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High-order Hamiltonian obtained by Foldy–Wouthuysen transformation up to the order of $m\alpha^8$

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Complete relativistic corrections of an effective Hamiltonian for a single-particle system in an external electromagnetic field and their unitary equivalent form up to the order of $m\alpha^8$ are obtained. The derivation is based on two approaches applying Foldy–Wouthuysen (FW) transformation to the Dirac Hamiltonian for a particle in an external electromagnetic field. The results are consistent with the previous work at the $m\alpha^6$ and $m\alpha^8$ order correction [*Phys. Rev. A* **71** 012503 (2005); *Phys. Rev. A* **100** 012513 (2019)]. We also further consider the effect of anomalous magnetic moments, namely, the Dirac–Pauli equation, and obtain FW-Hamiltonians at the same order. The results obtained can be used for the subsequent calculation of relativistic and radiation effects in simple atomic and molecular systems.

Keywords: high-order correction, relativistic corrections, Foldy–Wouthuysen (FW) transformation, effective Hamiltonians

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1. Introduction

Precision spectrum calculations for simple atoms such as hydrogen and helium have important theoretical value for testing quantum electrodynamics (QED) and finding new physics beyond the standard model by comparison with the values from high-precision experimental measurements.[1–3] Sven Sturm and colleagues measured the magnetic moment of a single electron bound to a hydrogen-like carbon ion with the relative precision of 3×10^{-11},[4] which is matched by theoretical calculations based on quantum electrodynamics.[5,6] Experiment and theoretical calculations are in excellent agreement so far.

In theoretical calculations, with nonrelativistic approximation (low-energy), the energy level of a simple atom system can be expanded in a series of powers of fine-structure constant α

$$E = E_{(2)} + \Delta E_{(4)} + \Delta E_{(5)} + \Delta E_{(6)} + \Delta E_{(7)} + \Delta E_{(8)} + \cdots, \quad (1)$$

where the number in the subscript indicates the order is $m\alpha^n$. The leading term $E_{(2)}$ can be derived through resolving the time-independent Schrödinger equation $\hat{H}_0|\psi\rangle = E|\psi\rangle$, where $\hat{H}_0 = \hat{p}^2/(2m) + eA^0$. The rest of the terms of Eq. (1) are high-order corrections, such as relativistic, radiative, and recoil corrections. For a light hydrogen-like system, the energy level was calculated up to the order of mα^7.[7] For helium, the complete formula for the $m\alpha^7$ contribution to energy levels was derived recently.[8] At the order of $m\alpha^8$, the derivation of the high-order correction operators has already begun by different methods,[9–11] but the correctness of the results has yet to be verified.

In order to obtain high-order correction, the derivation of an effective Hamiltonian is first needed. One of the practical methods to get relativistic and QED correction operators is Foldy–Wouthuysen (FW) transformation, which was proposed by Foldy and Wouthuysen in 1950.[12] This technique is widely used in deriving relativistic effects on low-energy atomic and molecular systems.[13–15] For Dirac particles with free and weak electromagnetic field approximations, high-order expansion with the FW transformation for the Hamiltonian has been obtained up to the order of $m\alpha^{14}$.[16] However, the approximation condition of weak electromagnetic field cannot apply to atomic and molecular systems. In the field of calculation of atomic and molecular systems, FW transformation is often used to obtain the correction of the low-energy part in the Lamb shift,[17] which contributes to the hyperfine structure of helium, H_2^+, and HD^+.[18–20] At present, with the application of the FW transformation, the relativistic corrections of a Dirac particle in an external electromagnetic field are evaluated to the order of $m\alpha^8$,[9] but there are some numerical errors in the coefficients, which are corrected in this paper.

In this paper, by applying the FW transformation in two different approaches, we obtain the complete relativistic correction operators in unitary equivalent form for the effective Hamiltonian up to $m\alpha^8$, as well as the corrections for Pauli anomalous magnetic moments. In Section 2, the traditional approach to FW transformation is introduced, which is covered

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in many textbooks.[21] In Section 3, two approaches of the FW transformation are applied to the Dirac equation for a particle in electromagnetic field. The different forms for relativistic corrections up to $m\alpha^8$ are obtained. In Section 4, considering Pauli anomalous magnetic moments, the FW transformation of the Dirac–Pauli equation up to the same order is performed.

2. Formalism

The system of single-electron atoms in an external electromagnetic field can be described by the following Dirac Hamiltonian:

$$\begin{aligned} H_{\text{Dirac}} &= \hat{\alpha}\cdot\boldsymbol{\pi}+\hat{\beta}m+eA^0 \\ &= \hat{\alpha}\cdot(\boldsymbol{p}-e\boldsymbol{A})+\hat{\beta}m+eA^0 \\ &= \begin{pmatrix} m+eA^0 & \hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi} \\ \hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi} & -m+eA^0 \end{pmatrix}, \end{aligned} \tag{2}$$

where $\hat{\alpha}$ and $\hat{\beta}$ are 4×4 matrices under the Dirac representation

$$\hat{\alpha}=\begin{pmatrix} 0 & \hat{\sigma} \\ \hat{\sigma} & 0 \end{pmatrix}, \quad \hat{\beta}=\begin{pmatrix} 1_{2\times2} & 0 \\ 0 & -1_{2\times2} \end{pmatrix}, \tag{3}$$

and $\hat{\sigma}$ is the Pauli matrix, while A^0 and $\boldsymbol{A}$ are the scalar and vector potentials of the electromagnetic field, respectively. And the wave function is

$$\phi=\begin{pmatrix} \phi^{\text{L}} \\ \phi^{\text{S}} \end{pmatrix},$$

where ϕ^{L} denotes large component and ϕ^{S} denotes small component. Due to the existence of the $\hat{\alpha}$ operator, the positive energy states of the Hamiltonian couple with the negative energy states, which means the states cannot be dealt with by non-relativistic quantum mechanics. Theoretically, one can find a unitary transformation that transforms all positive energy states into positive energy subspaces with a certain precision.

The Foldy–Wouthuysen transformation is an excellent method to decouple large and small components of the wave function. By this decoupling, such a transformation allows one to get the low-energy approximation of relativistic corrections to a non-relativistic system, such as an electron surrounding a light atomic nucleus. The transformed Hamiltonian is called H_{FW},

$$H_{\text{FW}}=UH_0U^{\dagger}. \tag{4}$$

Here H_0 is the Dirac Hamiltonian (Eq. (2)). In principle, the transformation can be applied to other forms of Hamiltonian, such as spin-0 and spin-1. Only the spin-1/2 case is considered in this work. For the time-dependent Hamiltonian,

$$H_{\text{FW}}=U\left(H_0-\mathrm{i}\partial_t\right)U^{\dagger}+\mathrm{i}\partial_t, \tag{5}$$

where $U=\mathrm{e}^{\mathrm{i}\hat{S}}$.

The aim of FW transformation is to transform the Dirac Hamiltonian into the following form:

$$H_{\text{FW}}=\begin{pmatrix} h_+ & 0 \\ 0 & h_- \end{pmatrix}, \tag{6}$$

where h_+ is the positive energy part of the Hamiltonian and h_- is the negative. Each of them is a 2×2 matrix. Unfortunately no energy-independent closed-form solutions for the transformation U are known in general. Therefore, the form expanded in terms of $m\alpha^n$ is the final result that people usually pursue.

