(\begin{array}{c}\dfrac{(\boldsymbol{\sigma},\boldsymbol{H})}{2}\\ -\dfrac{3i}{2mc}\sum_{j,k=1}^{3}\sigma^j\pi_k\dfrac{\partial A^k}{\partial_{x^j}}-\dfrac{i(\nabla_x,\mathbf{A})(\boldsymbol{\sigma},\boldsymbol{\pi})}{2m}+\dfrac{3(\boldsymbol{\sigma},\boldsymbol{\pi})(\boldsymbol{\sigma},\boldsymbol{H})}{4mc}\end{array}\right)+O(\boldsymbol{\pi}^2).
$$

Hence, taking the equalities

$$
(\nabla_x,\boldsymbol{E})=-\Delta\Phi-\frac{1}{c}\frac{\partial(\nabla_x,\mathbf{A})}{\partial t},\qquad \operatorname{rot}\boldsymbol{E}=-\boldsymbol{H}_t,\qquad \boldsymbol{H}^2=\sum_{j,k=1}^{3}\frac{\partial A^j}{\partial x^k}\frac{\partial A^j}{\partial x^k}-\frac{\partial A^j}{\partial x^k}\frac{\partial A^k}{\partial x^j}
$$

into account, we finally obtain

$$
\begin{aligned}
L_2|_{\boldsymbol{\pi}=0}={}&\frac{e}{8m^2c^2}\Delta\Phi+\frac{e^2\boldsymbol{E}^2}{8m^3c^3}+\frac{e^2}{8m^3c^3}\sum_{j,k=1}^{3}\left(\frac{\partial A^j}{\partial x^k}\frac{\partial A^j}{\partial x^k}+\frac{\partial A^j}{\partial x^k}\frac{\partial A^k}{\partial x^j}+\frac{\partial A^k}{\partial x^k}\frac{\partial A^j}{\partial x^j}\right)+\\
&+\frac{ie}{4m^3c^3}(\nabla_x,\mathbf{A})(\boldsymbol{\sigma},\boldsymbol{H})-\frac{ie}{8m^2c^2}(\boldsymbol{\sigma},\operatorname{rot}\boldsymbol{E}).
\end{aligned}\tag{4.10}
$$

4.3. The Feynman–Maslov symbol of the essential part of the effective Hamiltonian. Collecting the formulas for L_0^+, L_1^+, and L_2^+, we obtain the following fact.

Statement 1. *The Feynman–Maslov symbol of the essential part of the quantum effective Hamiltonian of the electron term is given by*

$$
\begin{aligned}
L_0^++\hbar L_1^++\hbar^2L_2^+={}&\varepsilon^+(\boldsymbol{\pi})-\hbar\left\{\frac{i}{2}\sum_{j=1}^{3}\varepsilon^+_{p^jx^j}-\frac{e(\boldsymbol{\sigma},\boldsymbol{H})}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}}-\frac{e\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}\left(\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc\right)}\right\}+\\
&+\hbar^2\left\{\frac{\hbar^2e}{8m^2c^2}\Delta\Phi+\frac{e^2\boldsymbol{E}^2}{8m^3c^3}+\frac{e^2}{8m^3c^3}\sum_{j,k=1}^{3}\left(\frac{\partial A^j}{\partial x^k}\frac{\partial A^j}{\partial x^k}+\frac{\partial A^j}{\partial x^k}\frac{\partial A^k}{\partial x^j}+\frac{\partial A^k}{\partial x^k}\frac{\partial A^j}{\partial x^j}\right)+\right.\\
&\left.+\frac{ie}{4m^3c^3}(\nabla_x,\mathbf{A})(\boldsymbol{\sigma},\boldsymbol{H})-\frac{ie}{8m^2c^2}(\boldsymbol{\sigma},\operatorname{rot}\boldsymbol{E})\right\}.
\end{aligned}\tag{4.11}
$$

