



How to approximate the Dirac equation with the Mauser method

Klaus Renziehausen · Kunlong Liu · Ingo Barth

Received: 24 November 2021 / Accepted: 21 March 2022
© The Author(s) 2022

Abstract Mauser and coworkers discussed in a series of papers an ansatz how to split the Dirac equation and the wave function appearing therein into a part related to a free moving electron and another part related to a free moving positron. This ansatz includes an expansion of these quantities into orders of the reciprocal of the speed of light $\epsilon = 1/c$. In particular, in Mauser (VLSI Design 9:415, 1999) it is discussed how to apply this expansion up to the second order in the reciprocal of the speed of light ϵ . As an expansion of this analysis, we show in this work how all three well-known terms that appear in an expansion of the Dirac equation in second order on the reciprocal of the speed of light, namely, a relativistic correction to the kinetic energy, the Darwin term, and the spin-orbit interaction, can be found using the ansatz of Mauser—and doing so, we close a gap between this ansatz to approximate the Dirac equation and other approximative results found using the Foldy–Wouthuysen transformation.

Keywords Quantum mechanics · Relativistic physics · Dirac equation · Atomic physics

K. Renziehausen (✉) · I. Barth
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle (Saale), Germany
e-mail: klaus.renziehausen@mpi-halle.mpg.de

K. Renziehausen
Institute of Physical Chemistry and Abbe School of Photonics, Friedrich Schiller University Jena, Helmholtzweg 4, 07743 Jena, Germany

K. Liu
School of Physics, Huazhong University of Science and Technology, Wuhan 430074, China
e-mail: liukunlong@hust.edu.cn

I. Barth
School of Science, Technology, Accessibility, Mathematics, and Public Health (STAMP), Gallaudet University, 800 Florida Ave NE, Washington, D.C. 20002, USA
e-mail: ingo.barth@gallaudet.edu

1 Introduction

In 1928, Dirac found the famous Dirac equation for the description of the relativistic quantum theory of an electron [1]. According to the relativistic aspect of this equation, the question arises how the Dirac equation can be approximated in a semi-classical approach, so that one finds an equation which has the form of a Schrödinger equation plus small relativistic corrections.

This approximation can be made using the reciprocal of the the speed of light $\epsilon = 1/c$ as a parameter—this ansatz was discussed already in several works [2–11]. In particular, in [8–11] Mauser and his coworkers applied such an approximation of the Dirac equation within an ansatz, where the Dirac equation and the wave function are both split into a part related to a free moving electron and a part related to a free moving positron, and hereby, Mauser demonstrates in [9, 10] how to apply this expansion up to second order in the reciprocal of the speed of light ϵ for the differential equation being related to the free moving electron.

However, within this calculation the question remains unclear how to find the relativistic corrections to the Schrödinger equation in second order in the reciprocal of the speed of light ϵ —namely, a relativistic correction to the kinetic energy, the spin–orbit interaction, and the Darwin term—in the form which can be found elsewhere in the literature [12–15] derived with the Foldy–Wouthuysen scheme [16]. Within this work, we address this question and show how to derive these terms if one uses the ansatz of Mauser. Hereby, a careful discussion must be made how the electromagnetic quantities and their spatial derivatives depend in leading order on the reciprocal of the speed of light ϵ for the chosen system—we analyse in our discussion dependencies which are typical for atomic or molecular systems containing one electron, such as the interaction of a hydrogen atom or a dihydrogen cation with a laser pulse.

This paper is structured as follows: in Sect. 2, we explain how the electromagnetic quantities depend in leading order on the reciprocal of the speed of light ϵ . In Sect. 3, a brief review of the Dirac equation is given, and then, in Sect. 4, it is discussed how the splitting of the Dirac equation is made into one differential equation for a free moving electron and another part related to a free moving positron with the Mauser method. After that, we show in Sect. 5, how we can derive from these two equations another differential equation with the form of the Schrödinger equation plus relativistic corrections up to second order in ϵ . In addition, we analyze in Sect. 5 how the differential equations derived there can be related to prior findings of Mauser and his coworkers, where they derived within their ansatz the Pauli equation [8–11]. Some longish side calculations of this section are presented in the Appendices. Finally, we close this paper with a summary in Sect. 6.

2 Properties of the electromagnetic quantities

In this chapter, we will discuss how some electromagnetic quantities—these are the electric field \mathbf{E} , the magnetic field \mathbf{B} , the scalar potential V , the vector potential \mathbf{A} and spatial derivatives of these four quantities—depend in leading order on the reciprocal of the speed of light

$$\epsilon = 1/c. \quad (1)$$

In general, all these quantities depend on the position \mathbf{r} and the time t . The position \mathbf{r} is described in Cartesian coordinates with according coordinates $r_1 \equiv x$, $r_2 \equiv y$, $r_3 \equiv z$, basis vectors $\mathbf{e}_1 \equiv \mathbf{e}_x$, $\mathbf{e}_2 \equiv \mathbf{e}_y$, $\mathbf{e}_3 \equiv \mathbf{e}_z$, and coordinate derivatives $\partial_1 \equiv \partial_x$, $\partial_2 \equiv \partial_y$, $\partial_3 \equiv \partial_z$. Moreover, we use Gaussian units throughout this paper.

We analyze a system, where an atom or molecule that contains one electron interacts with a laser pulse (so, the atom or molecule might be a hydrogen atom H or a hydrogen cation H_2^+). In the following, we will use the position \mathbf{r} as the position of the electron, while the positions of all other particles will not appear in the following calculations explicitly—so we omit to use formula symbols for these positions. For this system, the scalar potential V is related to the attractive Coulomb forces that pull the electron towards the nuclei. These Coulomb forces are zero-order

quantities in ϵ —thus, the vector potential V itself and its spatial and time derivatives are zero-order quantities in ϵ , too:

$$V = \mathcal{O}(\epsilon^0), \tag{2}$$

$$\left(\prod_{a=1}^n \partial_{i_a} \right) V = \mathcal{O}(\epsilon^0), \tag{3}$$

$$\partial_t^n V = \mathcal{O}(\epsilon^0), \tag{4}$$

where in the equations above and below $i_a \in \{1, 2, 3\}$ and $n \in \mathbb{N}$.

Here, due to the form of Eq. (3), the left side of this equation can take for an appropriate choice of the parameter n and the indices i_a all forms of mixed derivatives of the Cartesian coordinates of the position \mathbf{r} —for instance for the special choice $n = 3$, $i_1 = i_2 = 1$ and $i_3 = 3$, the left side of Eq. (3) becomes

$$\partial_1^2 \partial_3 V \equiv \partial_x^2 \partial_z V. \tag{5}$$

Moreover, the effects of the laser pulse on the electron are induced by the vector potential \mathbf{A} . We use for the vector potential \mathbf{A} the Coulomb gauge:

$$\nabla \mathbf{A} = 0 \tag{6}$$

and assume that it has the following form:

$$\mathbf{A} = \frac{A_0}{\epsilon} \mathbf{f}(\eta), \tag{7}$$

where the prefactor A_0 does not depend on the position \mathbf{r} or the time t , and the vector function $\mathbf{f}(\eta)$ depends on the quantity:

$$\eta = \omega t - \mathbf{k} \mathbf{r} = \omega (t - \epsilon \boldsymbol{\kappa} \mathbf{r}), \tag{8}$$

where ω is the angular frequency of the laser pulse, and

$$\mathbf{k} = \omega \epsilon \boldsymbol{\kappa} = \mathcal{O}(\epsilon), \tag{9}$$

is the wave vector of the pulse, where $\boldsymbol{\kappa}$ is a unit vector being independent of ϵ , so $|\boldsymbol{\kappa}| = 1$.

A typical example, which form the vector function $\mathbf{f}(\eta)$ appearing in Eq. (7) could take for a laser pulse propagating in z direction (so that $\boldsymbol{\kappa} = \mathbf{e}_z$) is

$$\mathbf{f}(\eta) = \sin^2 \left(\frac{\pi \eta}{\omega N T} \right) \left[-\sin(\eta + \phi_{CE}) \mathbf{e}_x + p \cos(\eta + \phi_{CE}) \mathbf{e}_y \right] \tag{10}$$

for $0 \leq \eta \leq \omega N T$ and $\mathbf{f}(\eta) = \mathbf{0}$ for all other values of η .

Here, $T = 2\pi/\omega$ is the oscillation period, N is the number of oscillation cycles of the pulse, $p \in [-1, 1]$ is the ellipticity parameter, ϕ_{CE} is the carrier-envelope phase (CEP). Now, we continue our discussion for any general form of the function $\mathbf{f}(\eta)$ for which

$$\mathbf{f}(\eta) = \mathcal{O}(\epsilon^0), \tag{11}$$

$$\frac{\partial^n \mathbf{f}(\eta)}{\partial \eta^n} = \mathcal{O}(\epsilon^0) \quad (12)$$

is valid.

Then, the vector potential \mathbf{A} multiplied by ϵ , that is

$$\mathcal{A} := \epsilon \mathbf{A} = A_0 \mathbf{f}(\eta), \quad (13)$$

is a zero-order term in ϵ because of Eqs. (7) and (11) and the constancy of the prefactor A_0 :

$$\mathcal{A} := \mathcal{O}(\epsilon^0). \quad (14)$$

In the following, we call the vector \mathcal{A} as the scaled vector potential and substitute the vector potential \mathbf{A} in all equations by \mathcal{A}/ϵ .

Moreover, using Eqs. (8) and (13), we find for spatial derivatives of the k -th component of the scaled vector potential \mathcal{A} (where $k \in \{1, 2, 3\}$ here and in all following calculations):

$$\begin{aligned} \left(\prod_{a=1}^n \partial_{i_a} \right) \mathcal{A}_k &= \left(\prod_{a=1}^{n-1} \partial_{i_a} \right) \partial_{i_n} [A_0 f_k(\eta)] \\ &= \left(\prod_{a=1}^{n-1} \partial_{i_a} \right) A_0 \left(\frac{\partial \eta}{\partial r_{i_n}} \right) \frac{\partial f_k(\eta)}{\partial \eta} \\ &= -\omega \epsilon A_0 \kappa_{i_n} \left(\prod_{a=1}^{n-1} \partial_{i_a} \right) \frac{\partial f_k(\eta)}{\partial \eta} \\ &= (-1)^n \omega^n \epsilon^n A_0 \left(\prod_{a=1}^n \kappa_{i_a} \right) \frac{\partial^n f_k(\eta)}{\partial \eta^n}. \end{aligned} \quad (15)$$

The important consequence of the result (15) for the spatial derivatives of the vector component \mathcal{A}_k is

$$\left(\prod_{a=1}^n \partial_{i_a} \right) \mathcal{A}_k = \mathcal{O}(\epsilon^n). \quad (16)$$

Here, after comparing Eqs. (3) and (16), we note that each spatial derivative increases the leading order in ϵ of a vector component \mathcal{A}_k by one, whereas these spatial derivatives have no effect on the leading order in ϵ of the scalar potential V .

However, time derivatives have no effect on the leading order in ϵ of a vector component \mathcal{A}_k , which can be proven using Eqs. (8), (12) and (13) within the following calculation:

$$\begin{aligned} \partial_t^n \mathcal{A}_k &= \partial_t^n [A_0 f_k(\eta)] \\ &= \partial_t^{n-1} \left[A_0 \left(\frac{\partial \eta}{\partial t} \right) \frac{\partial f_k(\eta)}{\partial \eta} \right] \\ &= A_0 \omega \partial_t^{n-1} \frac{\partial f_k(\eta)}{\partial \eta} \\ &= A_0 \omega^n \frac{\partial^n f_k(\eta)}{\partial \eta^n} \\ &= \mathcal{O}(\epsilon^0). \end{aligned} \quad (17)$$

For all other electromagnetic quantities discussed in this publication, time derivatives have no impact on the leading order in ϵ as well.

Now, we turn our discussion to the electric field \mathbf{E} and the magnetic field \mathbf{B} . They depend in this manner on the potentials V and \mathcal{A} :

$$\mathbf{E} = -\nabla V - \frac{\partial \mathcal{A}}{\partial t}, \tag{18}$$

$$\mathbf{B} = \frac{1}{\epsilon} \nabla \times \mathcal{A}. \tag{19}$$

Then, by combing Eqs. (3), (16), and (17) with Eqs. (18) and (19) we find that both the electric field \mathbf{E} and the magnetic field \mathbf{B} have in lowest order a zero-order term in ϵ :

$$\mathbf{E} := \mathcal{O}(\epsilon^0), \tag{20}$$

$$\mathbf{B} := \mathcal{O}(\epsilon^0). \tag{21}$$

As a further consequence of Eqs. (16) and (19), we find for spatial derivatives of the magnetic field \mathbf{B} :

$$\left(\prod_{a=1}^n \partial_{i_a} \right) B_k = \mathcal{O}(\epsilon^n). \tag{22}$$

Moreover, because of Eqs. (3), (17) and (18), we find for spatial derivatives of the electric field \mathbf{E} in contrast to Eq. (22) for \mathbf{B} :

$$\left(\prod_{a=1}^n \partial_{i_a} \right) E_k = \mathcal{O}(\epsilon^0). \tag{23}$$

As an additional comment for all equations in this paper, where the symbol $\mathcal{O}(\epsilon^q)$ with a $q \in \mathbb{N}_0$ is used, we note that there exist special cases for which in some of these equations the value of q is higher than in our more general calculations.

In particular, if the electron is so far away from all nuclei that their Coulomb forces on the electron can be neglected and we can use $V = 0$, then from Eqs. (16) and (18) follows that on the right side of Eq. (23) appears the symbol $\mathcal{O}(\epsilon^n)$ instead of $\mathcal{O}(\epsilon^0)$.

As another special case, we find for the rotation of the electric field $\nabla \times \mathbf{E}$ using Eqs. (16), (18) and regarding that for all quantities analyzed in this work time derivatives have no effect on the leading order in ϵ :

$$\nabla \times \mathbf{E} = -\nabla \times \left(\nabla V + \frac{\partial \mathcal{A}}{\partial t} \right) = -\frac{\partial}{\partial t} (\nabla \times \mathcal{A}) = \mathcal{O}(\epsilon), \tag{24}$$

so this is in contrast to Eq. (23) in the leading order in ϵ a first order term.

However, for the discussions in the following sections, these special cases are not problematic, because then the order of approximation is even higher if we neglect terms described by the symbol $\mathcal{O}(\epsilon^q)$.

Here, we mention that in [11] a discussion about how the electromagnetic fields and potentials depend on the quantity ϵ is performed, too. However, in Ref. [11] a different ansatz for this discussion is made that leads to a magnetic field $\mathbf{B} = \mathcal{O}(\epsilon)$, while in our work, we have $\mathbf{B} = \mathcal{O}(\epsilon^0)$. Moreover, in this work the additional point appears that due to Eq. (22), applying spatial derivatives on the magnetic field \mathbf{B} increases the leading expansion order in the quantity ϵ , which is not included in [11].

Now, we have completed our discussion about the properties of the electromagnetic fields \mathbf{E} , \mathbf{B} and the potentials V and \mathcal{A} and will turn now to the analysis of the Dirac equation.

3 The Dirac equation

In the following equations, we use the Einstein summation convention. Thus, when an index variable which is related to time or a spacial coordinate appears twice in a single term, it implies summation of that term over all the values of the index.

Therefore, with this convention, the Dirac equation is given by [1, 13–15]¹

$$i\hbar \partial_t \Psi^\epsilon = \left(\frac{m_e}{\epsilon^2} \beta + \frac{1}{\epsilon} \alpha^k \hat{p}_k \right) \Psi^\epsilon + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \Psi^\epsilon - eV \Psi^\epsilon. \quad (25)$$

Here, $i = \sqrt{-1}$ is the unit imaginary number, \hbar is the reduced Planck constant, e is the elementary charge and m_e is the mass of the electron. The wave function Ψ^ϵ is a four-dimensional spinor wave function depending on ϵ . Here and below, an upper index ϵ of a quantity does not denote a power but that this quantity depends on ϵ . Moreover, α^k and β are 4×4 matrices given by

$$\alpha^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix} \quad (26)$$

and

$$\beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \quad (27)$$

where $\mathbb{1}_2$ is the 2×2 unit matrix and σ^k are the 2×2 Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (28)$$

$$\sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad (29)$$

$$\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (30)$$

In addition,

$$\hat{p}_k = -i\hbar \partial_k \quad (31)$$

is the k -th vector component of the momentum operator $\hat{\mathbf{p}}$. As an additional quantity, we will use in the following the kinematic momentum operator $\hat{\Pi}$. Its components $\hat{\Pi}_k$ are given by

$$\hat{\Pi}_k = \hat{p}_k + e\mathcal{A}_k. \quad (32)$$

¹ In the Refs. [1, 13–15], in the Dirac equation the vector potential \mathbf{A} appears, for which we use \mathcal{A}/ϵ instead.

Using Eq. (32), the Dirac equation (25) can be rewritten into this form:

$$i\hbar \partial_t \Psi^\epsilon = \left(\frac{m_e}{\epsilon^2} \beta + \frac{1}{\epsilon} \alpha^k \hat{\Pi}_k - eV \right) \Psi^\epsilon. \tag{33}$$

4 The Mauser method

Having rewritten the Dirac equation (33) and discussed how the quantities depend on ϵ , we can start to transform it within the Mauser method developed by Mauser and his coworkers [8–11]. This means that we will split the Dirac equation into two differential equations: One differential equation in which appears the eigenfunction of the free moving electron, and another differential equation in which the eigenfunction of the free moving positron appears.

Here, we mention as a detail that in [8] this point, which is deviating to our following calculations, is explained: there, the Dirac equation (33) is rescaled in a manner so that in this equation the natural constants m_e , \hbar and c are eliminated—and the quantity ϵ is introduced there not as the reciprocal of the speed of light, but as the dimensionless quotient v/c of a reference speed v and the speed of light c . However, we will keep these nature constants in the Dirac equation (33) for a better comparability of our results to other literature, such as [12–15], where this equation is discussed within Gaussian units like in our work.

Now, the first step for the application of the Mauser method is to introduce the operator \hat{Q}^ϵ as

$$\hat{Q}^\epsilon = m_e \beta + \epsilon \alpha^k \hat{p}_k = \begin{pmatrix} m_e & 0 & \epsilon \hat{p}_3 & \epsilon (\hat{p}_1 - i \hat{p}_2) \\ 0 & m_e & \epsilon (\hat{p}_1 + i \hat{p}_2) & -\epsilon \hat{p}_3 \\ \epsilon \hat{p}_3 & \epsilon (\hat{p}_1 - i \hat{p}_2) & -m_e & 0 \\ \epsilon (\hat{p}_1 + i \hat{p}_2) & -\epsilon \hat{p}_3 & 0 & -m_e \end{pmatrix}. \tag{34}$$

Therefore, the Dirac equation of the free electron, which is not coupling to the potentials \mathcal{A} and V and which is described by a wave function Ψ_f^ϵ , is given by

$$i\hbar \partial_t \Psi_f^\epsilon := \frac{1}{\epsilon^2} \hat{Q}^\epsilon \Psi_f^\epsilon. \tag{35}$$

In the momentum space, we have to substitute the operator $\hat{p}_k = -i\hbar \partial_k$ by the real-valued vector component p_k . Then, in momentum space, we find that the operator \hat{Q}^ϵ has eigenfunctions $\tilde{\Psi}_\pm^\epsilon(\mathbf{p}, t)$ and eigenvalues $\pm \lambda^\epsilon(\mathbf{p})$. The according equation is

$$\hat{Q}^\epsilon \tilde{\Psi}_\pm^\epsilon(\mathbf{p}, t) = \pm \lambda^\epsilon(\mathbf{p}) \tilde{\Psi}_\pm^\epsilon(\mathbf{p}, t), \tag{36}$$

and the function $\lambda^\epsilon(\mathbf{p})$ is given by

$$\lambda^\epsilon(\mathbf{p}) = \sqrt{m_e^2 + \epsilon^2 \mathbf{p}^2}. \tag{37}$$

Therefore, we can interpret the eigenfunction $\tilde{\Psi}_+^\epsilon(\mathbf{p}, t)$ as the electronic wave function and the eigenfunction $\tilde{\Psi}_-^\epsilon(\mathbf{p}, t)$ as the positronic wave function. With respect to the indices \pm of the wave functions $\tilde{\Psi}_\pm^\epsilon(\mathbf{p}, t)$, we here follow the notation of Mauser and his coworkers in [8–10] pointing out that these indices \pm do not refer to the charge of the associated particles. Instead, they refer to the sign of the eigenvalues $\pm \lambda^\epsilon(\mathbf{p})$. As a further consequence, these indices also refer to whether the particle assigned to the wave function $\tilde{\Psi}_\pm^\epsilon(\mathbf{p}, t)$ is matter (+) or antimatter (–).