For simplicity and without losing generality, we refer to operators which cause two-component coupling to the wave function as odd operators, such as $\hat{\alpha}\cdot\boldsymbol{\pi}$, and even operators, such as $\hat{\beta}$, A^0, etc. Defining $\hat{O}$ and $\hat{\mathcal{E}}$ as abstract odd–even operators

$$\begin{aligned} \hat{O} &\equiv \hat{\alpha}\cdot\boldsymbol{\pi}, \\ \hat{\mathcal{E}} &\equiv eA^0. \end{aligned} \tag{7}$$

$\hat{\mathcal{E}}$ can be changed to $(eA^0-\mathrm{i}\partial_t)$ in the time-dependent case. Then the Dirac Hamiltonian can be divided into

$$H_0=\hat{\beta}m+\hat{O}+\hat{\mathcal{E}}, \tag{8}$$

where the following commutative relations are satisfied:

$$\left\{\hat{\beta},\hat{O}\right\}=0, \quad \left[\hat{\beta},\hat{\mathcal{E}}\right]=0. \tag{9}$$

For the sake of simplicity, only the time-independent Hamiltonian will be considered here.

For the unitary transformation of H_0,

$$\begin{aligned} H' &= UH_0U^{\dagger}=\mathrm{e}^{\mathrm{i}\hat{S}}H_0\mathrm{e}^{-\mathrm{i}\hat{S}} \\ &= H_0+\frac{\mathrm{i}}{1!}\left[\hat{S},H_0\right]+\frac{\mathrm{i}^2}{2!}\left[\hat{S},\left[\hat{S},H_0\right]\right]+\cdots \\ &\quad +\frac{\mathrm{i}^n}{n!}\overbrace{\left[\left[\hat{S},\left[\hat{S},\cdots\left[\hat{S},H_0\right]\cdots\right]\right]\right]}^{n}+\cdots, \end{aligned} \tag{10}$$

here, using the following formula:

$$\begin{aligned} \mathrm{e}^{A}B\mathrm{e}^{-A} &= \sum_{n=0}^{\infty}\frac{1}{n!}\left[A^{(n)},B\right] \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\overbrace{[A,[A,\cdots[A,B]\cdots]]}^{n}. \end{aligned}$$

$\hat{S}$ can be chosen as: $\hat{S}=-\frac{\mathrm{i}\hat{\beta}\hat{O}}{2m}$. Substituting $\hat{S}$ and H_0 from their own expressions into the equation and simplifying, H' can be derived as

$$\begin{aligned} H' &= m\hat{\beta}+\hat{\mathcal{E}}+\frac{1}{2m}\hat{O}^2\hat{\beta}-\frac{1}{8m^3}\hat{O}^4\hat{\beta}-\frac{1}{8m^2}\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right] \\ &\quad +\frac{1}{384m^4}\left[\hat{O},\left[\hat{O},\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]\right] \\ &\quad -\frac{1}{3m^2}\hat{O}^3+\frac{1}{30m^4}\hat{O}^5+\frac{1}{2m}\hat{\beta}\left[\hat{O},\hat{\mathcal{E}}\right] \\ &\quad -\frac{1}{48m^3}\hat{\beta}\left[\hat{O},\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]+\cdots. \end{aligned} \tag{11}$$

The term multiplying an odd (even) number of odd operators is an odd (even) operator. It can be seen that the lowest level of odd operator is from $1/m^0$ up to $1/m^1$ according to the term $\frac{1}{2m}\hat{\beta}\left[\hat{O},\hat{\mathcal{E}}\right]$. As long as one chooses the proper form of $\hat{S}$ operator, $H_{\rm FW}$ will contain only even operators of the desired order after a finite number of transformations. Therefore, all the odd(even) operators can be defined as $\hat{O}'\left(\hat{\mathcal{E}}'\right)$, and Hamiltonian (11) will become

$$H' = \hat{\beta}m + \hat{O}' + \hat{\mathcal{E}}'.$$

And a new operator $\hat{S}$ can be chosen from

$$\hat{S}' = -\frac{\mathrm{i}\hat{\beta}\hat{O}'}{2m}.$$

Repeating the same process, $H'' = \mathrm{e}^{\mathrm{i}\hat{S}}H'\mathrm{e}^{-\mathrm{i}\hat{S}}$ can be evaluated with the lowest level of the odd operator up to $1/m^2$.

Repeating the process until the lowest order of the odd terms exceeds the desired order, one can obtain a full-even Hamiltonian.

In atomic precision spectroscopy, the fine-structure constant α is used as an order for the magnitude scale to represent contributions to energy level in the electromagnetic interaction. The magnitude of every operator mentioned in our work is listed below:

$$\begin{aligned}\langle\hat{p}\rangle \sim m(v/c),\ \langle\partial_t\rangle \sim m(v/c)^2,\ \langle eA^0\rangle \sim m(v/c)^2,\\ \langle e\boldsymbol{A}\rangle \sim m(v/c)^3,\ \langle\boldsymbol{E}\rangle \sim m^2(v/c)^3,\end{aligned} \tag{12}$$

where $(v/c) \sim \alpha$.

3. FW transformation for Dirac Hamiltonian

The approach described in the previous section is known as the traditional approach to FW transformation. This approach is easy to understand but hard to implement in high-order cases. With the help of a computer program, we get the FW Hamiltonian up to $m\alpha^8$ order. However, the algorithm is rather complicated and time-consuming. Pachucki proposed a new approach to do the transformation, which simplifies the complexity of calculations. To distinguish this from the traditional approach, the FW transformation developed by Pachucki is called the "new approach".

In this section, all relativistic correction operators of the effective Hamiltonian in an external electromagnetic field with an order of $m\alpha^8$ are derived using both approaches mentioned above. Furthermore, the arbitrary form of the effective Hamiltonian is derived by combining the two methods. Each result expressed by the even and odd operators is also given here, and they can be used in wider equations.

3.1. Traditional approach

Based on the traditional approach, with the help of a computer program, we apply FW transformation successively several times to increase the order of the odd operators beyond $m\alpha^8$, and the results obtained are as follows:

$$\begin{aligned}H_{\rm FW} =\ & \hat{\mathcal{E}} + \frac{\hat{O}^2\hat{\beta}}{2m} - \frac{\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]}{8m^2} - \frac{\hat{O}^4\hat{\beta}}{8m^3}\\ & - \frac{\left[\hat{O},\hat{\mathcal{E}}\right]^2\hat{\beta}}{8m^3} - \frac{\left[\hat{O},\left[\hat{O},\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]\right]}{128m^4} + \frac{\left\{\hat{O}^2,\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right\}}{16m^4} - \frac{\left[\hat{O}^2,\left[\hat{O}^2,\hat{\mathcal{E}}\right]\right]}{32m^4} + \frac{\hat{O}^6\hat{\beta}}{16m^5}\\ & + \frac{\left[\left[\hat{\mathcal{E}},\left[\hat{O},\hat{\mathcal{E}}\right]\right],\left[\hat{O},\hat{\mathcal{E}}\right]\right]}{32m^4} + \frac{\left\{\hat{O}^3,\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right\}\hat{\beta} + 2\left\{\left[\hat{O},\hat{\mathcal{E}}\right],\left\{\hat{O}^2,\left[\hat{O},\hat{\mathcal{E}}\right]\right\}\right\}\hat{\beta}}{48m^5}\\ & + \frac{\left(\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}\right)^2\hat{\beta} + \left(\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\right)^2\hat{\beta}}{96m^5} - \frac{49\left[\hat{O}^4,\left\{\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right\}\right]}{1536m^6} - \frac{77\left\{\hat{O}^4,\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right\}}{3072m^6}\\ & + \frac{43\left\{\left[\hat{O}^2,\hat{O}^3\left[\hat{O},\hat{\mathcal{E}}\right]\right] - \left[\hat{O}^3,\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right\}}{1536m^6} - \frac{5\hat{O}^8\hat{\beta}}{128m^7}.\end{aligned} \tag{13}$$

