

## Hyperfine Structure of Positronium\*

Thomas Fulton†

*CERN, Geneva, Switzerland*

and

David A. Owen‡ and Wayne W. Repko§

*Department of Physics, The Johns Hopkins University, Baltimore, Maryland 21218*

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We present the details of a calculation of the  $m\alpha^6 \ln\alpha^{-1}$  contributions to the triplet-singlet splitting of the positronium ground state. Our result  $\Delta\nu(\alpha^6 \ln\alpha^{-1}) = \frac{3}{4}\alpha^4 R_\infty \ln\alpha^{-1} = 34$  MHz places the theoretical value for the transition frequency  $\nu$  approximately 1 standard deviation above the most recent experimental value. The calculation is performed using a perturbation theory based on the Bethe-Salpeter equation and on a wave function obtained by a single iteration from the nonrelativistic Pauli wave function. After a study of all relevant terms, we conclude that the only diagrams which contribute to our order are those involving the exchange of one or two virtual transverse photons. These contributions are explicitly evaluated, and we show that other possible contributions actually vanish.

### I. INTRODUCTION

Potentially, the splitting between the triplet and singlet levels of the positronium ground state affords a very accurate test of quantum electrodynamics. This follows since the bound electron-positron system, perhaps more than any other, presents a very nearly pure quantum electrodynamical problem, which to our order of approximation is free from contamination by hadronic effects or unusual leptonic corrections. Therefore, an agreement between the experimental and theoretical determinations of the triplet-singlet splitting is necessary in any systematic check of the predictive power of quantum electrodynamics. Furthermore, positronium is the only experimentally accessible bound system which must be described by using the relativistic two-body equations for interacting fermions. Agreement between theory and experiment is, therefore, also a check of the treatment of bound states in field theory.

Motivated by these considerations, we have calculated the corrections to the triplet-singlet transition frequency  $\nu$  of order  $\alpha^2 \ln\alpha^{-1}$ . This calculation is necessary since the accuracy of the previous theoretical value for this separation<sup>1-3</sup> has been exceeded by that of the most recent experimental value.<sup>4</sup> Hence, a meaningful comparison between theory and experiment could not be made until higher-order corrections were taken into account.

Our result for the  $\alpha^2 \ln\alpha^{-1}$  correction to the transition frequency is

$$\Delta\nu(\alpha^6 \ln\alpha^{-1}) = \frac{3}{4} \alpha^4 R_\infty \ln\alpha^{-1}, \quad (1)$$

where  $\hbar=c=1$ , and where  $R$  is a frequency rydberg. Combining this contribution with the order  $\alpha$  correction of Karplus and Klein,<sup>3</sup> the total triplet-

singlet transition frequency becomes

$$\nu = \alpha^2 R_\infty \left[ \frac{7}{8} - \left( \frac{46}{9} + \ln 2 \right) (\alpha/\pi) + \frac{3}{4} \alpha^2 \ln\alpha^{-1} + O(\alpha^2) \right]. \quad (2)$$

The contributions of order  $m\alpha^6 \ln\alpha^{-1}$  represent recoil corrections arising from low-momentum components of the wave function associated with the Bethe-Salpeter (BS) equation<sup>5</sup> for positronium. The perturbation techniques used by Karplus and Klein<sup>3</sup> and Fulton and Martin<sup>6</sup> prove sufficiently accurate to this order. We obtain the necessary wave function from the BS equation, containing only the Coulomb interaction, by a single iteration from the nonrelativistic Pauli wave function. This wave function is expressed to a higher order in the wave-function momentum than was previously necessary. We must also keep other momentum contributions to a higher order. Wave-function retardation effects are only important in the one-photon exchange process, while wave-function pair effects can be neglected. It is, however, essential that these two effects are taken into account in the interaction kernels.

In Sec. II, we review the necessary portions of the perturbation theory for the BS equation, and obtain the approximate wave function. Sections III and IV contain, respectively, the calculations of the one and two virtual transverse photon contributions, and Sec. V is devoted to a discussion of the noncontributing diagrams. Finally, we summarize our results and compare them with the latest experimental data.

In the following, we denote the space-time coordinates by  $x_\mu = (\vec{x}, ix_0)$  and take the  $\gamma_\mu$  to be Hermitian matrices satisfying  $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ .

### II. PERTURBATION THEORY AND APPROXIMATE WAVE FUNCTION

We begin by presenting a brief account of the

perturbation theory as developed by Fulton and Karplus.<sup>7</sup> The essential idea is to separate the instantaneous Coulomb interaction, which accounts for the major part of the binding, from the total interaction. With the aid of an approximate solution to the BS equation containing only a Coulomb interaction, we can then treat the contributions of the remaining time-dependent interaction terms by perturbation theory.