Then, we find projectors [8–10]

$$\pi_{\pm}^{\epsilon} = \frac{1}{2} \left(1 \pm \frac{\hat{Q}^{\epsilon}}{\lambda^{\epsilon}(\mathbf{p})} \right). \quad (38)$$

For these projectors, the following equations are valid:

$$\pi_{\pm}^{\epsilon} \tilde{\Psi}_{\pm}^{\epsilon}(\mathbf{p}, t) = \tilde{\Psi}_{\pm}^{\epsilon}(\mathbf{p}, t), \quad (39)$$

$$\pi_{\pm}^{\epsilon} \tilde{\Psi}_{\mp}^{\epsilon}(\mathbf{p}, t) = 0, \quad (40)$$

$$\pi_{+}^{\epsilon} + \pi_{-}^{\epsilon} = 1. \quad (41)$$

For the non-relativistic case $\epsilon = 0$, we find the according projectors π_{\pm}^0 using Eqs. (34), (37), and (38):

$$\pi_{\pm}^0 = \frac{1}{2} (1 \pm \beta). \quad (42)$$

We note that because of Eqs. (26), (27) and (42), these equations are valid:

$$\pi_{\pm}^0 \alpha^k = \alpha^k \pi_{\mp}^0, \quad (43)$$

$$\pi_{\pm}^0 \beta = \pm \pi_{\pm}^0. \quad (44)$$

As the next step, using Eqs. (37), (38), (42) and the expansion

$$\frac{1}{\lambda^{\epsilon}(\mathbf{p})} = \frac{1}{m_e} - \frac{1}{2} \frac{\epsilon^2 \mathbf{p}^2}{m_e^3} + \mathcal{O}(\epsilon^4), \quad (45)$$

we find for the projectors π_{\pm}^{ϵ} the following third-order expansion:

$$\begin{aligned} \pi_{\pm}^{\epsilon} &= \frac{1}{2} \left[1 \pm \left(m_e \beta + \epsilon \alpha^k p_k \right) \left(\frac{1}{m_e} - \frac{1}{2} \frac{\epsilon^2 \mathbf{p}^2}{m_e^3} + \mathcal{O}(\epsilon^4) \right) \right] \\ &= \pi_{\pm}^0 \pm \frac{1}{2} \frac{\epsilon}{m_e} \alpha^k p_k \mp \frac{1}{4} \frac{\epsilon^2}{m_e^2} \beta \mathbf{p}^2 \mp \frac{1}{4} \frac{\epsilon^3}{m_e^3} \alpha^k p_k \mathbf{p}^2 + \mathcal{O}(\epsilon^4). \end{aligned} \quad (46)$$

Since in the position space, the vector components p_k transform into the operators $-i\hbar \partial_k$, there, this expansion turns into the following equation:

$$\pi_{\pm}^{\epsilon} = \pi_{\pm}^0 \mp \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k \pm \frac{\hbar^2}{4} \frac{\epsilon^2}{m_e^2} \beta \Delta \mp \frac{i\hbar^3}{4} \frac{\epsilon^3}{m_e^3} \alpha^k \partial_k \Delta + \mathcal{O}(\epsilon^4). \quad (47)$$

In the following equations, we will take into account often only the first two orders of this approximation, so we will use:

$$\pi_{\pm}^{\epsilon} = \pi_{\pm}^0 \mp \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k \pm \frac{\hbar^2}{4} \frac{\epsilon^2}{m_e^2} \beta \Delta + \mathcal{O}(\epsilon^3). \quad (48)$$

Sometimes, also a rewritten form of the equation above for the projectors π_{\pm}^0 is useful:

$$\pi_{\pm}^0 = \pi_{\pm}^{\epsilon} \pm \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k \mp \frac{\hbar^2}{4} \frac{\epsilon^2}{m_e^2} \beta \Delta + \mathcal{O}(\epsilon^3). \quad (49)$$

In addition, we can transform the function $\lambda^{\epsilon}(\mathbf{p})$ given in Eq. (37) from the momentum space into the position space. Then, we find:

$$\lambda^{\epsilon}(\hat{\mathbf{p}}) = \sqrt{m_e^2 + \epsilon^2 \hat{\mathbf{p}}^2} = \sqrt{m_e^2 - \hbar^2 \epsilon^2 \Delta}. \quad (50)$$

Here, the operator Δ under the square root can be evaluated using an expansion in ϵ —up to the fifth order, this expansion is given by

$$\lambda^{\epsilon}(\hat{\mathbf{p}}) = m_e - \frac{\hbar^2}{2} \frac{\epsilon^2}{m_e} \Delta - \frac{\hbar^4}{8} \frac{\epsilon^4}{m_e^3} \Delta^2 + \mathcal{O}(\epsilon^6). \quad (51)$$

Then, the eigenvalue equation (36) can be transformed into the position space—there, it takes the following form:

$$\hat{Q}^{\epsilon} \Psi_{\pm}^{\epsilon} = \pm \lambda^{\epsilon}(\hat{\mathbf{p}}) \Psi_{\pm}^{\epsilon}. \quad (52)$$

Moreover, Eqs. (39) and (40) can be transformed into the position space in the following manner:

$$\pi_{\pm}^{\epsilon} \Psi_{\pm}^{\epsilon} = \Psi_{\pm}^{\epsilon}, \quad (53)$$

$$\pi_{\pm}^{\epsilon} \Psi_{\mp}^{\epsilon} = 0. \quad (54)$$

In addition, we assume that the wave functions Ψ_{\pm}^{ϵ} are scaled in a manner so that for the wave function Ψ^{ϵ} holds

$$\Psi^{\epsilon} = \Psi_{+}^{\epsilon} + \Psi_{-}^{\epsilon}, \quad (55)$$

where the wave function Ψ^{ϵ} is normalized as

$$\int d\mathbf{r} (\Psi^{\epsilon})^{\dagger} \Psi^{\epsilon} = 1, \quad (56)$$

where $\int d\mathbf{r}$ means an integration over the three-dimensional space. In contrast, the wave functions Ψ_{\pm}^{ϵ} are not normalized to unity.

Now, we rewrite the Dirac equation (33) using Eqs. (34), (52) and (55). Then, we find:

$$\begin{aligned} i\hbar \partial_t \Psi^{\epsilon} &= \frac{1}{\epsilon^2} \hat{Q}^{\epsilon} \Psi^{\epsilon} + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \Psi^{\epsilon} - eV \Psi^{\epsilon} \\ &= \frac{1}{\epsilon^2} \hat{Q}^{\epsilon} (\Psi_{+}^{\epsilon} + \Psi_{-}^{\epsilon}) + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \Psi^{\epsilon} - eV \Psi^{\epsilon} \\ &= \frac{\lambda^{\epsilon}(\hat{\mathbf{p}})}{\epsilon^2} (\Psi_{+}^{\epsilon} - \Psi_{-}^{\epsilon}) + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \Psi^{\epsilon} - eV \Psi^{\epsilon}. \end{aligned} \quad (57)$$

Then, we apply the projectors π_{\pm}^{ϵ} on Eq. (57).

When we execute this projection, we regard that the projectors π_{\pm}^{ϵ} depend on the momentum operator $\hat{\mathbf{p}}$ but not on the position vector \mathbf{r} , which means that the following commutators hold:

$$[\pi_{\pm}^{\epsilon}, \partial_t] = 0, \quad (58)$$

$$[\pi_{\pm}^{\epsilon}, \lambda^{\epsilon}(\hat{\mathbf{p}})] = 0, \quad (59)$$

$$[\pi_{\pm}^{\epsilon}, \mathbf{r}] \neq 0. \quad (60)$$

Thus, the projectors π_{\pm}^{ϵ} do not commute with the potentials V and \mathcal{A} .

Therefore, using the projectors π_{\pm}^{ϵ} on Eq. (57), we find that

$$i\hbar \partial_t \Psi_{\pm}^{\epsilon} = \pm \frac{1}{\epsilon^2} \lambda^{\epsilon}(\hat{\mathbf{p}}) \Psi_{\pm}^{\epsilon} + \pi_{\pm}^{\epsilon} \left(\frac{e}{\epsilon} \mathcal{A}_k \alpha^k \Psi^{\epsilon} - eV \Psi^{\epsilon} \right). \quad (61)$$

Now, we define the wave functions ϕ_{\pm}^{ϵ} and ϕ^{ϵ} as

$$\phi_{\pm}^{\epsilon} := \exp\left(i \frac{m_e t}{\epsilon^2 \hbar}\right) \Psi_{\pm}^{\epsilon}, \quad (62)$$

$$\phi^{\epsilon} := \phi_{+}^{\epsilon} + \phi_{-}^{\epsilon}. \quad (63)$$

As a consequence, we can express the wave functions Ψ_{\pm}^{ϵ} and Ψ^{ϵ} as

$$\Psi_{\pm}^{\epsilon} = \exp\left(-i \frac{m_e t}{\epsilon^2 \hbar}\right) \phi_{\pm}^{\epsilon}, \quad (64)$$

$$\Psi^{\epsilon} = \exp\left(-i \frac{m_e t}{\epsilon^2 \hbar}\right) \phi^{\epsilon}. \quad (65)$$

Then, by combining Eqs. (56) and (65) we find that the wave function ϕ^{ϵ} is normalized:

$$\int d\mathbf{r} (\phi^{\epsilon})^{\dagger} \phi^{\epsilon} = 1. \quad (66)$$

Since

$$\left[\pi_{\pm}^{\epsilon}, \exp\left(-i \frac{m_e t}{\epsilon^2 \hbar}\right) \right] = 0, \quad (67)$$

we can find for the functions ϕ_{\pm}^{ϵ} analogous equations to Eqs. (53) and (54):

$$\pi_{\pm}^{\epsilon} \phi_{\pm}^{\epsilon} = \phi_{\pm}^{\epsilon}, \quad (68)$$

$$\pi_{\pm}^{\epsilon} \phi_{\mp}^{\epsilon} = 0. \quad (69)$$

As a next step, we find for the left side of Eq. (61):

$$i\hbar \partial_t \Psi_{\pm}^{\epsilon} = \frac{m_e}{\epsilon^2} \exp\left(-i \frac{m_e t}{\epsilon^2 \hbar}\right) \phi_{\pm}^{\epsilon} + \exp\left(-i \frac{m_e t}{\epsilon^2 \hbar}\right) i\hbar \partial_t \phi_{\pm}^{\epsilon}. \quad (70)$$

Using Eq. (67), we find the following equation, too:

$$\pi_{\pm}^{\epsilon} \left[\frac{e}{\epsilon} \mathcal{A}_k \alpha^k \Psi^{\epsilon} - eV \Psi^{\epsilon} \right] = \exp \left(-i \frac{m_e t}{\epsilon^2 \hbar} \right) \pi_{\pm}^{\epsilon} \left[\frac{e}{\epsilon} \mathcal{A}_k \alpha^k \phi^{\epsilon} - eV \phi^{\epsilon} \right]. \quad (71)$$

Thus, using Eqs. (70) and (71), we find the following differential equation for the wave functions:

$$i\hbar \partial_t \phi_{\pm}^{\epsilon} = \pm \frac{1}{\epsilon^2} \lambda^{\epsilon}(\hat{\mathbf{p}}) \phi_{\pm}^{\epsilon} - \frac{m_e}{\epsilon^2} \phi_{\pm}^{\epsilon} + \pi_{\pm}^{\epsilon} \left(\frac{e}{\epsilon} \mathcal{A}_k \alpha^k \phi^{\epsilon} - eV \phi^{\epsilon} \right). \quad (72)$$

Therefore, as a result of the Mauser ansatz, we find that this differential equation splits into two differential equations, one for ϕ_{+}^{ϵ} and one for ϕ_{-}^{ϵ} [8–10]:

$$i\hbar \partial_t \phi_{+}^{\epsilon} = \frac{1}{\epsilon^2} (\lambda^{\epsilon}(\hat{\mathbf{p}}) - m_e) \phi_{+}^{\epsilon} + \pi_{+}^{\epsilon} \left(\frac{e}{\epsilon} \mathcal{A}_k \alpha^k \phi^{\epsilon} - eV \phi^{\epsilon} \right), \quad (73)$$

$$i\hbar \partial_t \phi_{-}^{\epsilon} = \frac{1}{\epsilon^2} (-\lambda^{\epsilon}(\hat{\mathbf{p}}) - m_e) \phi_{-}^{\epsilon} + \pi_{-}^{\epsilon} \left(\frac{e}{\epsilon} \mathcal{A}_k \alpha^k \phi^{\epsilon} - eV \phi^{\epsilon} \right). \quad (74)$$

5 Approximation of the Dirac equation

In this section, we will analyze how to derive a differential equation that has the form of the Schödinger equation plus relativistic corrections up to the second order in the reciprocal of the speed of light ϵ from the two differential equations (73) and (74). For the following discussion, we use this expansion for the wave functions ϕ_{\pm}^{ϵ} [9, 10]

$$\phi_{\pm}^{\epsilon} := \sum_{n=0}^{\infty} \epsilon^n \phi_{\pm}^n. \quad (75)$$

The upper index of the wave functions ϕ_{\pm}^n is not a power but it is related to the n -th expansion order of ϕ_{\pm}^{ϵ} in ϵ . The wave functions ϕ_{\pm}^{ϵ} and ϕ_{\pm}^n can be distinguished by the fact that for the wave function ϕ_{\pm}^{ϵ} the upper index has the dimension of a reciprocal velocity, but for the wave function ϕ_{\pm}^n , the upper index is an integer greater than or equal to zero. However, for the special case $\{\epsilon = 0, n = 0\}$, the wave functions ϕ_{\pm}^{ϵ} and ϕ_{\pm}^n cannot be distinguished—but this is not a problem, since it follows from Eq. (75) that for this case, the wave functions ϕ_{\pm}^{ϵ} and ϕ_{\pm}^n are equal.

For other wave functions discussed below, where either an upper index ϵ or n is used, an analogous argumentation is valid.

Now, the next step of our derivations of the differential equation mentioned above is to calculate the positronic wave function ϕ_{-}^{ϵ} up to third order in ϵ .

5.1 Positronic wave function ϕ_{-}^{ϵ} up to third order in ϵ

Using Eqs. (51) and (63), we obtain from the differential equation for ϕ_{-}^{ϵ} (74):

$$\begin{aligned} \phi_{-}^{\epsilon} = & \frac{\epsilon}{2m_e} \pi_{-}^{\epsilon} \left(e \mathcal{A}_k \alpha^k \phi_{+}^{\epsilon} \right) + \frac{\epsilon}{2m_e} \pi_{-}^{\epsilon} \left(e \mathcal{A}_k \alpha^k \phi_{-}^{\epsilon} \right) \\ & - \frac{\epsilon^2}{2m_e} \pi_{-}^{\epsilon} \left(eV \phi_{+}^{\epsilon} \right) - \frac{\epsilon^2}{2m_e} \pi_{-}^{\epsilon} \left(eV \phi_{-}^{\epsilon} \right) \\ & - \frac{\epsilon^2}{2m_e} \frac{\hat{\mathbf{p}}^2}{2m_e} \phi_{-}^{\epsilon} - \frac{i\hbar \epsilon^2}{2m_e} \partial_t \phi_{-}^{\epsilon} + \mathcal{O}(\epsilon^5). \end{aligned} \quad (76)$$

Now, we realize that only the lowest order function ϕ_-^0 vanishes, that is

$$\phi_-^0 = 0, \quad (77)$$

$$\implies \phi_-^\epsilon = \epsilon \phi_-^1 + \epsilon^2 \phi_-^2 + \epsilon^3 \phi_-^3 + \mathcal{O}(\epsilon^4). \quad (78)$$

For the following transformations, Eqs. (48), (49), (68), and (69) for the projectors π_\pm^ϵ and π_\pm^0 will be useful. In addition, we need the following equations [13]:²

$$\alpha^k \alpha^l = \delta_{kl} \mathbb{1}_4 + i \varepsilon_{klm} \Sigma^m, \quad (79)$$

$$\alpha^k \alpha^l = 2\delta_{kl} \mathbb{1}_4 - \alpha^l \alpha^k, \quad (80)$$

$$\beta \beta = \mathbb{1}_4, \quad (81)$$

$$\alpha^k \beta = -\beta \alpha^k. \quad (82)$$

Here, $\mathbb{1}_4$ is the 4×4 unit matrix, Σ^k is the following 4×4 matrix

$$\Sigma^k = \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix} \quad (83)$$

being an extension of the 2×2 Pauli matrices σ^k . In addition, δ_{kl} is the Kronecker delta, where

$$\delta_{kl} = \begin{cases} 1 & \text{if } k = l \\ 0 & \text{if } k \neq l \end{cases}, \quad (84)$$

and ε_{klm} is the Levi–Cevita symbol given by

$$\varepsilon_{klm} = \begin{cases} 1 & \text{if } (k, l, m) \text{ is an even permutation of } (1, 2, 3) \\ -1 & \text{if } (k, l, m) \text{ is an odd permutation of } (1, 2, 3) \\ 0 & \text{if at least two indices are equal} \end{cases}. \quad (85)$$

Moreover, for the operator Σ^k , the following calculation rule applies:

$$\pi_\pm^0 \Sigma^k = \Sigma^k \pi_\pm^0. \quad (86)$$

As the next step, the six summands in Eq. (76) have to be evaluated and then the sum of these summands has to be simplified to find the final result for ϕ_-^ϵ up to third order in ϵ . Since these calculations are quite long and cumbersome, we execute them in the Appendix A and state here just the final result:

$$\begin{aligned} \phi_-^\epsilon &= \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} - \epsilon^2 \alpha^k \frac{2\hat{\mathbf{\Pi}}^2 - e^2 \mathcal{A}^2}{4m_e^2} \right) \phi_+^\epsilon \\ &\quad - \frac{\epsilon^3 e \hbar}{4m_e^2} \left(\mathbf{\Sigma} \mathbf{B} - i E_k \alpha^k \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^4). \end{aligned} \quad (87)$$

² In [13], Eq. (79) is given in an analogous form $\sigma^k \sigma^l = \delta_{kl} \mathbb{1}_2 + i \varepsilon_{klm} \sigma^m$ for the 2×2 matrices σ^k instead of the 4×4 matrices α^k and Σ^k . However, using Eqs. (26) and (83), one can easily verify that from this form follows, Eq. (79).

The quantity Σ appearing in Eq. (A.27) is just $\Sigma = \Sigma^k \mathbf{e}_k$. As an analogous quantity, we use below $\sigma = \sigma^k \mathbf{e}_k$, too.

5.2 Differential equation for ϕ_+^ϵ up to second order in ϵ

As the next step, we now derive the differential equation for ϕ_+^ϵ up to second order in ϵ . Therefore, we use Eqs. (51), (63), and (73) to get

$$\begin{aligned} i\hbar \partial_t \phi_+^\epsilon &= -\frac{\hbar^2}{2m_e} \Delta \phi_+^\epsilon - \frac{\epsilon^2 \hbar^4}{8m_e^3} \Delta^2 \phi_+^\epsilon + \pi_+^\epsilon \left(\frac{1}{\epsilon} e \mathcal{A}_k \alpha^k \phi_+^\epsilon - eV \phi_+^\epsilon \right) + \mathcal{O}(\epsilon^4) \\ &= -\frac{\hbar^2}{2m_e} \Delta \phi_+^\epsilon - \frac{\epsilon^2 \hbar^4}{8m_e^3} \Delta^2 \phi_+^\epsilon + \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) \\ &\quad - \pi_+^\epsilon (eV \phi_+^\epsilon) - \pi_+^\epsilon (eV \phi_-^\epsilon) + \mathcal{O}(\epsilon^4). \end{aligned} \tag{88}$$

On the right side of Eq. (88), six summands appear in front of the $\mathcal{O}(\epsilon^4)$ term. The first two of these six summands do not need to be simplified. Moreover, in the Appendix B, we explain how the last four of these six summands can be simplified. Then, we sum up in this appendix these six summands, simplify the resulting sum, and find the following final differential equation for ϕ_+^ϵ up to second order in ϵ :

$$\begin{aligned} i\hbar \partial_t \phi_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \phi_+^\epsilon + \frac{i \epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \phi_+^\epsilon + \frac{\epsilon^2 e}{2m_e^2} \alpha^k \left[\left(\frac{1}{\epsilon} \hat{p}_k \mathcal{A}_l \right) e \mathcal{A}_l + \beta \left(\frac{1}{\epsilon} \hat{p}_l \mathcal{A}_k \right) \hat{p}_l \right] \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\mathbf{E} - (\nabla V))] + i \mathcal{A} (\partial_t \mathcal{A}) \} \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{89}$$

We mention here that Mauser also gives a differential equation for ϕ_+^ϵ up to second order in ϵ in [9, 10]. However, Mauser’s differential equation deviates from our differential equation, because he uses in his calculation the vector potential \mathbf{A} as a quantity which is independent of ϵ , while we use the scaled vector potential $\mathcal{A} = \epsilon \mathbf{A}$ instead as a quantity which is in leading order independent from ϵ (see Eq. (14)). As an additional contrast to [9, 10], we regard in our calculations that spatial derivatives increase the leading order for an expansion in ϵ of the scaled vector potential \mathcal{A} and the magnetic field \mathbf{B} (see Eqs. (16) and (22)).

