Relativistic Corrections to the Fine Structure of Helium*

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(Received 2 December 1964; revised manuscript received 17 June 1965)

Relativistic corrections to the fine structure of the hydrogen atom have been calculated by many authors, but the experimental confirmation of the theory, or alternatively the determination of the numerical value of the fine-structure constant α, is limited to an accuracy of $1/10^5$ because of the short lifetime of 2^2P states of hydrogen. However, in view of the fact that 2^3P states of helium have a longer lifetime, we expect that the fine-structure intervals of the 2^3P states of helium can be measured to an accuracy of $1/10^6$ or better. With this expectation, we attempted to evaluate semirelativistically the theoretical formula for the helium fine structure to the order α^4 Ry.

I. INTRODUCTION

ONE of the simplest fields of application of quantum mechanics is the theory of atoms with one or two electrons, which also provides a fairly accurate test of the validity of quantum electrodynamics. The simplest of all the applications involving radiative corrections is the calculation of the hydrogen fine structure $(2P_{1/2}-2P_{3/2})$, and its best experimental data at present come from the work by Dayhoff, Triebwasser, and Lamb,[1] which is uncertain to about one part in 10^5. The best available data for α, the fine-structure constant, comes from this work with the same accuracy. But from the consideration of the short lifetime of $2P$ states of

hydrogen, it is unlikely that we can better the existing experimental data any further than the accuracy of $1/10^5$, and this makes the further confirmation of the theory to higher order very difficult. However, in view of the fact that 2^3P states of helium have a longer lifetime (which is about 10^{-7} sec compared with about 10^{-9} sec for $2P$ states of hydrogen), we expect that the fine structure of 2^3P states of helium *can* be measured to an accuracy of up to $1/10^6$ or even better.[2] This experimental prospect and the existing need[3,4] for a better value of α make it necessary to improve the theoretical data for the helium fine structure up to the same order.

The study of the helium fine structure has historically played a very important role because it provides the test for the validity of the quantum mechanics of a many-electron system, not only in its nonrelativistic form, but also in its semirelativistic part. An earlier attempt in this direction was made by Breit[5] by introducing into the Hamiltonian the so-called "Breit interaction term," which essentially comes from a one-photon exchange between the two electrons of helium, and, by using a two-term wave function, Breit calculated ν_{01} (see Fig. 1) to an accuracy of several percent.[6] The Breit term, when transformed into Pauli form, is of order α^2 Ry (which we denote by $\mathfrak{IC}_2$, whereas the unperturbed Schrödinger Hamiltonian is denoted by $\mathfrak{IC}_0$) and should give more accurate results than Breit initially obtained if a more accurate wave function is used.[7] Breit's results were improved this way and also by including in the Hamiltonian the terms[8,9] of order α^3 Ry (which we denote by $\mathfrak{IC}_3$ and which is sometimes called the "Schwinger term" because it is obtained by introducing into $\mathfrak{IC}_2$ the anomalous magnetic moment first suggested by Schwinger[10]). For example, by using
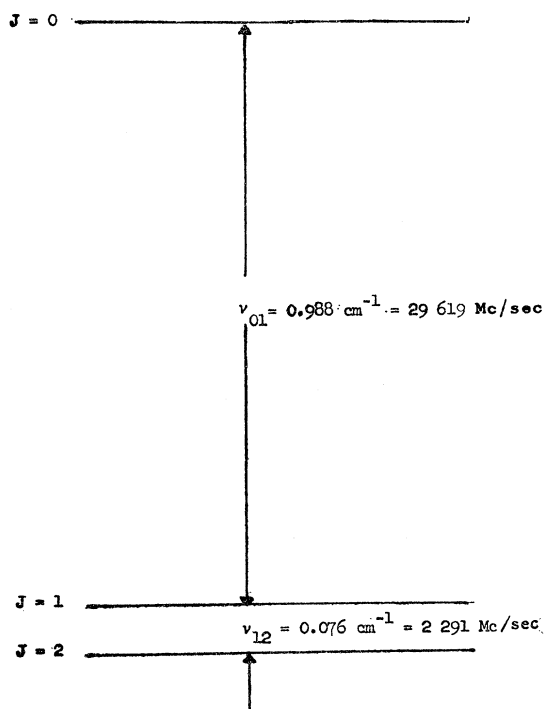

FIG. 1. Energy levels of the $1S2P\ ^3P$ state of helium.

$\nu_{01} = 0.988\ cm^{-1} = 29\ 619\ Mc/sec$

$\nu_{12} = 0.076\ cm^{-1} = 2\ 291\ Mc/sec$

J = 0

J = 1

J = 2

[1] E. S. Dayhoff, S. Triebwasser, and W. E. Lamb, Phys. Rev. 89, 106 (1953).

[2] See footnote 6 of Ref. 15.
[3] C. K. Iddings and P. M. Platzman, Phys. Rev. 115, 919 (1959).
[4] D. Zwanziger, Bull. Am. Phys. Soc. 6, 514 (1961).
[5] G. Breit, Phys. Rev. 34, 553 (1929); 39, 616 (1932).
[6] G. Breit, Phys. Rev. 36, 383 (1930).
[7] G. Araki and S. Huzinaga, Progr. Theoret. Phys. (Kyoto) 6, 673 (1951).
[8] H. Fukuda, Y. Miyamoto, and S. Tomonaga, Progr. Theoret. Phys. (Kyoto) 4, 121 (1949).
[9] T. Fulton and P. C. Martin, Phys. Rev. 95, 811 (1954).
[10] J. Schwinger, Phys. Rev. 73, 416 (1948).

an 8-parameter wave function, Araki, Ohta, and Mano[11] obtained ν_{01} with an accuracy of 1%; by using an 18-parameter wave function, Traub and Foley[12] came within $1/10^3$; and by using a 220-term trial wave function, Pekeris, Schiff, and Lifson[13] reached the accuracy[14] of $1/10^4$, which is just about the order of accuracy needed to see the presence of $\mathcal{K}_3$ in the Hamiltonian. In order to improve the theoretical data further to the accuracy of $1/10^6$, we need to have:

(1) the wave function of $\mathcal{K}_0$ in 2^3P states, which gives the expectation value of $\mathcal{K}_2$ with an accuracy of $1/10^6$;

and

(2) the Hamiltonian term of order α^4 Ry (which we denote by $\mathcal{K}_4$) and perhaps the terms of order $\alpha^5 \ln\alpha$ Ry.