After mass and charge renormalization, the BS equation for the wave function  $\psi(x_1, x_2)$  of a system of two interacting equal-mass fermions is

$$\psi(x_1, x_2) = S_F^{(1)}(x_1 - x'_1) S_F^{(2)}(x_2 - x'_2) \times \bar{I}(x'_1, x'_2; x_3, x_4) \psi(x_3, x_4), \quad (3)$$

where

$$S_F^{(j)}(x) = \frac{1}{(2\pi)^4} \int d^4p S_F^{(j)}(p) e^{ip \cdot x} \\ = \frac{1}{(2\pi)^4} \int d^4p \frac{(i\gamma^{(j)} p - m) e^{ip \cdot x}}{p^2 + m^2 - i\epsilon}, \quad j = 1, 2 \quad (4)$$

and we use the convention that repeated four-vector arguments are integrated over. The interaction kernel  $\bar{I}(x_1, x_2; x_3, x_4)$  is extracted from the expansion of the electron-positron Green's function  $G(x_1, x_2; x_3, x_4)$  in a perturbation series. This Green's function is defined as

$$G_{\alpha\beta, \gamma\delta}(x_1, x_2; x_3, x_4) \\ = \langle 0 | T \{ \psi_\alpha(x_1) \phi_\beta(x_2) \bar{\psi}_\gamma(x_3) \bar{\phi}_\delta(x_4) \} | 0 \rangle \\ - \langle 0 | T \{ \psi_\alpha(x_1) \phi_\beta(x_2) \} | 0 \rangle \langle 0 | T \{ \bar{\psi}_\gamma(x_3) \bar{\phi}_\delta(x_4) \} | 0 \rangle, \quad (5)$$

with

$$\phi = C \bar{\psi}^T. \quad (6)$$

$\bar{I}(x_1, x_2; x_3, x_4)$  is obtained by writing the summed perturbation series as

$$G(x_1, x_2; x_3, x_4) = S_F^{(1)}(x_1 - x_3) S_F^{(2)}(x_2 - x_4) \\ + S_F^{(1)}(x_1 - x'_1) S_F^{(2)}(x_2 - x'_2) \\ \times \bar{I}(x'_1, x'_2; x_3, x_4) G(x'_3, x'_4; x_3, x_4). \quad (7)$$

In the following, it is convenient to introduce the center-of-mass and relative coordinates  $X$  and  $x$  defined by

$$X = \frac{1}{2}(x_1 + x_2), \quad x = x_1 - x_2. \quad (8)$$

Then, observing that  $S_F^{(1)}(x_1 - x'_1) S_F^{(2)}(x_2 - x'_2)$  and  $\bar{I}(x_1, x_2; x'_1, x'_2)$  are functions of  $x, x'$  and  $X - X'$ , we can write Eq. (3) in the form

$$\varphi_K(x) = G_K(x, x') I_K(x', x'') \varphi_K(x''), \quad (9)$$

with

$$\varphi_K(x) = e^{-iK \cdot X} \psi(x_1, x_2), \quad (10)$$

$$G_K(x, x') = \int d^4X' e^{-iK \cdot (X - X')} S_F^{(1)}[(X - X') + \frac{1}{2}(x - x')] \\ \times S_F^{(2)}[(X - X') - \frac{1}{2}(x - x')] \\ = (2\pi)^{-4} \int d^4p S_F^{(1)}(p + \frac{1}{2}K) S_F^{(2)}(-p + \frac{1}{2}K) e^{ip \cdot x}, \quad (11)$$

$$I_K(x, x') = \int d^4X' e^{-iK \cdot (X - X')} \bar{I}(x, x'; X - X'). \quad (12)$$

For the development which follows, it is useful to factorize  $G_K(x, x')$  in the form

$$G_K(x, x') = \mathcal{G}_K(x, y) \Lambda_K(y, x') \gamma_4^{(1)} \gamma_4^{(2)} \\ = \Lambda_K(x, y) \mathcal{G}_K(y, x') \gamma_4^{(1)} \gamma_4^{(2)}, \quad (13)$$

where

$$\mathcal{G}_K(x, y) = (2\pi)^{-4} \int d^4p e^{ip \cdot (x - y)} [H^{(1)}(p) + H^{(2)}(-\vec{p}) - K_0]^{-1}, \quad (14)$$

$$\Lambda_K(y, x') = (2\pi)^{-4} \int d^4p e^{ip \cdot (y - x')} \{ [H^{(1)}(\vec{p}) - (p_0 + \frac{1}{2}K_0)]^{-1} \\ + [H^{(2)}(-\vec{p}) - (-p_0 + \frac{1}{2}K_0)]^{-1} \}, \quad (15)$$

where  $H^{(j)}(\vec{p})$  is the Dirac Hamiltonian  $\vec{\alpha}^{(j)} \cdot \vec{p} + \beta^{(j)} m$ , and we work in the rest system of the center of mass so that  $K_\mu = (0, iK_0)$ . For completeness, we note that the differential operator

$$F_K(x, x') = (\gamma^{(1)} \cdot \partial + \frac{1}{2} i \gamma^{(1)} \cdot K + m) \\ \times (-\gamma^{(2)} \cdot \partial + \frac{1}{2} i \gamma^{(2)} \cdot K + m) \delta(x - x') \quad (16)$$

obeys the relation

$$F_K(x, x') G_K(x', y) = \delta(x - y), \quad (17)$$

so that the relative coordinate-dependent wave function  $\varphi_K(x)$  satisfies the differential equation

$$[F_K(x, x') - I_K(x, x')] \varphi_K(x') = 0. \quad (18)$$

We begin the development of the perturbation theory by writing the interaction kernel as

$$I_K(x, x') = I^c(x, x') + I'_K(x, x'), \quad (19)$$

where

$$I^c(x, x') = -i \alpha \delta(x - x') \delta(x_0) \gamma_4^{(1)} \gamma_4^{(2)} / r \quad (20)$$