4.4. Weyl symbol of the essential part of the effective Hamiltonian. As noted above, more suitable formulas for the electron and positron operators $\hat{L}^{\pm}$ follow based on the Weyl ordering, which expresses them directly in a self-adjoint or at least symmetric form. We pass from the Feynman–Maslov symbol to the Weyl symbol of the same operator $\operatorname{mod}\bigl(O(\hbar^3)+O(\hbar^2|\boldsymbol{\pi}|)\bigr)$. In accordance with (2.7), the Weyl symbol $L_{\mathrm{w}}=L_0^++\hbar L_1^++\hbar^2L_2^+$ is

$$
\begin{aligned}
L_{\mathrm{w}}(\mathbf{p},\mathbf{x},t,\hbar)={}&L_0^++\frac{i\hbar}{2}\sum_{j=1}^{3}\frac{\partial^2L_0^+}{\partial x^j\,\partial p_j}+\hbar L_1^+-\\
&-\frac{\hbar^2}{8}\sum_{j,k=1}^{3}\frac{\partial^4L_0^+}{\partial x^j\,\partial x^k\,\partial p_j\,\partial p_k}\bigg|_{\boldsymbol{\pi}=0}+\frac{i\hbar^2}{2}\sum_{j=1}^{3}\frac{\partial^2L_1^+}{\partial x^j\,\partial p_j}\bigg|_{\boldsymbol{\pi}=0}+\hbar^2L_2^+|_{\boldsymbol{\pi}=0}.
\end{aligned}\tag{4.12}
$$

After appropriate calculations, we obtain

$$\sum_{j=1}^{3}\frac{\partial^2 L_0^+}{\partial x^j\,\partial p_j}=\sum_{j=1}^{3}\frac{\partial^2 \varepsilon_0^+}{\partial x^j\,\partial p_j},$$

$$\sum_{j,k=1}^{3}\frac{\partial^4 L_0^+}{\partial x^j\,\partial x^k\,\partial p_j\,\partial p_k}\bigg|_{\boldsymbol{\pi}=0}=\frac{1}{m^3c^3}\sum_{j,k=1}^{3}\left(\frac{\partial A^j}{\partial x^k}\frac{\partial A^j}{\partial x^k}+\frac{\partial A^j}{\partial x^k}\frac{\partial A^k}{\partial x^j}+\frac{\partial A^k}{\partial x^k}\frac{\partial A^j}{\partial x^j}\right)+O(|\boldsymbol{\pi}|+\hbar),$$

$$\sum_{j=1}^{3}\frac{\partial^2 L_1^+}{\partial x^j\,\partial p_j}=\frac{e(\nabla_x,\mathbf{A})(\boldsymbol{\sigma},\boldsymbol{H})}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}}+O(|\boldsymbol{\pi}|+\hbar).$$

Substituting these expressions in (4.11) and (4.12), we finally obtain the following fact.

Statement 2. *The Weyl symbols of the essential parts of the quantum effective electron and positron matrix Hamiltonians are given by*

$$L_{\mathrm{W}}^+(\mathbf{p},\mathbf{r},\hbar)=c\sqrt{m^2c^2+\boldsymbol{\pi}^2}+e\Phi-\frac{e\hbar(\boldsymbol{\sigma},\boldsymbol{H})}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}}-$$
$$-\frac{e\hbar\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big(\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc\big)}+\frac{e\hbar^2}{8m^2c^2}\Delta\Phi+\frac{e^2\hbar^2\boldsymbol{E}^2}{8m^3c^3}+O(\hbar^2|\boldsymbol{\pi}|), \tag{4.13}$$

$$L_{\mathrm{W}}^-(\mathbf{p},\mathbf{r},\hbar)=-c\sqrt{m^2c^2+\boldsymbol{\pi}^2}+e\Phi-\frac{e\hbar(\boldsymbol{\sigma},\boldsymbol{H})}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}}+$$
$$+\frac{e\hbar\bar{\boldsymbol{\sigma}}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2\sqrt{m^2c^2+\boldsymbol{\pi}^2}\big(\sqrt{m^2c^2+\boldsymbol{\pi}^2}+mc\big)}+\frac{e\hbar^2}{8m^2c^2}\Delta\Phi-\frac{e^2\hbar^2\boldsymbol{E}^2}{8m^3c^3}+O(\hbar^2|\boldsymbol{\pi}|). \tag{4.14}$$

Along with (2.3) and (2.6), these formulas determine the corresponding quantum dynamics of the electron and positron in a certain approximation.

4.5. Nonrelativistic limit. As noted above, it is sometimes useful to allow a regular dependence of the potentials $\mathbf{A}$ and Φ on the parameter μ, which allows considering the case of sufficiently weak magnetic fields and studying the nonrelativistic limit. In this case, all the previous arguments remain valid, but the final equations can be simplified by expanding the potentials $\mathbf{A}$ and Φ in the symbols $L_{\mathrm{W}}^{\pm}$. We give the simplified formulas.