C. Schwartz[15] worked out (1) by using the same technique he had successfully applied for the helium ground-state ($1S$) wave function.[16] Our objective in this paper is to deal with at least part of (2); that is, to find $\mathcal{K}_4$.

Our approach in this paper is basically nothing new. In our Dirac-type Hamiltonian the photon field is quantized, whereas the number of electrons is fixed. In order to simplify our task and to avoid the difficulties which will arise from the self-energy terms, we introduced a form-factor in our Hamiltonian. Terms corresponding to the emission and re-absorption of photons by the same electron, the effect of which is included in the form factor, will be omitted in the later process of calculations. This Hamiltonian, which is expanded in terms of α, is then transformed into the Schrödinger-type Hamiltonian. Then by using a generalized perturbation theory we get the Hamiltonian term $\mathcal{K}_4$ as well as $\mathcal{K}_0$, $\mathcal{K}_2$, and $\mathcal{K}_3$. Here the $\mathcal{K}$'s are to be understood as their expectation values with respect to the wave function of $\mathcal{K}_0$ giving the corresponding terms in the expansion of the energy. In $\mathcal{K}_3$ and $\mathcal{K}_4$ only terms contributing to the fine structure are considered (many spin-independent terms have been dropped).

Finally, our attempt to find $\mathcal{K}_4$ is not intended to be complete (because we have not started from the complete relativistic quantized theory), but we hope that the main parts of $\mathcal{K}_4$ are included in our results and will serve for later improvement.

[11] G. Araki, M. Ohta, and K. Mano, Phys. Rev. **116**, 651 (1959).
[12] J. Traub and H. M. Foley, Phys. Rev. **116**, 914 (1959).
[13] C. L. Pekeris, B. Schiff, and H. Lifson, Phys. Rev. **126**, 1057 (1962).
[14] When the more accurate theoretical data was compared with the more accurate experimental data (of Ref. 15), the accuracy here was still $1/10^4$. This shows that the inclusion of one of the higher order terms, namely $\mathcal{K}_{42}$, alone does not improve the theoretical data, but more or less changes the sign of discrepancies.
[15] C. Schwartz, Phys. Rev. **134**, A1181 (1964).
[16] C. Schwartz, Phys. Rev. **128**, 1146 (1962).

II. HAMILTONIAN

We start with the Hamiltonian for the two-electron system consisting of three parts, given by

$$H = H_r + H_e + H_i, \qquad (\text{II-1})$$

with

$$H_r = \int d^3k k \hbar c \sum_{\lambda=1}^{2} a_\lambda^*(\mathbf{k}) a_\lambda(\mathbf{k}); \quad k = |\mathbf{k}|; \qquad (\text{II-2})$$

$$H_e = (c\boldsymbol{\alpha}_1 \cdot \mathbf{P}_1 + \beta_1 mc^2 - e\varphi_1)$$
$$+ (c\boldsymbol{\alpha}_2 \cdot \mathbf{P}_2 + \beta_2 mc^2 - e\varphi_2) + e\varphi_{12}; \qquad (\text{II-3})$$

$$H_i = e\boldsymbol{\alpha}_1 \cdot \mathbf{A}_1 + e\boldsymbol{\alpha}_2 \cdot \mathbf{A}_2; \qquad (\text{II-4})$$

$$\mathbf{A}(x) = \frac{(\hbar c)^{1/2}}{2\pi} \int \frac{d^3k}{\sqrt{k}} \sum_{\lambda=1}^{2} \boldsymbol{\varepsilon}_\lambda(\mathbf{k}) [a_\lambda(\mathbf{k}) e^{-ik\cdot x}$$
$$+ a_\lambda^*(\mathbf{k}) e^{ik\cdot x}]; \qquad (\text{II-5})$$

$$k \cdot x = kct - \mathbf{k} \cdot \mathbf{r};$$

$$[a_\lambda(\mathbf{k}), a_{\lambda'}^*(\mathbf{k}')]_- = \delta_{\lambda\lambda'} \delta(\mathbf{k} - \mathbf{k}'), \qquad (\text{II-6})$$

where H_r is the Hamiltonian for the radiation field; H_e is the Dirac Hamiltonian for a two-electron system; and H_i represents the interaction between the electron and the radiation field. $\mathbf{A}(x)$ is the radiation field vector in gaussian units, and (II-6) is the usual commutation relation for the creation (a^*) and destruction (a) operators of a photon.

Then, by a perturbation method, it is rather straightforward in principle to evaluate the relativistic corrections involving electron self-energy, but it is difficult in practice. We will sidetrack this difficulty by replacing $\varphi_1(\varphi_2)$, φ_{12}, and $\boldsymbol{\alpha}_1 \cdot \mathbf{A}_1(\boldsymbol{\alpha}_2 \cdot \mathbf{A}_2)$ in (II-1) by $\gamma_1^0 \Gamma_1^0 \varphi_1 \times (\gamma_2^0 \Gamma_2^0 \varphi_2)$, $\Gamma_{12}\varphi_{12}$, and $\gamma_1^0 \boldsymbol{\Gamma}_1 \cdot \mathbf{A}_1(\gamma_2^0 \boldsymbol{\Gamma}_2 \cdot \mathbf{A}_2)$, respectively. Here Γ^μ, the so-called form factor, is given by

$$\Gamma^\mu(P^2) = [1 + F(P^2)]\gamma^\mu + (i/2m)G(P^2)P_\nu\sigma^{\nu\mu}, \quad (\text{II-7})$$

and was derived by several authors.[17,18] Γ_{12} is given by

$$\Gamma_{12}\varphi_{12} = (\gamma^0\Gamma^0)_1(\gamma^0\Gamma^0)_2\varphi_{12}, \qquad (\text{II-8})$$

which will be obtained if we calculate the matrix element of an S matrix corresponding to one-photon exchange through the interaction $-e\Gamma^\mu A_\mu(x)$ and take the contribution of the time-like photon neglecting the retardation effect.