is the instantaneous Coulomb interaction kernel and  $I'_K(x, x')$  denotes the remaining part of the interaction kernel. With this separation, Eq. (9) can be written

$$\varphi_K(x) = \mathcal{G}_K(x, y) [-\Lambda_K(y, x') (i\alpha/r') \delta(x'_0) \varphi_K(x') \\ + \Lambda_K(y, y') \gamma_4^{(1)} \gamma_4^{(2)} I'_K(y', x') \varphi_K(x')], \quad (21)$$

so that the unperturbed system, having total energy  $K_0^c$ , will satisfy the equation

$$\varphi_{K^c}(x) = -i \alpha \mathcal{G}_{K^c}(x, y) \Lambda_{K^c}(y, x') [\delta(x'_0)/r'] \varphi_{K^c}(x'). \quad (22)$$

In order to obtain an expression for the energy shift  $\Delta E = K_o - K_o^c$ , it proves convenient to introduce a wave function  $\varphi'_K(x)$  by the equation

$$\begin{aligned} \varphi'_K(x) &= -i\alpha \mathcal{G}_{Kc}(x, y) \Lambda_K(y, x') [\delta(x'_o)/r'] \varphi_{Kc}(x') \\ &= -i\Lambda_K(x, y) \delta(y_o) \chi(y), \end{aligned} \quad (23)$$

where  $\chi(y)$  is defined as

$$\delta(y_o) \chi(y) = \alpha \mathcal{G}_{Kc}(y, x') [\delta(x'_o)/r'] \varphi_{Kc}(x'). \quad (24)$$

Using the relations<sup>8</sup>

$$\begin{aligned} \mathcal{G}_{Kc}(x, y) \Lambda_K(y, x') &= G_K(x, x') \gamma_4^{(1)} \gamma_4^{(2)} \\ &\quad - \Delta E G_K(x, y) \gamma_4^{(1)} \gamma_4^{(2)} \mathcal{G}_{Kc}(y, x'), \end{aligned} \quad (25)$$

$$[\delta(x_o)/r'] \varphi'_K(x) = [\delta(x_o)/r'] \varphi_{Kc}(x) \quad (26)$$

together with Eq. (17), it is easily seen that  $\varphi'_K(x)$  satisfies the equation

$$[F_K(x, x') - I^c(x, x')] \varphi'_K(x) = i\Delta E \gamma_4^{(1)} \gamma_4^{(2)} \delta(x_o) \chi(x), \quad (27)$$

which has as an adjoint

$$\bar{\varphi}'_K(x') [F_K(x', x) - I^c(x', x)] = i\Delta E \chi^*(x) \delta(x_o), \quad (28)$$

where  $\bar{\varphi}'_K(x) = \varphi'^*_K(x) \gamma_4^{(1)} \gamma_4^{(2)}$ . Multiplying Eq. (28) by  $\varphi_K(x)$ , and using Eqs. (18) and (19), we obtain

$$\bar{\varphi}'_K(x) I'_K(x, x') \varphi_K(x') = i\Delta E, \quad (29)$$

where the normalization is chosen so that

$$\chi^*(x) \delta(x_o) \varphi_K(x) = 1. \quad (30)$$

As can be seen by comparing Eqs. (22) and (23),  $\varphi'_K(x)$  and  $\varphi_{Kc}(x)$  differ by terms of order  $\Delta E$ , and this difference is negligible to our order of accuracy. Thus, if we can express Eq. (29) in terms of  $\varphi'_K(x)$ , it is permissible to replace  $\varphi'_K(x)$  by  $\varphi_{Kc}(x)$ . In view of Eq. (27), the connection between  $\varphi'_K(x)$  and  $\varphi_K(x)$  is seen to be

$$\begin{aligned} \varphi_K(x) &= \varphi'_K(x) + \bar{G}_K(x, x') [I'_K(x', x') \varphi'_K(x') \\ &\quad - i\Delta E \gamma_4^{(1)} \gamma_4^{(2)} \delta(x'_o) \chi(x')], \end{aligned} \quad (31)$$

where  $\bar{G}_K(x, x')$  is the Green's function for Eq. (18), which can be expanded in terms of the Coulomb Green's function as

$$\bar{G}_K(x, x') = G_K^c(x, x') + G_K^c(x, y) I'(y, y') G_K^c(y', x') + \dots \quad (32)$$

Hence, neglecting the term involving  $\Delta E$  in Eq. (31), we finally obtain, to our order of accuracy,

$$\begin{aligned} \Delta E &= -i \bar{\varphi}_{Kc}(x) [I'_K(x, x') \\ &\quad + I'_K(x, y) G_K^c(y, y') I'(y', x')] \varphi_{Kc}(x'). \end{aligned} \quad (33)$$