The differential equation for ϕ_+^ϵ (Eq. (89)) has already the form of a Schrödinger equation plus relativistic corrections up to second order in ϵ . Within this equation, there appear two relativistic correction terms which have already a form that one could expect from literature [12–15]:

These two terms are first the coupling term $\frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \phi_+^\epsilon$ of the magnetic field \mathbf{B} with the operator Σ , and second a relativistic correction to the kinetic energy which is $-\frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \phi_+^\epsilon$.³

However, two other relativistic corrections to the Schrödinger equation in second order in the reciprocal of the speed of light ϵ , namely, these are the spin–orbit interaction and the Darwin term, cannot be found in Eq. (89) in the form we would expect them from the references [12–15]. However, for two reasons, these deviations are not too surprising:

³ As a detail, here and in [12] the kinematic momentum operator $\hat{\Pi}$ is regarded for this relativistic correction to the kinetic energy, while in [13–15] in this term the kinematic momentum operator $\hat{\Pi}$ is approximated using just the momentum operator $\hat{\mathbf{p}}$ instead. Among these references, this approximation is explained in the most detail in Ref. [13].

The first reason is that the differential equation (89) is only a differential equation for the electronic wave function ϕ_+^ϵ , but not for the full wave function ϕ^ϵ being the sum of the electronic wave function ϕ_+^ϵ and the positronic wave function ϕ_-^ϵ (see Eq. (63)).

The second reason is that the above mentioned spin-orbit interaction and the Darwin term do not appear in a differential equation for a four-dimensional spinor like Eq. (89) but a two-dimensional one—so we have to search for a differential equation, where a two-dimensional spinor appears. As the first step for that, we define below several two-dimensional wave functions.

5.3 Introduction of different two-spinors

We begin with the introduction of the two-dimensional spinors φ_\pm^ϵ and χ_\pm^ϵ —using these spinors we can write the four-dimensional spinors ϕ_\pm^ϵ as

$$\phi_\pm^\epsilon = \begin{pmatrix} \varphi_\pm^\epsilon \\ \chi_\pm^\epsilon \end{pmatrix}, \quad (90)$$

and then, we define the four-dimensional spinors $\tilde{\varphi}_\pm^\epsilon$ and $\tilde{\chi}_\pm^\epsilon$ as

$$\tilde{\varphi}_\pm^\epsilon := \begin{pmatrix} \varphi_\pm^\epsilon \\ 0 \end{pmatrix} \quad (91)$$

and

$$\tilde{\chi}_\pm^\epsilon := \begin{pmatrix} 0 \\ \chi_\pm^\epsilon \end{pmatrix}. \quad (92)$$

Thus, we can calculate these spinors $\tilde{\varphi}_\pm^\epsilon$ and $\tilde{\chi}_\pm^\epsilon$ using the projectors π_\pm^0 and Eqs. (27) and (42) as

$$\tilde{\varphi}_\pm^\epsilon = \pi_+^0 \phi_\pm^\epsilon, \quad (93)$$

$$\tilde{\chi}_\pm^\epsilon = \pi_-^0 \phi_\pm^\epsilon. \quad (94)$$

Analogously to Eq. (75), we expand the functions $\tilde{\varphi}_\pm^\epsilon$ and $\tilde{\chi}_\pm^\epsilon$ in this way:

$$\tilde{\varphi}_\pm^\epsilon := \sum_{n=0}^{\infty} \epsilon^n \tilde{\varphi}_\pm^n, \quad (95)$$

$$\tilde{\chi}_\pm^\epsilon := \sum_{n=0}^{\infty} \epsilon^n \tilde{\chi}_\pm^n. \quad (96)$$

Of course, such two-dimensional spinors can not only be defined like in Eq. (90) for the four-dimensional electronic spinor ϕ_+^ϵ or the according positronic spinor ϕ_-^ϵ , but for the total four-dimensional wave function $\phi^\epsilon = \phi_+^\epsilon + \phi_-^\epsilon$ (see also Eq. (63)), too. Therefore, within the following equation, we introduce the two-dimensional spinors φ^ϵ and χ^ϵ :

$$\phi^\epsilon = \begin{pmatrix} \varphi^\epsilon \\ \chi^\epsilon \end{pmatrix}, \quad (97)$$

and also these four-spinors:

$$\tilde{\varphi}^\epsilon = \begin{pmatrix} \varphi^\epsilon \\ 0 \end{pmatrix}, \tag{98}$$

$$\tilde{\chi}^\epsilon := \begin{pmatrix} 0 \\ \chi^\epsilon \end{pmatrix}. \tag{99}$$

In analogy to Eqs. (93)–(96), for the four-spinors $\tilde{\varphi}^\epsilon$ and $\tilde{\chi}^\epsilon$, these equations hold:

$$\tilde{\varphi}^\epsilon = \pi_+^0 \phi^\epsilon, \tag{100}$$

$$\tilde{\chi}^\epsilon = \pi_-^0 \phi^\epsilon. \tag{101}$$

Moreover, the four-spinors $\tilde{\varphi}^\epsilon$ and $\tilde{\chi}^\epsilon$ can be expanded as

$$\tilde{\varphi}^\epsilon := \sum_{n=0}^{\infty} \epsilon^n \tilde{\varphi}^n, \tag{102}$$

$$\tilde{\chi}^\epsilon := \sum_{n=0}^{\infty} \epsilon^n \tilde{\chi}^n. \tag{103}$$

As the next step, we derive a differential equation for φ_+^ϵ up to second order in ϵ .

5.4 Differential equation for φ_+^ϵ up to second order in ϵ

To obtain the differential equation for φ_+^ϵ up to second order in ϵ , we use Eqs. (43), (44), (86), and apply the projector π_+^0 on the differential equation for the electronic wave function ϕ_+^ϵ up to second order in ϵ for interaction with laser fields (89) according to

$$\begin{aligned} i\hbar \partial_t \pi_+^0 \phi_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \pi_+^0 \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \pi_+^0 \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \pi_-^0 \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \pi_+^0 \phi_+^\epsilon + \frac{\epsilon^2 e}{2m_e^2} \alpha^k \left[\left(\frac{1}{\epsilon} \hat{p}_k \mathcal{A}_l \right) e \mathcal{A}_l - \left(\frac{1}{\epsilon} \hat{p}_l \mathcal{A}_k \right) \hat{p}_l \right] \pi_-^0 \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\mathbf{E} - (\nabla V))] + i \mathcal{A} (\partial_t \mathcal{A}) \} \pi_+^0 \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} (\Delta V - V \Delta) \pi_+^0 \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{104}$$

Now, we derive first a differential equation for $\tilde{\varphi}_+^\epsilon$ up to second order in ϵ —since these calculations are a bit cumbersome, we give them in the Appendix C and here just state their result:

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma \left[(\nabla V) \times \hat{\Pi} + e \mathcal{A} \times \mathbf{E} \right] \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} [\hbar \nabla (\nabla V) + ie \mathcal{A} (\partial_t \mathcal{A})] \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{105}$$

In this equation, only terms appear, in which the upper two components of the wave function $\tilde{\varphi}_+^\epsilon$ are not coupled to its lower two components. Moreover, the lower two components of the wave function $\tilde{\varphi}_+^\epsilon$ are zero (see Eq. (91)). Therefore, we can substitute in Eq. (105) all the four-dimensional spinors $\tilde{\varphi}_+^\epsilon$ by the two-dimensional spinors φ_+^ϵ and the operator Σ —being a 4×4 extension of the spinor operator σ , which is a 2×2 matrix—by the spinor operator σ itself. Taking this into account and using Eq. (31), we find

$$\begin{aligned} i\hbar \partial_t \varphi_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \varphi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \sigma \mathbf{B} \varphi_+^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \varphi_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \sigma \left[(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} \right] \varphi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar}{4m_e^2} \left[\hat{\mathbf{p}} (\nabla V) + e\mathcal{A} (\partial_t \mathcal{A}) \right] \varphi_+^\epsilon + \mathcal{O}(\epsilon^3) \end{aligned} \quad (106)$$

as the differential equation for the wave function φ_+^ϵ up to second order in ϵ .

5.5 Differential equation for φ^ϵ up to second order in ϵ

We derived the differential equation (106) for φ_+^ϵ up to second order in ϵ . However, the wave function φ_+^ϵ contains just the electronic part of the total upper two-spinor φ^ϵ , and now we derive an according differential equation for this upper two-spinor φ^ϵ .

In the following, we apply $\pi_+^0 i\hbar \partial_t$ on Eq. (63), i.e., $\phi^\epsilon = \phi_+^\epsilon + \phi_-^\epsilon$. In addition, we use Eq. (93) and that the limit $\epsilon \rightarrow 0$ of the $+$ -case of Eq. (58) is $[\pi_+^0, \partial_t] = 0$. Then, we find

$$\begin{aligned} \pi_+^0 i\hbar \partial_t \phi^\epsilon &= \pi_+^0 i\hbar \partial_t (\phi_+^\epsilon + \phi_-^\epsilon) \\ \implies \pi_+^0 i\hbar \partial_t \phi^\epsilon &= \pi_+^0 i\hbar \partial_t \phi_+^\epsilon + \pi_+^0 i\hbar \partial_t \phi_-^\epsilon \\ \implies i\hbar \partial_t \pi_+^0 \phi^\epsilon &= i\hbar \partial_t \pi_+^0 \phi_+^\epsilon + i\hbar \partial_t \pi_+^0 \phi_-^\epsilon \\ \implies i\hbar \partial_t \tilde{\varphi}^\epsilon &= i\hbar \partial_t \tilde{\varphi}_+^\epsilon + i\hbar \partial_t \tilde{\varphi}_-^\epsilon. \end{aligned} \quad (107)$$

Now, we have to bring the right side of Eq. (107) into the form of an operator acting on $\tilde{\varphi}^\epsilon$ (where we will neglect terms of higher order than $\mathcal{O}(\epsilon^2)$). This right side of Eq. (107) contains two terms, namely, $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ and $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$. We will focus first on the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ in this equation, for which we can use Eq. (105). However, on the right side of Eq. (105), the wave function $\tilde{\varphi}_+^\epsilon$ appears, but not φ^ϵ . Therefore, we need a formula to rewrite the wave function $\tilde{\varphi}_+^\epsilon$ as an expression, where φ^ϵ appears. In the Appendix D, we show first how to derive this equation. It is

$$\tilde{\varphi}_+^\epsilon = \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} \left[\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}}) \right] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \quad (108)$$

Using Eq. (108), we rewrite then in Appendix D the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ and find:

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon \\ &\quad + \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \left[\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}}) \right] \tilde{\varphi}^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma \left[(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} \right] \tilde{\varphi}^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \left[\hbar \nabla (\nabla V) + i e \mathcal{A} (\partial_t \mathcal{A}) \right] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (109)$$

Having found the result (109) for the first term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ on the right side of Eq. (107), we turn now to the second term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$.

Since the calculus of this term is long, we discuss it in Appendix E and state here just the result of this calculation:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi}_-^\epsilon &= -\frac{i\epsilon^2 e\hbar}{4m_e^2} [(\partial_t \mathcal{A})\hat{\mathbf{p}} + \mathcal{A}(\nabla V)] \tilde{\varphi}^\epsilon \\
 &\quad - \frac{\epsilon^2 e\hbar}{4m_e^2} \Sigma [(\partial_t \mathcal{A}) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\nabla V)] \tilde{\varphi}^\epsilon \\
 &\quad - \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\mathbf{P}}^2 - eV \right) [\mathcal{A}\hat{\mathbf{p}} - i\Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{110}$$

As the next step, we insert into Eq. (107) the result (109) for the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ and the result (110) for the term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$. Then a differential equation for the wave function $\tilde{\varphi}^\epsilon$ can be calculated. The corresponding calculations are given in detail in Appendix F—here we give just the result:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi}^\epsilon &= \frac{1}{2m_e} \hat{\mathbf{P}}^2 \tilde{\varphi}^\epsilon - eV \tilde{\varphi}^\epsilon + \frac{\epsilon e\hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\mathbf{P}}^4 \tilde{\varphi}^\epsilon \\
 &\quad + \frac{\epsilon^2 e\hbar}{4m_e^2} \hat{\mathbf{P}} (\Sigma \times \mathbf{E}) \tilde{\varphi}^\epsilon + \frac{i\epsilon^2 e\hbar}{4m_e^2} \hat{\mathbf{P}} \mathbf{E} \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{111}$$

Since all of the operators that act in Eq. (111) on the wave function $\tilde{\varphi}^\epsilon$ do not couple its upper two components with its lower two components, and the lower two components of the wave function $\tilde{\varphi}^\epsilon$ are due to Eq. (98) just zero, we can substitute in (111) the four-spinor $\tilde{\varphi}^\epsilon$ everywhere it appears by its upper two-spinor φ^ϵ , and the 4×4 matrix Σ , which is an extension of the 2×2 spinor operator σ , by the spinor operator σ itself. Then, we find:

$$\begin{aligned}
 i\hbar \partial_t \varphi^\epsilon &= \frac{1}{2m_e} \hat{\mathbf{P}}^2 \varphi^\epsilon - eV \varphi^\epsilon + \frac{\epsilon e\hbar}{2m_e} \sigma \mathbf{B} \varphi^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\mathbf{P}}^4 \varphi^\epsilon \\
 &\quad + \frac{\epsilon^2 e\hbar}{4m_e^2} \hat{\mathbf{P}} (\sigma \times \mathbf{E}) \varphi^\epsilon + \frac{i\epsilon^2 e\hbar}{4m_e^2} \hat{\mathbf{P}} \mathbf{E} \varphi^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{112}$$

Now, we have derived the differential equation for the wave function φ^ϵ up to second order in ϵ .

However, one problem remains: while the operators

$$\hat{H}_1 := \frac{1}{2m_e} \hat{\mathbf{P}}^2, \tag{113}$$

$$\hat{H}_2 := -eV, \tag{114}$$

$$\hat{H}_3 := \frac{\epsilon e\hbar}{2m_e} \sigma \mathbf{B}, \tag{115}$$

$$\hat{H}_4 := -\frac{\epsilon^2}{8m_e^3} \hat{\mathbf{P}}^4, \tag{116}$$

which act in the first line of Eq. (112) on the wave function φ^ϵ , are Hermitian, the operators

$$\hat{H}_5 := \frac{\epsilon^2 e\hbar}{4m_e^2} \hat{\mathbf{P}} (\sigma \times \mathbf{E}), \tag{117}$$

$$\hat{H}_6 := \frac{i\epsilon^2 e\hbar}{4m_e^2} \hat{\mathbf{P}} \mathbf{E}, \tag{118}$$

which act in the second line of Eq. (112) on the wave function φ^ϵ , are non-Hermitian. Because of these non-Hermitian operators \hat{H}_5 and \hat{H}_6 , in general, the norm of the wave function φ^ϵ is not conserved during its propagation in time.

The reason why these norm deviations occur during the propagation of the wave function φ^ϵ is:

According to Eq. (97), the four-dimensional spinor ϕ^ϵ can be represented with a two-dimensional upper spinor φ^ϵ and a two-dimensional lower spinor χ^ϵ . As given in Eq. (66), the four-dimensional spinor ϕ^ϵ is normalized but it still allows the two-dimensional spinors φ^ϵ and χ^ϵ to exchange population between each other during their propagation in time. Because of this exchange of population, the norms of the two-dimensional spinors φ^ϵ and χ^ϵ are not conserved.

5.6 Differential equation for the normalized upper wave function φ_n^ϵ

In the following, we will discuss how to bring the differential equation (112) for the non-normalized wave function φ^ϵ in a form with a normalized wave-function φ_n^ϵ . To do that, we have to make the operators \hat{H}_5 and \hat{H}_6 on the right side of (112) Hermitian.

Therefore, we regard that the Hermitian part \hat{O}_h of any operator \hat{O} is

$$\hat{O}_h = \frac{1}{2} (\hat{O} + \hat{O}^\dagger). \quad (119)$$

The adjoint operators to the operators \hat{H}_5 and \hat{H}_6 are

$$\hat{H}_5^\dagger = \frac{\epsilon^2 e \hbar}{4m_e^2} (\boldsymbol{\sigma} \times \mathbf{E}) \hat{\Pi}, \quad (120)$$

$$\hat{H}_6^\dagger = -\frac{i\epsilon^2 e \hbar}{4m_e^2} \mathbf{E} \hat{\Pi}, \quad (121)$$

hence

$$\hat{H}_{5h} = \frac{\epsilon^2 e \hbar}{8m_e^2} [\hat{\Pi} (\boldsymbol{\sigma} \times \mathbf{E}) + (\boldsymbol{\sigma} \times \mathbf{E}) \hat{\Pi}], \quad (122)$$

$$\begin{aligned} \hat{H}_{6h} &= \frac{i\epsilon^2 e \hbar}{8m_e^2} (\hat{\Pi} \mathbf{E} - \mathbf{E} \hat{\Pi}) \\ &= \frac{i\epsilon^2 e \hbar}{8m_e^2} (-i\hbar \nabla \mathbf{E} + e\mathcal{A} \mathbf{E} + i\hbar \mathbf{E} \nabla - e\mathbf{E}\mathcal{A}) \\ &= \frac{\epsilon^2 e \hbar^2}{8m_e^2} (\nabla \mathbf{E} - \mathbf{E} \nabla) \\ &= \frac{\epsilon^2 e \hbar^2}{8m_e^2} [(\nabla \mathbf{E}) + \mathbf{E} \nabla - \mathbf{E} \nabla] \\ &= \frac{\epsilon^2 e \hbar^2}{8m_e^2} (\nabla \mathbf{E}). \end{aligned} \quad (123)$$

As an additional detail, we mention that the term \hat{H}_{5h} given in (122) can be rewritten using Eqs. (31), (32) in the following form:

$$\hat{H}_{5h} = \frac{\epsilon^2 e \hbar}{8m_e^2} \epsilon_{klm} (\hat{\Pi}_k \sigma_l E_m + \sigma_l E_m \hat{\Pi}_k)$$

$$\begin{aligned}
 &= \frac{\epsilon^2 e \hbar}{8m_e^2} \epsilon_{klm} \left[2\hat{\Pi}_k \sigma_l E_m + i\hbar \sigma_l (\partial_k E_m) \right] \\
 &= \frac{\epsilon^2 e \hbar}{4m_e^2} \hat{\Pi} (\boldsymbol{\sigma} \times \mathbf{E}) - \frac{i\epsilon^2 e \hbar^2}{8m_e^2} \boldsymbol{\sigma} (\nabla \times \mathbf{E}) \\
 &= \hat{H}_5 - \frac{i\epsilon^2 e \hbar}{8m_e^2} \boldsymbol{\sigma} (\nabla \times \mathbf{E}).
 \end{aligned} \tag{124}$$

Now, we regard Eq. (24) for the rotation of the electric field $\nabla \times \mathbf{E}$ and find:

$$\hat{H}_{5h} = \hat{H}_5 + \mathcal{O}(\epsilon^3). \tag{125}$$

If the rotation of the electric fields vanishes, from Eq. (124) follows that we have even $\hat{H}_{5h} = \hat{H}_5$ then.

Nevertheless, for electric fields with a non-vanishing rotation, it is still advisable to use the term \hat{H}_{5h} instead of the term \hat{H}_5 as a summand in the Hamiltonian, because the Hermitian term \hat{H}_{5h} does not cause norm violations for all kind of electric fields \mathbf{E} , while this applies for the term \hat{H}_5 only for electric fields with a vanishing rotation.

Having discussed this detail related to the term \hat{H}_{5h} , using the results (122) and (123), we finally obtain the differential equation for the normalized upper wave function φ_n^ϵ :

$$\begin{aligned}
 i\hbar \partial_t \varphi_n^\epsilon &= \frac{1}{2m_e} \hat{\Pi}^2 \varphi_n^\epsilon - eV \varphi_n^\epsilon + \frac{\epsilon e \hbar}{2m_e} \boldsymbol{\sigma} \mathbf{B} \varphi_n^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \varphi_n^\epsilon \\
 &+ \frac{\epsilon^2 e \hbar}{8m_e^2} \left[\hat{\Pi} (\boldsymbol{\sigma} \times \mathbf{E}) + (\boldsymbol{\sigma} \times \mathbf{E}) \hat{\Pi} \right] \varphi_n^\epsilon + \frac{\epsilon^2 e \hbar^2}{8m_e^2} (\nabla \mathbf{E}) \varphi_n^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{126}$$

The result (126) is the Schrödinger equation with the relativistic corrections we searched for, and it coincides with the result in [12]. In detail, these relativistic corrections can be split into four different terms; one term scaling with ϵ in first order and three terms scaling with ϵ in second order. Due to [12], these terms can be described in the following way:

The single first-order term is \hat{H}_3 (see Eq. (115)), which can be related to the Zeeman splitting in the magnetic field.

The first second-order term is \hat{H}_4 (see Eq. (116)), which can be related to a relativistic correction of the kinetic energy; the following second-order term is \hat{H}_{5h} (see Eq. (122)), which is proportional for the special case of static electromagnetic central fields with

$$\mathcal{A} = \mathbf{B} = \mathbf{0}, \tag{127}$$

$$\mathbf{E} = -\frac{\mathbf{r}}{r} \frac{\partial V}{\partial r} \tag{128}$$

to an operator $\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$, where $\hat{\mathbf{S}} = \frac{\hbar}{2} \boldsymbol{\sigma}$ is the so-called spin operator and $\hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}}$ is the angular momentum. Therefore, this operator \hat{H}_{5h} is called the spin-orbit interaction.