The results listed above are in the form of odd–even operators. The expression of $H_{\rm FW}$ in terms of specific operators can be derived using the following commutation relation:

$$\begin{aligned}\left[\hat{O},\hat{\mathcal{E}}\right] &= \left[\hat{\alpha}\cdot\hat{\pi}, eA^0 - \mathrm{i}\partial_t\right] = \mathrm{i}e\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\begin{pmatrix}0 & 1_{2\times2}\\ 1_{2\times2} & 0\end{pmatrix},\\ \left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\hat{\mathcal{E}}\right] &= \left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}, eA^0 - \mathrm{i}\partial_t\right] = \mathrm{i}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}},\\ \left[\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}},\hat{\mathcal{E}}\right] &= \left[\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}, eA^0 - \mathrm{i}\partial_t\right] = \mathrm{i}\hat{\boldsymbol{\sigma}}\cdot\ddot{\boldsymbol{E}},\end{aligned} \tag{14}$$

where $\boldsymbol{E}$ is electric field

$$\boldsymbol{E} = -\nabla A^0 - \frac{\partial\boldsymbol{A}}{\partial t}. \tag{15}$$

Using the relation above, the effective Hamiltonian can be derived as

$$\begin{aligned}H_{\rm eff} &= H_0 + H_{\rm FW}^{(4)} + H_{\rm FW}^{(6)} + H_{\rm FW}^{(8)},\\ H_0 &= m + eA^0 + \frac{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^2}{2m},\\ H_{\rm FW}^{(4)} &= -\frac{\mathrm{i}e}{8m^2}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right] - \frac{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^4}{8m^3},\\ H_{\rm FW}^{(6)} &= \frac{e^2(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})^2}{8m^3} + \frac{5\mathrm{i}e}{128m^4}\left[(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2,\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right]\end{aligned}$$

$$
\begin{aligned}
&+\frac{3\mathrm{i}e}{64m^4}\left\{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^2,[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}]\right\}+\frac{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^6}{16m^5},\\
H_{\mathrm{FW}}^{(8)} &= \frac{\mathrm{i}e^2}{32m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]-\frac{e}{48m^5}\left\{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^3,\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right\}\\
&-\frac{e^2}{24m^5}\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\left\{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^2,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right\}\\
&-\frac{e^2}{96m^5}\left[(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}))^2+(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}))^2\right]\\
&-\frac{49\mathrm{i}e}{1536m^6}\left[(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^4,\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\}\right]\\
&-\frac{77\mathrm{i}e}{3072m^6}\left\{(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^4,[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}]\right\}\\
&+\frac{43\mathrm{i}e}{1536m^6}\left\{\left[(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^2,(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^3\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right.\\
&\left.-\left[(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^3,(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right\}-\frac{5(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}})^8}{128m^7}. \qquad (16)
\end{aligned}
$$

$H_{\mathrm{FW}}^{(n)}$ represents the order $m\alpha^n$. This result is consistent with previous work on $m\alpha^6$ done by Zhou[10] but has two different terms compared to Pachucki's work. Actually, they are equivalent, and we will discuss this later.

3.2. New approach

The difference between this approach and the traditional approach is the choice of $\hat{S}$ operator:

$$
\begin{aligned}
\hat{S} &= -\frac{\mathrm{i}}{2m}\left\{\hat{\beta}\hat{O}-\frac{1}{3m^2}\hat{\beta}\hat{O}^3+\frac{1}{2m}\left[\hat{O},\hat{\mathcal{E}}-\mathrm{i}\partial_t\right]+\hat{Y}\right\}\\
&= -\frac{\mathrm{i}}{2m}\left\{\hat{\beta}\boldsymbol{\alpha}\cdot\boldsymbol{\pi}-\frac{1}{3m^2}\hat{\beta}(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})^3\right.\\
&\left.+\frac{1}{2m}\left[\boldsymbol{\alpha}\cdot\boldsymbol{\pi},eA^0-\mathrm{i}\partial_t\right]+\hat{Y}\right\}, \qquad (17)
\end{aligned}
$$

where $\hat{Y}$ is an unspecified odd operator and has following commutation relation:

$$\left\{\hat{\beta},\hat{Y}\right\}=0.$$

The purpose of introducing the $\hat{Y}$ operator is to cancel all high-order odd terms at the end of the calculation. Thus, after manually eliminating the odd operators in the $\hat{Y}$ operator, only one FW transformation is required to obtain the Hamiltonian of Eq. (6).

According to this idea, we choose the form of the $\hat{S}$ operator as follows instead of Eq. (17):

$$
\begin{aligned}
\hat{S} = &\frac{-\mathrm{i}\hat{\beta}}{2m}\left\{\hat{O}+\frac{\left(c_{11}\hat{O}\hat{\mathcal{E}}+c_{12}\hat{\mathcal{E}}\hat{O}\right)\hat{\beta}}{m}+\frac{c_{21}\hat{O}^3}{m^2}+\frac{c_{22}\hat{O}\hat{\mathcal{E}}^2+c_{23}\hat{\mathcal{E}}\hat{O}\hat{\mathcal{E}}+c_{24}\hat{\mathcal{E}}^2\hat{O}}{m^2}\right.\\
&+\frac{\left(c_{31}\hat{O}^3\hat{\mathcal{E}}+c_{32}\hat{O}^2\hat{\mathcal{E}}\hat{O}+c_{33}\hat{O}\hat{\mathcal{E}}\hat{O}^2+c_{34}\hat{\mathcal{E}}\hat{O}^3\right)\hat{\beta}}{m^3}+\frac{\left(c_{35}\hat{O}\hat{\mathcal{E}}^3+c_{36}\hat{\mathcal{E}}\hat{O}\hat{\mathcal{E}}^2+c_{37}\hat{\mathcal{E}}^2\hat{O}\hat{\mathcal{E}}+c_{38}\hat{\mathcal{E}}^3\hat{O}\right)\hat{\beta}}{m^3}\\
&+\frac{c_{40}\hat{O}^5}{m^4}+\frac{1}{m^4}\left[c_{41}\hat{O}^3\hat{\mathcal{E}}^2+c_{42}\hat{O}\left(\hat{O}\hat{\mathcal{E}}\right)^2+c_{43}\hat{O}^2\hat{\mathcal{E}}^2\hat{O}+c_{44}\hat{O}\hat{\mathcal{E}}\hat{O}^2\hat{\mathcal{E}}+c_{45}\hat{O}\left(\hat{\mathcal{E}}\hat{O}\right)^2\right.\\
&\left.+c_{46}\hat{O}\hat{\mathcal{E}}^2\hat{O}^2+c_{47}\hat{\mathcal{E}}\hat{O}^3\hat{\mathcal{E}}+c_{48}\hat{\mathcal{E}}\hat{O}^2\hat{\mathcal{E}}\hat{O}+c_{49}\left(\hat{\mathcal{E}}\hat{O}\right)^2\hat{O}+c_{4,10}\hat{\mathcal{E}}^2\hat{O}^3\right]\\
&\left.+\frac{1}{m^5}\left(c_{51}\hat{O}^5\hat{\mathcal{E}}+c_{52}\hat{O}^4\hat{\mathcal{E}}\hat{O}+c_{53}\hat{O}^3\hat{\mathcal{E}}\hat{O}^2+c_{54}\hat{O}^2\hat{\mathcal{E}}\hat{O}^3+c_{55}\hat{O}\hat{\mathcal{E}}\hat{O}^4+c_{56}\hat{\mathcal{E}}\hat{O}^5\right)\hat{\beta}+\frac{c_6\hat{O}^7}{m^6}\right\}. \qquad (18)
\end{aligned}
$$