The nonrelativistic limit formally follows as the result of a Taylor expansion of symbol (4.13) with respect to the parameter mc, with the $O(mc)$, $O(1)$, and $O\big((mc)^{-1}\big)$ terms kept. All the other terms are corrections. We present the final formulas, also keeping the terms $O\big((mc)^{-2}\big)$:

$$L_{\mathrm{W}}^+(\mathbf{p},\mathbf{r},\hbar)=mc^2\sqrt{1+\frac{\boldsymbol{\pi}^2}{m^2c^2}}+e\Phi-\frac{e\hbar(\boldsymbol{\sigma},\boldsymbol{H})}{2mc\sqrt{1+\boldsymbol{\pi}^2/(m^2c^2)}}-$$
$$-\frac{e\hbar\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2m^2c^2\sqrt{1+\boldsymbol{\pi}^2/(m^2c^2)}\big(\sqrt{1+\boldsymbol{\pi}^2/(m^2c^2)}+1\big)}+$$
$$+\frac{e\hbar^2}{8m^2c^2}\Delta\Phi+\frac{e^2\hbar^2\boldsymbol{E}^2}{8m^3c^3}+O(\hbar^2|\boldsymbol{\pi}|)=$$
$$=mc^2+\left[\frac{\boldsymbol{\pi}^2}{2m}+e\Phi-\frac{e\hbar(\boldsymbol{\sigma},\boldsymbol{H})}{2m}\right]+\left[\frac{e\hbar^2}{8m^2c}\operatorname{div}\boldsymbol{E}-\frac{e\hbar\boldsymbol{\sigma}[\boldsymbol{E}\times\boldsymbol{\pi}]}{2m^2c}\right]+O(\hbar^2|\boldsymbol{\pi}|). \tag{4.15}$$

The first term here defines the symbol of the standard Pauli operator, and the other terms define corrections to it.

5. Estimates and the accuracy of the presented transformations

We next discuss the accuracy of the presented transformations. Formal expansions of form (3.4) are known formulas for the composition of μ-pseudodifferential operators. Such formulas for different classes of symbols are justified in [4], [9], [11]–[13]. We need formulas for composition with an estimate of the error term for symbols of the class S^m consisting of smooth functions $a(\mathbf{p},\mathbf{x})$ such that both these functions and their derivatives have a powerlike growth as $(\mathbf{p},\mathbf{x})\to\infty$ of the order at most m, i.e., with some constants $C_{\alpha,\beta}$, the inequalities

$$\left|\frac{\partial^{|\alpha|}}{\partial p^\alpha}\frac{\partial^{|\beta|}}{\partial x^\beta}a(\mathbf{p},\mathbf{x})\right|\le C_{\alpha,\beta}\big(1+|\mathbf{p}|+|\mathbf{x}|\big)^m$$

are satisfied for all multi-indices $\alpha=(\alpha_1,\alpha_2,\alpha_3)$ and $\beta=(\beta_1,\beta_2,\beta_3)$ with integer nonnegative components. For example, the class S^0 consists of functions that are bounded together with all their derivatives. In the space S^m, we can introduce the system of norms

$$\|a(\mathbf{p},\mathbf{x})\|_{k,m}=\sum_{|\alpha|+|\beta|\le k}\sup\frac{|(\partial^{|\alpha|}/\partial p^\alpha)(\partial^{|\beta|}/\partial x^\beta)a(\mathbf{p},\mathbf{x})|}{(1+|\mathbf{p}|+|\mathbf{x}|)^m},\tag{5.1}$$

and S^m then becomes a countably normalized space. We write $a(\mathbf{p},\mathbf{x},\mu)=O(\mu^N)$ with respect to S^m if each norm $\|a(\mathbf{p},\mathbf{x},\mu)\|_{k,m}$ is of the order $O(\mu^N)$ as $\mu\to0$.

A simple derivation of the composition formula for class-S^m symbols can be given based on Theorem 2.2 in [13]; namely, the following statement holds.