The explicit formulas for $\gamma^0\Gamma^0$, $\gamma^0\boldsymbol{\Gamma}$, and Γ_{12}, when expressed in atomic units, give

$$(\gamma^0\Gamma^0)_{1,2} = (1 + \alpha^3 F + \tfrac{1}{2}\alpha G \mathbf{P} \cdot \boldsymbol{\gamma})_{1,2};$$

$$(\gamma^0\boldsymbol{\Gamma})_{1,2} = [(1 + \alpha^3 F)\boldsymbol{\alpha} + \tfrac{1}{2}\alpha^2(i\gamma^0\boldsymbol{\sigma} \times \mathbf{P} + \alpha P^0\boldsymbol{\gamma})]_{1,2};$$

$$\Gamma_{12} = [1 + \alpha^3 f_0 + \alpha^2 f_1 \boldsymbol{\gamma}_1 \cdot \mathbf{P}_1 + \alpha^2 f_2 \boldsymbol{\gamma}_2 \cdot \mathbf{P}_2 \qquad (\text{II-9})$$
$$+ \alpha^4 f_3 \boldsymbol{\gamma}_1 \cdot \mathbf{P}_1 \boldsymbol{\gamma}_2 \cdot \mathbf{P}_2],$$

[17] L. L. Foldy, Phys. Rev. **87**, 688 (1952).
[18] S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson and Company, Evanston, Illinois, 1961), pp. 543 and 702.

where

$$f_0 = F_1 + F_2 + \alpha^3 F_1 F_2;$$
$$f_1 = \tfrac{1}{2}(1 + \alpha^3 F_2)G_1;$$
$$f_2 = \tfrac{1}{2}(1 + \alpha^3 F_1)G_2; \tag{II-10}$$
$$f_3 = \tfrac{1}{4}G_1 G_2.$$

Thus we have the desired Hamiltonian in atomic units:

$$H = \alpha H_r + [\alpha \boldsymbol{\alpha}_1 \cdot \mathbf{P}_1 + \beta_1 - \alpha^2(1 + \alpha^3 F_1 + \alpha\tfrac{1}{2}G_1 \boldsymbol{\gamma}_1 \cdot \mathbf{P}_1)\varphi_1] + [\alpha \boldsymbol{\alpha}_2 \cdot \mathbf{P}_2 + \beta_2 - \alpha^2(1 + \alpha^3 F_2 + \alpha\tfrac{1}{2}G_2 \boldsymbol{\gamma}_2 \cdot \mathbf{P}_2)\varphi_2]$$
$$+ \alpha^2[1 + \alpha^3 f_0 + \alpha^2 f_1 \boldsymbol{\gamma}_1 \cdot \mathbf{P}_1 + \alpha^2 f_2 \boldsymbol{\gamma}_2 \cdot \mathbf{P}_2 + \alpha^4 f_3 \boldsymbol{\gamma}_1 \cdot \mathbf{P}_1 \boldsymbol{\gamma}_2 \cdot \mathbf{P}_2]\varphi_{12} + \alpha(\sqrt{\alpha})[(1 + \alpha^3 F_1)\boldsymbol{\alpha}_1$$
$$+ \tfrac{1}{2}\alpha^2 G_1(i\boldsymbol{\gamma}_1{}^0 \boldsymbol{\sigma}_1 \times \mathbf{P}_1 + \alpha P_1{}^0 \boldsymbol{\gamma}_1)] \cdot \mathbf{A}_1 + \alpha(\sqrt{\alpha})[(1 + \alpha^3 F_2)\boldsymbol{\alpha}_2 + \alpha^2\tfrac{1}{2}G_2(i\boldsymbol{\gamma}_2{}^0 \boldsymbol{\sigma}_2 \times \mathbf{P}_2 + \alpha P_2{}^0 \boldsymbol{\gamma}_2)] \cdot \mathbf{A}_2. \tag{II-11}$$

In regard to the Hamiltonian (II-11):

(1) In the process of calculating energy, the terms involving emission and re-absorption of photons by the same electron should be omitted because what is left after mass and charge renormalization is supposed to be already included in the form factor.

(2) We will expand the Hamiltonian in powers of α, and we need to expand the form factor likewise as

$$G = {}^0G + \alpha\,{}^1G + \alpha^2\,{}^2G \cdots;$$
$$F = {}^0F + \alpha\,{}^1F + \alpha^2\,{}^2F \cdots; \tag{II-12}$$

where

$${}^0G = {}^0G_1 = {}^0G_2 = 1/2\pi;$$
$${}^1G = {}^1G_1 = {}^1G_2 = -0.328/\pi^2,$$

which[19] was obtained from the field-theory calculations for the free electron. In actual numerical calculations for helium, where the electrons are bound, we will use these data hoping that the error is not significant.

We expect that the corrections to the above static values for G would be of relative order p^2/m^2 which is, in the atomic state, of order α^2 and thus negligible. The leading terms of F, which give the Lamb shift, etc., will enter into our calculation independent of the spin variables, and so will not contribute to the fine structure to the desired order.

(3) Our Hamiltonian does not allow creation, nor destruction, of electrons (and positrons), and corresponding effects are excluded from our consideration, though some of these effects (vacuum polarization) are included in the form factor.

Now that we have the Hamiltonian (II-11), our next step is to convert this into a Schrödinger-type Hamil-

tonian involving the Pauli spin matrix $\boldsymbol{\sigma}$ but independent of the Dirac matrices. We proceed as follows:

We know very well that we can decompose the wave function for one Dirac particle (electron), which is a 1×4 spinor, into a large and a small component, namely,

$$\begin{pmatrix} A \\ B \end{pmatrix}.$$

The operators α, β, γ, etc.,[20] acting on it have the effect

$$\alpha\begin{pmatrix} A \\ B \end{pmatrix} = \sigma\begin{pmatrix} B \\ A \end{pmatrix};$$

$$\beta\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ -B \end{pmatrix}; \tag{II-13}$$

$$\gamma\begin{pmatrix} A \\ B \end{pmatrix} = \sigma\begin{pmatrix} B \\ -A \end{pmatrix}, \text{ etc.,}$$

where $\boldsymbol{\sigma}$ is the Pauli spin matrix and can be treated as a c number. We do likewise for the two-electron system, and express the wave function ψ as

$$\psi = \begin{pmatrix} U & V \\ W & X \end{pmatrix}, \tag{II-14}$$

where the upper row (left column) denotes the large component for the electron "1" ("2") and the lower row (right column) denotes the small component for the same electron. In other words, U is the large-large component; X is the small-small component; and finally $V(W)$ is the large-small (small-large) component for electron "1" and electron "2", respectively. Then

[19] C. Sommerfield, Phys. Rev. **107**, 328 (1957), and several earlier papers referred to therein.