In order to make use of Eq. (33), we need an approximation to the Coulomb wave function  $\varphi_{Kc}(x)$ . This may be obtained by using Eq. (22) as the basis of an iteration procedure<sup>9</sup> beginning with the non-relativistic Pauli wave function  $\varphi_P(x)$ . Specifically,

ly, we write

$$\varphi_{Kc}^{(1)}(x) = G_K(x, x') I^c(x', x'') \varphi_P(\vec{x}'')$$

or

$$\begin{aligned} \varphi_{Kc}^{(1)}(x) &= -\frac{i\alpha}{2\pi^2} \frac{1}{(2\pi)^{5/2}} \\ &\quad \times \int d^4p e^{ip \cdot x} S_F^{(1)}(p + \frac{1}{2}K) S_F^{(2)}(-p + \frac{1}{2}K) \gamma_4^{(1)} \gamma_4^{(2)} \\ &\quad \times \int \frac{d^3k \varphi_P(\vec{k})}{|\vec{k} - \vec{p}|^2}, \end{aligned} \quad (34)$$

where

$$\varphi_P(\vec{k}) = \frac{4\pi\alpha}{(2\pi)^{3/2}} \frac{m\varphi_P(0)}{(\vec{k}^2 + \gamma^2)^2}, \quad (35)$$

$$\begin{aligned} \varphi_P(0) &= \varphi(0) \times (\text{spin function}) \\ &= \pi^{-1/2} \gamma^{3/2} \times (\text{spin function}), \end{aligned} \quad (36)$$

$$\gamma = \frac{1}{2} m \alpha. \quad (37)$$

After performing the  $k$  integration, the expression for  $\varphi_{Kc}^{(1)}(x)$  becomes

$$\begin{aligned} \varphi_{Kc}^{(1)}(x) &= \frac{-4\pi i \alpha}{(2\pi)^4} \\ &\quad \times \int d^4p e^{ip \cdot x} \frac{S_F^{(1)}(p + \frac{1}{2}K) S_F^{(2)}(-p + \frac{1}{2}K) \gamma_4^{(1)} \gamma_4^{(2)}}{(\vec{p}^2 + \gamma^2)} \\ &\quad \times \varphi_P(0). \end{aligned} \quad (38)$$

It is useful to write  $\varphi_{Kc}^{(1)}(x)$  in the form

$$\varphi_{Kc}^{(1)}(x) = \varphi_c(x) + \delta\varphi_c(x) + \delta\varphi'_c(x), \quad (39)$$

where  $\varphi_c(x)$  is the wave function used to obtain the  $\alpha^5$  contributions,<sup>3</sup> while  $\delta\varphi_c(x)$  and  $\delta\varphi'_c(x)$  represent higher-order correction terms. Explicit expressions for these wave functions are given in the Appendix.

### III. SINGLE TRANSVERSE PHOTON CONTRIBUTIONS

#### A. Pure One-Photon Exchange

The simplest correction term which produces a  $\alpha^8 \ln \alpha^{-1}$  contribution to the triplet-singlet splitting is the single transverse photon exchange kernel  $I_B(x, x')$ . This (Breit) interaction kernel has the form

$$\begin{aligned} I_B(x, x') &= \frac{ie^2 \delta(x - x') \gamma_4^{(1)} \gamma_4^{(2)}}{(2\pi)^4} \\ &\quad \times \int d^4k \frac{[\vec{\alpha}^{(1)} \cdot \vec{\alpha}^{(2)} - (\vec{\alpha}^{(1)} \cdot \hat{k})(\vec{\alpha}^{(2)} \cdot \hat{k})]}{k^2} e^{ik \cdot x}, \end{aligned} \quad (40)$$

where  $\hat{k} = \vec{k}/|\vec{k}|$  and  $k^2 = \vec{k}^2 - k_0^2$ . Denoting the single transverse photon exchange contribution to the triplet-singlet splitting by  $\Delta E_1$ , we may use Eqs. (33) and (39) to obtain

$$\Delta E_1 = -i\bar{\varphi}_c(x)I_B(x, x')\varphi_c(x') - i\delta\bar{\varphi}_c(x)I_B(x, x') \times \varphi_c(x') - i\bar{\varphi}_c(x)I_B(x, x')\delta\varphi_c(x'), \quad (41)$$

where we have omitted the  $\delta\varphi'_c$  terms, which can easily be shown to yield no  $\alpha^6 \ln\alpha^{-1}$  contributions.

The relevant spin-dependent part of the first term in Eq. (41) has been computed previously,<sup>3</sup> and may be written in the form

$$\begin{aligned} & -i\bar{\varphi}_c(x)I_B(x, x')\varphi_c(x') \\ &= \frac{1}{3} \frac{\alpha^3 |\varphi(0)|^2}{(2\pi)^3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3p d^3p'}{E E' (p^2 + \gamma^2)^2 (p'^2 + \gamma^2)^2} \\ & \times \left( 4m^2 - \frac{[p^2(E' + m) + p'^2(E + m)]}{k + E + E' - K_0} \right. \\ & \left. + \frac{2(p^2 E' + p'^2 E)}{k + E + E'} - \frac{[p^2(E' - m) + p'^2(E - m)]}{k + E + E' + K_0} \right), \end{aligned} \quad (42)$$

where

$$E = (p^2 + m^2)^{1/2}, \quad k = |\vec{p} - \vec{p}'|, \quad K_0 \simeq 2m - \frac{1}{4}m\alpha^2, \quad (43)$$