Lemma 3. *Let $a_1(\mathbf{p},\mathbf{x})$ and $a_2(\mathbf{p},\mathbf{x})$ belong to the respective classes S^{m_1} and S^{m_2} with $m_1\ge0$ and $m_2\ge0$. Then the composition $a_2\big(\overset{1}{\hat{\mathbf{p}}},\overset{2}{\mathbf{x}}\big)a_1\big(\overset{1}{\hat{\mathbf{p}}},\overset{2}{\mathbf{x}}\big)$ has a symbol $b(\mathbf{p},\mathbf{x},\mu)$ belonging to the class $S^{m_1+m_2}$ for each $0\le\mu\le1$ for which the asymptotic expansion*

$$b(\mathbf{p},\mathbf{x},\mu)=\sum_{\nu=0}^{\infty}\frac{1}{\nu!}(-i\mu)^{|\nu|}\frac{\partial^{|\nu|}a_2}{\partial p^\nu}(\mathbf{p},\mathbf{x})\frac{\partial^{|\nu|}a_1}{\partial x^\nu}(\mathbf{p},\mathbf{x})$$

holds. The error term $b_N(\mathbf{p},\mathbf{x},\mu)$ that follows from the terms with $|\nu|<N$ in this sum is of the order $O(\mu^N)$ with respect to $S^{m_1+m_2}$, and for any integers $N\ge0$ and $k\ge0$, there exist integers $k_1\ge0$ and $k_2\ge0$ such that the estimates

$$\|b_N(\mathbf{p},\mathbf{x},\mu)\|_{k,m_1+m_2}\le C_{N,k,m_1,m_2}\mu^N\|a_1(\mathbf{p},\mathbf{x})\|_{k_1,m_1}\|a_2(\mathbf{p},\mathbf{x})\|_{k_2,m_2}\tag{5.2}$$

hold.

We recall some facts from the theory of pseudodifferential operators. It is known (see [4]) that a μ-pseudodifferential operator $a\big(\overset{1}{\hat{\mathbf{p}}},\overset{2}{\mathbf{x}}\big)$ with a symbol $a(\mathbf{p},\mathbf{x})$ can be written as

$$a\big(\overset{1}{\hat{\mathbf{p}}},\overset{2}{\mathbf{x}}\big)u=\frac{1}{(2\pi\mu)^3}\iint e^{(i/\mu)(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}}a(\mathbf{p},\mathbf{x})u(\mathbf{y})\,dy\,dp.\tag{5.3}$$

If $a(\mathbf{p},\mathbf{x})$ and $u(\mathbf{x})$ respectively sufficiently rapidly decrease in $\mathbf{p}$ and $\mathbf{x}$, then the integral in (5.3) can be understood in the standard sense, but we also use formula (5.3) in this case, where $a(\mathbf{p},\mathbf{x})\in S^m$ and $u(\mathbf{x})$ belong to the space S (the space S consists of functions decreasing together with their derivatives faster than any negative power of $|\mathbf{x}|$ as $\mathbf{x}\to\infty$) or $S^{m'}$ (the space S^m of functions of $\mathbf{x}$ is defined similarly to the spaces S^m of functions of $(\mathbf{p},\mathbf{x})$). The integral in (5.3) is then understood as an oscillatory integral (see, e.g., [13]) that can be defined as the $\varepsilon \to 0$ limit of the same integrals where the symbol $a(\mathbf{p}, \mathbf{x})$ is replaced with $a^\varepsilon(\mathbf{p}, \mathbf{x})\rho(\varepsilon\mathbf{p})$ and where $u(\mathbf{y})$ with $u \in S^{m'}$ is replaced with $u(\mathbf{y})\rho(\varepsilon\mathbf{y})$. Here, $\rho(\mathbf{x})$ is a finitary function equal to unity in a neighborhood of the origin. In the oscillatory integral, we can integrate by parts based on the relations

$$\frac{\partial}{\partial p_j} e^{(i/\mu)(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}} = \frac{i}{\mu}(x_j - y_j) e^{(i/\mu)(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}}, \qquad \frac{\partial}{\partial y_j} e^{(i/\mu)(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}} = -\frac{i}{\mu} p_j e^{(i/\mu)(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}}.$$

Such integrations allow transforming (5.3) into an absolutely convergent integral. The operator $a\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big)$ with $a(\mathbf{p}, \mathbf{x}) \in S^m$ for each $\mu \neq 0$ maps the space S to itself continuously, and the map $\big(a(\mathbf{p}, \mathbf{x}), u(\mathbf{x})\big) \to a\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big)u$ maps $S^m \times S$ to S continuously, which is easily established by integrating by parts in (5.3). This same map for $m \geq 0$ and $m' \geq 0$ can be considered a continuous map from $S^m \times S^{m'}$ to $S^{m+m'}$, as can be seen from Theorem 2.2 in [13].