After the transformation, there will be a Hamiltonian with both odd and even terms. Combining similar terms and making the coefficients of the odd terms equal to 0, parameters in the $\hat{S}$ operator can be determined as

$$
\begin{aligned}
&c_{11}=-\frac{1}{2},\quad c_{12}=\frac{1}{2},\quad c_{21}=-\frac{1}{3},\quad c_{22}=\frac{1}{4},\\
&c_{23}=-\frac{1}{2},\quad c_{24}=\frac{1}{4},\quad c_{31}=\frac{7}{24},\quad c_{32}=-\frac{5}{24},\\
&c_{33}=\frac{5}{24},\quad c_{34}=-\frac{7}{24},\quad c_{35}=-\frac{1}{8},\quad c_{36}=\frac{3}{8},\\
&c_{37}=-\frac{3}{8},\quad c_{38}=\frac{1}{8},\quad c_{40}=\frac{1}{5},\quad c_{41}=-\frac{5}{24},\\
&c_{42}=\frac{1}{4},\quad c_{43}=-\frac{1}{8},\quad c_{44}=-\frac{1}{6},\quad c_{45}=\frac{1}{6},\\
&c_{46}=-\frac{1}{8},\quad c_{47}=\frac{1}{3},\quad c_{48}=-\frac{1}{6},\quad c_{49}=\frac{1}{4},\\
&c_{4,10}=-\frac{5}{24},\quad c_{51}=-\frac{49}{240},\quad c_{52}=\frac{11}{80},\quad c_{53}=-\frac{19}{120},\\
&c_{54}=\frac{19}{120},\quad c_{55}=-\frac{11}{80},\quad c_{56}=\frac{49}{240},\quad c_6=-\frac{1}{7}. \qquad (19)
\end{aligned}
$$

Then, the $\hat{S}$ operator can be determined as

$$
\begin{aligned}
\hat{S} = &\frac{\mathrm{i}\hat{O}\hat{\beta}}{2m}-\frac{\mathrm{i}\left[\hat{O},\hat{\mathcal{E}}\right]}{4m^2}-\frac{\mathrm{i}\hat{O}^3\hat{\beta}}{6m^3}-\frac{\mathrm{i}\left[\hat{\mathcal{E}},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\hat{\beta}}{8m^3}\\
&+\frac{\mathrm{i}}{48m^4}\left\{7\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^2+2\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}+7\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\right\}-\frac{\mathrm{i}}{16m^4}\left[\hat{\mathcal{E}},\left[\hat{\mathcal{E}},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]+\frac{24\mathrm{i}\hat{O}^5\hat{\beta}}{240m^5}\\
&+\frac{\mathrm{i}}{48m^5}\left(-2\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{\mathcal{E}}\hat{O}-5\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\hat{\mathcal{E}}+2\hat{\mathcal{E}}\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}+5\hat{\mathcal{E}}\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\right)\hat{\beta}
\end{aligned}
$$

$$+\frac{\mathrm{i}}{48m^5}\left\{5\left[\hat{\mathcal{E}},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\hat{O}^2-2\left[\hat{O},\hat{\mathcal{E}}\right]\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}-3\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]+\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\left[\hat{O},\hat{\mathcal{E}}\right]\right\}\hat{\beta}$$
$$-\frac{\mathrm{i}}{480m^6}\left\{49\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^4+16\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^3+54\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^2+16\hat{O}^3\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}+49\hat{O}^4\left[\hat{O},\hat{\mathcal{E}}\right]\right\}-\frac{\mathrm{i}\hat{O}^7\hat{\beta}}{14m^7}. \tag{20}$$

Finally, H_{FW} is obtained as

$$\begin{aligned}
H_{\mathrm{FW}} =\ & \hat{\mathcal{E}}+\frac{\hat{O}^2\hat{\beta}}{2m}-\frac{\hat{O}^4\hat{\beta}}{8m^3}-\frac{\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]}{8m^2}\\
&+\frac{\hat{O}^6\hat{\beta}}{16m^5}+\frac{\left\{\hat{O},\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right\}\hat{\beta}}{16m^3}-\frac{\left[\hat{O},\left[\hat{O},\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]\right]}{128m^4}+\frac{\left\{\hat{O}^2,\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right\}}{16m^4}\\
&-\frac{5\hat{O}^8\hat{\beta}}{128m^7}+\frac{\left[\left[\hat{O},\hat{\mathcal{E}}\right],\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right]}{32m^4}-\frac{\left[\hat{O},\left[\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right]-\left[\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right],\left[\hat{O},\hat{\mathcal{E}}\right]\right]}{32m^4}\\
&-\frac{5\left\{\left[\hat{O},\hat{\mathcal{E}}\right],\left\{\hat{O},\left\{\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right\}\right\}\right\}\hat{\beta}+\left\{\left[\hat{O},\hat{\mathcal{E}}\right],\left\{\hat{O}^2,\left[\hat{O},\hat{\mathcal{E}}\right]\right\}\right\}\hat{\beta}}{128m^5}+\frac{11\left[\left\{\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right\},\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]\hat{\beta}}{256m^5}\\
&+\frac{-\left[\hat{O}^2,\left[\hat{O},\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right]\right]\hat{\beta}}{64m^5}+\frac{-11\left\{\hat{O},\left\{\hat{O},\left\{\hat{O},\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right\}\right\}\right\}\hat{\beta}}{256m^5}\\
&-\frac{5\left\{\hat{O}^4,\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right\}}{128m^6}-\frac{\left[\hat{O}^4,\left\{\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right\}\right]}{512m^6}+\frac{11\left[\hat{O}^2,\left[\hat{O}^2,\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]\right]\right]}{1024m^6}.
\end{aligned} \tag{21}$$

After substituting each odd (even) operator with its relevant operator in the Dirac equation and using the commutator relation described in Eq. (14), the transformation on the Dirac Hamiltonian can be obtained as

$$\begin{aligned}
H_{\mathrm{eff}} =\ & H_0+H_{\mathrm{FW}}^{(4)}+H_{\mathrm{FW}}^{(6)}+H_{\mathrm{FW}}^{(8)},\\
H_0 =\ & m+eA^0+\frac{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2}{2m},\\
H_{\mathrm{FW}}^{(4)} =\ & -\frac{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^4}{8m^3}-\frac{\mathrm{i}e}{8m^2}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right],\\
H_{\mathrm{FW}}^{(6)} =\ & \frac{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^6}{16m^5}-\frac{e}{16m^3}\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right\}\\
&-\frac{\mathrm{i}e}{128m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right]\right]\\
&+\frac{\mathrm{i}e}{16m^4}\left\{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2,\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right\},\\
H_{\mathrm{FW}}^{(8)} =\ & -\frac{5\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^8}{128m^7}-\frac{\mathrm{i}e^2}{32m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right]\\
&-\frac{\mathrm{i}e^2}{32m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]+\frac{\mathrm{i}e}{32m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\ddot{\boldsymbol{E}}\right]\\
&+\frac{5e^2}{128m^5}\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right\}\right\}\\
&+\frac{e^2}{128m^5}\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\left\{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right\}\\
&-\frac{11e^2}{256m^5}\left[\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\},\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right]\\
&+\frac{e}{64m^5}\left[\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2,\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right]\right]\\
&+\frac{11e}{256m^5}\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right\}\right\}\right\}\\
&-\frac{5\mathrm{i}e}{128m^6}\left\{\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^4,\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right\}\\
&-\frac{\mathrm{i}e}{512m^6}\left[\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^4,\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right]\\
&+\frac{11\mathrm{i}e}{1024m^6}\left[\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2,\left[\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2,\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right]\right].
\end{aligned} \tag{22}$$