and  $p$  denotes the magnitude of the vector  $\vec{p}$ . As we shall see, the  $\alpha^6 \ln\alpha^{-1}$  contributions arise from integrands which behave as (momentum)<sup>-2</sup> in the region of small wave-function momenta, provided there is a coupling between the  $d^3p$  and  $d^3p'$  integrations. Using these criteria, the  $4m^2$  term in large parentheses should yield no  $\alpha^6 \ln\alpha^{-1}$  terms, and this is confirmed by a direct evaluation which gives the well-known  $\alpha^4$  contribution<sup>1,2</sup> together with an  $\alpha^5$  correction.<sup>3</sup> Of the remaining terms in Eq. (42), only the second in the large parentheses gives an  $\alpha^6 \ln\alpha^{-1}$  contribution. It may be extracted by using the relations

$$\begin{aligned} \frac{p^2}{k + E + E' - K_0} &= \frac{p^2}{k + E - E'} \left( 1 - \frac{2(E' - m)}{k + E + E' - K_0} \right) \\ &\simeq \frac{p^2}{k} \left( 1 - \frac{p'^2}{mk} \right), \\ \frac{p'^2}{k + E + E' - K_0} &= \frac{p'^2}{k + E' - E} \left( 1 - \frac{2(E - m)}{k + E + E' - K_0} \right) \\ &\simeq \frac{p'^2}{k} \left( 1 - \frac{p^2}{mk} \right), \end{aligned} \quad (44)$$

which produce a correction term of order  $\alpha^6 \ln\alpha^{-1}$  given by

$$\frac{4}{3} \frac{\alpha^3 |\varphi(0)|^2}{(2\pi)^3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3p d^3p' p^2 p'^2}{E (p^2 + \gamma^2)^2 (p'^2 + \gamma^2)^2 k^2}. \quad (45)$$

The integration involving  $k^{-2}$  may be evaluated with the aid of the formula

$$\int \frac{d^3p' p'^2}{(p'^2 + \gamma^2)^2 |\vec{p}' - \vec{p}|^2} = \pi^2 \left( \frac{2}{p} \tan^{-1} \frac{p}{\gamma} - \frac{\gamma}{p^2} + \frac{\gamma^3}{p^2(p^2 + \gamma^2)} \right), \quad (46)$$

and hence the leading contribution of Eq. (45) is

$$\frac{1}{3} \frac{\alpha^3 |\varphi(0)|^2}{2\pi m} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3p 2p \tan^{-1}(p/\gamma)}{E (p^2 + \gamma^2)^2}. \quad (47)$$

The  $\ln\alpha^{-1}$  term in the remaining integral can be obtained by setting  $\tan^{-1}(p/\gamma) \simeq \frac{1}{2}\pi$  and noting that

$$\int \frac{d^3p p}{E (p^2 + \gamma^2)^2} = \frac{4\pi}{m} \ln\alpha^{-1} + O(\alpha). \quad (48)$$

Hence, the  $\alpha^6 \ln\alpha^{-1}$  portion of Eq. (42) is

$$-i\bar{\varphi}_c(x)I_B(x, x')\varphi_c(x') = \frac{1}{12} m \alpha^6 \ln\alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle, \quad (49)$$

where we have used Eqs. (36) and (37).

Using the expression for  $\delta\varphi_c(x)$  given in the Appendix, the remaining terms in Eq. (41) can be shown to give

$$\begin{aligned} & \frac{1}{24} \frac{\alpha^3 |\varphi(0)|^2}{(2\pi)^3 m^2} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3p d^3p'}{(p^2 + \gamma^2)^2 (p'^2 + \gamma^2)^2 E E' k} \\ & \left[ 4p^2 p'^2 \left( \frac{(m^2 - E E')}{k + E + E' - K_0} + \frac{2(m^2 + E E')}{k + E + E'} + \frac{(m^2 - E E')}{k + E + E' + K_0} \right) \right. \\ & - \frac{|\vec{p} \times \vec{p}'|^2}{k^2} \left( \frac{p^2(m - E)(m + E')}{k + E + E' - K_0} + \frac{2p^2(m^2 + E E')}{k + E + E'} \right. \\ & \left. \left. + \frac{p^2(m + E)(m - E')}{k + E + E' + K_0} + (p - p') \right) \right]. \end{aligned} \quad (50)$$

In contrast to Eq. (42), where the denominator  $(k + E + E' - K_0)$  gave the most singular low-momentum behavior, the corresponding term in Eq. (50) is not dominant at low momentum owing to a factor  $(m^2 - E E')$  in its numerator.<sup>10</sup> Instead, the denominator  $(k + E + E')$  gives the leading low-momentum behavior of Eq. (50). Keeping only the leading terms, Eq. (50) reduces to

$$\begin{aligned} & \frac{1}{6} \frac{\alpha^3 |\varphi(0)|^2}{(2\pi)^3 m} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3p d^3p'}{(p^2 + \gamma^2)^2 (p'^2 + \gamma^2)^2 E E' k} \\ & \times \left( 4p^2 p'^2 - (p^2 + p'^2) \frac{|\vec{p} \times \vec{p}'|^2}{k^2} \right). \end{aligned} \quad (51)$$

For small  $p$  and  $p'$ , the integrand of Eq. (51) behaves as (momentum)<sup>-1</sup> and we therefore expect no  $\alpha^6 \ln\alpha^{-1}$  contribution. Explicit evaluation of the integrals shows this to be the case.