Finally, the last second-order term is \hat{H}_{6h} , which is the Darwin term: a relativistic correction that can be related to the charge density $\rho = \nabla \mathbf{E} / (4\pi)$ in the system.

As an additional comment to Eq. (126), we mention that it also corresponds to the according results in [13–15]—whereas in these references, the spin-orbit interaction is given in the above-mentioned form for the special case of static electromagnetic fields, where \hat{H}_{5h} is proportional to the operator $\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$.⁴

⁴ Moreover, in the Refs. [13–15], the kinematic momentum operator $\hat{\Pi}$ is approximated by the momentum operator $\hat{\mathbf{p}}$ in the term \hat{H}_4 (see also Footnote 3 in Sect. 5.2).

Thus, using the Mauser method, we could derive the differential equation (126) in the Schrödinger form containing relativistic corrections up to the second order in ϵ that coincides with other literature results [12–15] derived with the Foldy–Wouthuysen scheme [16].

5.7 Relation of the discussed differential equations to the Pauli equation

As a final part of Sect. 5, we discuss how the Pauli equation [13–15, 17] is related to the differential equations (106), (112), and (126) derived in Sects. 5.4, 5.5, and 5.6, because Mauser and his coworkers derived the Pauli equation from a differential equation for the wave function φ_+^ϵ in [8–10] already.

At first sight, one might wonder why they found the Pauli equation from an equation related to the electronic part φ_+^ϵ of the upper two-spinor φ^ϵ and not from an equation related to the wave function φ_n^ϵ , since we needed in this work the differential equation (126) related to the wave function φ_n^ϵ to derive a differential equation in the Schrödinger form containing relativistic corrections up to the second order in ϵ that coincides with other literature results. As an addition to the works of Mauser [8–10], we will clarify this point with the discussion below about Eqs. (106), (112), and (126):

If we regard on the left side of the differential equation (126) for φ_n^ϵ only all the expansion terms up to the first expansion order $\mathcal{O}(\epsilon)$, Eq. (126) is approximated as a Pauli equation that takes this form (where we note the approximative wave function solving this equation as φ_p^ϵ):

$$i\hbar \partial_t \varphi_p^\epsilon = \frac{1}{2m_e} \hat{\mathbf{P}}^2 \varphi_p^\epsilon - eV \varphi_p^\epsilon + \frac{\epsilon e \hbar}{2m_e} \boldsymbol{\sigma} \mathbf{B} \varphi_p^\epsilon. \quad (129)$$

Moreover, if we take into account on the right side of the differential equation (112) for the wave function φ^ϵ just all the expansion terms up to the first expansion order $\mathcal{O}(\epsilon)$ and approximate the wave function φ^ϵ as φ_p^ϵ , we find again the Pauli equation (129). This result can be explained in this way:

As discussed in Sect. 5.6, on the right side of Eq. (112) the operators \hat{H}_a , $a \in \{1, 2, \dots, 6\}$, act on the wave function φ^ϵ and on the right side of Eq. (126) their Hermitian parts \hat{H}_{ah} act on the wave function φ_n^ϵ . Among these six operators \hat{H}_a , three operators are $\mathcal{O}(\epsilon^0)$ or $\mathcal{O}(\epsilon)$ —these three operators are \hat{H}_1 , \hat{H}_2 , \hat{H}_3 , and all three of them are Hermitian. Thus, they appear in the same form in Eqs. (112) and (126). In addition, the operators \hat{H}_4 , \hat{H}_5 , \hat{H}_6 and their respective Hermitian parts are $\mathcal{O}(\epsilon^2)$ —so, these operators are neglected if we take into account just operators up to the order $\mathcal{O}(\epsilon)$.

Therefore, it is comprehensible that Eq. (112) becomes the Pauli equation (129), too, if we approximate it analogously to the derivation of the Pauli equation starting from Eq. (126), where we took into account only all the expansion terms up to the first expansion order $\mathcal{O}(\epsilon)$.

Furthermore, if we regard on the right side of Eq. (106) only the expansion terms up to the expansion order $\mathcal{O}(\epsilon)$ and substitute the electronic part φ_+^ϵ of the upper two-spinor φ^ϵ by the wave function φ_p^ϵ , then we find the Pauli equation (129) again. This finding can be cleared up in the following way: using Eqs. (91), (98), and (108), we realize that

$$\begin{aligned} \varphi_+^\epsilon &= \varphi^\epsilon + \frac{\epsilon^2 e}{4m_e^2} [\mathcal{A} \hat{\mathbf{p}} - i \boldsymbol{\sigma} (\mathcal{A} \times \hat{\mathbf{p}})] \varphi^\epsilon + \mathcal{O}(\epsilon^3), \\ \implies \varphi_+^\epsilon &= \varphi^\epsilon + \mathcal{O}(\epsilon^2). \end{aligned} \quad (130)$$

Thus, we find this consequence of the transformations from the differential equation (106) for the wave function φ_+^ϵ to the differential equation (112) for the wave function φ^ϵ :

Because of Eq. (130), these transformations modify only the kind of operators on the right side of these equations, which are at least $\mathcal{O}(\epsilon^2)$. Therefore, both on the right side of Eq. (106) and on the right side of Eq. (112), up to the expansion order $\mathcal{O}(\epsilon)$ just the same operators \hat{H}_1 , \hat{H}_2 and \hat{H}_3 act on the wave functions φ_+^ϵ and φ^ϵ , respectively.

Therefore, both Eqs. (106) and (112) can be transformed into the Pauli equation (129) within the approximations for these equations described above.

Thus, the discussion above clarifies why we can derive the Pauli equation from all three differential equations (106) for φ_+^ϵ , (112) for φ^ϵ , and (126) for φ_n^ϵ —and so, we could verify the result of Mauser and his coworkers given in [8–10], where they derived the Pauli equation from a differential equation for the wave function φ_+^ϵ .

However, if we are interested to find a differential equation in the Schrödinger form containing relativistic corrections up to the second order in ϵ that coincides with the literature results derived with the Foldy–Wouthuysen scheme [16], it is not sufficient to take into account just the electronic part φ_+^ϵ for the wave function in this differential equation. Instead, we have to take into account both the electronic part φ_+^ϵ and the positronic part φ_-^ϵ of the upper two-spinor φ^ϵ . This is done in this work within the derivation from Eqs. (106) to (112) in Sect. 5.5. Furthermore, we have to make an another transformation to obtain a normalized wave function φ_n^ϵ , what can be found in this work within the derivation from Eqs. (112) to (126) in Sect. 5.6.

6 Summary

In this paper, we further developed the works [8–11] of Mauser and his coworkers, where they developed an ansatz how to split the Dirac equation into a set of two differential equations: there is one equation, where an eigenfunction for a free moving electron and another equation including an eigenfunction for a free moving positron appears. In our work, we addressed the question how to find a differential equation of the Schrödinger form plus relativistic corrections using the ansatz of Mauser. Here, we regard all relativistic corrections up to second order in the reciprocal of the speed of light—and we find for these corrections, in coincidence with other literature results derived with the Foldy–Wouthuysen scheme, a first order term related to the Zeeman splitting and three second-order terms: a relativistic correction to the kinetic energy, the spin–orbit interaction and the Darwin term.

To find these results, we had to regard several aspects in our calculations.

The first point is that one has to regard carefully how the electromagnetic potentials and their spatial derivatives depend on the reciprocal of the speed of light—we analyze a scenario which is typical for the interaction of a laser pulse with a molecular system, where the scalar potential and its spatial derivations of it do not depend in general in the lowest expansion order on the reciprocal of the speed of light. However, not the vector potential itself but another quantity, which we call the scaled vector potential being the vector potential divided by the speed of light, is independent in lowest expansion order of the reciprocal of the speed of light. In addition, each spatial derivative applied on the scaled vector potential increases its leading lowest expansion order related to the reciprocal of the speed of light by one.

The next critical question is which wave function does one analyze: we analyze in our work the complete upper two-spinor of the four-spinor appearing in the Dirac equation. In particular, we realized as a further development to the analysis in [9, 10] that it is not sufficient for the reproduction of the literature results derived using the Foldy–Wouthuysen scheme for all relativistic corrections of the Schrödinger equation up to second order in the reciprocal of the speed of light if one regards only the part of the wave function related to a free moving electron. At least, regarding just this part of the wave function is sufficient to derive the Pauli equation that contains the relativistic corrections of the Schrödinger equation up to first order in the reciprocal of the speed of light.

As a last point, one has to regard for the derivation of relativistic corrections of the Schrödinger equation up to second order in the reciprocal of the speed of light to bring the Hamiltonian into a Hermitian, norm-conserving form.

Therefore, with our calculations, we have found the missing link between the ansatz of Mauser and the approximation of the Dirac equation derived in the literature using the Foldy–Wouthuysen scheme.

Appendix A: The positronic wave function ϕ_-^ϵ

In this Appendix A, we transform the six summands in Eq. (76) that we give here again for clarity:

$$\begin{aligned} \phi_-^\epsilon &= \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e\mathcal{A}_k \alpha^k \phi_-^\epsilon \right) \\ &\quad - \frac{\epsilon^2}{2m_e} \pi_-^\epsilon (eV\phi_+^\epsilon) - \frac{\epsilon^2}{2m_e} \pi_-^\epsilon (eV\phi_-^\epsilon) \\ &\quad - \frac{\epsilon^2}{2m_e} \frac{\hat{\mathbf{p}}^2}{2m_e} \phi_-^\epsilon - \frac{i\hbar\epsilon^2}{2m_e} \partial_l \phi_-^\epsilon + \mathcal{O}(\epsilon^5). \end{aligned}$$

Then, we simplify the sum of these six summands and doing so, we derive a result for the positronic wave function ϕ_-^ϵ up to the third order in ϵ .

Now, we start with the calculation of the first summand.

Analysis for the first summand:

The first summand in Eq. (76) is rewritten as

$$\begin{aligned} \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{\epsilon}{2m_e} \left(\pi_-^0 + \frac{i\hbar}{2m_e} \epsilon \alpha^l \partial_l - \frac{\hbar^2}{4m_e^2} \epsilon^2 \beta \Delta \right) \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \mathcal{O}(\epsilon^4) \\ &= \frac{1}{2} \frac{\epsilon}{m_e} e\mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon + \frac{i\hbar}{4} \frac{\epsilon^2}{m_e^2} \alpha^l \partial_l \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) \\ &\quad - \frac{\hbar^2}{8} \frac{\epsilon^3}{m_e^3} \beta \Delta \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \mathcal{O}(\epsilon^4) \\ &= \frac{1}{2} \frac{\epsilon}{m_e} e\mathcal{A}_k \alpha^k \left(\pi_+^\epsilon + \frac{i\hbar}{2m_e} \epsilon \alpha^l \partial_l - \frac{\hbar^2}{4m_e^2} \epsilon^2 \beta \Delta \right) \phi_+^\epsilon \\ &\quad + \frac{i\hbar}{4} \frac{\epsilon^2}{m_e^2} \alpha^l \partial_l \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) - \frac{\hbar^2}{8} \frac{\epsilon^3}{m_e^3} \beta \Delta \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \mathcal{O}(\epsilon^4), \end{aligned} \tag{A.1}$$

hence

$$\begin{aligned} \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e\mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon + \frac{i\epsilon^2 e\hbar}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \partial_l \phi_+^\epsilon - \frac{\epsilon^3 e\hbar^2}{8m_e^3} \alpha^k \beta \mathcal{A}_k \Delta \phi_+^\epsilon \\ &\quad + \frac{i\epsilon^2 e\hbar}{4m_e^2} \alpha^l \alpha^k \partial_l \mathcal{A}_k \phi_+^\epsilon - \frac{\epsilon^3 e\hbar^2}{8m_e^3} \beta \alpha^k \Delta \mathcal{A}_k \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\ &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon + \frac{i\epsilon^2 e\hbar}{4m_e^2} \left(\alpha^k \alpha^l \mathcal{A}_k \partial_l + \alpha^l \alpha^k \partial_l \mathcal{A}_k \right) \phi_+^\epsilon \\ &\quad - \frac{\epsilon^3 e\hbar^2}{8m_e^3} \left(\alpha^k \beta \mathcal{A}_k \Delta + \beta \alpha^k \Delta \mathcal{A}_k \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\ &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon \\ &\quad + \frac{i\epsilon^2 e\hbar}{4m_e^2} \left[\left(\alpha^k \alpha^l + \alpha^l \alpha^k \right) \mathcal{A}_k \partial_l + \alpha^l \alpha^k \left(\partial_l \mathcal{A}_k \right) \right] \phi_+^\epsilon \\ &\quad - \frac{\epsilon^3 e\hbar^2}{8m_e^3} \left[\left(\alpha^k \beta + \beta \alpha^k \right) \mathcal{A}_k \Delta \right. \\ &\quad \left. + 2\beta \alpha^k \left(\partial_n \mathcal{A}_k \right) \partial_n + \beta \alpha^k \left(\Delta \mathcal{A}_k \right) \right] \phi_+^\epsilon + \mathcal{O}(\epsilon^4), \end{aligned} \tag{A.2}$$

where in the last step

$$\Delta f g = (\Delta f) g + 2(\partial_n f) \partial_n g + f \Delta g \tag{A.3}$$

was used.

For the further transformation of Eq. (A.2), we apply Eqs. (79), (80), (82), and regard that because of Eq. (19) the following formula is true for m -th component of the magnetic field vector \mathbf{B} :

$$B_m = \frac{1}{\epsilon} [\nabla \times \mathcal{A}]_m = \frac{1}{\epsilon} \varepsilon_{lkm} (\partial_l \mathcal{A}_k). \tag{A.4}$$

In addition, we take into account Eq. (31) and that for the k -th component of the scaled vector potential \mathcal{A} because of the Coulomb gauge (6) and because of Eq. (16) these equations are true:

$$\partial_k \mathcal{A}_k = 0, \tag{A.5}$$

$$\partial_n \mathcal{A}_k = \mathcal{O}(\epsilon), \tag{A.6}$$

$$\Delta \mathcal{A}_k = \mathcal{O}(\epsilon^2). \tag{A.7}$$

Then, we transform Eq. (A.2) in the following way:

$$\begin{aligned} \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon + \frac{i\epsilon^2 e \hbar}{4m_e^2} [2\mathcal{A}_k \partial_k + (\partial_k \mathcal{A}_k) + i\varepsilon_{lkm} \Sigma^m (\partial_l \mathcal{A}_k)] \phi_+^\epsilon \\ &\quad - \frac{\epsilon^3 e \hbar^2}{8m_e^3} \beta \alpha^k [2(\partial_n \mathcal{A}_k) \partial_n + (\Delta \mathcal{A}_k)] \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\ &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon - \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon + \mathcal{O}(\epsilon^4), \end{aligned} \tag{A.8}$$

and finally, we find for the first summand in Eq. (76):

$$\frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) = \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon + \mathcal{O}(\epsilon^4). \tag{A.9}$$

Analysis for the second summand:

Using $\phi_-^\epsilon = \mathcal{O}(\epsilon)$, see Eq. (78), the second summand in Eq. (76) is rewritten as

$$\begin{aligned} \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) &= \frac{\epsilon}{2m_e} \left(\pi_-^0 + \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^l \partial_l \right) \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) + \mathcal{O}(\epsilon^4) \\ &= \frac{1}{2} \frac{\epsilon}{m_e} e \mathcal{A}_k \alpha^k \pi_+^0 \phi_-^\epsilon + \frac{i\hbar}{4} \frac{\epsilon^2}{m_e^2} \alpha^l \partial_l \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) + \mathcal{O}(\epsilon^4) \\ &= \frac{1}{2} \frac{\epsilon}{m_e} e \mathcal{A}_k \alpha^k \left(\pi_+^\epsilon + \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^l \partial_l \right) \phi_-^\epsilon \\ &\quad + \frac{i\hbar}{4} \frac{\epsilon^2}{m_e^2} \alpha^l \partial_l \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) + \mathcal{O}(\epsilon^4), \end{aligned} \tag{A.10}$$

hence

$$\begin{aligned} \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) &= \frac{i\epsilon^2 e \hbar}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \partial_l \phi_-^\epsilon + \frac{i\epsilon^2 e \hbar}{4m_e^2} \alpha^l \alpha^k \partial_l \mathcal{A}_k \phi_-^\epsilon + \mathcal{O}(\epsilon^4) \\ &= \frac{i\epsilon^2 e \hbar}{4m_e^2} \left(\alpha^k \alpha^l \mathcal{A}_k \partial_l + \alpha^l \alpha^k \partial_l \mathcal{A}_k \right) \phi_-^\epsilon + \mathcal{O}(\epsilon^4) \\ &= \frac{i\epsilon^2 e \hbar}{4m_e^2} \left[\left(\alpha^k \alpha^l + \alpha^l \alpha^k \right) \mathcal{A}_k \partial_l + \alpha^l \alpha^k (\partial_l \mathcal{A}_k) \right] \phi_-^\epsilon + \mathcal{O}(\epsilon^4). \end{aligned} \tag{A.11}$$

Using Eqs. (31), (79), (80), (A.4), (A.5), and $\phi_-^\epsilon = \mathcal{O}(\epsilon)$, we get

$$\frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) = \frac{i\epsilon^2 e \hbar}{4m_e^2} [2\mathcal{A}_k \partial_k + (\partial_k \mathcal{A}_k) + i\varepsilon_{lkm} \Sigma^m (\partial_l \mathcal{A}_k)] \phi_-^\epsilon + \mathcal{O}(\epsilon^4)$$

$$\begin{aligned}
&= -\frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi_-^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \mathbf{\Sigma} \mathbf{B} \phi_-^\epsilon + \mathcal{O}(\epsilon^4) \\
&= -\frac{\epsilon^2 e \mathcal{A}_k}{2m_e} \frac{\hat{p}_k}{m_e} \phi_-^\epsilon + \mathcal{O}(\epsilon^4).
\end{aligned} \tag{A.12}$$

Using Eqs. (76), (A.8), i.e.

$$\begin{aligned}
\phi_-^\epsilon &= \frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_l \alpha^l \phi_+^\epsilon \right) + \mathcal{O}(\epsilon^2) \\
&= \frac{\epsilon e \mathcal{A}_l}{2m_e} \alpha^l \phi_+^\epsilon + \mathcal{O}(\epsilon^2),
\end{aligned} \tag{A.13}$$

Equations (31), and (A.6), we finally obtain

$$\begin{aligned}
\frac{\epsilon}{2m_e} \pi_-^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) &= -\frac{\epsilon^2 e \mathcal{A}_k}{2m_e} \frac{\hat{p}_k}{m_e} \frac{\epsilon e \mathcal{A}_l}{2m_e} \alpha^l \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= \frac{i\epsilon^3 e^2 \hbar \mathcal{A}_k}{4m_e^3} \alpha^l \partial_k \mathcal{A}_l \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= \frac{i\epsilon^3 e^2 \hbar \mathcal{A}_k}{4m_e^3} \alpha^l [\mathcal{A}_l \partial_k + (\partial_k \mathcal{A}_l)] \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= \frac{i\epsilon^3 e^2 \hbar \mathcal{A}_k \mathcal{A}_l}{4m_e^3} \partial_k \alpha^l \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= -\frac{\epsilon^3 e^2 \mathcal{A}_k \mathcal{A}_l}{4m_e^2} \frac{\hat{p}_k}{m_e} \alpha^l \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= -\frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{e \mathcal{A}_l \hat{p}_l}{2m_e^2} \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
\end{aligned} \tag{A.14}$$

Analysis for the third summand:

The third summand in Eq. (76) is rewritten as

$$\begin{aligned}
-\frac{\epsilon^2}{2m_e} \pi_-^\epsilon (eV\phi_+^\epsilon) &= -\frac{\epsilon^2}{2m_e} \left(\pi_-^0 + \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k \right) (eV\phi_+^\epsilon) + \mathcal{O}(\epsilon^4) \\
&= -\frac{1}{2} \frac{\epsilon^2}{m_e} eV\pi_-^0 \phi_+^\epsilon - \frac{i\hbar}{4} \frac{\epsilon^3}{m_e^2} \alpha^k \partial_k (eV\phi_+^\epsilon) + \mathcal{O}(\epsilon^4) \\
&= -\frac{1}{2} \frac{\epsilon^2}{m_e} eV \left(\pi_-^\epsilon - \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k \right) \phi_+^\epsilon - \frac{i\hbar}{4} \frac{\epsilon^3}{m_e^2} \alpha^k \partial_k (eV\phi_+^\epsilon) + \mathcal{O}(\epsilon^4),
\end{aligned} \tag{A.15}$$

hence

$$\begin{aligned}
-\frac{\epsilon^2}{2m_e} \pi_-^\epsilon (eV\phi_+^\epsilon) &= \frac{i\epsilon^3 e \hbar}{4m_e^2} \alpha^k V \partial_k \phi_+^\epsilon - \frac{i\epsilon^3 e \hbar}{4m_e^2} \alpha^k \partial_k V \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= \frac{i\epsilon^3 e \hbar}{4m_e^2} \alpha^k (V \partial_k - \partial_k V) \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= \frac{i\epsilon^3 e \hbar}{4m_e^2} \alpha^k [V \partial_k - V \partial_k - (\partial_k V)] \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
&= -\frac{i\epsilon^3 e \hbar}{4m_e^2} (\partial_k V) \alpha^k \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
\end{aligned} \tag{A.16}$$