This result is consistent with Puchucki's work at the order of $m\alpha^6$.[22]

At the order of $m\alpha^8$, this result corrected the coefficient error in the work by Mei.[9] By comparing the two results item by item, one can see that their difference is only in the coefficients of some items. By subtracting one equation from the other, we get the different terms

$$\begin{aligned}
\Delta H =\ & -\frac{e^2}{96m^5}\left\{\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right]\right\}\right.\\
&\left.+2\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\left\{\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right)^2,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right\}\right\}\\
&-\frac{\mathrm{i}e}{23040m^6}\left\{148\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right)^5\right]\right.\\
&+765\left[\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right)^4,\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right]\\
&+865\left[\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right)^5,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\\
&\left.-100\left[\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right)^3,\left\{\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right)^2,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right\}\right]\right\}.
\end{aligned} \tag{23}$$

As one can see, the coefficient errors occur to terms containing one or two $(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})$, while terms containing the first or second derivatives of $(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})$ with respect to time are the same. Since the same approach is applied, the differences are mostly due to the miscalculation of Ref. [9].

Compared with the result Eq. (16) obtained by the traditional approach, we find that there are several formal differences. Subtracting Eq. (22) from Eq. (16) to get the difference

$$\begin{aligned}
\Delta H_{\mathrm{FW}} =\ & \frac{e}{16m^3}\left\{2e\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)^2+\left\{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right\}\right\}\\
&-\frac{\mathrm{i}e^2}{32m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right]-\frac{\mathrm{i}e}{32m^4}\left[\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}},\hat{\boldsymbol{\sigma}}\cdot\ddot{\boldsymbol{E}}\right]
\end{aligned}$$

$$
\begin{aligned}
&-\frac{\mathrm{i}e}{32m^4}\left[\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^3+\hat{\sigma}\cdot\hat{\pi}\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\right.\\
&\left.-\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\hat{\sigma}\cdot\boldsymbol{E}\hat{\sigma}\cdot\hat{\pi}-\left(\hat{\sigma}\cdot\hat{\pi}\right)^3\hat{\sigma}\cdot\boldsymbol{E}\right]\\
&-\frac{e}{768m^5}\left[17\hat{\sigma}\cdot\dot{\boldsymbol{E}}\left(\hat{\sigma}\cdot\hat{\pi}\right)^3+51\hat{\sigma}\cdot\hat{\pi}\hat{\sigma}\cdot\dot{\boldsymbol{E}}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\right.\\
&\left.+51\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\hat{\sigma}\cdot\dot{\boldsymbol{E}}\hat{\sigma}\cdot\hat{\pi}+17\left(\hat{\sigma}\cdot\hat{\pi}\right)^3\hat{\sigma}\cdot\dot{\boldsymbol{E}}\right]\\
&-\frac{e^2}{768m^5}\left[68\left(\hat{\sigma}\cdot\boldsymbol{E}\right)^2\left(\hat{\sigma}\cdot\hat{\pi}\right)^2+68\left(\hat{\sigma}\cdot\boldsymbol{E}\hat{\sigma}\cdot\hat{\pi}\right)^2\right.\\
&+70\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\hat{\sigma}\cdot\boldsymbol{E}\\
&+66\hat{\sigma}\cdot\hat{\pi}\left(\hat{\sigma}\cdot\boldsymbol{E}\right)^2\hat{\sigma}\cdot\hat{\pi}+68\left(\hat{\sigma}\cdot\hat{\pi}\hat{\sigma}\cdot\boldsymbol{E}\right)^2\\
&\left.+68e\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\left(\hat{\sigma}\cdot\boldsymbol{E}\right)^2\right]\\
&+\frac{\mathrm{i}e}{1536m^6}\left[41\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^5+51\hat{\sigma}\cdot\hat{\pi}\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^4\right.\\
&+10\hat{\sigma}\cdot\hat{\pi}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^3\\
&-10\left(\hat{\sigma}\cdot\hat{\pi}\right)^3\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2-51\left(\hat{\sigma}\cdot\hat{\pi}\right)^4\hat{\sigma}\cdot\boldsymbol{E}\hat{\sigma}\cdot\hat{\pi}\\
&\left.-41\left(\hat{\sigma}\cdot\hat{\pi}\right)^5\hat{\sigma}\cdot\boldsymbol{E}\right]. \qquad (24)
\end{aligned}
$$

As one can see, the operators of $m\alpha^4$ are the same, but $m\alpha^6$ (the first term in Eq. (24)) and $m\alpha^8$ operators are not. This is because of the arbitrariness of unitary transformation. In the next subsection, we give the Hamiltonian with unitary transformation of the arbitrary form.

3.3. Arbitrary form of H_{FW}

As shown by the results above, different forms can be obtained by using different approaches. We hope to find a form of H_{FW} with some undetermined parameters to include all the forms we can get from FW transformation.

For this purpose, we start from the $\hat{S}$ operator in Eq. (18), and perform multiple FW transformations on H_0 successively to "push" the odd operators beyond the considered order, just as we did with the traditional approach, except that in each transformation we use an arbitrary form of odd operators with undetermined parameters during the iteration. Noticing that only the term corresponding to the lowest power of $1/m$ in the $\hat{S}$ operator affects the lowest order of the odd operator after transformation, we choose the lowest order of the odd operators in H as the first term in the $\hat{S}$ operator before the next transformation. Other terms in the $\hat{S}$ operator are arbitrary.