Hence, the  $\alpha^6 \ln\alpha^{-1}$  contribution to  $\Delta E_1$  is given by

$$\Delta E_1(\alpha^6 \ln\alpha^{-1}) = \frac{1}{12} m \alpha^6 \ln\alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle. \quad (52)$$

#### B. Coulomb-Transverse Exchange

In computing the effects of a single transverse

exchange, it is important to remember that, because of retardation, the exchange of a single transverse photon can be accompanied by the exchange of instantaneous Coulomb photons. This is evident in the  $\alpha^5$  calculation, where an important cancellation occurs between the one transverse photon exchange diagram and the diagram containing one transverse and one Coulomb photon.<sup>3</sup> A similar cancellation will be seen to occur in the present calculation.

If we denote the Coulomb-transverse kernel by  $I_{CT}(x, x')$ , and the corresponding energy shift by  $\Delta E_{CT}$ , then the  $\alpha^6 \ln \alpha^{-1}$  spin-dependent part of  $\Delta E_{CT}$  is given by

$$\Delta E_{CT} = -i \int d^4x d^4x' [\bar{\varphi}_P(0) I_{CT}(x, x') \varphi_c(\vec{x}') + \varphi_c(\vec{x}) I_{CT}(x, x') \varphi_P(0)]. \quad (53)$$

Since the evaluation of  $\Delta E_{CT}$  is quite similar to the evaluation of the crossed two-transverse photon contribution, which is given in detail in Sec. IV, we will merely outline the calculation. After transforming to momentum space, the spin-spin content of Eq. (53) is made explicit by repeated use of the relation

$$\alpha_i \alpha_j = \delta_{ij} + i \epsilon_{ijk} \sigma_k \quad (54)$$

to obtain, for example,

$$\langle \vec{\alpha}^{(1)} \cdot \vec{k}' \vec{\alpha}^{(2)} \cdot \vec{k} \vec{\alpha}^{(1)} \cdot \vec{\alpha}^{(2)} \rangle = - \langle \vec{k}' \cdot \vec{k} \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} - \vec{\sigma}^{(1)} \cdot \vec{k}' \vec{\sigma}^{(2)} \cdot \vec{k} \rangle, \quad (55)$$

where the angular brackets indicate that we have retained only spin-spin terms. Further, apart from terms such as those in Eq. (55), the integrand of Eq. (53) is invariant under a simultaneous rotation of all momentum vectors. Since such a rotation is nothing but a change of integration variables, we obtain the result

$$\langle \vec{\sigma}^{(1)} \cdot \vec{A} \vec{\sigma}^{(2)} \cdot \vec{B} \rangle = \frac{1}{3} \vec{A} \cdot \vec{B} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle, \quad (56)$$

so that Eq. (55) may be written

$$\langle \vec{\alpha}^{(1)} \cdot \vec{k}' \vec{\alpha}^{(2)} \cdot \vec{k} \vec{\alpha}^{(1)} \cdot \vec{\alpha}^{(2)} \rangle = - \frac{2}{3} \vec{k} \cdot \vec{k}' \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle. \quad (57)$$

In this way, the spin dependence of Eq. (53) may be separated from the momentum dependence and, retaining the leading low-momentum contributions, we find

$$\Delta E_{CT}(\alpha^6 \ln \alpha^{-1}) = \frac{1}{3} \frac{\alpha^3 |\varphi(0)|^2}{\pi^3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \times \int \frac{d^3k d^3p \vec{k} \cdot \vec{p}}{k^2 (k^2 + m^2) (p^2 + \gamma^2)^2 |\vec{k} + \vec{p}|^2}. \quad (58)$$

The remaining integrations can be performed with the aid of the formulas

$$\int \frac{d^3p \vec{k} \cdot \vec{p}}{(p^2 + \gamma^2)^2 |\vec{k} + \vec{p}|^2} = - \frac{\pi^2}{k} \left( \tan^{-1} \frac{k}{\gamma} - \frac{\gamma k}{(k^2 + \gamma^2)} \right), \quad (59)$$

$$\int_{-\infty}^{\infty} \frac{dk}{(k^2 + m^2)k} \tan^{-1} \frac{k}{\gamma} = \frac{\pi}{m^2} \ln \alpha^{-1}. \quad (60)$$

Hence, we finally obtain

$$\Delta E_{CT}(\alpha^6 \ln \alpha^{-1}) = - \frac{1}{12} m \alpha^6 \ln \alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle. \quad (61)$$

#### IV. DOUBLE TRANSVERSE PHOTON EXCHANGE

Recalling Eq. (33), we see that contributions to  $\Delta E$  involving two transverse photons can arise in two ways. First, there is the contribution from the irreducible crossed two-photon kernel  $\tilde{I}_K(x, x')$ ,

$$\tilde{I}_K(x, x') = - [(4\pi\alpha)^2 / (2\pi)^8] \int d^4k d^4k' (\delta_{ij} - \hat{k}_i \hat{k}_j) \times (\delta_{lm} - \hat{k}_l \hat{k}'_m) \gamma_i^{(1)} \gamma_j^{(2)} G_{\tilde{K}}(x, x') \gamma_m^{(1)} \gamma_l^{(2)} (1/k^2) (1/k'^2) \times e^{i(\mathbf{k}-\mathbf{k}') \cdot (\mathbf{x}+\mathbf{x}')/2}, \quad (62)$$

$$\vec{K} = K - k - k',$$

where  $G_K(x, x')$  is given by Eq. (11). Secondly, there is the effective uncrossed two-photon kernel  $I_K(x, x')$ , corresponding to the iteration of the single transverse exchange kernel  $I_B(x, x')$ . Explicitly, we have

$$I_K(x, x') = I_B(x, y) G_K(y, y') I_B(y', x'), \quad (63)$$

where we have approximated  $G_K^c(x, x')$  in Eq. (33) by  $G_K(x, x')$ .