[20] See pp. 26 and 69 of Ref. 18 for the definitions of the Dirac α and γ matrices.

we have the relations:

$$\alpha_1 \begin{pmatrix} U & V \\ W & X \end{pmatrix} = \sigma_1 \begin{pmatrix} W & X \\ U & V \end{pmatrix};$$

$$\alpha_2 \begin{pmatrix} U & V \\ W & X \end{pmatrix} = \sigma_2 \begin{pmatrix} V & U \\ X & W \end{pmatrix};$$

$$\beta_1 \begin{pmatrix} U & V \\ W & X \end{pmatrix} = \begin{pmatrix} U & V \\ -W & -X \end{pmatrix};$$

$$\beta_2 \begin{pmatrix} U & V \\ W & X \end{pmatrix} = \begin{pmatrix} U & -V \\ W & -X \end{pmatrix};$$

$$\gamma_1 \begin{pmatrix} U & V \\ W & X \end{pmatrix} = \sigma_1 \begin{pmatrix} W & X \\ -U & -V \end{pmatrix};$$

$$\gamma_2 \begin{pmatrix} U & V \\ W & X \end{pmatrix} = \sigma_2 \begin{pmatrix} V & -U \\ X & -W \end{pmatrix}; \text{ etc.}$$

(II-15)

Here, again, σ's can be treated as c numbers. Hence, by using the properties of (II-15), the wave equation $(H-E)\Psi=0$ [where H is given by (II-11)] can be transformed into a form of

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = 0,$$

which is equivalent to four coupled linear equations: $A=0$, $B=0$, $C=0$, and $D=0$. Here A, B, C, and D are linear equations with respect to U, V, W, and X. Then by eliminating X, W, and V, we will obtain the single Schrödinger-type equation for U, the large-large component:

$$\mathfrak{K}U = WU. \qquad \text{(II-16)}$$

Obviously $\mathfrak{K}$, the Schrödinger-type Hamiltonian, is a function of α, the fine-structure constant. We expand $\mathfrak{K}$ as

$$\mathfrak{K} = \mathfrak{K}_0 + (\sqrt{\alpha})\mathfrak{K}_{1/2} + \alpha\,\mathfrak{K}_1 + \cdots + \alpha^3(\sqrt{\alpha})\mathfrak{K}_{7/2}$$
$$+ \alpha^4\mathfrak{K}_4 + \cdots. \qquad \text{(II-17)}$$

The processes of obtaining the explicit forms of each term of $\mathfrak{K}$ is very tedious and we merely give the results for $\mathfrak{K}_l(l=0, \frac{1}{2}, \cdots, 4)$ in the Appendix A.

III. ENERGY FORMULAS

For convenience we will use the notations

$$U_i \equiv |U_i\rangle; \qquad \text{(III-1)}$$

$$\int d\tau U_i^+ \mathfrak{K}_l U_j \equiv \langle U_i | \mathfrak{K}_l | U_j \rangle. \qquad \text{(III-2)}$$

Following the usual procedure of perturbation theory,

we put

$$|U\rangle \equiv |U_0\rangle + (\sqrt{\alpha})|U_{1/2}\rangle + \alpha|U_1\rangle$$
$$+ \cdots + \alpha^4|U_4\rangle; \qquad \text{(III-3)}$$

$$W \equiv W_0 + (\sqrt{\alpha})W_{1/2} + \alpha W_1 + \cdots + \alpha^4 W_4. \qquad \text{(III-4)}$$

Then we know from the standard perturbation theory that $\mathfrak{K}_0$ satisfies $(\mathfrak{K}_0 - W_0)|U_0\rangle = 0$; $\mathfrak{K}_0$ has discrete eigenvalues E_n, with corresponding eigenfunctions, $|n\rangle$; and $\{|n\rangle\}$ form a complete set, i.e., $\sum_n |n\rangle\langle n| = 1$. We choose $n=0$ as the initial (and final) unperturbed state. Then $W_0 = E_0$, $|U_0\rangle \equiv |0\rangle$, and

$$(\mathfrak{K}_0 - E_0)|0\rangle = 0, \qquad \text{(III-5)}$$

where it is understood that $|0\rangle$ also includes the photon vacuum-state vector. Then by a standard perturbation theory we will get

$$W = W_0 + \alpha\,W_1 + \alpha^2 W_2 + \alpha^3 W_3 + \alpha^4 W_4, \qquad \text{(III-6)}$$

where W_0, W_1, W_2, W_3, and W_4 are given as the expectation values with respect to the state vector $|0\rangle$. [It will turn out that $W_{l+1/2}(l=0, 1, 2, \cdots)$ vanishes.] However, $W_l(l=1, 2, 3, 4)$ still depends on α through

$$Q_s^t \equiv \sideset{}{'}\sum_{nk_1\lambda_1\cdots k_s\lambda_s} \frac{|nk_1\lambda_1\cdots k_s\lambda_s\rangle\langle nk_1\lambda_1\cdots k_s\lambda_s|}{[E_n - E_0 + (k_1 + \cdots + k_s)/\alpha]^t}, \qquad \text{(III-7)}$$

where $|nk_1\lambda_1\cdots k_s\lambda_s\rangle$ is an s-photon state with momenta $k_1, \cdots, k_s$. Then, by expanding Q_s^t in terms of α and by regrouping terms of W according to the order of α, we will get the energy in terms of

$$\,^lR_s^t \equiv \sideset{}{'}\sum_{nk_1\lambda_1\cdots k_s\lambda_s} \frac{|nk_1\lambda_1\cdots k_s\lambda_s\rangle\langle nk_1\lambda_1\cdots k_s\lambda_s|}{(k_1 + k_2 + \cdots + k_s)^t}$$
$$\times (E_n - E_0)^l \qquad \text{(III-8)}$$

as follows:

$$W = \mathcal{E}_0 + \alpha\mathcal{E}_1 + \cdots + \alpha^4\mathcal{E}_4. \qquad \text{(III-9)}$$

The results for $\mathcal{E}_i$'s obtained in this manner are given in Appendix B.