We now pass to the proof of Lemma 3. We first obtain a formula for the symbol of the composition of operators with finitary symbols and $u \in S$. Writing the corresponding operators using formula (5.3), we obtain

$$\begin{aligned} a_2\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big) a_1\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big)u &= \frac{1}{(2\pi\mu)^6} \iint e^{(i/\mu)(\mathbf{x}-\mathbf{z})\cdot\eta} a_2(\eta, \mathbf{x}) \iint e^{(i/\mu)(\mathbf{z}-\mathbf{y})\cdot\xi} a_1(\xi, \mathbf{z}) u(\mathbf{y})\, dy\, d\xi\, dz\, d\eta = \\ &= \frac{1}{(2\pi\mu)^3} \iint e^{(i/\mu)(\mathbf{x}-\mathbf{y})\cdot\xi} b(\xi, \mathbf{x}, \mu) u(\mathbf{y})\, dy\, d\xi, \end{aligned} \tag{5.4}$$

where

$$b(\xi, \mathbf{x}, \mu) = \frac{1}{(2\pi\mu)^3} \iint e^{(i/\mu)(\mathbf{z}-\mathbf{x}\cdot(\xi-\eta)} a_2(\eta, \mathbf{x}) a_1(\xi, \mathbf{z})\, dz\, d\eta. \tag{5.5}$$

Passing from the variables $\mathbf{z}$ and η to $\tilde{\mathbf{z}} = \mathbf{z} - \mathbf{x}$ and $\tilde{\eta} = \eta - \xi$ and replacing ξ with $\mathbf{p}$ yields

$$b(\mathbf{p}, \mathbf{x}, \mu) = \frac{1}{(2\pi\mu)^3} \iint e^{-(i/\mu)\tilde{\mathbf{z}}\cdot\tilde{\eta}} a_2(\tilde{\eta} + \mathbf{p}, \mathbf{x}) a_1(\mathbf{p}, \tilde{\mathbf{z}} + \mathbf{x})\, d\tilde{z}\, d\tilde{\eta}. \tag{5.6}$$

Formula (5.4) shows that $b(\mathbf{p}, \mathbf{x}, \mu)$ is a symbol of the composition of $\hat{a}_1$ and $\hat{a}_2$. We must now pass to arbitrary symbols $a_1(\mathbf{p}, \mathbf{x}) \in S^{m_1}$ and $a_2(\mathbf{p}, \mathbf{x}) \in S^{m_2}$ and establish that formula (5.5) defines the symbol of the composition of the corresponding operator, with the integral in that formula understood as an oscillatory integral. Theorem 2.2 in [13] implies estimate (5.2). In the particular case where $N = 0$, it then follows that $\big(a_1(\mathbf{p}, \mathbf{x}), a_2(\mathbf{p}, \mathbf{x})\big) \to b(\mathbf{p}, \mathbf{x}, \mu)$ is a continuous map $S^{m_1} \times S^{m_2} \to S^{m_1+m_2}$ for any $m_1 \geq 0$, $m_2 \geq 0$, and $0 < \mu \leq 1$, and it is therefore also continuous as a map $S^{m_1+1} \times S^{m_2+1} \to S^{m_1+m_2+2}$.

We consider finitary approximations $a^\varepsilon_{1,2}(\mathbf{p}, \mathbf{x}) = \rho(\varepsilon\mathbf{x})\rho(\varepsilon\mathbf{p})a_{1,2}(\mathbf{p}, \mathbf{x})$. Let $b^\varepsilon(\mathbf{p}, \mathbf{x}, \mu)$ be the symbol of the composition of operators $\hat{a}^\varepsilon_1$ and $\hat{a}^\varepsilon_2$. It is easy to see that as $\varepsilon \to 0$, these approximations respectively converge to the symbols $a_1(\mathbf{p}, \mathbf{x})$ and $a_2(\mathbf{p}, \mathbf{x})$ in S^{m_1+1} and S^{m_2+1} themselves, and therefore $b^\varepsilon(\mathbf{p}, \mathbf{x}, \mu) \to b(\mathbf{p}, \mathbf{x}, \mu)$ in $S^{m_1+m_2+2}$, whence

$$b^\varepsilon\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, \mu\big)u \to b\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, \mu\big)u \quad \forall u(\mathbf{x}) \in S \tag{5.7}$$