Analysis for the fourth summand:

Using $\phi_-^\epsilon = \mathcal{O}(\epsilon)$, see Eq. (78), the fourth summand in Eq. (76) is rewritten as

$$-\frac{\epsilon^2}{2m_e} \pi_-^\epsilon (eV\phi_-^\epsilon) = -\frac{\epsilon^2}{2m_e} \pi_-^0 (eV\phi_-^\epsilon) + \mathcal{O}(\epsilon^4)$$

$$\begin{aligned}
 &= -\frac{1}{2} \frac{\epsilon^2}{m_e} eV \pi_-^0 \phi_-^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= -\frac{1}{2} \frac{\epsilon^2}{m_e} eV \pi_-^\epsilon \phi_-^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= -\frac{\epsilon^2 eV}{2m_e} \phi_-^\epsilon + \mathcal{O}(\epsilon^4).
 \end{aligned} \tag{A.17}$$

Using Eq. (A.13), we finally obtain

$$\begin{aligned}
 -\frac{\epsilon^2}{2m_e} \pi_-^\epsilon (eV \phi_-^\epsilon) &= -\frac{\epsilon^3 e^2 V \mathcal{A}_k}{4m_e^2} \alpha^k \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= -\frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{eV}{2m_e} \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
 \end{aligned} \tag{A.18}$$

Analysis for the fifth summand:

Using Eq. (31), $\hat{\mathbf{p}}^2 = \hat{p}_k^2 = -\hbar^2 \partial_k^2$, and Eqs. (A.6), (A.7), and (A.13), the fifth summand in Eq. (76) is rewritten as

$$\begin{aligned}
 -\frac{\epsilon^2}{2m_e} \frac{\hat{\mathbf{p}}^2}{2m_e} \phi_-^\epsilon &= \frac{\epsilon^2 \hbar^2}{4m_e^2} \partial_k^2 \phi_-^\epsilon \\
 &= \frac{\epsilon^3 e \hbar^2}{8m_e^3} \alpha^l \partial_k^2 \mathcal{A}_l \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= \frac{\epsilon^3 e \hbar^2 \mathcal{A}_l}{8m_e^3} \alpha^l \partial_k^2 \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= -\frac{\epsilon^3 e \mathcal{A}_k}{8m_e} \alpha^k \frac{\hat{p}_l^2}{m_e^2} \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
 \end{aligned} \tag{A.19}$$

Analysis for the sixth summand:

Using Eq. (A.13), the sixth summand in Eq. (76) is rewritten as

$$\begin{aligned}
 -\frac{i\hbar\epsilon^2}{2m_e} \partial_t \phi_-^\epsilon &= -\frac{i\epsilon^3 e \hbar}{4m_e^2} \alpha^k \partial_t \mathcal{A}_k \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= -\frac{i\epsilon^3 e \hbar}{4m_e^2} (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon - \frac{i\epsilon^3 e \hbar \mathcal{A}_k}{4m_e^2} \alpha^k \partial_t \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
 \end{aligned} \tag{A.20}$$

To obtain the differential equation for ϕ_+^ϵ up to zeroth order in ϵ , we use Eqs. (51), (63), and (74) to get

$$\begin{aligned}
 i\hbar \partial_t \phi_+^\epsilon &= -\frac{\hbar^2}{2m_e} \Delta \phi_+^\epsilon + \pi_+^\epsilon \left(\frac{1}{\epsilon} e \mathcal{A}_k \alpha^k \phi_+^\epsilon - eV \phi_+^\epsilon \right) + \mathcal{O}(\epsilon^2) \\
 &= -\frac{\hbar^2}{2m_e} \Delta \phi_+^\epsilon + \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) \\
 &\quad - \pi_+^\epsilon (eV \phi_+^\epsilon) - \pi_+^\epsilon (eV \phi_-^\epsilon) + \mathcal{O}(\epsilon^2).
 \end{aligned} \tag{A.21}$$

Using Eqs. (31), (80) and (A.6), we obtain for the second term

$$\begin{aligned}
 \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \left[\frac{1}{\epsilon} \pi_+^0 - \frac{i\hbar}{2m_e} \alpha^l \partial_l + \mathcal{O}(\epsilon) \right] \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) \\
 &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon - \frac{ie\hbar}{2m_e} \alpha^l \alpha^k \partial_l \mathcal{A}_k \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
 &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon - \frac{ie\hbar}{2m_e} \alpha^l \alpha^k \mathcal{A}_k \partial_l \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
 &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon - \frac{ie\hbar}{2m_e} \left(2\delta_{kl} - \alpha^k \alpha^l \right) \mathcal{A}_k \partial_l \phi_+^\epsilon + \mathcal{O}(\epsilon)
 \end{aligned}$$

$$\begin{aligned}
&= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon + \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \frac{i\epsilon \hbar}{2m_e} \alpha^l \partial_l \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \left(\pi_-^0 + \frac{i\epsilon \hbar}{2m_e} \alpha^l \partial_l \right) \phi_+^\epsilon + \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_-^\epsilon \phi_+^\epsilon + \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= e \mathcal{A}_k \frac{\hat{p}_k}{m_e} \phi_+^\epsilon + \mathcal{O}(\epsilon).
\end{aligned} \tag{A.22}$$

For the third term, we obtain with $\phi_-^\epsilon = \mathcal{O}(\epsilon)$, Eqs. (79), (A.13), and $\mathcal{A} \times \mathcal{A} = \mathbf{0}$

$$\begin{aligned}
\frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) &= \frac{1}{\epsilon} \pi_+^0 \left(e \mathcal{A}_k \alpha^k \phi_-^\epsilon \right) + \mathcal{O}(\epsilon) \\
&= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_-^0 \phi_-^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_-^\epsilon \phi_-^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \phi_-^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e^2 \mathcal{A}_k \mathcal{A}_l}{2m_e} \alpha^k \alpha^l \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e^2 \mathcal{A}_k \mathcal{A}_l}{2m_e} (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{e^2 \mathcal{A}_k^2}{2m_e} \phi_+^\epsilon + \mathcal{O}(\epsilon).
\end{aligned} \tag{A.23}$$

Furthermore, we easily get for both last terms:

$$\begin{aligned}
-\pi_+^\epsilon (eV\phi_+^\epsilon) &= -\pi_+^0 (eV\phi_+^\epsilon) + \mathcal{O}(\epsilon) \\
&= -eV\pi_+^0 \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= -eV\pi_+^\epsilon \phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= -eV\phi_+^\epsilon + \mathcal{O}(\epsilon),
\end{aligned} \tag{A.24}$$

$$\begin{aligned}
-\pi_+^\epsilon (eV\phi_-^\epsilon) &= -\pi_+^0 (eV\phi_-^\epsilon) + \mathcal{O}(\epsilon) \\
&= -eV\pi_+^0 \phi_-^\epsilon + \mathcal{O}(\epsilon) \\
&= -eV\pi_+^\epsilon \phi_-^\epsilon + \mathcal{O}(\epsilon) \\
&= \mathcal{O}(\epsilon).
\end{aligned} \tag{A.25}$$

Then, along with these equations and Eq. (31), the differential equation (74) for ϕ_+^ϵ up to zeroth order in ϵ is rewritten as

$$\begin{aligned}
i\hbar \partial_t \phi_+^\epsilon &= \frac{1}{2m_e} \left(\hat{p}_k^2 + 2e\mathcal{A}_k \hat{p}_k + e^2 \mathcal{A}_k^2 \right) \phi_+^\epsilon - eV\phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{1}{2m_e} \left[\hat{p}_k^2 + e(\hat{p}_k \mathcal{A}_k) + 2e\mathcal{A}_k \hat{p}_k + e^2 \mathcal{A}_k^2 \right] \phi_+^\epsilon - eV\phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{1}{2m_e} \left(\hat{p}_k^2 + e\hat{p}_k \mathcal{A}_k + e\mathcal{A}_k \hat{p}_k + e^2 \mathcal{A}_k^2 \right) \phi_+^\epsilon - eV\phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{1}{2m_e} (\hat{p}_k + e\mathcal{A}_k)^2 \phi_+^\epsilon - eV\phi_+^\epsilon + \mathcal{O}(\epsilon) \\
&= \frac{1}{2m_e} \hat{\Pi}^2 \phi_+^\epsilon - eV\phi_+^\epsilon + \mathcal{O}(\epsilon),
\end{aligned} \tag{A.26}$$

where in the last steps we used Eq. (A.5), i.e., $\partial_k \mathcal{A}_k = \hat{p}_k \mathcal{A}_k = 0$, Eq. (32), and $\hat{\Pi}^2 = \hat{\Pi}_k^2$. Then, the sixth summand in Eq. (76) is obtained from Eq. (A.20) as

$$\begin{aligned}
 -\frac{i\hbar\epsilon^2}{2m_e} \partial_t \phi_-^\epsilon &= -\frac{i\epsilon^3 e\hbar}{4m_e^2} (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon - \frac{\epsilon^3 e \mathcal{A}_k}{8m_e^3} \alpha^k \left(\hat{p}_l^2 + 2e \mathcal{A}_l \hat{p}_l + e^2 \mathcal{A}_l^2 \right) \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{eV}{2m_e} \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
 \end{aligned}
 \tag{A.27}$$

Result:

With Eqs. (A.9), (A.14), (A.16), (A.18), (A.19), (A.27), the positronic wave function ϕ_-^ϵ (74) up to third order in ϵ is rewritten as

$$\begin{aligned}
 \phi_-^\epsilon &= \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon - \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{e \mathcal{A}_l \hat{p}_l}{2m_e^2} \phi_+^\epsilon \\
 &\quad - \frac{i\epsilon^3 e \hbar}{4m_e^2} (\partial_k V) \alpha^k \phi_+^\epsilon - \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{eV}{2m_e} \phi_+^\epsilon - \frac{\epsilon^3 e \mathcal{A}_k}{8m_e} \alpha^k \frac{\hat{p}_l^2}{m_e^2} \phi_+^\epsilon \\
 &\quad - \frac{i\epsilon^3 e \hbar}{4m_e^2} (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon - \frac{\epsilon^3 e \mathcal{A}_k}{8m_e^3} \alpha^k \left(\hat{p}_l^2 + 2e \mathcal{A}_l \hat{p}_l + e^2 \mathcal{A}_l^2 \right) \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{eV}{2m_e} \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon - \frac{i\epsilon^3 e \hbar}{4m_e^2} (\partial_k V + \partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^3 e \mathcal{A}_k}{8m_e^3} \alpha^k \left(2\hat{p}_l^2 + 4e \mathcal{A}_l \hat{p}_l + e^2 \mathcal{A}_l^2 \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^4).
 \end{aligned}
 \tag{A.28}$$

Using Eq. (18), i.e. $E_k = -(\partial_k V + \partial_t \mathcal{A}_k)$ and Eq. (32) with $\hat{p}_l \mathcal{A}_l = 0$, we get

$$\begin{aligned}
 \phi_-^\epsilon &= \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon + \frac{i\epsilon^3 e \hbar}{4m_e^2} E_k \alpha^k \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^3 e \mathcal{A}_k}{4m_e^3} \alpha^k \left(\hat{p}_l^2 + 2e \mathcal{A}_l \hat{p}_l + e^2 \mathcal{A}_l^2 \right) \phi_+^\epsilon + \frac{\epsilon^3 e \mathcal{A}_k}{8m_e^3} \alpha^k e^2 \mathcal{A}_l^2 \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon + \frac{i\epsilon^3 e \hbar}{4m_e^2} E_k \alpha^k \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^3 e \mathcal{A}_k}{4m_e^3} \alpha^k \left(\hat{p}_l^2 + 2e \mathcal{A}_l \hat{p}_l + e^2 \mathcal{A}_l^2 \right) \phi_+^\epsilon + \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{e^2 \mathcal{A}_l^2}{4m_e^2} \phi_+^\epsilon + \mathcal{O}(\epsilon^4) \\
 &= \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \Sigma \mathbf{B} \phi_+^\epsilon + \frac{i\epsilon^3 e \hbar}{4m_e^2} E_k \alpha^k \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{\hat{\Pi}^2}{2m_e^2} \phi_+^\epsilon + \frac{\epsilon^3 e \mathcal{A}_k}{2m_e} \alpha^k \frac{e^2 \mathcal{A}^2}{4m_e^2} \phi_+^\epsilon + \mathcal{O}(\epsilon^4)
 \end{aligned}
 \tag{A.29}$$

and obtain the final result

$$\phi_-^\epsilon = \frac{\epsilon e \mathcal{A}_k}{2m_e} \left(\alpha^k - \epsilon \frac{\hat{p}_k}{m_e} - \epsilon^2 \alpha^k \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{4m_e^2} \right) \phi_+^\epsilon - \frac{\epsilon^3 e \hbar}{4m_e^2} \left(\Sigma \mathbf{B} - i E_k \alpha^k \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^4). \quad (\text{A.30})$$

Appendix B: The differential equation for the wave function ϕ_+^ϵ

In this Appendix B, we derive an differential equation for the wave function ϕ_+^ϵ up to second order in ϵ . As the starting point for our calculation, we use Eq. (88):

$$\begin{aligned} i\hbar \partial_t \phi_+^\epsilon &= -\frac{\hbar^2}{2m_e} \Delta \phi_+^\epsilon - \frac{\epsilon^2 \hbar^4}{8m_e^3} \Delta^2 \phi_+^\epsilon + \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) + \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) \\ &\quad - \pi_+^\epsilon \left(e V \phi_+^\epsilon \right) - \pi_+^\epsilon \left(e V \phi_-^\epsilon \right) + \mathcal{O}(\epsilon^4). \end{aligned}$$

As we mention in Sec. 5.2, as a first step, we simplify now the last four of the six summands on the right side of Eq. (88) in front of the $\mathcal{O}(\epsilon^4)$ term. After that, we sum up these six summands, bring their sum in a compact form and doing so, we will find the result for the differential equation for ϕ_+^ϵ up to second order in ϵ .

Therefore, we begin our calculations with the simplification of the third of the above-mentioned six summands.

Analysis for the third summand:

We use Eqs. (43) and (47) to rewrite the third summand of Eq. (88) as

$$\begin{aligned} \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \left[\frac{1}{\epsilon} \pi_+^0 - \frac{i\hbar}{2m_e} \alpha^l \partial_l + \frac{\epsilon \hbar^2}{4m_e^2} \beta \Delta - \frac{i\epsilon^2 \hbar^3}{4m_e^3} \alpha^l \partial_l \Delta + \mathcal{O}(\epsilon^3) \right] \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) \\ &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon - \frac{i e \hbar}{2m_e} \alpha^l \alpha^k \partial_l \mathcal{A}_k \phi_+^\epsilon + \frac{\epsilon e \hbar^2}{4m_e^2} \beta \alpha^k \Delta \mathcal{A}_k \phi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar^3}{4m_e^3} \alpha^l \alpha^k \Delta \partial_l \mathcal{A}_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon - \frac{i e \hbar}{2m_e} \alpha^l \alpha^k \mathcal{A}_k \partial_l \phi_+^\epsilon - \frac{i e \hbar}{2m_e} \alpha^l \alpha^k (\partial_l \mathcal{A}_k) \phi_+^\epsilon \\ &\quad + \frac{\epsilon e \hbar^2}{4m_e^2} \beta \alpha^k \Delta \mathcal{A}_k \phi_+^\epsilon - \frac{i\epsilon^2 e \hbar^3}{4m_e^3} \alpha^l \alpha^k \Delta \mathcal{A}_k \partial_l \phi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar^3}{4m_e^3} \alpha^l \alpha^k \Delta (\partial_l \mathcal{A}_k) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{B.1})$$

Then, we use Eqs. (31), (79), (80), (A.4), and (A.5) to obtain

$$\begin{aligned} \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_+^0 \phi_+^\epsilon - \frac{i e \hbar}{2m_e} (2\delta_{kl} - \alpha^k \alpha^l) \mathcal{A}_k \partial_l \phi_+^\epsilon \\ &\quad - \frac{i e \hbar}{2m_e} (\delta_{kl} + i\epsilon_{lkm} \Sigma^m) (\partial_l \mathcal{A}_k) \phi_+^\epsilon + \frac{\epsilon e \hbar^2}{4m_e^2} \beta \alpha^k \Delta \mathcal{A}_k \phi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar^3}{4m_e^3} (2\delta_{kl} - \alpha^k \alpha^l) \Delta \mathcal{A}_k \partial_l \phi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar^3}{4m_e^3} (\delta_{kl} + i\epsilon_{lkm} \Sigma^m) \Delta (\partial_l \mathcal{A}_k) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \end{aligned}$$

$$\begin{aligned}
 &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon + \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \frac{i\epsilon\hbar}{2m_e} \alpha^l \partial_l \phi_+^\epsilon \\
 &\quad + \frac{\epsilon e\hbar}{2m_e} \mathbf{\Sigma} \mathbf{B} \phi_+^\epsilon + \frac{\epsilon e\hbar^2}{4m_e^2} \beta \alpha^k \Delta \mathcal{A}_k \phi_+^\epsilon - \frac{i\epsilon^2 e\hbar^3}{2m_e^3} \Delta \mathcal{A}_k \partial_k \phi_+^\epsilon \\
 &\quad + \frac{i\epsilon^2 e\hbar^3}{4m_e^3} \alpha^k \alpha^l \Delta \mathcal{A}_k \partial_l \phi_+^\epsilon + \frac{\epsilon^3 e\hbar^3}{4m_e^3} \Sigma^m \Delta B_m \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{B.2}$$

With Eqs. (82) and (A.3), we get

$$\begin{aligned}
 \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon + \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon \\
 &\quad + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \frac{i\epsilon\hbar}{2m_e} \alpha^l \partial_l \phi_+^\epsilon + \frac{\epsilon e\hbar}{2m_e} \mathbf{\Sigma} \mathbf{B} \phi_+^\epsilon \\
 &\quad + \frac{\epsilon e\hbar^2}{4m_e^2} (\Delta \mathcal{A}_k) \beta \alpha^k \phi_+^\epsilon + \frac{\epsilon e\hbar^2}{2m_e^2} (\partial_n \mathcal{A}_k) \beta \alpha^k \partial_n \phi_+^\epsilon \\
 &\quad - \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \frac{\epsilon^2 \hbar^2}{4m_e^2} \beta \Delta \phi_+^\epsilon - \frac{i\epsilon^2 e\hbar^3}{2m_e^3} (\Delta \mathcal{A}_k) \partial_k \phi_+^\epsilon \\
 &\quad - \frac{i\epsilon^2 e\hbar^3}{m_e^3} (\partial_n \mathcal{A}_k) \partial_k \partial_n \phi_+^\epsilon - \frac{i\epsilon^2 e\hbar^3}{2m_e^3} \mathcal{A}_k \partial_k \Delta \phi_+^\epsilon \\
 &\quad + \frac{i\epsilon^2 e\hbar^3}{4m_e^3} (\Delta \mathcal{A}_k) \alpha^k \alpha^l \partial_l \phi_+^\epsilon + \frac{i\epsilon^2 e\hbar^3}{2m_e^3} (\partial_n \mathcal{A}_k) \alpha^k \alpha^l \partial_l \partial_n \phi_+^\epsilon \\
 &\quad + \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \frac{i\epsilon^3 \hbar^3}{4m_e^3} \alpha^l \partial_l \Delta \phi_+^\epsilon + \frac{\epsilon^3 e\hbar^3}{4m_e^3} \Sigma^m (\Delta B_m) \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^3 e\hbar^3}{2m_e^3} \Sigma^m (\partial_n B_m) \partial_n \phi_+^\epsilon + \frac{\epsilon^3 e\hbar^3}{4m_e^3} \mathbf{\Sigma} \mathbf{B} \Delta \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{B.3}$$

Now, we use the fact that for the kind of systems which we analyze Eqs. (A.6), (A.7) hold, and because of Eq. (22), the following equations are true, too:

$$\partial_n B_m = \mathcal{O}(\epsilon), \tag{B.4}$$

$$\Delta B_m = \mathcal{O}(\epsilon^2). \tag{B.5}$$

Then, Eq. (B.3) is simplified to

$$\begin{aligned}
 \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{e}{\epsilon} \mathcal{A}_k \alpha^k \left(\pi_-^0 + \frac{i\epsilon\hbar}{2m_e} \alpha^l \partial_l - \frac{\epsilon^2 \hbar^2}{4m_e^2} \beta \Delta + \frac{i\epsilon^3 \hbar^3}{4m_e^3} \alpha^l \partial_l \Delta \right) \phi_+^\epsilon \\
 &\quad + \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \frac{\epsilon e\hbar}{2m_e} \mathbf{\Sigma} \mathbf{B} \phi_+^\epsilon + \frac{\epsilon e\hbar^2}{2m_e^2} (\partial_l \mathcal{A}_k) \beta \alpha^k \partial_l \phi_+^\epsilon \\
 &\quad - \frac{i\epsilon^2 e\hbar^3}{2m_e^3} \mathcal{A}_k \partial_k \Delta \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{B.6}$$

Using the definition for π_-^ϵ , see Eq. (47), and Eqs. (31), (69), we obtain the final result for the third summand of Eq. (88) as

$$\begin{aligned}
 \frac{1}{\epsilon} \pi_+^\epsilon \left(e \mathcal{A}_k \alpha^k \phi_+^\epsilon \right) &= \frac{e}{m_e} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \frac{\epsilon e\hbar}{2m_e} \mathbf{\Sigma} \mathbf{B} \phi_+^\epsilon - \frac{\epsilon e}{2m_e^2} \beta \alpha^k (\hat{p}_l \mathcal{A}_k) \hat{p}_l \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2 e}{2m_e^3} \mathcal{A}_k \hat{p}_k \hat{\mathbf{p}}^2 \phi_+^\epsilon + \mathcal{O}(\epsilon^3)
 \end{aligned}$$

$$\begin{aligned}
&= e\mathcal{A}_k \frac{\hat{p}_k}{m_e} \left(1 - \frac{\epsilon^2 \hat{\mathbf{p}}^2}{2m_e^2}\right) \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \boldsymbol{\Sigma} \mathbf{B} \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2}{2} \beta \alpha^k \left(\frac{1}{\epsilon} \frac{\hat{p}_l}{m_e} e\mathcal{A}_k\right) \frac{\hat{p}_l}{m_e} \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
\end{aligned} \tag{B.7}$$

Note that we should always remind that because of Eq. (A.6), $\hat{p}_l \mathcal{A}_k = -i\hbar \partial_l \mathcal{A}_k = \mathcal{O}(\epsilon)$, hence $\hat{p}_l \mathcal{A}_k / \epsilon = \mathcal{O}(\epsilon^0)$.