After doing FW transformation several times, H_{FW} is obtained as

$$
\begin{aligned}
H_{\mathrm{FW}} =\ & \frac{\hat{O}^2\hat{\beta}}{2m}+\hat{\mathcal{E}}-\frac{\left[\hat{O},\left[\hat{O},\hat{\mathcal{E}}\right]\right]}{8m^2}-\frac{\hat{O}^4\hat{\beta}}{8m^3}\\
&+\frac{-C_1\left(\left[\hat{O},\hat{\mathcal{E}}\right]\right)^2-C_4\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\hat{O}-C_6\hat{O}\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]}{8m^3}\hat{\beta}-\frac{C_9\hat{\mathcal{E}}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}+C_{11}\hat{\mathcal{E}}\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]}{4m^3}\hat{\beta}\\
&+\frac{1}{128m^4}\left\{C_{13}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^3+C_{16}\hat{O}^3\left[\hat{O},\hat{\mathcal{E}}\right]+C_{14}\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^2+C_{15}\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}\right\}+\frac{\hat{O}^6}{16m^5}\hat{\beta}\\
&+\frac{1}{32m^4}\left\{-C_2\left[\hat{O},\hat{\mathcal{E}}\right]\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]-C_3\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\left[\hat{O},\hat{\mathcal{E}}\right]\right\}-\frac{C_8\mathcal{E}\left[\hat{O},\hat{\mathcal{E}}\right]^2}{4m^4}\\
&+\frac{-C_5\left[\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\hat{O}-2C_7\hat{O}\left[\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]}{16m^4}+\frac{\mathcal{E}\left(-C_{10}\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\hat{O}+C_{12}\hat{O}\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\right)}{16m^4}\\
&+\frac{1}{384m^5}\left\{-C_{34}\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\hat{O}^3-C_{30}\hat{O}^3\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]-C_{32}\hat{O}\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\hat{O}^2-C_{27}\hat{O}^2\left[\left[\hat{O},\hat{\mathcal{E}}\right],\hat{\mathcal{E}}\right]\hat{O}\right\}\hat{\beta}\\
&-\frac{1}{384m^5}\left\{C_{33}\left[\hat{O},\hat{\mathcal{E}}\right]^2\hat{O}^2+C_{35}\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]^2+C_{36}\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]^2\hat{O}\right.\\
&\left.+C_{31}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]+4C_{23}\left(\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}\right)^2+4C_{24}\left(\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\right)^2\right\}\hat{\beta}\\
&-\frac{\mathcal{E}}{48m^5}\left\{C_{22}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^3+C_{19}\hat{O}^3\left[\hat{O},\hat{\mathcal{E}}\right]+C_{21}\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^2+C_{20}\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}\right\}\hat{\beta}\\
&+\frac{1}{3072m^6}\left\{C_{28}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^5+C_{25}\hat{O}^5\left[\hat{O},\hat{\mathcal{E}}\right]+C_{26}\hat{O}\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^4\right.\\
&\left.+C_{29}\hat{O}^4\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}+2C_{17}\hat{O}^2\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^3-2C_{18}\hat{O}^3\left[\hat{O},\hat{\mathcal{E}}\right]\hat{O}^2\right\}-\frac{5\hat{O}^8\hat{\beta}}{128m^7}. \qquad (25)
\end{aligned}
$$

Using Eq. (14), it can be concretized into the Dirac Hamiltonian operators

$$
\begin{aligned}
H_{\mathrm{eff,arb}} =\ & H_0+H_{\mathrm{FW}}^{(4)}+H_{\mathrm{FW,arb}}^{(6)}+H_{\mathrm{FW,arb}}^{(8)},\\
H_{\mathrm{FW,arb}}^{(6)} =\ & \frac{e}{8m^3}\left[C_1e\left(\hat{\sigma}\cdot\boldsymbol{E}\right)^2+C_4\hat{\sigma}\cdot\dot{\boldsymbol{E}}\hat{\sigma}\cdot\hat{\pi}+C_6\hat{\sigma}\cdot\hat{\pi}\hat{\sigma}\cdot\dot{\boldsymbol{E}}\right]-\frac{\mathrm{i}eC_9\left(eA^0-\mathrm{i}\partial_t\right)}{4m^3}\left\{\hat{\sigma}\cdot\hat{\pi},\hat{\sigma}\cdot\boldsymbol{E}\right\}\\
&+\frac{\mathrm{i}e}{128m^4}\left[C_{13}\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^3+C_{14}\hat{\sigma}\cdot\hat{\pi}\hat{\sigma}\cdot\boldsymbol{E}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2+C_{15}\left(\hat{\sigma}\cdot\hat{\pi}\right)^2\hat{\sigma}\cdot\boldsymbol{E}\hat{\sigma}\cdot\hat{\pi}+C_{16}\left(\hat{\sigma}\cdot\hat{\pi}\right)^3\hat{\sigma}\cdot\boldsymbol{E}\right]+\frac{\left(\hat{\sigma}\cdot\hat{\pi}\right)^6}{16m^5},
\end{aligned}
$$

$$
\begin{aligned}
H_{\mathrm{eff,arb}}^{(8)} = & \frac{\mathrm{i}e^2}{32m^4}\left(C_2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}+C_3\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)+\frac{e^2C_8}{4m^4}\left(eA^0-\mathrm{i}\partial_t\right)\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)^2 \\
& +\frac{\mathrm{i}e}{16m^4}\left(C_5\hat{\boldsymbol{\sigma}}\cdot\ddot{\boldsymbol{E}}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}+2C_7\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\hat{\boldsymbol{\sigma}}\cdot\ddot{\boldsymbol{E}}\right)+\frac{e\left(eA^0-\mathrm{i}\partial_t\right)}{16m^4}\left(C_{10}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}-C_{12}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right) \\
& +\frac{e}{384m^5}\left[C_{34}e\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^3+C_{30}e\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^3\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}+C_{32}e\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2+C_{27}e\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right] \\
& +\frac{e^2}{384m^5}\left[C_{33}\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)^2\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2+C_{35}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)^2+C_{36}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)^2\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right. \\
& \left.+C_{31}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}+4C_{23}\left(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2+4C_{24}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right)^2\right] \\
& -\frac{\mathrm{i}e\left(eA^0-\mathrm{i}\partial_t\right)}{48m^5}\left[C_{22}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^3+C_{19}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^3\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}+C_{21}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2+C_{20}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)\right] \\
& +\frac{\mathrm{i}e}{3072m^6}\left[C_{28}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^5+C_{25}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^5\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}+C_{26}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^4\right. \\
& \left.+C_{29}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^4\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}+2C_{17}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^3-2C_{18}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^3\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^2\right]-\frac{5\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\pi}}\right)^8}{128m^7}, \qquad (26)
\end{aligned}
$$

H_0 and $H_{\mathrm{FW}}^{(4)}$ are the same as previous results above. Every coefficient C_n in Eqs. (25) and (26) is listed in Table 1.

Table 1. The parameters in Eqs. (25) and (26).