in the space S. On the other hand, the map $a_{1,2}(\mathbf{p}, \mathbf{x}) \to a_{1,2}\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big)$ can be regarded as a continuous map of the respective spaces S^{m_1} and S^{m_2} to the space of continuous operators from S to S, whence it follows that

$$b^\varepsilon\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, \mu\big)u = a^\varepsilon_2\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big) a^\varepsilon_1\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big)u \to a_2\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big) a_1\big(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}\big)u \quad \forall u(\mathbf{x}) \in S \tag{5.8}$$

in the space S. It follows from relations (5.7) and (5.8) that

$$b(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}}, \mu)u = a_2(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}})a_1(\overset{1}{\hat{\mathbf{p}}}, \overset{2}{\mathbf{x}})u \quad \forall u(\mathbf{x}) \in S,$$

i.e., the function $b(\mathbf{p}, \mathbf{x}, \mu)$ is defined by integral (5.5) and is the symbol of the composition of $\hat{a}_1$ and $\hat{a}_2$. The statement of Lemma 3 and estimate (5.2) now follow from Theorem 2.2 in [13] applied to integral (5.6).

We pass to the analysis of the symbols $\chi_j^\pm$ and $L_j^\pm$ obtained in Sec. 3.3. We assume that on the relevant bounded time interval, the potentials $\mathbf{A}(\mathbf{x}, t)$ and $\Phi(\mathbf{x}, t)$ belong to the class S^1 and their derivatives of any order with respect to $(\mathbf{x}, t)$ belong to S^0 uniformly in t. We here assume that these potentials and the variables $(\mathbf{x}, t)$ themselves are represented in dimensionless form (as in Sec. 2). It follows from formulas (1.3) and (1.4) and Lemma 2 that $\chi_0^\pm \in S^0$ and $L_0^\pm \in S^1$. Next, from the formulas in Sec. 3.3, it is easy to see by induction that $\chi_j^\pm \in S^0$ and $L_j^\pm \in S^0$ for all $j \geq 1$. We next construct functions $\Psi_N^\pm$ using an approximate intertwining operator:

$$\Psi_N^\pm = (\widehat{\chi}_0^\pm + \mu\widehat{\chi}_1^\pm + \cdots + \mu^N\widehat{\chi}_N^\pm)\varphi^\pm. \tag{5.9}$$

From the recurrence relation (see Sec. 3.3) and Lemma 3, we then obtain

$$\begin{aligned}\widehat{\mathcal{H}}\Psi_N - i\mu\frac{\partial\Psi_N}{\partial t} = \Bigg(&\widehat{\mathcal{H}}(\widehat{\chi}_0^\pm + \cdots + \mu^N\widehat{\chi}_N^\pm) - \\ &- (\widehat{\chi}_0^\pm + \cdots + \mu^N\widehat{\chi}_N^\pm)(\hat{L}_0^\pm + \cdots + \mu^N\hat{L}_N^\pm) - i\mu\frac{\partial(\widehat{\chi}_0^\pm + \cdots + \mu^N\widehat{\chi}_N^\pm)}{\partial t}\Bigg)\varphi^\pm - \\ &- (\widehat{\chi}_0^\pm + \cdots + \mu^N\widehat{\chi}_N^\pm)\left(i\mu\frac{\partial}{\partial t} - \hat{L}_0^\pm - \cdots - \mu^N\hat{L}_N^\pm\right)\varphi^\pm + \mu^{N+1}\widehat{R}_N\varphi^\pm,\end{aligned} \tag{5.10}$$

where the symbol $R_N(\mathbf{p}, \mathbf{x}, t, \mu)$ belongs to S^1 with uniform estimates of the corresponding norms (5.1) for all $0 \leq \mu \leq 1$ and t in the relevant time interval. We thus obtain the following result.

Statement 3. *Let the reduced equation*

$$i\mu\frac{\partial}{\partial t}\varphi^\pm = (\hat{L}_0^\pm + \mu\hat{L}_1^\pm + \cdots + \mu^N\hat{L}_N^\pm)\varphi^\pm \tag{5.11}$$

be satisfied. Then function (5.9) *satisfies Dirac equation* (2.1) *approximately with an error of the order* $O(\mu^{N+1})$*. If reduced equation* (5.11) *is satisfied up to* $O(h^\alpha)$*, then Eq.* (5.10) *and the error in reduced equation* (5.11) *allow finding the error in the original Eq.* (2.1).

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