Analysis for the fourth summand:

We use Eqs. (31), (43), (48), (79), (80), (86), (87), and (A.6), to obtain the fourth summand of Eq. (88) as

$$\begin{aligned}
\frac{1}{\epsilon} \pi_+^\epsilon \left(e\mathcal{A}_k \alpha^k \phi_-^\epsilon\right) &= \left[\pi_+^0 - \frac{i\epsilon \hbar}{2m_e} \alpha^m \partial_m + \frac{\epsilon^2 \hbar^2}{4m_e^2} \beta \Delta + \mathcal{O}(\epsilon^3)\right] e\mathcal{A}_k \alpha^k \\
&\quad \cdot \left[\frac{e\mathcal{A}_l}{2m_e} \left(\alpha^l - \epsilon \frac{\hat{p}_l}{m_e} - \epsilon^2 \alpha^l \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{4m_e^2}\right) - \frac{\epsilon^2 e \hbar}{4m_e^2} (\boldsymbol{\Sigma} \mathbf{B} - iE_l \alpha^l) + \mathcal{O}(\epsilon^3)\right] \phi_+^\epsilon \\
&= \frac{e^2}{2m_e} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \pi_+^0 \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \left(\mathcal{A}_l \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{2m_e} - i\hbar E_l\right) \alpha^k \alpha^l \pi_+^0 \phi_+^\epsilon \\
&\quad + \frac{i\epsilon e^2 \hbar}{2m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \partial_l \pi_+^0 \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \boldsymbol{\Sigma} \mathbf{B} \mathcal{A}_k \pi_+^0 \phi_+^\epsilon \\
&\quad - \frac{i\epsilon e^2 \hbar}{4m_e^2} \alpha^m \alpha^k \alpha^l \partial_m \mathcal{A}_k \mathcal{A}_l \phi_+^\epsilon + \frac{\epsilon^2 e^2 \hbar^2}{4m_e^3} \alpha^m \alpha^k \partial_m \mathcal{A}_k \mathcal{A}_l \partial_l \phi_+^\epsilon \\
&\quad + \frac{\epsilon^2 e^2 \hbar^2}{8m_e^3} \beta \alpha^k \alpha^l \Delta \mathcal{A}_k \mathcal{A}_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= \frac{e^2}{2m_e} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \pi_+^0 \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \left(\mathcal{A}_l \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{2m_e} - i\hbar E_l\right) \alpha^k \alpha^l \pi_+^0 \phi_+^\epsilon \\
&\quad + \frac{i\epsilon e^2 \hbar}{2m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \partial_l \pi_+^0 \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \boldsymbol{\Sigma} \mathbf{B} \mathcal{A}_k \pi_+^0 \phi_+^\epsilon \\
&\quad - \frac{i\epsilon e^2 \hbar}{4m_e^2} (\partial_m \mathcal{A}_k \mathcal{A}_l) \alpha^m \alpha^k \alpha^l \phi_+^\epsilon - \frac{i\epsilon e^2 \hbar}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^m \alpha^k \alpha^l \partial_m \phi_+^\epsilon \\
&\quad + \frac{\epsilon^2 e^2 \hbar^2}{4m_e^3} \mathcal{A}_k \mathcal{A}_l \alpha^m \alpha^k \partial_l \partial_m \phi_+^\epsilon + \frac{\epsilon^2 e^2 \hbar^2}{8m_e^3} \mathcal{A}_k \mathcal{A}_l \beta \alpha^k \alpha^l \Delta \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= \frac{e^2}{2m_e} \mathcal{A}_k \mathcal{A}_l (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \pi_+^0 \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \left(\mathcal{A}_l \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{2m_e} - i\hbar E_l\right) (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \pi_+^0 \phi_+^\epsilon \\
&\quad + \frac{i\epsilon e^2 \hbar}{2m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \partial_l \pi_+^0 \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \boldsymbol{\Sigma} \mathbf{B} \mathcal{A}_k \pi_+^0 \phi_+^\epsilon
\end{aligned}$$

$$\begin{aligned}
 & -\frac{i\epsilon e^2 \hbar}{4m_e^2} (\partial_m \mathcal{A}_k \mathcal{A}_l) \alpha^m (\delta_{kl} + i\epsilon_{klm} \Sigma^n) \phi_+^\epsilon \\
 & -\frac{i\epsilon e^2 \hbar}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^m (\delta_{kl} + i\epsilon_{klm} \Sigma_n) \partial_m \phi_+^\epsilon \\
 & +\frac{\epsilon^2 e^2 \hbar^2}{4m_e^3} \mathcal{A}_k \mathcal{A}_l (2\delta_{km} - \alpha^k \alpha^m) \partial_l \partial_m \phi_+^\epsilon \\
 & +\frac{\epsilon^2 e^2 \hbar^2}{8m_e^3} \mathcal{A}_k \mathcal{A}_l \beta (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \Delta \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{B.8}$$

With $\mathcal{A} \times \mathcal{A} = \mathbf{0}$, we then get

$$\begin{aligned}
 \frac{1}{\epsilon} \pi_+^\epsilon (e \mathcal{A}_k \alpha^k \phi_-^\epsilon) &= \frac{e^2}{2m_e} \mathcal{A}^2 \pi_+^0 \phi_+^\epsilon \\
 & -\frac{\epsilon^2 e^2}{4m_e^2} \left[\mathcal{A}^2 \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{2m_e} - i\hbar \mathcal{A} \mathbf{E} + \hbar \Sigma (\mathcal{A} \times \mathbf{E}) \right] \pi_+^0 \phi_+^\epsilon \\
 & +\frac{i\epsilon e^2 \hbar}{2m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \partial_l \pi_-^0 \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \Sigma \mathbf{B} \mathcal{A}_k \pi_-^0 \phi_+^\epsilon \\
 & -\frac{i\epsilon e^2 \hbar}{4m_e^2} (\partial_k \mathcal{A}^2) \alpha^k \phi_+^\epsilon - \frac{i\epsilon e^2 \hbar}{4m_e^2} \mathcal{A}^2 \alpha^k \partial_k \phi_+^\epsilon \\
 & +\frac{\epsilon^2 e^2 \hbar^2}{2m_e^3} \mathcal{A}_k \mathcal{A}_l \partial_k \partial_l \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar^2}{4m_e^3} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^m \partial_l \partial_m \phi_+^\epsilon \\
 & +\frac{\epsilon^2 e^2 \hbar^2}{8m_e^3} \mathcal{A}^2 \beta \Delta \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 & = \frac{e^2 \mathcal{A}^2}{2m_e} \left(\pi_+^0 - \frac{i\epsilon \hbar}{2m_e} \alpha^k \partial_k + \frac{\epsilon^2 \hbar^2}{4m_e^2} \beta \Delta \right) \phi_+^\epsilon \\
 & -\frac{\epsilon^2 e^2}{4m_e^2} \left[\mathcal{A}^2 \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{2m_e} - i\hbar \mathcal{A} \mathbf{E} + \hbar \Sigma (\mathcal{A} \times \mathbf{E}) \right] \pi_+^0 \phi_+^\epsilon \\
 & +\frac{i\epsilon e^2 \hbar}{2m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \partial_l \left(\pi_-^0 + \frac{i\epsilon \hbar}{2m_e} \alpha^m \partial_m \right) \phi_+^\epsilon \\
 & -\frac{\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \Sigma \mathbf{B} \mathcal{A}_k \pi_-^0 \phi_+^\epsilon - \frac{i\epsilon e^2 \hbar}{4m_e^2} (\partial_k \mathcal{A}^2) \alpha^k \phi_+^\epsilon \\
 & +\frac{\epsilon^2 e^2 \hbar^2}{2m_e^3} \mathcal{A}_k \mathcal{A}_l \partial_k \partial_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{B.9}$$

Using Eqs. (31), (48), (49), (68), (69), and (A.6), it is simplified to

$$\begin{aligned}
 \frac{1}{\epsilon} \pi_+^\epsilon (e \mathcal{A}_k \alpha^k \phi_-^\epsilon) &= \frac{e^2 \mathcal{A}^2}{2m_e} \phi_+^\epsilon \\
 & -\frac{\epsilon^2 e^2}{4m_e^2} \left[\mathcal{A}^2 \frac{2\hat{\Pi}^2 - e^2 \mathcal{A}^2}{2m_e} - i\hbar \mathcal{A} \mathbf{E} + \hbar \Sigma (\mathcal{A} \times \mathbf{E}) \right] \phi_+^\epsilon \\
 & -\frac{i\epsilon e^2 \hbar}{4m_e^2} (\partial_k \mathcal{A}^2) \alpha^k \phi_+^\epsilon + \frac{\epsilon^2 e^2 \hbar^2}{2m_e^3} \mathcal{A}_k \partial_k \mathcal{A}_l \partial_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3)
 \end{aligned}$$

$$\begin{aligned}
&= \frac{e^2 \mathcal{A}^2}{2m_e} \phi_+^\epsilon - \frac{\epsilon^2 e^2 \mathcal{A}^2}{8m_e^3} \left(2\hat{\Pi}^2 - e^2 \mathcal{A}^2 \right) \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} [\boldsymbol{\Sigma} (\boldsymbol{\mathcal{A}} \times \mathbf{E}) - i\boldsymbol{\mathcal{A}}\mathbf{E}] \phi_+^\epsilon - \frac{\epsilon^2}{2m_e} \left(e\boldsymbol{\mathcal{A}} \frac{\hat{\mathbf{p}}}{m_e} \right)^2 \phi_+^\epsilon \\
&\quad + \frac{\epsilon^2}{4m_e} \alpha^k \left(\frac{1}{\epsilon} \frac{\hat{p}^k}{m_e} e^2 \mathcal{A}^2 \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3),
\end{aligned} \tag{B.10}$$

where we note that because of Eq. (A.6), $\hat{p}_k \mathcal{A}^2 = -i\hbar \partial_k \mathcal{A}^2 = -2i\hbar \mathcal{A}_l \partial_k \mathcal{A}_l = \mathcal{O}(\epsilon)$.

Equation (B.10) is the final result of the fourth summand of Eq. (88).

Analysis for the fifth summand:

Using Eqs. (48) and (68), we calculate for the fifth summand of Eq. (88):

$$\begin{aligned}
- \pi_+^\epsilon (eV \phi_+^\epsilon) &= - \left(\pi_+^0 - \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k + \frac{\hbar^2}{4} \frac{\epsilon^2}{m_e^2} \beta \Delta \right) (eV \phi_+^\epsilon) + \mathcal{O}(\epsilon^3) \\
&= -eV \left(\pi_+^0 - \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k + \frac{\hbar^2}{4} \frac{\epsilon^2}{m_e^2} \beta \Delta \right) \phi_+^\epsilon \\
&\quad + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= -eV \pi_+^\epsilon \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= -eV \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon \\
&\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
\end{aligned} \tag{B.11}$$

Analysis for the sixth summand:

We use Eqs. (31), (43), (48), (49), (68), (69), (79), (80), (87), and (A.6) to obtain the sixth summand of Eq. (88) as

$$\begin{aligned}
- \pi_+^\epsilon (eV \phi_-^\epsilon) &= - \left(\pi_+^0 - \frac{i\epsilon \hbar}{2m_e} \alpha^k \partial_k \right) eV \frac{\epsilon e \mathcal{A}_l}{2m_e} \left(\alpha^l - \epsilon \frac{\hat{p}_l}{m_e} \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= - \frac{\epsilon e^2}{2m_e} V \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon - \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} V \mathcal{A}_k \partial_k \pi_-^0 \phi_+^\epsilon \\
&\quad + \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \alpha^l \partial_k V \mathcal{A}_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= - \frac{\epsilon e^2}{2m_e} V \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon - \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} V \mathcal{A}_k \partial_k \pi_-^0 \phi_+^\epsilon \\
&\quad + \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} (\partial_k V) \alpha^k \alpha^l \mathcal{A}_l \phi_+^\epsilon + \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \alpha^l V \mathcal{A}_l \partial_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
&= - \frac{\epsilon e^2}{2m_e} V \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon - \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} V \mathcal{A}_k \partial_k \pi_-^0 \phi_+^\epsilon \\
&\quad + \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} (\partial_k V) (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \mathcal{A}_l \phi_+^\epsilon \\
&\quad + \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} (2\delta_{kl} - \alpha^l \alpha^k) V \mathcal{A}_l \partial_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3)
\end{aligned}$$

$$\begin{aligned}
 &= -\frac{\epsilon e^2}{2m_e} V \mathcal{A}_k \alpha^k \pi_-^0 \phi_+^\epsilon - \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} V \mathcal{A}_k \partial_k \pi_+^0 \phi_+^\epsilon \\
 &\quad + \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} (\nabla V) \mathcal{A} \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \Sigma [(\nabla V) \times \mathcal{A}] \phi_+^\epsilon \\
 &\quad + \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} V \mathcal{A}_k \partial_k \phi_+^\epsilon - \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \alpha^l V \mathcal{A}_k \partial_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{\epsilon e^2}{2m_e} V \mathcal{A}_k \alpha^k \left(\pi_-^0 + \frac{i\epsilon \hbar}{2m_e} \alpha^l \partial_l \right) \phi_+^\epsilon \\
 &\quad - \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} V \mathcal{A}_k \partial_k \left(\pi_+^0 - 1 \right) \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\nabla V)] + i\mathcal{A} (\nabla V) \} \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{B.12}
 \end{aligned}$$

Thus, we find for the sixth summand:

$$-\pi_+^\epsilon (eV\phi_-^\epsilon) = \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\nabla V)] + i\mathcal{A} (\nabla V) \} \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{B.13}$$

Result:

With Eqs. (31), (82), (B.7), (B.10), (B.11), and (B.13), the differential equation for the electronic wave function ϕ_+^ϵ (88) up to second order in ϵ is rewritten as

$$\begin{aligned}
 i\hbar \partial_t \phi_+^\epsilon &= \frac{\hat{\mathbf{p}}^2}{2m_e} \phi_+^\epsilon - \frac{\epsilon^2 \hat{\mathbf{p}}^4}{8m_e^3} \phi_+^\epsilon + e\mathcal{A}_k \frac{\hat{p}_k}{m_e} \left(1 - \frac{\epsilon^2 \hat{\mathbf{p}}^2}{2m_e^2} \right) \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2}{2} \beta \alpha^k \left(\frac{1}{\epsilon} \frac{\hat{p}_l}{m_e} e\mathcal{A}_k \right) \frac{\hat{p}_l}{m_e} \phi_+^\epsilon + \frac{e^2 \mathcal{A}^2}{2m_e} \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2 e^2 \mathcal{A}^2}{8m_e^3} \left(2\hat{\Pi}^2 - e^2 \mathcal{A}^2 \right) \phi_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} [\Sigma (\mathcal{A} \times \mathbf{E}) - i\mathcal{A} \mathbf{E}] \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^2}{4m_e} \alpha^k \left(\frac{1}{\epsilon} \frac{\hat{p}_k}{m_e} e^2 \mathcal{A}^2 \right) \phi_+^\epsilon - \frac{\epsilon^2}{2m_e} \left(e\mathcal{A} \frac{\hat{\mathbf{p}}}{m_e} \right)^2 \phi_+^\epsilon \\
 &\quad - eV \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\nabla V)] + i\mathcal{A} (\nabla V) \} \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= \left[\frac{1}{2m_e} \left(\hat{\mathbf{p}}^2 + 2e\mathcal{A}\hat{\mathbf{p}} + e^2 \mathcal{A}^2 \right) - eV \right] \phi_+^\epsilon \\
 &\quad + \frac{\epsilon e \hbar}{2m_e} \left[\Sigma \mathbf{B} + i\alpha^k (\partial_k V) \right] \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2}{8m_e^3} \left[\hat{\mathbf{p}}^4 + e^2 \mathcal{A}^2 \left(2\hat{\Pi}^2 - e^2 \mathcal{A}^2 \right) + 4e\mathcal{A}\hat{\mathbf{p}}\hat{\mathbf{p}}^2 + 4e^2 (\mathcal{A}\hat{\mathbf{p}})^2 \right] \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^2 e}{2m_e^2} \alpha^k \left[\left(\frac{1}{\epsilon} \hat{p}_k \mathcal{A}_l \right) e\mathcal{A}_l + \beta \left(\frac{1}{\epsilon} \hat{p}_l \mathcal{A}_k \right) \hat{p}_l \right] \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times ((\nabla V) - \mathbf{E})] + i\mathcal{A} [\mathbf{E} + (\nabla V)] \} \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{B.14}
 \end{aligned}$$

Using Eq. (18), i.e. $E_k = -(\partial_k V + \partial_t A_k)$ and Eq. (32)—here we regard that $\hat{p}_k \mathcal{A}_k = 0$ because of the Coulomb gauge given in Eq. (6)—we get

$$\begin{aligned}
 i\hbar \partial_t \phi_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2}{8m_e^3} \left[\hat{\mathbf{p}}^4 + 4e \mathcal{A} \hat{\mathbf{p}} \hat{\mathbf{p}}^2 + 2e^2 \mathcal{A}^2 \hat{\mathbf{p}}^2 \right. \\
 &\quad \left. + 4e^2 (\mathcal{A} \hat{\mathbf{p}})^2 + 4e^3 \mathcal{A}^2 \mathcal{A} \hat{\mathbf{p}} + e^4 \mathcal{A}^4 \right] \phi_+^\epsilon \\
 &\quad + \frac{\epsilon^2 e}{2m_e^2} \alpha^k \left[\left(\frac{1}{\epsilon} \hat{p}_k \mathcal{A}_l \right) e \mathcal{A}_l + \beta \left(\frac{1}{\epsilon} \hat{p}_l \mathcal{A}_k \right) \hat{p}_l \right] \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\mathbf{E} - (\nabla V))] + i \mathcal{A} (\partial_t \mathcal{A}) \} \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{B.15}
 \end{aligned}$$

Now, we evaluate $\hat{\Pi}^4$ using Eq. (32), regarding $\hat{p}_k \mathcal{A}_k = 0$ because of Eq. (6) and $\hat{p}_k \mathcal{A}_l = \mathcal{O}(\epsilon)$ because of Eq. (A.6), as

$$\begin{aligned}
 \hat{\Pi}^4 &= \left(\hat{\Pi}^2 \right)^2 \\
 &= \left[(\hat{p}_k + e \mathcal{A}_k)^2 \right]^2 \\
 &= \left(\hat{\mathbf{p}}^2 + 2e \mathcal{A} \hat{\mathbf{p}} + e^2 \mathcal{A}^2 \right)^2 \\
 &= \hat{\mathbf{p}}^4 + 2e \hat{\mathbf{p}}^2 \mathcal{A} \hat{\mathbf{p}} + 2e \mathcal{A} \hat{\mathbf{p}} \hat{\mathbf{p}}^2 + e^2 \hat{\mathbf{p}}^2 \mathcal{A}^2 + e^2 \mathcal{A}^2 \hat{\mathbf{p}}^2 \\
 &\quad + 4e^2 (\mathcal{A} \hat{\mathbf{p}})^2 + 2e^3 \mathcal{A} \hat{\mathbf{p}} \mathcal{A}^2 + 2e^3 \mathcal{A}^2 \mathcal{A} \hat{\mathbf{p}} + e^4 \mathcal{A}^4 \\
 &= \hat{\mathbf{p}}^4 + 4e \mathcal{A} \hat{\mathbf{p}} \hat{\mathbf{p}}^2 + 2e^2 \mathcal{A}^2 \hat{\mathbf{p}}^2 + 4e^2 (\mathcal{A} \hat{\mathbf{p}})^2 + 4e^3 \mathcal{A}^2 \mathcal{A} \hat{\mathbf{p}} + e^4 \mathcal{A}^4 + \mathcal{O}(\epsilon) \tag{B.16}
 \end{aligned}$$

to obtain the final result of the differential equation for the electronic wave function ϕ_+^ϵ up to second order in ϵ as

$$\begin{aligned}
 i\hbar \partial_t \phi_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \phi_+^\epsilon + \frac{\epsilon^2 e}{2m_e^2} \alpha^k \left[\left(\frac{1}{\epsilon} \hat{p}_k \mathcal{A}_l \right) e \mathcal{A}_l + \beta \left(\frac{1}{\epsilon} \hat{p}_l \mathcal{A}_k \right) \hat{p}_l \right] \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \Sigma [\mathcal{A} \times (\mathbf{E} - (\nabla V))] + i \mathcal{A} (\partial_t \mathcal{A}) \} \phi_+^\epsilon - \frac{\epsilon^2 e \hbar^2}{4m_e^2} \beta (\Delta V - V \Delta) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{B.17}
 \end{aligned}$$