C_n	The value determined by c_n
C_1	$3c_{11}+c_{12}+1$
C_2	$12c_{22}+4c_{23}-1$
C_3	$2c_{11}+2c_{12}+8c_{22}+8c_{23}+4c_{24}+1$
C_4	$2c_{11}+c_{12}$
C_5	$c_{11}+c_{12}+2(c_{23}+c_{24})$
C_6	c_{11}
C_7	c_{22}
C_8	$c_{22}+c_{23}+c_{24}$
C_9	$c_{11}+c_{12}$
C_{10}	$c_{11}+c_{12}+2c_{23}+4c_{24}$
C_{11}	$c_{11}+c_{12}$
C_{12}	$c_{11}+c_{12}-2(2c_{22}+c_{23})$
C_{13}	$8c_{12}-11$
C_{14}	$8c_{11}+16c_{12}+1$
C_{15}	$16c_{11}+8c_{12}-1$
C_{16}	$8c_{11}+11$
C_{17}	$8c_{11}(12c_2+12c_{21}-7)+48c_2-60c_{12}+96c_{21}+96c_{32}+192c_{33}+96c_{34}+59$
C_{18}	$-8c_{12}(12c_2+12c_{21}-7)+48c_2+60c_{11}+96c_{21}-96c_{31}-192c_{32}-96c_{33}+59$
C_{19}	$(c_{11}+c_{12})(12c_2+12c_{21}-1)-3(2c_{22}+c_{23}-4(c_{31}+c_{32}+c_{33}+c_{34}))$
C_{20}	$(c_{11}+c_{12})(12c_2+12c_{21}-1)-3(c_{23}+2c_{24}-4(c_{31}+c_{32}+c_{33}+c_{34}))$
C_{21}	$(c_{11}+c_{12})(12c_2+12c_{21}-1)+3(2c_{22}+c_{23}+4(c_{31}+c_{32}+c_{33}+c_{34}))$
C_{22}	$(c_{11}+c_{12})(12c_2+12c_{21}-1)+3(c_{23}+2c_{24}+4(c_{31}+c_{32}+c_{33}+c_{34}))$
C_{23}	$6c_{11}(6c_2+6c_{21}-1)+c_{12}(24c_2+24c_{21}-5)+6c_2+12c_{21}-6c_{23}-12c_{24}+48c_{31}+36c_{32}+24c_{33}+12c_{34}+1$
C_{24}	$c_{11}(24c_2+24c_{21}+1)+2c_{12}(6c_2+6c_{21}+1)+6c_2+12c_{21}-12c_{22}-6c_{23}+36c_{31}+24c_{32}+12c_{33}+1$
C_{25}	$4c_{11}(48c_2+48c_{21}-13)+96c_2+192c_{21}+192c_{31}-143$
C_{26}	$4c_{11}(48c_2+48c_{21}-13)+16c_{12}(12c_2+12c_{21}-7)+3(64c_{33}+128c_{34}+7)$
C_{27}	$16c_{11}(3c_2+3c_{21}-1)+c_{12}(48c_2+48c_{21}-13)-24(c_{23}+c_{24}-4c_{31}-2c_{32})$
C_{28}	$4c_{12}(48c_2+48c_{21}-13)-96c_2-192c_{21}+192c_{34}+143$
C_{29}	$16c_{11}(12c_2+12c_{21}-7)+4c_{12}(48c_2+48c_{21}-13)+3(128c_{31}+64c_{32}-7)$
C_{30}	$c_{11}(48c_2+48c_{21}-1)+8(3c_2+6c_{21}-3c_{22}+6c_{31}+2)$
C_{31}	$3c_{11}(48c_2+48c_{21}-5)+c_{12}(48c_2+48c_{21}-1)+8(6c_2+12c_{21}-6c_{22}-3c_{23}+18c_{31}+12c_{32}+12c_{33}+6c_{34}-2)$
C_{32}	$c_{11}(48c_2+48c_{21}+5)+8c_{12}(6c_2+6c_{21}+1)+24(c_{22}+4c_{31}+4c_{32}+2c_{33})$
C_{33}	$3c_{11}(48c_2+48c_{21}-5)+c_{12}(96c_2+96c_{21}-11)+8(3c_2+6c_{21}+6c_{22}+3c_{23}+24c_{31}+24c_{32}+18c_{33}+6c_{34}-1)$
C_{34}	$c_{11}(96c_2+96c_{21}-8)+c_{12}(48c_2+48c_{21}-7)+8(3c_2+6c_{21}+3c_{23}+3c_{24}+12c_{31}+12c_{32}+12c_{33}+6c_{34}+2)$
C_{35}	$c_{11}(96c_2+96c_{21}-5)+c_{12}(48c_2+48c_{21}-1)+8(3c_2+6c_{21}-6c_{22}-3c_{23}+18c_{31}+6c_{32}-1)$
C_{36}	$c_{11}(96c_2+96c_{21}-5)+c_{12}(96c_2+96c_{21}-11)-24(c_{23}+2c_{24}-8c_{31}-6c_{32}-2c_{33})$

Each of the numbered, lowercase values c_n in the table above is an undetermined parameter and can be chosen as any real number.

If parameters in Eq. (26) take the following values, $H_{\rm FW}$ can then be obtained by using the traditional approach Eq. (16):

$$\begin{aligned}
&c_{11}=0,\quad c_{12}=0,\quad c_{22}=0,\quad c_{23}=0,\\
&c_{24}=0,\quad c_{31}=-\frac{1}{2}c_2-c_{21}-\frac{1}{6},\\
&c_{32}=c_2+2c_{21}+\frac{1}{3},\quad c_{33}=-c_2-2c_{21}-\frac{1}{3},\\
&c_{34}=\frac{1}{2}c_2+c_{21}+\frac{1}{6},
\end{aligned}\tag{27}$$

and for the new approach (Eq. (22)):

$$\begin{aligned}
&c_{11}=-\frac{1}{2},\quad c_{12}=\frac{1}{2},\quad c_{22}=\frac{1}{4},\\
&c_{23}=-\frac{1}{2},\quad c_{24}=\frac{1}{4},\\
&c_{31}=\frac{1}{8}-\frac{c_{21}}{2},\quad c_{32}=c_{21}+\frac{1}{8},\\
&c_{33}=-c_{21}-\frac{1}{8},\quad c_{34}=\frac{c_{21}}{2}-\frac{1}{8}.
\end{aligned}\tag{28}$$

By comparison with the previous work by Zhou[10] (Eq. (57)), which reached to $m\alpha^8$ by scattering matching, it can be seen that the two results are perfectly matched, with the list of parameters as follows:

$$\begin{aligned}
&c_{11}=0,\quad c_{32}=\frac{1}{3}(6c_{21}+3c_2+2),\\
&c_{33}=\frac{1}{3}(-6c_{21}-3c_2-2),\\
&c_{31}=\frac{1}{6}(-6c_{21}-3c_2-2).
\end{aligned}\tag{29}$$

This verifies the correctness of our results.

4. FW transformation for the Dirac–Pauli Hamiltonian

In the previous section, higher-order relativistic corrections of the effective Hamiltonian were obtained by applying the FW transformation to the Dirac equation. By adding certain additional factors to the Dirac equation, one can obtain partial corrections for QED effects through the FW transformation.

In this section, the anomalous magnetic moment of the Dirac particle is considered. A Dirac particle with the Pauli anomalous magnetic moment can be described by Dirac–Pauli Hamiltonian. In addition to the Dirac Hamiltonian, there is an anomalous electric interaction $V_{\rm E}$ and an anomalous magnetic interaction $V_{\rm B}$,

$$\begin{aligned}
H_{\rm DP} &= H_{\rm D}+H_{\rm P},\\
H_{\rm P} &= -{\rm i}V_{\rm E}\begin{pmatrix}0 & 1_{2\times2}\\ 1_{2\times2} & 0\end{pmatrix}\cdot\hat{\beta}+V_{\rm B}\hat{\beta}\\
&= \begin{pmatrix}V_{\rm B} & {\rm i}V_{\rm E}\\ -{\rm i}V_{\rm E} & -V_{\rm B}\end{pmatrix},
\end{aligned}\tag{30}$$

where $H_{\rm D}$ is given by Eq. (2), $V_{\rm B}=-\mu'\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}$, $V_{\rm B}=\mu'\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}$, and the coefficient μ' is defined as follows:

$$\mu'=\frac{e}{2m}\left(\frac{g}{2}-1\right).$$

For the case of an electron with $g=2$, $H_{\rm P}=0$, the Dirac–Pauli Hamiltonian degenerates to the Dirac Hamiltonian.