When evaluating the contributions of  $I_K(x, x')$  and  $\tilde{I}_K(x, x')$ , it is important to note that the addition of another photon introduces a factor  $\alpha$  into the expression for  $\Delta E$ . This allows us to replace one of the wave functions in Eq. (33) by  $\varphi_P(x)$ , while using  $\varphi'_c(x) = \varphi_c(x) + \delta\varphi_c(x)$  as the other wave function. We have also found, by explicit calculation, that it is permissible to neglect the spatial dependence of  $\varphi_P(x)$  to our order of accuracy. In implementing these two simplifications, it can be seen that  $\varphi'_c(x)$  will appear on the right-hand as well as on the left-hand side of the kernel, i. e.,

$$\Delta E_2 = -i \int d^4x d^4x' \{ \bar{\varphi}'_c(\vec{x}) [I_K(x, x') + \tilde{I}_K(x, x')] \varphi_P(\vec{x}') + \bar{\varphi}_P(\vec{x}) [I_K(x, x') + \tilde{I}_K(x, x')] \varphi'_c(\vec{x}') - \bar{\varphi}_P(\vec{x}) [I_K(x, x') + \tilde{I}_K(x, x')] \varphi_P(\vec{x}') \}, \quad (64)$$

where  $\Delta E_2$  denotes the energy shift associated with the two transverse photon exchange. After some effort, it can be shown that the first two terms in Eq. (64) make equal contributions, and we choose to work with the term in which  $\varphi'_c(x)$  appears on the right. We further separate the leading  $\alpha^5$  contribution by writing  $\Delta E_2$  in the form

$$\begin{aligned}
\Delta E_2 = & -2i \int d^4x d^4x' \bar{\varphi}_P(0) I_K(x, x') [\varphi'_c(\vec{x}') - \varphi_P(\vec{x}')] \\
& - 2i \int d^4x d^4x' \bar{\varphi}_P(0) \bar{I}_K(x, x') [\varphi'_c(\vec{x}') - \varphi_P(\vec{x}')] \\
& - i \int d^4x d^4x' \{2\bar{\varphi}_P(0) [I_K(x, x') + \bar{I}_K(x, x')] \varphi_P(\vec{x}') \\
& \quad - \bar{\varphi}_P(0) [I_K(x, x') + \bar{I}_K(x, x')] \varphi_P(0)\} \\
= & \epsilon + \bar{\epsilon} + \epsilon_P, \tag{65}
\end{aligned}$$

where, as we shall see,  $\epsilon_P$  contains the  $\alpha^5$  con-

$$\begin{aligned}
\epsilon = & \frac{4i\alpha^3 |\varphi(0)|^2}{(2\pi)^4} \int d^3p d^3k' d^4k \delta_{ij}^T(\hat{k}) \delta_{im}^T(\hat{k}') \frac{\delta(\vec{k}' - \vec{k} - \vec{p})}{(p^2 + \gamma^2)^2 E(p)} \frac{1}{\vec{k}^2 - k_0^2} \frac{1}{\vec{k}'^2 - k_0^2} \\
& \times \langle \alpha_i^{(1)} \alpha_j^{(2)} S_F^{(1)}(-k + \frac{1}{2}K) S_F^{(2)}(k + \frac{1}{2}K) \gamma_4^{(1)} \gamma_4^{(2)} \alpha_i^{(1)} \alpha_m^{(2)} [2m(\vec{\alpha}^{(1)} - \vec{\alpha}^{(2)}) \cdot \vec{p} - p^2 - \vec{\alpha}^{(1)} \cdot \vec{p} \vec{\alpha}^{(2)} \cdot \vec{p}] \rangle, \tag{67}
\end{aligned}$$

where

$$\delta_{ij}^T(\hat{k}) = \delta_{ij} - \hat{k}_i \hat{k}_j. \tag{68}$$

The  $k_0$  dependence of the fermion propagators can be made explicit by using the decomposition

$$S_F(k) = \left( \frac{\Lambda_+(\vec{k})}{k_0 - E(k)} + \frac{\Lambda_-(\vec{k})}{k_0 + E(k)} \right) \gamma_4, \tag{69}$$

where

$$\Lambda_{\pm}(\vec{k}) = [E(k) \pm H(\vec{k})] / 2E(k). \tag{70}$$

Using Eq. (69), we encounter the contour integrals  $I_{\pm\pm}(k, k')$  defined by

$$\begin{aligned}
I_{\pm\pm}(\vec{k}, \vec{k}') = & \int_{-\infty}^{\infty} dk_0 \frac{1}{k_0^2 - \vec{k}^2} \frac{1}{k_0^2 - \vec{k}'^2} \\
& \times \frac{1}{-k_0 + \frac{1}{2}K_0 \mp E(k)} \frac{1}{k_0 + \frac{1}{2}K_0 \mp E(k)}. \tag{71}
\end{aligned}$$