Appendix C: The differential equation for the wave function $\tilde{\varphi}_+^\epsilon$

At the beginning of Sect. (5.4), we derived Eq. (104), which is

$$\begin{aligned}
 i\hbar \partial_t \pi_+^0 \phi_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \pi_+^0 \phi_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \pi_+^0 \phi_+^\epsilon + \frac{i\epsilon e \hbar}{2m_e} \alpha^k (\partial_k V) \pi_+^0 \phi_+^\epsilon \\
 &\quad - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \pi_+^0 \phi_+^\epsilon + \frac{\epsilon^2 e}{2m_e^2} \alpha^k \left[\left(\frac{1}{\epsilon} \hat{p}_k \mathcal{A}_l \right) e \mathcal{A}_l - \left(\frac{1}{\epsilon} \hat{p}_l \mathcal{A}_k \right) \hat{p}_l \right] \pi_+^0 \phi_+^\epsilon
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \boldsymbol{\Sigma} [\boldsymbol{\mathcal{A}} \times (\mathbf{E} - (\nabla V))] + i\boldsymbol{\mathcal{A}} (\partial_t \boldsymbol{\mathcal{A}}) \} \pi_+^0 \phi_+^\epsilon \\
 & -\frac{\epsilon^2 e \hbar^2}{4m_e^2} (\Delta V - V \Delta) \pi_+^0 \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned}$$

In this Appendix C, we use this equation as a starting point to derive a differential equation for the wave function $\tilde{\varphi}_+^\epsilon$ up to the second order in ϵ . But as a preparation of the transformations of Eq. (104), we take into account first that from Eqs. (49) and (69) follows that

$$\pi_-^0 = \pi_-^\epsilon - \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^k \partial_k + \frac{\hbar^2}{4} \frac{\epsilon^2}{m_e^2} \beta \Delta + \mathcal{O}(\epsilon^3) \tag{C.1}$$

$$\begin{aligned}
 \implies \epsilon \pi_-^0 \phi_+^\epsilon &= \epsilon \pi_-^\epsilon \phi_+^\epsilon - \frac{i\hbar}{2} \frac{\epsilon^2}{m_e} \alpha^k \partial_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{i\hbar}{2} \frac{\epsilon^2}{m_e} \alpha^k \partial_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{C.2}$$

From Eq. (C.2) directly follows by multiplication with ϵ :

$$\epsilon^2 \pi_-^0 \phi_+^\epsilon = \mathcal{O}(\epsilon^3). \tag{C.3}$$

Using Eqs. (79), (93), (C.2), and (C.3), we then transform Eq. (104) in the following manner:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi}_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \boldsymbol{\Sigma} \mathbf{B} \tilde{\varphi}_+^\epsilon + \frac{\epsilon^2 e \hbar^2}{4m_e^2} \alpha^k \alpha^l (\partial_k V) \partial_l \phi_+^\epsilon \\
 & -\frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \boldsymbol{\Sigma} [\boldsymbol{\mathcal{A}} \times (\mathbf{E} - (\nabla V))] + i\boldsymbol{\mathcal{A}} (\partial_t \boldsymbol{\mathcal{A}}) \} \tilde{\varphi}_+^\epsilon \\
 & -\frac{\epsilon^2 e \hbar^2}{4m_e^2} (\Delta V - V \Delta) \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \boldsymbol{\Sigma} \mathbf{B} \tilde{\varphi}_+^\epsilon + \frac{\epsilon^2 e \hbar^2}{4m_e^2} (\delta_{kl} + i\epsilon_{klm} \Sigma^m) (\partial_k V) \partial_l \phi_+^\epsilon \\
 & -\frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \boldsymbol{\Sigma} [\boldsymbol{\mathcal{A}} \times (\mathbf{E} - (\nabla V))] + i\boldsymbol{\mathcal{A}} (\partial_t \boldsymbol{\mathcal{A}}) \} \tilde{\varphi}_+^\epsilon \\
 & -\frac{\epsilon^2 e \hbar^2}{4m_e^2} (\Delta V - V \Delta) \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \boldsymbol{\Sigma} \mathbf{B} \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon \\
 & + \frac{\epsilon^2 e \hbar^2}{4m_e^2} (\nabla V) \nabla \phi_+^\epsilon - \frac{\epsilon^2 e \hbar}{4m_e^2} \boldsymbol{\Sigma} [(\nabla V) \times \hat{\mathbf{p}}] \phi_+^\epsilon \\
 & -\frac{\epsilon^2 e^2 \hbar}{4m_e^2} \{ \boldsymbol{\Sigma} [\boldsymbol{\mathcal{A}} \times (\mathbf{E} - (\nabla V))] + i\boldsymbol{\mathcal{A}} (\partial_t \boldsymbol{\mathcal{A}}) \} \tilde{\varphi}_+^\epsilon \\
 & -\frac{\epsilon^2 e \hbar^2}{4m_e^2} (\Delta V - V \Delta) \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{C.4}$$

Before we continue to transform Eq. (C.4), we first make the following side calculation, where we derive an equation that relates terms of the form $\epsilon^2 \phi_+^\epsilon$ and $\epsilon^2 \tilde{\varphi}_+^\epsilon$:

We start this derivation by taking the limit $\epsilon \rightarrow 0$ of Eq. (68) and get

$$\pi_{\pm}^0 \phi_{\pm}^0 = \phi_{\pm}^0. \quad (\text{C.5})$$

Using Eq. (C.5) and taking the limit $\epsilon \rightarrow 0$ for the +-case of Eq. (93), we find that

$$\tilde{\varphi}_+^0 = \pi_+^0 \phi_+^0 = \phi_+^0. \quad (\text{C.6})$$

Therefore, using Eq. (C.6) the following result can be found for terms of the form $\epsilon^2 \phi_+^\epsilon$:

$$\begin{aligned} \epsilon^2 \phi_+^\epsilon &= \epsilon^2 \phi_+^0 + \mathcal{O}(\epsilon^3) \\ &= \epsilon^2 \tilde{\varphi}_+^0 + \mathcal{O}(\epsilon^3) \\ &= \epsilon^2 \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{C.7})$$

Having finished the side calculation, now we use Eq. (C.7) for the following transformation of Eq. (C.4):

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma [(\nabla V) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\mathbf{E} - (\nabla V))] \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar^2}{4m_e^2} [\Delta V - (\nabla V) \nabla - V \Delta] \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} [ie\mathcal{A}(\partial_t \mathcal{A})] \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{C.8})$$

Using Eq. (32),

$$\begin{aligned} [(\nabla V) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\mathbf{E} - (\nabla V))] \tilde{\varphi}_+^\epsilon &= [(\nabla V) \times (\hat{\Pi} - e\mathcal{A}) \\ &\quad + e\mathcal{A} \times (\mathbf{E} - (\nabla V))] \tilde{\varphi}_+^\epsilon \\ &= [(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E}] \tilde{\varphi}_+^\epsilon \end{aligned} \quad (\text{C.9})$$

and

$$\begin{aligned} [\Delta V - (\nabla V) \nabla - V \Delta] \tilde{\varphi}_+^\epsilon &= [(\Delta V) + 2(\nabla V) \nabla + V \Delta - (\nabla V) \nabla - V \Delta] \tilde{\varphi}_+^\epsilon \\ &= [(\Delta V) + (\nabla V) \nabla] \tilde{\varphi}_+^\epsilon \\ &= \nabla (\nabla V) \tilde{\varphi}_+^\epsilon. \end{aligned} \quad (\text{C.10})$$

we get the differential equation for $\tilde{\varphi}_+^\epsilon$ up to second order in ϵ as

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma [(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E}] \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} [\hbar \nabla (\nabla V) + ie\mathcal{A}(\partial_t \mathcal{A})] \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{C.11})$$

Appendix D: Calculation of the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$

In Sect. 5.5 is discussed that we have to transform the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ into a term, where the wave function $\tilde{\varphi}^\epsilon$ appears, and for this calculation, we have to find an equation that expresses the electronic wave function $\tilde{\varphi}_+^\epsilon$ by the wave function $\tilde{\varphi}^\epsilon$.

As a first step for this task, we calculate another formula that rewrites the wave function ϕ_+^ϵ as an expression, where the wave function ϕ^ϵ appears:

If we regard just terms up to second order in ϵ , we find that from Eq. (87) follows:

$$\phi_-^\epsilon = \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon - \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{D.1}$$

Therefore, we realize that using the abbreviations

$$\hat{f}_1 = \frac{e}{2m_e} \mathcal{A}_k \alpha^k, \tag{D.2}$$

$$\hat{f}_2 = -\frac{e}{2m_e^2} \mathcal{A}_k \hat{p}_k, \tag{D.3}$$

Eq. (D.1) for the wave function ϕ_-^ϵ can be rewritten as

$$\phi_-^\epsilon = \epsilon \hat{f}_1 \phi_+^\epsilon + \epsilon^2 \hat{f}_2 \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \tag{D.4}$$

Then, we derive the following formula using Eq. (63), i.e., $\phi^\epsilon = \phi_+^\epsilon + \phi_-^\epsilon$, and (78), i.e. $\phi_-^\epsilon = \mathcal{O}(\epsilon)$:

$$\begin{aligned} \epsilon^2 \phi_+^\epsilon &= \epsilon^2 \phi^\epsilon - \epsilon^2 \phi_-^\epsilon \\ &= \epsilon^2 \phi^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.5}$$

Now, we add ϕ_+^ϵ to Eq. (D.4) and use Eqs. (63) and (D.5). Thus, we get:

$$\begin{aligned} \phi_+^\epsilon + \phi_-^\epsilon &= \phi_+^\epsilon + \epsilon \hat{f}_1 \phi_+^\epsilon + \epsilon^2 \hat{f}_2 \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ \implies \phi^\epsilon &= \phi_+^\epsilon + \epsilon \hat{f}_1 \phi_+^\epsilon + \epsilon^2 \hat{f}_2 \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ \implies \phi_+^\epsilon &= \phi^\epsilon - \epsilon \hat{f}_1 \phi_+^\epsilon - \epsilon^2 \hat{f}_2 \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.6}$$

Then, we further transform the equation above using Eqs. (63), (D.4), and (D.5)

$$\begin{aligned} \phi_+^\epsilon &= \phi^\epsilon - \epsilon \hat{f}_1 (\phi^\epsilon - \phi_-^\epsilon) - \epsilon^2 \hat{f}_2 \phi^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \phi^\epsilon - \epsilon \hat{f}_1 \phi^\epsilon + \epsilon \hat{f}_1 (\epsilon \hat{f}_1 \phi_+^\epsilon + \epsilon^2 \hat{f}_2 \phi_+^\epsilon) - \epsilon^2 \hat{f}_2 \phi^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \phi^\epsilon - \epsilon \hat{f}_1 \phi^\epsilon + \epsilon^2 \hat{f}_1^2 \phi_+^\epsilon - \epsilon^2 \hat{f}_2 \phi^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \phi^\epsilon - \epsilon \hat{f}_1 \phi^\epsilon + \epsilon^2 (\hat{f}_1^2 - \hat{f}_2) \phi^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.7}$$

Now we insert into Eq. (D.7) the abbreviations (D.2) and (D.3) for the operators \hat{f}_1 and \hat{f}_2 . Then, we find the following result to express the wave function ϕ_+^ϵ with ϕ^ϵ :

$$\phi_+^\epsilon = \phi^\epsilon - \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi^\epsilon + \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \phi^\epsilon + \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi^\epsilon + \mathcal{O}(\epsilon^3). \tag{D.8}$$

As a side result, by combining Eqs. (63) and (D.8), we directly find the following equation to express the wave function ϕ_-^ϵ with ϕ^ϵ :

$$\phi_-^\epsilon = \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi^\epsilon - \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \phi^\epsilon - \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi^\epsilon + \mathcal{O}(\epsilon^3). \tag{D.9}$$

As the next step, we transform Eq. (D.8) into an equation, where the wave function $\tilde{\varphi}_+$ is expressed by a formula containing the wave function $\tilde{\varphi}$. Therefore, we apply the projector π_+^0 on Eq. (D.8) and regard Eqs. (43), (63), (93), and (100). Therefore, we find:

$$\begin{aligned} \pi_+^0 \phi_+^\epsilon &= \pi_+^0 \phi^\epsilon - \pi_+^0 \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi^\epsilon + \pi_+^0 \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \phi^\epsilon \\ &\quad + \pi_+^0 \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi^\epsilon + \mathcal{O}(\epsilon^3) \\ \implies \tilde{\varphi}_+^\epsilon &= \tilde{\varphi}^\epsilon - \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \pi_+^0 (\phi_+^\epsilon + \phi_-^\epsilon) + \frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \tilde{\varphi}^\epsilon \\ &\quad + \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.10}$$

Now, we make a separate discussion for the term $-\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \pi_+^0 (\phi_+^\epsilon + \phi_-^\epsilon)$ appearing in Eq. (D.10). Therefore, we use Eqs. (49) and (D.9). Then, we find:

$$\begin{aligned} -\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \pi_+^0 (\phi_+^\epsilon + \phi_-^\epsilon) &= -\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k (\pi_-^\epsilon - \frac{i\hbar}{2} \frac{\epsilon}{m_e} \alpha^l \partial_l) (\phi_+^\epsilon + \phi_-^\epsilon) + \mathcal{O}(\epsilon^3) \\ &= -\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_-^\epsilon + \frac{i\epsilon^2 e \hbar}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \partial_l \phi^\epsilon + \mathcal{O}(\epsilon^3) \\ &= -\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \left(\frac{\epsilon e \mathcal{A}_l}{2m_e} \alpha^l \phi^\epsilon \right) \\ &\quad + \frac{i\epsilon^2 e \hbar}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \partial_l \phi^\epsilon + \mathcal{O}(\epsilon^3) \\ &= -\frac{\epsilon^2 e^2}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \mathcal{A}_l \phi^\epsilon \\ &\quad + \frac{i\epsilon^2 e \hbar}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \partial_l \phi^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.11}$$

In addition, from Eq. (D.11) follows

$$-\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \pi_+^0 (\phi_+^\epsilon + \phi_-^\epsilon) = \mathcal{O}(\epsilon^2), \tag{D.12}$$

thus, Eq. (D.10) has the consequence

$$\tilde{\varphi}_+^\epsilon = \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^2). \tag{D.13}$$

Now, we regard that using Eqs. (63), (78), (C.7), and (D.13), we find these side results:

$$\begin{aligned} \epsilon^2 \phi^\epsilon &= \epsilon^2 (\phi_+^\epsilon + \phi_-^\epsilon) \\ &= \epsilon^2 \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \epsilon^2 \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \epsilon^2 \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.14}$$

Then, we insert Eq. (D.14) into Eq. (D.11). In addition, we use Eq. (31) and get this result:

$$-\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \pi_-^0 (\phi_+^\epsilon + \phi_-^\epsilon) = -\frac{\epsilon^2 e^2}{4m_e^2} \mathcal{A}_k \mathcal{A}_l \alpha^k \alpha^l \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \hat{p}_l \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{D.15}$$

As the next step, we insert the result from Eq. (D.15) for the term $-\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \pi_-^0 (\phi_+^\epsilon + \phi_-^\epsilon)$ into Eq. (D.10), and apply then Eq. (79). Therefore, we get

$$\begin{aligned} \tilde{\varphi}_+^\epsilon &= \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e^2}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \mathcal{A}_l \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \hat{p}_l \tilde{\varphi}^\epsilon \\ &\quad + \frac{\epsilon^2 e^2}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \mathcal{A}_l \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} \left(2\mathcal{A}_k \hat{p}_k - \alpha^k \alpha^l \mathcal{A}_k \hat{p}_l \right) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} \left[2\mathcal{A}_k \hat{p}_k - (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \mathcal{A}_k \hat{p}_l \right] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} (\mathcal{A}_k \hat{p}_k - i\epsilon_{klm} \Sigma^m \mathcal{A}_k \hat{p}_l) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.16}$$

Therefore, we find this result that transforms the wave function $\tilde{\varphi}_+^\epsilon$ into a expression that contains the wave function $\tilde{\varphi}^\epsilon$:

$$\tilde{\varphi}_+^\epsilon = \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} [\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{D.17}$$

Now, we can evaluate the first term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ on the right side of Eq. (107) by combining Eqs. (105) and (D.17):

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_+^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}_+^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}_+^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma \left[(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} \right] \tilde{\varphi}_+^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} [\hbar \nabla (\nabla V) + i e \mathcal{A} (\partial_t \mathcal{A})] \tilde{\varphi}_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \left\{ \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} [\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon \right\} \\ &\quad + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma \left[(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} \right] \tilde{\varphi}^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} [\hbar \nabla (\nabla V) + i e \mathcal{A} (\partial_t \mathcal{A})] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) [\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon \\ &\quad - \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma \left[(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} \right] \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e \hbar}{4m_e^2} [\hbar \nabla (\nabla V) + i e \mathcal{A} (\partial_t \mathcal{A})] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{D.18}$$

With Eq. (D.18), we have found now the result for the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$, which we were looking for.

Appendix E: Calculation of the term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$

In this Appendix E, the second term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$ on the right side of Eq. (107) is rewritten in a form, where the wave function $\tilde{\varphi}_-^\epsilon$ appears.