However, the $\mathcal{E}_i$'s given by Appendix B are not of workable form because they involve the photon operators. By eliminating photon operators and also by carrying out the integrations over the photon momentum, we will get the final expressions for $\mathcal{E}_i$'s as given in the following

(1) $\mathcal{E}_0$ and $\mathcal{E}_1$ [21]:

$$\mathcal{E}_0 = \langle 0 | \mathfrak{K}_0 | 0 \rangle; \quad \mathcal{E}_1 = 0, \qquad \text{(III-10)}$$

with

$$\mathfrak{K}_0 = \tfrac{1}{2}(\mathbf{P}_1^2 + \mathbf{P}_2^2) - V; \qquad \text{(III-11)}$$

$$V = \varphi_1 + \varphi_2 - \varphi_{12} = \frac{Z_1}{r_1} + \frac{Z_2}{r_2} - \frac{1}{r_{12}}, \qquad \text{(III-12)}$$

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[21] Actually $\mathcal{E}_1 = \langle 0 | \mathfrak{K}_1^{(2)} | 0 \rangle$. However, $\mathfrak{K}_1^{(2)}$, along with $\mathfrak{K}_{1/2}$, will be obtained by applying a gauge transformation, $\mathbf{P} \to \mathbf{P} + (\sqrt{\alpha})\mathbf{A}$, to $\mathfrak{K}_0$ and its expectation value $\mathcal{E}_1$ contributes to an uninteresting (spin-, momentum-independent) constant self-energy of the electrons. So we will omit $\mathcal{E}_1$ (i.e., $\mathcal{E}_1 = 0$).

where $\mathcal{3C}_0$ is the ordinary Schrödinger Hamiltonian for the two-electron system, as is expected.

(2) $\mathcal{E}_2$:

$$\mathcal{E}_2 = \langle 0|\mathcal{3C}_2|0\rangle = \langle 0|\mathcal{3C}_{21}+\mathcal{3C}_{22}+\mathcal{3C}_{23}$$
$$+\mathcal{3C}_{24}+\mathcal{3C}_{25}+\mathcal{3C}_{26}|0\rangle, \quad \text{(III-13)}$$

with

$$\mathcal{3C}_{21} = -\tfrac{1}{8}(\mathbf{P}_1{}^4+\mathbf{P}_2{}^4); \quad \text{(III-14)}$$

$$\mathcal{3C}_{22} = \tfrac{1}{8}(\boldsymbol{\nabla}_1\cdot\mathbf{E}_1+\boldsymbol{\nabla}_2\cdot\mathbf{E}_2); \quad \text{(III-15)}$$

$$\mathcal{3C}_{23} = \tfrac{1}{4}(\boldsymbol{\sigma}_1\cdot\mathbf{E}_1\times\mathbf{P}_1+\boldsymbol{\sigma}_2\cdot\mathbf{E}_2\times\mathbf{P}_2)\equiv\mathcal{3C}_{so}{}^s; \quad \text{(III-16)}$$

$$\mathcal{3C}_{24} = -\frac{1}{2r}\left[\mathbf{P}_1\cdot\mathbf{P}_2+\frac{1}{r^2}\mathbf{r}\cdot(\mathbf{r}\cdot\mathbf{P}_1)\mathbf{P}_2\right]; \quad \text{(III-17)}$$

$$\mathcal{3C}_{25} = \frac{1}{2r^3}(\boldsymbol{\sigma}_1\cdot\mathbf{r}\times\mathbf{P}_2-\boldsymbol{\sigma}_2\cdot\mathbf{r}\times\mathbf{P}_1)\equiv\mathcal{3C}_{so}{}^m; \quad \text{(III-18)}$$

$$\mathcal{3C}_{26} = \tfrac{1}{4}\left[-\frac{8\pi}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r})\right.$$
$$\left.+\frac{1}{r^3}\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2-3\frac{\boldsymbol{\sigma}_1\cdot\mathbf{r}\boldsymbol{\sigma}_2\cdot\mathbf{r}}{r^2}\right)'\right]\equiv\mathcal{3C}_{ss}; \quad \text{(III-19)}$$

$$\mathbf{E}_1 = -\boldsymbol{\nabla}_1 V, \quad \text{and} \quad \mathbf{E}_2 = -\boldsymbol{\nabla}_2 V,$$

where $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$, and the prime in $\mathcal{3C}_{26}$ indicates that when ( )$'$ occurs in any integral over position space, replace ( )$'$ by zero for $r<\epsilon$, evaluate the integral for $\epsilon<r<\infty$, and then take the limit of $\epsilon\to 0$.

These are the familiar results and were derived by several authors.[11,22,23] Actually only $\mathcal{3C}_{23}$, $\mathcal{3C}_{25}$, and $\mathcal{3C}_{26}$ contribute to the fine structure. But $\mathcal{3C}_{21}$, $\mathcal{3C}_{22}$, and $\mathcal{3C}_{24}$, as well as the spin-dependent parts, will contribute to the fine structure through $\mathcal{E}_4$, as we will see later. The physical significance of the various terms of $\mathcal{3C}_2$ have been discussed by Bethe and others.[24]

(3) $\mathcal{E}_3$:

$$\mathcal{E}_3 = \langle 0|\mathcal{3C}_3|0\rangle, \quad \text{(III-20)}$$

with

$$\mathcal{3C}_3 = 2\,{}^0G(\mathcal{3C}_{23}+\tfrac{1}{2}\mathcal{3C}_{25}+\mathcal{3C}_{26})$$
$$= 2\,{}^0G(\mathcal{3C}_{so}{}^s+\tfrac{1}{2}\mathcal{3C}_{so}{}^m+\mathcal{3C}_{ss}). \quad \text{(III-21)}$$

These also are the familiar results,[11,23,24] and their presence here has been discussed by Araki and others.[8,23]

(4) $\mathcal{E}_4$:

$$\mathcal{E}_4 = \langle 0|\mathcal{3C}_4|0\rangle = \langle 0|\mathcal{3C}_{41}+\mathcal{3C}_{42}+\mathcal{3C}_{43}$$
$$+\mathcal{3C}_{44}+\mathcal{3C}_{45}+\mathcal{3C}_{46}|0\rangle, \quad \text{(III-22)}$$

with

$$\mathcal{3C}_{41} = 2\,{}^1G(\mathcal{3C}_{23}+\tfrac{1}{2}\mathcal{3C}_{25}+\mathcal{3C}_{26})+({}^0G)^2\mathcal{3C}_{26}; \quad \text{(III-23)}$$

$$\mathcal{3C}_{42} = -\sum_n{}' \mathcal{3C}_2|n\rangle\langle n|\mathcal{3C}_2/(E_n-E_0); \quad \text{(III-24)}$$