For an FW transformation U, the effective Hamiltonian corresponding to the Dirac–Pauli Hamiltonian has the following form:

$$\begin{aligned}
H_{\rm eff} &= U\left(H_{\rm DP}-{\rm i}\partial_t\right)U^{\dagger}+{\rm i}\partial_t\\
&= U\left(H_{\rm D}+H_{\rm P}-{\rm i}\partial_t\right)U^{\dagger}+{\rm i}\partial_t.
\end{aligned}\tag{31}$$

Defining

$$\hat{\eta}=\begin{pmatrix}0 & 1_{2\times2}\\ 1_{2\times2} & 0\end{pmatrix},\tag{32}$$

this is an odd operator, so the term $\left(-{\rm i}V_{\rm E}\hat{\eta}\cdot\hat{\beta}\right)$ in $H_{\rm P}$ is also an odd operator. The term $V_{\rm B}\hat{\beta}$ is an even operator. It is easy to obtain the following relations:

$$\begin{aligned}
&\left\{-{\rm i}V_{\rm E}\hat{\eta}\cdot\hat{\beta},\hat{\beta}\right\}=0,\\
&\left[V_{\rm B}\hat{\beta},\hat{\beta}\right]=0.
\end{aligned}\tag{33}$$

This relation is same as Eq. (9). Therefore, when FW transformation of the Dirac–Pauli Hamiltonian is performed, Eq. (26), obtained previously, can be applied directly. Substitute the odd and even operators in Eq. (26) into the following form:

$$\begin{aligned}
&\hat{O}\to\hat{O}-{\rm i}V_{\rm E}\hat{\eta}\cdot\hat{\beta},\\
&\hat{\mathcal{E}}\to\hat{\mathcal{E}}+V_{\rm B}\hat{\beta}.
\end{aligned}\tag{34}$$

By expanding all the terms, we obtain the following effective Hamiltonian expression for the Dirac–Pauli Hamiltonian:

$$\begin{aligned}
&H_{\rm eff,DP}=H_{\rm eff,arb}+H_{\rm FW,P},\\
&H_{\rm FW,P}=H^{(4)}_{\rm FW,P}+H^{(6)}_{\rm FW,P}+H^{(8)}_{\rm FW,P},
\end{aligned}\tag{35}$$

where $H_{\rm eff,arb}$ is given by Eq. (26). $H_{\rm FW,P}$ is the part of the effective Hamiltonian that relates to the Pauli anomalous magnetic moment. The specific form of $H_{\rm FW,P}$ is as follows:

$$H^{(4)}_{\rm FW,P}=-\frac{e(g-2)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B})}{4m}-\frac{{\rm i}e(g-2)[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}]}{8m^2},\tag{36a}$$

$$
\begin{aligned}
H^{(6)}_{\mathrm{FW,P}} &= \frac{e(g-2)}{32m^3}\left[eg(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})^2-\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right\}\right]+\frac{e(g-2)}{32m^3}\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\left\{\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\right\}\right\}+\frac{\mathrm{i}e(g-2)}{32m^4}\left\{(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2,\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\right\},\\
H^{(8)}_{\mathrm{FW,P}} &= \frac{\mathrm{i}e^2(g-2)}{128m^4}\left[(4C_9-8C_6+3g-2)\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}+(12C_9-8C_6-g-2)\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right.\\
&\quad\left.+(4C_1-8C_{11}+g-2)\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}+(8C_6-12C_9-3g+2)\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\\
&\quad+\frac{\mathrm{i}e^2(g-2)}{128m^4}\left[-(4C_6-4C_9+g+2)\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}+(4C_6-8C_{11}+g+2)\,\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\right]\\
&\quad+\frac{\mathrm{i}e(g-2)}{32m^4}\left[-(C_4-2C_9)\,\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{B}}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2+(C_6-2C_{11})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{B}}-C_9\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\left(\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{B}}\right)\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right]\\
&\quad+\frac{e^2(g-2)^2}{64m^4}\left[-2\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{E}\times\boldsymbol{B})\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}+\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\times\boldsymbol{B}\right]+\frac{\mathrm{i}eC_9(g-2)}{32m^4}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\ddot{\boldsymbol{E}}\\
&\quad-\frac{e^2(g-2)}{512m^5}\left[(-C_{13}+C_{14}+4g-8)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})^2(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2-(C_{15}-C_{16}-4g+8)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})^2\right.\\
&\quad+(C_{14}-C_{15}+4g-8)\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}-(C_{13}-C_{16}-4g+8)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})\\
&\quad\left.+(C_{13}+C_{15}-4g+8)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2-4(4C_9+g+1)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E})^2\right]\\
&\quad+\frac{e(g-2)}{512m^5}\left[C_{13}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^4-C_{16}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^4\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}+(C_{13}-C_{14})\,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^3\right.\\
&\quad\left.+(8C_9-12)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^3\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}-(C_{14}-C_{15})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2\right]\\
&\quad-\frac{e(g-2)}{512m^5}\left[C_{13}\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^3-C_{16}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^3\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}-C_{14}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})\,\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2+C_{15}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\right]\\
&\quad+\frac{\mathrm{i}e(g-2)}{64m^6}\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^5-(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^5\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}-\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^4\right.\\
&\quad\left.+(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^4\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi}+(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^3-(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^3\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2\right]\\
&\quad-\frac{C_9e(g-2)}{16m^4}\left\{\left[(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2,\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\right]+\left[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi},\hat{\boldsymbol{\sigma}}\cdot\dot{\boldsymbol{E}}\right]\right\}\left(eA^0-\mathrm{i}\partial_t\right), \qquad (36b)
\end{aligned}
$$

and the form of coefficient C_n is given by Table 1.

Since $\boldsymbol{B}\equiv\nabla\times\boldsymbol{A}=\mathrm{i}\boldsymbol{p}\times\boldsymbol{A}$, $\boldsymbol{B}$ is the order of $m^2\alpha^4$. The term $\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{E}\times\boldsymbol{B})$ is derived from the relation $[\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{E},\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}]=2\mathrm{i}\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{E}\times\boldsymbol{B})$, in which we used the following relation:

$$\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{a}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{b}=\boldsymbol{a}\cdot\boldsymbol{b}+\mathrm{i}\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{a}\times\boldsymbol{b}).$$

At the order of $m\alpha^8$, each $(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2$ can be substituted by $\boldsymbol{\pi}^2$, because $(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\pi})^2=\boldsymbol{\pi}^2-e\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}=\boldsymbol{\pi}^2+O(\alpha^4)$.

5. Conclusion

Foldy–Wouthuysen transformation is an excellent technology to obtain high-order correction of the effective Hamiltonian in the field of the high-precision calculations of atoms and molecules. In this work, under low-energy approximation, the higher order effective Hamiltonian that describes relativistic effects at the order of $m\alpha^8$ is derived through two ways of FW transformation (Eqs. (16) and (22)), and the unitary transformation of any form equivalent to them is further obtained by combining the two approaches (Eq. (26)).

Each result is consistent with previous work done by Pachucki and Zhou[10,22] up to the order of $m\alpha^6$. At the order of $m\alpha^8$, the result, Eq. (16), corrects the error of the coefficients from Mei.[9] After comparing the arbitrary unitary equivalent Hamiltonian (Eq. (26)) obtained in this paper with the result obtained by Zhou through scattering matching,[10] and taking appropriate values for the coefficients, it can be seen that they are in good agreement, which shows the correctness of the results in this paper.

And finally, the effect of Pauli anomalous magnetic moment is considered. The whole Hamiltonian with anomalous magnetic moment is also obtained up to the order of $m\alpha^8$ (Eq. (35)).

With the results from this paper, it is possible to derive the $m\alpha^8$ operators which can be used for numerical calculations. Although it is derived from single-particle Dirac and Dirac–Pauli equations, each result can also be used for a multi-particle system with additional terms of correlated interaction.

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