We start this calculation by applying $\pi_+^0 i\hbar \partial_t$ on Eq. (D.1). For the left side of this equation, we find because of Eqs. (58) and (93):

$$\pi_+^0 i\hbar \partial_t \phi_-^\epsilon = i\hbar \partial_t \tilde{\varphi}_-^\epsilon, \quad (\text{E.1})$$

what is just the term we want to calculate. Therefore, regarding Eq. (E.1), we find after applying $\pi_+^0 i\hbar \partial_t$ on Eq. (D.1):

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_-^\epsilon &= \pi_+^0 \left[i\hbar \partial_t \left(\frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \phi_+^\epsilon - \frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \phi_+^\epsilon \right) \right] + \mathcal{O}(\epsilon^3) \\ &= \frac{i\epsilon e \hbar}{2m_e} \pi_+^0 (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon + \frac{\epsilon e}{2m_e} \pi_+^0 \mathcal{A}_k \alpha^k i\hbar \partial_t \phi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar}{2m_e^2} \pi_+^0 (\partial_t \mathcal{A}_k) \hat{p}_k \phi_+^\epsilon - \frac{\epsilon^2 e}{2m_e^2} \pi_+^0 \mathcal{A}_k \hat{p}_k i\hbar \partial_t \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{E.2})$$

By inserting Eq. (89) into Eq. (E.2), we find:

$$\begin{aligned} i\hbar \partial_t \tilde{\varphi}_-^\epsilon &= \frac{i\epsilon e \hbar}{2m_e} \pi_+^0 (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon \\ &\quad + \frac{\epsilon e}{2m_e} \pi_+^0 \mathcal{A}_k \alpha^k \left\{ \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) + \frac{\epsilon e \hbar}{2m_e} \left[\boldsymbol{\Sigma} \mathbf{B} + i\alpha^l (\partial_l V) \right] \right\} \phi_+^\epsilon \\ &\quad - \frac{i\epsilon^2 e \hbar}{2m_e^2} \pi_+^0 (\partial_t \mathcal{A}_k) \hat{p}_k \phi_+^\epsilon - \frac{\epsilon^2 e}{2m_e^2} \pi_+^0 \mathcal{A}_k \hat{p}_k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{i\epsilon e \hbar}{2m_e} \pi_+^0 (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon + \frac{\epsilon e}{2m_e} \pi_+^0 \mathcal{A}_k \alpha^k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon \\ &\quad + \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \pi_+^0 \mathcal{A}_k \alpha^k \left[\boldsymbol{\Sigma} \mathbf{B} + i\alpha^l (\partial_l V) \right] \phi_+^\epsilon - \frac{i\epsilon^2 e \hbar}{2m_e^2} \pi_+^0 (\partial_t \mathcal{A}_k) \hat{p}_k \phi_+^\epsilon \\ &\quad - \frac{\epsilon^2 e}{2m_e^2} \pi_+^0 \mathcal{A}_k \hat{p}_k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{E.3})$$

In the intermediate result (E.3), five summands appear. In our next calculation step, we will evaluate them:

Analysis for the first summand:

For the calculation of the first summand, we apply Eqs. (43) and (49). Then, we find

$$\begin{aligned} \frac{i\epsilon e \hbar}{2m_e} \pi_+^0 (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon &= \frac{i\epsilon e \hbar}{2m_e} (\partial_t \mathcal{A}_k) \alpha^k \pi_-^0 \phi_+^\epsilon \\ &= \frac{i\epsilon e \hbar}{2m_e} (\partial_t \mathcal{A}_k) \alpha^k \left(\pi_-^\epsilon - \frac{i\epsilon \hbar}{2m_e} \alpha^l \partial_l \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{E.4})$$

As the next step, we combine Eqs. (C.7), (D.13) and get

$$\epsilon^2 \phi_+^\epsilon = \epsilon^2 \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{E.5}$$

Then, we transform Eq. (E.4) by applying Eqs. (31), (69), (79), and (E.5) and find the following result for the first summand:

$$\begin{aligned} \frac{i\epsilon e\hbar}{2m_e} \pi_+^0 (\partial_t \mathcal{A}_k) \alpha^k \phi_+^\epsilon &= \frac{i\epsilon^2 e\hbar}{4m_e^2} \alpha^k \alpha^l (\partial_t \mathcal{A}_k) \hat{p}_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{i\epsilon^2 e\hbar}{4m_e^2} \alpha^k \alpha^l (\partial_t \mathcal{A}_k) \hat{p}_l \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \\ &= \frac{i\epsilon^2 e\hbar}{4m_e^2} (\delta_{kl} + i\epsilon_{klm} \Sigma^m) (\partial_t \mathcal{A}_k) \hat{p}_l \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{i\epsilon^2 e\hbar}{4m_e^2} (\partial_t \mathcal{A}) \hat{\mathbf{p}} \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e\hbar}{4m_e^2} \Sigma [(\partial_t \mathcal{A}) \times \hat{\mathbf{p}}] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{E.6}$$

Analysis for the second summand:

For the analysis of the second summand, we take into account that because of Eqs. (31), (32) and (A.6) holds:

$$\begin{aligned} \epsilon^2 \mathcal{A}_k \hat{\Pi}_l &= \epsilon^2 \mathcal{A}_k (\hat{p}_l + e\mathcal{A}_l) \\ &= \epsilon^2 (\hat{p}_l + e\mathcal{A}_l) \mathcal{A}_k - i\hbar\epsilon^2 (\partial_l \mathcal{A}_k) \\ &= \epsilon^2 \hat{\Pi}_l \mathcal{A}_k + \mathcal{O}(\epsilon^3). \end{aligned} \tag{E.7}$$

Therefore, using Eqs. (31), (43), (49), (69), (79), (E.5), and (E.7), we get for the second summand:

$$\begin{aligned} \frac{\epsilon e}{2m_e} \pi_+^0 \mathcal{A}_k \alpha^k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \phi_+^\epsilon &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \pi_+^0 \phi_+^\epsilon \\ &= \frac{\epsilon e}{2m_e} \mathcal{A}_k \alpha^k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \left(\pi_-^\epsilon - \frac{i\epsilon\hbar}{2m_e} \alpha^l \partial_l \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{\epsilon^2 e}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \hat{p}_l \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{\epsilon^2 e}{4m_e^2} (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \mathcal{A}_k \hat{p}_l \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\ &= \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \mathcal{A} \hat{\mathbf{p}} \tilde{\varphi}^\epsilon \\ &\quad + \frac{i\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \Sigma (\mathcal{A} \times \hat{\mathbf{p}}) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \end{aligned} \tag{E.8}$$

Analysis for the third summand:

Applying Eqs. (43), (49), (68), (69), (79), (86), and (E.5), we derive for the third summand:

$$\begin{aligned}
 \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \pi_+^0 \mathcal{A}_k \alpha^k \left[\boldsymbol{\Sigma} \mathbf{B} + i\alpha^l (\partial_l V) \right] \phi_+^\epsilon &= \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \mathcal{A}_k \alpha^k \left[\boldsymbol{\Sigma} \mathbf{B} \pi_-^0 + i\alpha^l (\partial_l V) \pi_+^0 \right] \phi_+^\epsilon \\
 &= \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \mathcal{A}_k \alpha^k \left[\boldsymbol{\Sigma} \mathbf{B} \pi_-^\epsilon + i\alpha^l (\partial_l V) \pi_+^\epsilon \right] \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} \alpha^k \alpha^l \mathcal{A}_k (\partial_l V) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} (\delta_{kl} + i\epsilon_{klm} \Sigma^m) \mathcal{A}_k (\partial_l V) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} \mathcal{A} (\nabla V) \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \boldsymbol{\Sigma} [\mathcal{A} \times (\nabla V)] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{E.9}
 \end{aligned}$$

Analysis for the fourth summand:

Using Eqs. (49), (68), and (E.5), we calculate for the fourth summand:

$$\begin{aligned}
 -\frac{i\epsilon^2 e \hbar}{2m_e^2} \pi_+^0 (\partial_t \mathcal{A}_k) \hat{p}_k \phi_+^\epsilon &= -\frac{i\epsilon^2 e \hbar}{2m_e^2} (\partial_t \mathcal{A}_k) \hat{p}_k \pi_+^0 \phi_+^\epsilon \\
 &= -\frac{i\epsilon^2 e \hbar}{2m_e^2} (\partial_t \mathcal{A}_k) \hat{p}_k \pi_+^\epsilon \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{i\epsilon^2 e \hbar}{2m_e^2} (\partial_t \mathcal{A}_k) \hat{p}_k \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{i\epsilon^2 e \hbar}{2m_e^2} (\partial_t \mathcal{A}) \hat{\mathbf{p}} \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{E.10}
 \end{aligned}$$

Analysis for the fifth summand:

Taking into account Eqs. (31), (43), (49), (68), (E.5), and (E.7), we find for the fifth summand:

$$\begin{aligned}
 -\frac{\epsilon^2 e}{2m_e^2} \pi_+^0 \mathcal{A}_k \hat{p}_k \left(\frac{1}{2m_e} \hat{\mathbf{\Pi}}^2 - eV \right) \phi_+^\epsilon &= -\frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \left(\frac{1}{2m_e} \hat{\mathbf{\Pi}}^2 - eV \right) \pi_+^0 \phi_+^\epsilon \\
 &= -\frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \left(\frac{1}{2m_e} \hat{\mathbf{\Pi}}^2 - eV \right) \pi_+^\epsilon \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{\epsilon^2 e}{2m_e^2} \mathcal{A}_k \hat{p}_k \left(\frac{1}{2m_e} \hat{\mathbf{\Pi}}^2 - eV \right) \phi_+^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{\epsilon^2 e}{2m_e^2} \mathcal{A} \hat{\mathbf{p}} \left(\frac{1}{2m_e} \hat{\mathbf{\Pi}}^2 - eV \right) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\
 &= -\frac{\epsilon^2 e}{2m_e^2} \left(\frac{1}{2m_e} \hat{\mathbf{\Pi}}^2 - eV \right) \mathcal{A} \hat{\mathbf{p}} \tilde{\varphi}^\epsilon \\
 &\quad - \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} \mathcal{A} (\nabla V) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{E.11}
 \end{aligned}$$

Having calculated terms for the five summands, we insert the results (E.6), (E.8), (E.9), (E.10), and (E.11) into Eq. (E.3) for the term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$ and find:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi}_-^\epsilon &= \frac{i\epsilon^2 e\hbar}{4m_e^2} (\partial_t \mathcal{A}) \hat{\mathbf{p}} \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e\hbar}{4m_e^2} \Sigma [(\partial_t \mathcal{A}) \times \hat{\mathbf{p}}] \tilde{\varphi}^\epsilon \\
 &+ \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \mathcal{A} \hat{\mathbf{p}} \tilde{\varphi}^\epsilon \\
 &+ \frac{i\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \Sigma (\mathcal{A} \times \hat{\mathbf{p}}) \tilde{\varphi}^\epsilon \\
 &+ \frac{i\epsilon^2 e^2 \hbar}{4m_e^2} \mathcal{A} (\nabla V) \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e^2 \hbar}{4m_e^2} \Sigma [\mathcal{A} \times (\nabla V)] \tilde{\varphi}^\epsilon \\
 &- \frac{i\epsilon^2 e\hbar}{2m_e^2} (\partial_t \mathcal{A}) \hat{\mathbf{p}} \tilde{\varphi}^\epsilon \\
 &- \frac{\epsilon^2 e}{2m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \mathcal{A} \hat{\mathbf{p}} \tilde{\varphi}^\epsilon \\
 &- \frac{i\epsilon^2 e^2 \hbar}{2m_e^2} \mathcal{A} (\nabla V) \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{E.12}$$

After simplifying Eq. (E.12), we finally find this result for the term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi}_-^\epsilon &= -\frac{i\epsilon^2 e\hbar}{4m_e^2} [(\partial_t \mathcal{A}) \hat{\mathbf{p}} + \mathcal{A} (\nabla V)] \tilde{\varphi}^\epsilon - \frac{\epsilon^2 e\hbar}{4m_e^2} \Sigma [(\partial_t \mathcal{A}) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\nabla V)] \tilde{\varphi}^\epsilon \\
 &- \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) [\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned} \tag{E.13}$$

Appendix F: The differential equation for the wave function $\tilde{\varphi}^\epsilon$

In this Appendix F, we demonstrate how a differential equation for the wave function $\tilde{\varphi}^\epsilon$ up to the second order in ϵ can be calculated by inserting Eq. (109) for the term $i\hbar \partial_t \tilde{\varphi}_+^\epsilon$ into Eq. (107), and Eq. (110) for the term $i\hbar \partial_t \tilde{\varphi}_-^\epsilon$ into Eq. (107).

Therefore, by applying this insertions and simplifying the resulting equation, we find this intermediate result for the differential equation for the wave function $\tilde{\varphi}^\epsilon$:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi} &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}^\epsilon + \frac{\epsilon e\hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon \\
 &+ \frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) [\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon \\
 &- \frac{\epsilon^2 e\hbar}{4m_e^2} \Sigma [(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E}] \tilde{\varphi}^\epsilon \\
 &- \frac{\epsilon^2 e\hbar}{4m_e^2} [\hbar \nabla (\nabla V) + i e\mathcal{A} (\partial_t \mathcal{A})] \tilde{\varphi}^\epsilon \\
 &- \frac{i\epsilon^2 e\hbar}{4m_e^2} [(\partial_t \mathcal{A}) \hat{\mathbf{p}} + e\mathcal{A} (\nabla V)] \tilde{\varphi}^\epsilon
 \end{aligned}$$

$$\begin{aligned}
& -\frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma [(\partial_t \mathcal{A}) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\nabla V)] \tilde{\varphi}^\epsilon \\
& -\frac{\epsilon^2 e}{4m_e^2} \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) [\mathcal{A} \hat{\mathbf{p}} - i \Sigma (\mathcal{A} \times \hat{\mathbf{p}})] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3) \\
= & \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon \\
& -\frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma [(\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} + (\partial_t \mathcal{A}) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\nabla V)] \tilde{\varphi}^\epsilon \\
& -\frac{i\epsilon^2 e \hbar}{4m_e^2} [-i\hbar \nabla(\nabla V) + e\mathcal{A}(\partial_t \mathcal{A}) + (\partial_t \mathcal{A}) \hat{\mathbf{p}} + e\mathcal{A}(\nabla V)] \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3). \tag{F.1}
\end{aligned}$$

Now, we start an analysis for the two terms

$$\hat{\mathbf{T}}_1 := (\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} + (\partial_t \mathcal{A}) \times \hat{\mathbf{p}} + e\mathcal{A} \times (\nabla V), \tag{F.2}$$

$$\hat{T}_2 := -i\hbar \nabla(\nabla V) + e\mathcal{A}(\partial_t \mathcal{A}) + (\partial_t \mathcal{A}) \hat{\mathbf{p}} + e\mathcal{A}(\nabla V), \tag{F.3}$$

which appear both in [...] brackets in Eq. (F.1).

We start our calculations with the transformation of the term $\hat{\mathbf{T}}_1$. Therefore, we use Eqs. (18), (32), and (F.2)—then, we find:

$$\begin{aligned}
\hat{\mathbf{T}}_1 &= (\nabla V) \times \hat{\Pi} + e\mathcal{A} \times \mathbf{E} + e\mathcal{A} \times (\nabla V) + (\partial_t \mathcal{A}) \times \hat{\mathbf{p}} \\
&= [(\nabla V) + (\partial_t \mathcal{A}) - (\partial_t \mathcal{A})] \times \hat{\Pi} + e\mathcal{A} \times [\mathbf{E} + (\nabla V)] + (\partial_t \mathcal{A}) \times \hat{\mathbf{p}} \\
&= -\mathbf{E} \times \hat{\Pi} - (\partial_t \mathcal{A}) \times \hat{\Pi} - e\mathcal{A} \times (\partial_t \mathcal{A}) + (\partial_t \mathcal{A}) \times \hat{\mathbf{p}} \\
&= -\mathbf{E} \times \hat{\Pi} - (\partial_t \mathcal{A}) \times (\hat{\Pi} - e\mathcal{A} - \hat{\mathbf{p}}) \\
&= -\mathbf{E} \times \hat{\Pi}. \tag{F.4}
\end{aligned}$$

Having found the compact result (F.4) for the term $\hat{\mathbf{T}}_1$, we start now with the transformation of the term \hat{T}_2 .

For this task, we regard that because of Eqs. (31) and (A.6) the equation

$$(\partial_t \mathcal{A}) \hat{\mathbf{p}} = \hat{\mathbf{p}}(\partial_t \mathcal{A}) + \mathcal{O}(\epsilon) \tag{F.5}$$

holds.

Then, using Eqs. (18), (31), (32), (F.3), and (F.5), we find:

$$\begin{aligned}
\hat{T}_2 &= -i\hbar \nabla(\nabla V) + e\mathcal{A}(\partial_t \mathcal{A}) + (\partial_t \mathcal{A}) \hat{\mathbf{p}} + e\mathcal{A}(\nabla V) \\
&= \hat{\mathbf{p}}(\nabla V) + e\mathcal{A}(\partial_t \mathcal{A}) + \hat{\mathbf{p}}(\partial_t \mathcal{A}) + e\mathcal{A}(\nabla V) + \mathcal{O}(\epsilon) \\
&= (\hat{\mathbf{p}} + e\mathcal{A}) [(\nabla V) + (\partial_t \mathcal{A})] + \mathcal{O}(\epsilon) \\
&= -\hat{\Pi} \mathbf{E} + \mathcal{O}(\epsilon). \tag{F.6}
\end{aligned}$$

As the next step, we insert the results (F.4) and (F.6) into Eq. (F.1) and find:

$$\begin{aligned}
 i\hbar \partial_t \tilde{\varphi}^\epsilon &= \left(\frac{1}{2m_e} \hat{\Pi}^2 - eV \right) \tilde{\varphi}^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon \\
 &+ \frac{\epsilon^2 e \hbar}{4m_e^2} \Sigma (\mathbf{E} \times \hat{\Pi}) \tilde{\varphi}^\epsilon + \frac{i\epsilon^2 e \hbar}{4m_e^2} \hat{\Pi} \mathbf{E} \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3).
 \end{aligned}
 \tag{F.7}$$

Now, we make an intermediate calculation for the operator $\Sigma (\mathbf{E} \times \hat{\Pi})$ appearing in Eq. (F.7). Therefore, we use Eqs. (18), (31), (32), (A.6), $\nabla \times \nabla V = \mathbf{0}$, and find:

$$\begin{aligned}
 \Sigma (\mathbf{E} \times \hat{\Pi}) &= \varepsilon_{klm} \Sigma_k E_l \hat{\Pi}_m \\
 &= \varepsilon_{klm} \left[\hat{\Pi}_m \Sigma_k E_l - \Sigma_k (\hat{p}_m E_l) \right] \\
 &= \varepsilon_{klm} \hat{\Pi}_m \Sigma_k E_l + i\hbar \varepsilon_{klm} \Sigma_k \{ \partial_m [(\partial_l V) + (\partial_l \mathcal{A}_l)] \} \\
 &= \varepsilon_{klm} \hat{\Pi}_m \Sigma_k E_l + i\hbar \varepsilon_{klm} \Sigma_k (\partial_l \partial_m V) + \mathcal{O}(\epsilon) \\
 &= \hat{\Pi} (\Sigma \times \mathbf{E}) + i\hbar \Sigma (\nabla \times \nabla V) + \mathcal{O}(\epsilon) \\
 &= \hat{\Pi} (\Sigma \times \mathbf{E}) + \mathcal{O}(\epsilon).
 \end{aligned}
 \tag{F.8}$$

Inserting Eq. (F.8) into Eq. (F.7), we find as a result this differential equation for the wave function $\tilde{\varphi}^\epsilon$ up to the second order in ϵ :

$$i\hbar \partial_t \tilde{\varphi}^\epsilon = \frac{1}{2m_e} \hat{\Pi}^2 \tilde{\varphi}^\epsilon - eV \tilde{\varphi}^\epsilon + \frac{\epsilon e \hbar}{2m_e} \Sigma \mathbf{B} \tilde{\varphi}^\epsilon - \frac{\epsilon^2}{8m_e^3} \hat{\Pi}^4 \tilde{\varphi}^\epsilon + \frac{\epsilon^2 e \hbar}{4m_e^2} \hat{\Pi} (\Sigma \times \mathbf{E}) \tilde{\varphi}^\epsilon + \frac{i\epsilon^2 e \hbar}{4m_e^2} \hat{\Pi} \mathbf{E} \tilde{\varphi}^\epsilon + \mathcal{O}(\epsilon^3).
 \tag{F.9}$$

Funding Open Access funding enabled and organized by Projekt DEAL; National Natural Science Foundation of China (12174133).

Data availability statement Our manuscript has no associated data.

Declarations

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article’s Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article’s Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

1. Dirac, P.A.M.: The quantum theory of the electron. Proc. R. Soc. Lond. A **117**, 610 (1928). <https://doi.org/10.1098/rspa.1928.0023>
2. Hunziker, W.: On the nonrelativistic limit of the Dirac theory. Commun. Math. Phys. **40**, 215 (1975). <https://doi.org/10.1007/BF01609998>
3. Schoene, A. Y.: On the nonrelativistic limits of the Klein–Gordon and Dirac equations. J. Math. Anal. Appl. **71**, 36 (1979). [https://doi.org/10.1016/0022-247X\(79\)90216-6](https://doi.org/10.1016/0022-247X(79)90216-6)
4. Cirincione, R.J., Chernoff, P.R.: Dirac and Klein–Gordon equations: convergence of solutions in the nonrelativistic limit. Commun. Math. Phys. **79**, 33 (1981). <https://doi.org/10.1007/BF01208284>

5. Grigore, D.R., Nenciu, G., Purice, R.: On the nonrelativistic limit of the Dirac Hamiltonian. *Ann. Inst. Henri Poincaré Phys. Theor.* **51**, 231 (1989)
6. White, G.B.: Splitting of the Dirac operator in the nonrelativistic limit. *Ann. Inst. Henri Poincaré* **53**, 109 (1990)
7. Najman, B.: The nonrelativistic limit of the nonlinear Dirac equation. *Ann. Inst. Henri Poincaré* **9**, 3 (1992)
8. Bechouche, P., Mauser, N.J., Poupaud, F.: (Semi)-nonrelativistic limits of the Dirac equation with external time-dependent electromagnetic field. *Commun. Math. Phys.* **197**, 405 (1998). <https://doi.org/10.1007/s002200050457>
9. Mauser, N.J.: Rigorous derivation of the Pauli equation with time-dependent electromagnetic field. *VLSI Design* **9**, 415 (1999)
10. Mauser, N.J.: Semi-relativistic approximations of the Dirac equation: first and second order corrections. *Transp. Theor. Stat. Phys.* **29**, 449 (2000). <https://doi.org/10.1080/00411450008205884>
11. Masmoudi, N., Mauser, N.J.: The selfconsistent Pauli equation. *Monatsh. Math.* **132**, 19 (2001)
12. Fröhlich, F., Studer, U.M.: Gauge invariance and current algebra in nonrelativistic many-body theory. *Rev. Mod. Phys.* **65**, 733 (1993). <https://doi.org/10.1103/RevModPhys.65.733>
13. Schwabl, F.: *Advanced Quantum Mechanics*, 4th edn. Springer, Berlin (2008)
14. Bjorken, J.D., Drell, S.D.: *Relativistic Quantum Mechanics*. McGraw-Hill, New York (1964)
15. Greiner, W.: *Relativistic Quantum Mechanics: Wave Equations*, 3rd edn. Springer, Berlin (2000)
16. Foldy, L.L., Wouthuysen, S.A.: On the Dirac theory of spin 1/2 particles and its non-relativistic limit. *Phys. Rev.* **78**, 29 (1950). <https://doi.org/10.1103/PhysRev.78.29>
17. Pauli, W.: Zur Quantenmechanik des magnetischen Elektrons. *Z. Phys.* **43**, 601 (1927). <https://doi.org/10.1007/BF01397326>

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.