$$\mathcal{3C}_{43} = -\tfrac{1}{4}\mathcal{E}_2(\mathbf{P}_1{}^2+\mathbf{P}_2{}^2)-\tfrac{1}{8}[(\mathcal{3C}_{25}+\mathcal{3C}_{26})(\mathbf{P}_1{}^2+\mathbf{P}_2{}^2)+\text{H.c.}]; \quad \text{(III-25)}$$

$$\mathcal{3C}_{44} = \tfrac{1}{16}[2P_1T_0{}^2P_1-(P_1T_0P_1,P_2{}^2)_+-\tfrac{1}{2}P_1P_2T_0P_1P_2+\text{E.T.}]; \quad \text{(III-26)}$$

$$\mathcal{3C}_{45} = \frac{1}{16}\left[-\frac{3}{r}\left(\boldsymbol{\sigma}_1\times\mathbf{E}_1\cdot\mathbf{P}_2+\frac{\mathbf{r}\cdot\boldsymbol{\sigma}_1\times\mathbf{E}_1\mathbf{r}\cdot\mathbf{P}_2}{r^2}\right)-\frac{3}{r^3}\boldsymbol{\sigma}_1\times\mathbf{E}_1\cdot\boldsymbol{\sigma}_2\times\mathbf{r}-\frac{4}{r^4}\mathbf{r}\cdot\mathbf{P}_1\times\boldsymbol{\sigma}_1+\frac{1}{r}\left(\mathbf{E}_2\cdot\boldsymbol{\sigma}_1\times\mathbf{P}_1+\frac{\mathbf{r}\cdot\mathbf{E}_2\mathbf{r}\cdot\boldsymbol{\sigma}_1\times\mathbf{P}_1}{r^2}\right)\right.$$
$$\left.-\frac{4}{r}\left(\mathbf{E}_2\times\boldsymbol{\sigma}_1\cdot\mathbf{P}_1-\frac{\mathbf{r}\cdot\mathbf{E}_2\times\boldsymbol{\sigma}_1\mathbf{r}\cdot\mathbf{P}_1}{r^2}\right)-\frac{3i}{r^3}\mathbf{r}\cdot\mathbf{E}_2\times\boldsymbol{\sigma}_1+\text{E.T.}\right]; \quad \text{(III-27)}$$

$$\mathcal{3C}_{46} = \frac{1}{16}\left\{\left[-\frac{4}{r}\mathbf{r}\cdot\boldsymbol{\sigma}_2\times\mathbf{P}_1+\frac{1}{r}\left(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2+\frac{\boldsymbol{\sigma}_1\cdot\mathbf{r}\boldsymbol{\sigma}_2\cdot\mathbf{r}}{r^2}\right),\tfrac{1}{2}P_1{}^2\right]_-,\tfrac{1}{2}P_2{}^2\right\}_-+\frac{1}{16}\left[\frac{1}{r^3}\mathbf{r}\cdot\mathbf{P}_1\times\boldsymbol{\sigma}_2-\frac{i}{r^3}\boldsymbol{\sigma}_2\times\mathbf{r}\cdot\boldsymbol{\sigma}_1\times\mathbf{P}_1\right.$$
$$\left.-\frac{i}{r}\left(\boldsymbol{\sigma}_1\times\mathbf{P}_1\cdot\mathbf{P}_2+\frac{1}{r^2}\mathbf{r}(\mathbf{r}\cdot\mathbf{P}_2)\ \boldsymbol{\sigma}_1\times\mathbf{P}_1\right),\tfrac{1}{2}(P_1{}^2-P_2{}^2)\right]+\text{E.T.} \quad \text{(III-28)}$$

Notice here that:

(a) H.c. indicates the Hermitian conjugate terms, and E.T. the terms obtained by exchanging the two electrons;

(b) $T_0\equiv\mathcal{E}_0+V$, $P_1\equiv\boldsymbol{\sigma}_1\cdot\mathbf{P}_1$, $P_2\equiv\boldsymbol{\sigma}_2\cdot\mathbf{P}_2$, and $(A,B)_+=AB+BA$, in $\mathcal{3C}_{44}$;

(c) in $\mathcal{3C}_{45}$ the momentum operators $\mathbf{P}_1$ and $\mathbf{P}_2$ do not apply on the r's.

In the above, grouping terms by $\mathcal{3C}_{41}$, $\mathcal{3C}_{42}$, etc., is rather arbitrary except the first two. The physical interpretations for $\mathcal{3C}_{43}$ through $\mathcal{3C}_{46}$ are not obvious. It is

[22] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press Inc., New York, 1957); see Eq. (39.14) on p. 181.
[23] G. Araki, Phys. Rev. **101**, 1410 (1956).
[24] For example, see pp. 181 and 182 of Ref. 22.

quite likely that some terms grouped in one may also be found in others.

The physical interpretations for $\mathfrak{K}_{41}$ and $\mathfrak{K}_{42}$ are rather simple. The presence of $\mathfrak{K}_{41}$ here is due to the presence of anomalous magnetic moment, and can be understood similarly as the presence of $\mathfrak{K}_3$ in $\mathcal{E}_3$. The term $\mathfrak{K}_{42}$ is a rather expected one,[25] and is the second-order perturbation energy for the Hamiltonian $\mathfrak{K} = \mathfrak{K}_0 + \alpha^2 \mathfrak{K}_2 + \cdots$.

IV. CONCLUSION

We have obtained the energy formulas for the helium fine structure (i.e., the energy terms involving the spin) up to the order α^4 Ry:

$$\mathcal{E} = \langle 0 | \alpha^2 \mathfrak{K}_2 + \alpha^3 \mathfrak{K}_3 + \alpha^4 \mathfrak{K}_4 | 0 \rangle, \qquad \text{(IV-1)}$$

with $\mathfrak{K}_2$, $\mathfrak{K}_3$, and $\mathfrak{K}_4$ given by (III-13) through (III-19), (III-21), and (III-22) through (III-28), respectively. Our results for $\mathfrak{K}_2$ and $\mathfrak{K}_3$ check with the results obtained by others.[11,22,23] As for $\mathfrak{K}_4$, the first two terms $\mathfrak{K}_{41}$ and $\mathfrak{K}_{42}$ are rather expected results, but the presence of the rest of the terms is not obvious. One way to check our results is to carry out the numerical calculation of $\langle 0 | \alpha^4 \mathfrak{K}_4 | 0 \rangle$ and compare its contribution to the helium fine-structure intervals with the experimental data.

C. Schwartz[15] has carried out a very accurate calculation for the helium fine-structure intervals by using $\langle 0 | \alpha^2 \mathfrak{K}_2 + \alpha^3 \mathfrak{K}_3 | 0 \rangle$, with the results:

$$\nu_{01} = 0.987837 \text{ cm}^{-1};$$
$$\nu_{12} = 0.0765302 \text{ cm}^{-1}; \qquad \text{(IV-2)}$$
$$\nu_{02} = 1.064367 \text{ cm}^{-1},$$

which, when compared with the best available experimental data,[26]

$$\nu_{01} = 0.98791(4) \text{ cm}^{-1};$$
$$\nu_{10} = 0.076423(3) \text{ cm}^{-1}; \qquad \text{(IV-3)}$$
$$\nu_{02} = 1.06434(3) \text{ cm}^{-1},$$

show the differences of order 0.0001 cm^{-1}. This discrepancy is due, at least in part, to the exclusion of $\langle 0 | \alpha^4 \mathfrak{K}_4 | 0 \rangle$'s contribution to the interval. We should be able to improve the theoretical data by including its contribution to the interval.

Because the accurate calculation for $\langle 0 | \alpha^4 \mathfrak{K}_4 | 0 \rangle$ is outside the scope of this paper, we estimated it by

(1) using $u_{10}(\mathbf{r}_1) u_{21}(\mathbf{r}_2)$ as the unperturbed wave function, where $u_{10}(\mathbf{r}_1)$ and $u_{21}(\mathbf{r}_2)$ are the hydrogen-type wave functions for $1S$- and $2P$- states with charges $Z_1 = 2$, $Z_2 = 1$, respectively;
(2) expanding $1/r^n$ as $1/r^n = 1/r_2^n + \cdots$;

[25] For example, see Eq. (2) of Ref. 15.
[26] F. M. J. Pichanik, R. D. Swift, and V. W. Hughes, Bull. Am. Phys. Soc. 9, 90 (1964). Also data given in Ref. 15.

and

(3) taking the leading terms, which turn out to be of order $1/r_1 r_2^3$ and $1/r_2^3$, with the result:

$$\nu(\alpha^4 \mathfrak{K}_4 - \alpha^4 \mathfrak{K}_{42}) = \frac{\alpha^4}{48} \begin{pmatrix} -10 \\ -5 \end{pmatrix} \text{Ry} = \begin{pmatrix} -66 \\ -33 \end{pmatrix}$$
$$\times 10^{-6} \text{ cm}^{-1}, \qquad \text{(IV-4)}$$

where (and in the following) the upper (lower) row refers to ν_{01} (ν_{12}). If we use the result by Pekeris et al.[13] for $\alpha^4 \mathfrak{K}_{42}$:

$$\nu(\alpha^4 \mathfrak{K}_{42}) \approx \begin{pmatrix} 0.000158 \\ -0.000158 \end{pmatrix} \text{ cm}^{-1}, \qquad \text{(IV-5)}$$

and (IV-2) for $\alpha^2 \mathfrak{K}_2 + \alpha^3 \mathfrak{K}_3$:

$$\nu(\alpha^2 \mathfrak{K}_2 + \alpha^3 \mathfrak{K}_3) = \begin{pmatrix} 0.987837 \\ 0.076530 \end{pmatrix} \text{ cm}^{-1},$$

then we have

$$\nu(\alpha^2 \mathfrak{K}_2 + \alpha^3 \mathfrak{K}_3 + \alpha^4 \mathfrak{K}_{42}) = \begin{pmatrix} 0.987995 \\ 0.076372 \end{pmatrix} \text{ cm}^{-1}; \qquad \text{(IV-6)}$$

$$\nu(\alpha^2 \mathfrak{K}_2 + \alpha^3 \mathfrak{K}_3 + \alpha^4 \mathfrak{K}_4) = \begin{pmatrix} 0.987929 \\ 0.076339 \end{pmatrix} \text{ cm}^{-1}; \qquad \text{(IV-7)}$$

with

$$\nu_{\exp} = \begin{pmatrix} 0.98791(4) \\ 0.076473 \end{pmatrix} \text{ cm}^{-1}. \qquad \text{(IV-8)}$$

Our result (IV-7) looks very good for ν_{01}, although it does not look encouraging for ν_{12}. However, it is not conclusive for the following reasons:

(1) The convergence for the expansion $1/r^n = 1/r_2^n + \cdots$, is rather slow and the inclusion of terms of order $1/r_2^4$ alone could affect our result significantly [could even change the sign for ν_{12} in (IV-4)];
(2) the contribution from the mass correction, which we did not consider, is of the same order of $\nu(\alpha^4 \mathfrak{K}_4)$.

Therefore, we need a more accurate calculation for $\nu(\alpha^4 \mathfrak{K}_4)$ and the inclusion of the contribution from the mass correction to ν before we have a definite conclusion; but at least we now have an expression for $\mathfrak{K}_4$ to work with.

In summary, we re-emphasize that what we have accomplished in this work is quite some distance short of a complete calculation of the α^4 Ry terms in the helium fine structure. We envisage a plan for such a complete program as consisting of three major parts: First is a proper setting up of the problem starting from the full field theory of electromagnetic interactions; second is a reduction of the results of the first part to an effective Schrödinger Hamiltonian; and third is the evaluation of the expectation value of this Hamiltonian with good atomic wave functions. In this paper we have

not attempted to attack the first part of this program and have made only a very crude attempt at the third part. What we have presented here is what we believe to be a useful working out of the form, and many of the details, of the extensive algebra associated with the second part of the program described above.

ACKNOWLEDGMENT

The author wishes to express his gratitude to Professor C. Schwartz for suggesting this problem and for his guidance throughout the work.

APPENDIX A

$$\mathcal{H}_0 = (1/\alpha)H_r + \tfrac{1}{2}(P_1^2 + P_2^2) - V; \quad V = \varphi_1 + \varphi_2 - \varphi_{12}.$$

$$\mathcal{H}_{1/2} = \tfrac{1}{2}[(P_1, A_1)_+ + (P_2, A_2)_+].$$

$$\mathcal{H}_1 = \mathcal{H}_1^{(1)} + \mathcal{H}_1^{(2)};$$

$$\mathcal{H}_1^{(1)} = \tfrac{1}{4}[P_1 H_r P_1 + P_2 H_r P_2];$$

$$\mathcal{H}_1^{(2)} = \tfrac{1}{2}(A_1^2 + A_2^2).$$

$$\mathcal{H}_{3/2} = \mathcal{H}_{3/2}^{(1)} + \mathcal{H}_{3/2}^{(2)};$$

$$\mathcal{H}_{3/2}^{(1)} = \tfrac{1}{2}i[(^0G_1 P_1 \times A_1)_d + (^0G_2 P_2 \times A_2)_d];$$

$$\mathcal{H}_{/23}^{(2)} = \tfrac{1}{4}[(P_1, H_r, A_1)_+ + (P_2, H_r, A_2)_+].$$

$$\mathcal{H}_2 = \mathcal{H}_2^{(1)} + \cdots;$$

$$\mathcal{H}_2^{(1)} = \tfrac{1}{8}[-2(P_1 T_0 P_1 + P_2 T_0 P_2) + 2P_1^2 P_2^2].$$

$$\mathcal{H}_{5/2} = \mathcal{H}_{5/2}^{(1)} + \mathcal{H}_{5/2}^{(2)} + \mathcal{H}_{5/2}^{(3)} + \cdots;$$

$$\mathcal{H}_{5/2}^{(1)} = \tfrac{1}{2}i[(^1G_1 P_1 \times A_1)_d + (^1G_2 P_2 \times A_2)_d];$$

$$\mathcal{H}_{5/2}^{(2)} = -\tfrac{1}{4}[(P_1, T_0, A_1)_+ + (P_2, T_0, A_2)_+];$$

$$\mathcal{H}_{5/2}^{(3)} = \tfrac{1}{4}[(P_2, A_2)_+ P_1^2 + (P_1, A_1)_+ P_2^2].$$

$$\mathcal{H}_3 = \mathcal{H}_3^{(1)} + \cdots;$$

$$\mathcal{H}_3^{(1)} = -\tfrac{1}{4}\{[(^0G_1 P_1(\varphi_1 - \varphi_{12}))_d, P_1]_- + [(^0G_2 P_2(\varphi_2 - \varphi_{12}))_d, P_2]_-\}.$$

$$\mathcal{H}_4 = \mathcal{H}_4^{(1)} + \mathcal{H}_4^{(2)} + \cdots;$$

$$\mathcal{H}_4^{(1)} = -\tfrac{1}{4}\{[(^1G_1 P_1(\varphi_1 - \varphi_{12}))_d, P_1]_- + [(^1G_2 P_2(\varphi_2 - \varphi_{12}))_d, P_2]_-\};$$

$$\mathcal{H}_4^{(2)} = -\tfrac{1}{4}(P_1 T_2 P_1 + P_2 T_2 P_2) + \tfrac{1}{8}[P_1 T_0^2 P_1 + P_2 T_0^2 P_2] - \tfrac{1}{16}[P_1 P_2 T_0 P_2 P_1 + (P_1 T_0 P_1, P_2^2)_+ + (P_2 T_0 P_2, P_1^2)_+].$$

Notice here that

$$P \equiv \sigma \cdot p; \quad P^0 = P^0; \quad A \equiv \sigma \cdot A; \quad P \times A \equiv \sigma \cdot P \times A;$$

$$(\alpha, \gamma, \beta)_\pm \equiv \alpha\gamma\beta \pm \beta\gamma\alpha; \quad T_0 = \mathcal{E}_0 + V; \quad T_2 = \mathcal{E}_2.$$

"$(\ )_d$" indicates the limit of the differential operator. Also notice in $\mathcal{H}_0$ that we included the $1/\alpha$ order term. Because the unperturbed wave function should be of the order $\alpha^0 = 1$, this simplifies the perturbation theory.

APPENDIX B

$$\mathcal{E}_0 = \langle 0|\mathcal{H}_0|0\rangle; \quad \mathcal{E}_1 = 0; \quad \mathcal{E}_2 = \langle 0|(\mathcal{H}_2^{(1)} - \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_{1/2})|0\rangle;$$

$$\mathcal{E}_3 = \langle 0| - (\mathcal{H}_{3/2}^{(1)0} R_1^1 \mathcal{H}_{1/2} + \text{H.c.} - \mathcal{H}_3^{(1)})|0\rangle;$$

$$\mathcal{E}_4 = \langle 0|[\mathcal{H}_4^{(1)} - (\mathcal{H}_{5/2}^{(1)0} R_1^1 \mathcal{H}_{1/2} + \text{H.c.} - \mathcal{H}_4^{(1)} + \mathcal{H}_{3/2}^{(1)0} R_1^1 \mathcal{H}_{3/2}^{(1)})$$

$$+ (\mathcal{H}_2^{(1)} Q_0^1 \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_{1/2} + \text{H.c.} - \mathcal{H}_2^{(1)} Q_0^1 \mathcal{H}_2^{(1)} - \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_{1/2} Q_0^1 \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_{1/2})]$$

$$+ [\mathcal{H}_4^{(2)} - [(\mathcal{H}_{5/2}^{(2)} + \mathcal{H}_{5/2}^{(3)})^0 R_1^1 \mathcal{H}_{1/2} + \text{H.c.}] - \mathcal{H}_{1/2}^2 R_1^3 \mathcal{H}_{1/2}$$

$$+ (\mathcal{H}_1^{(2)0} R_2^1 \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_{1/2} + \text{H.c.} - \mathcal{E}_1 \mathcal{H}_{1/2}^0 R_1^2 \mathcal{H}_{1/2} + \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_1^{(2)0} R_1^1 \mathcal{H}_{1/2})$$

$$+ \mathcal{H}_{1/2}^0 R_1^1 \mathcal{H}_1^{(1)0} R_1^1 \mathcal{H}_{1/2} + (\mathcal{H}_{3/2}^{(2)1} R_1^2 \mathcal{H}_{1/2} + \text{H.c.})]|0\rangle.$$

Notice here that we only considered terms which contribute to the fine structure. Many terms which diverge but are spin independent have been omitted. As for $\mathcal{E}_1$, its exact expression is $\mathcal{E}_1 = \langle 0|\mathcal{H}_1^{(2)}|0\rangle$ and it diverges but is spin independent, hence is omitted (i.e., $\mathcal{E}_1 \equiv 0$). However, when we calculate $\mathcal{E}_4$, we have to use the exact expression for $\mathcal{E}_1$. Fortunately, it turns out that the spin-dependent diverging term $- \mathcal{E}_1\langle 0|\mathcal{H}_{1/2}^0 R_1^2 \mathcal{H}_{1/2}|0\rangle$ cancels out in $\mathcal{E}_4$.