The values<sup>11</sup> of these integrals are listed in Table I. After performing the  $k_0$  integration, the expression for  $\epsilon$  takes the form

$$\begin{aligned}
\bar{\epsilon} = & \frac{4i\alpha^3 |\varphi(0)|^2}{(2\pi)^4} \int d^3p d^3k' d^4k \delta_{ij}^T(\hat{k}') \delta_{im}^T(\hat{k}) \delta(\vec{k}' - \vec{k} - \vec{p}) \frac{1}{\vec{k}^2 - k_0^2} \frac{1}{\vec{k}'^2 - k_0^2} \\
& \times \langle \alpha_i^{(1)} \alpha_j^{(2)} S_F^{(1)}(k' + \frac{1}{2}K) S_F^{(2)}(k + \frac{1}{2}K) \gamma_4^{(1)} \gamma_4^{(2)} \alpha_m^{(1)} \alpha_j^{(2)} [2m(\vec{\alpha}^{(1)} - \vec{\alpha}^{(2)}) \cdot \vec{p} - p^2 - \vec{\alpha}^{(1)} \cdot \vec{p} \vec{\alpha}^{(2)} \cdot \vec{p}] \rangle, \tag{74}
\end{aligned}$$

where

$$k'_0 = k_0. \tag{75}$$

The  $k_0$  integration leads to the contour integrals  $\bar{I}_{\pm\pm}(k, k')$  defined by

$$\begin{aligned}
\bar{I}_{\pm\pm}(\vec{k}, \vec{k}') = & \int_{-\infty}^{\infty} dk_0 \frac{1}{\vec{k}^2 - k_0^2} \frac{1}{\vec{k}'^2 - k_0^2} \\
& \times \frac{1}{k_0 + \frac{1}{2}K_0 \mp E(k)} \frac{1}{k_0 + \frac{1}{2}K_0 \mp E(k)}. \tag{76}
\end{aligned}$$

tribution. For the purposes of computing  $\epsilon$  and  $\bar{\epsilon}$ , we note that, to the accuracy required,

$$\begin{aligned}
\varphi'_c(\vec{p}) - \varphi_P(\vec{p}) = & \pi\alpha(2\pi)^{-3/2} (p^2 + \gamma^2)^{-2} \\
& \times [2m(\vec{\alpha}^{(1)} - \vec{\alpha}^{(2)}) \cdot \vec{p} - p^2 - \vec{\alpha}^{(1)} \cdot \vec{p} \vec{\alpha}^{(2)} \cdot \vec{p}] \varphi_P(0). \tag{66}
\end{aligned}$$

A. Calculation of  $\epsilon$

From Eqs. (63) and (66), we find

$$\begin{aligned}
\epsilon = & \frac{i\alpha^3 |\varphi(0)|^2}{(2\pi)^4} \int \frac{d^3p d^3k' d^3k \delta(\vec{k}' - \vec{k} - \vec{p})}{(p^2 + \gamma^2)^2 E(p) E^2(k)} \\
& \times [J_{++}(\vec{k}, \vec{k}') + J_{+-}(\vec{k}, \vec{k}') + J_{--}(\vec{k}, \vec{k}')], \tag{72}
\end{aligned}$$

where

$$\begin{aligned}
J_{++} = & \{-p^2 [E(k) - m]^2 A - 2m [E(k) - m] B + C\} I_{++}, \\
J_{+-} = & (2p^2 k^2 A - 4m^2 B - 2C) I_{+-}, \\
J_{--} = & \{p^2 [E(k) + m]^2 A + 2m [E(k) + m] B + C\} I_{--}, \tag{73}
\end{aligned}$$

and the spin averages  $A$ ,  $B$ , and  $C$  are given in Table II. Since extensive cancellations occur between the expressions for  $\epsilon$  and  $\bar{\epsilon}$ , it is best to defer the evaluation of Eq. (72) until the corresponding expression for  $\bar{\epsilon}$  is obtained.

B. Calculation of  $\bar{\epsilon}$

From Eqs. (62) and (66), we find

The values of these integrals are listed in Table III. After performing the  $k_0$  integration, the expression for  $\bar{\epsilon}$  takes the form

$$\begin{aligned}
\bar{\epsilon} = & \frac{i\alpha^3 |\varphi(0)|^2}{(2\pi)^4} \int \frac{d^3p d^3k' d^3k \delta(\vec{k}' - \vec{k} - \vec{p})}{(p^2 + \gamma^2)^2 E(p) E(k) E(k')} \\
& \times [\bar{J}_{++}(\vec{k}, \vec{k}') + \bar{J}_{+-}(\vec{k}, \vec{k}') + \bar{J}_{--}(\vec{k}, \vec{k}')], \tag{77}
\end{aligned}$$

where

TABLE I. Integrals  $I_{\pm\pm}(\vec{k}, \vec{k}')$ .

Signature	Contribution
++	$2\pi i \left( \frac{m}{ \vec{k} ^4  \vec{k}' ^2} - \frac{1}{2} \frac{( \vec{k}' ^2 +  \vec{k}  \vec{k}'  +  \vec{k} ^2)}{( \vec{k}'  +  \vec{k} ) \vec{k}' ^3  \vec{k} ^3} \right)$
+ - & - +	$2\pi i \left( \frac{-1}{4m \vec{k} ^2  \vec{k}' ^2} \right)$
--	$2\pi i \left( \frac{1}{8m^2( \vec{k}'  +  \vec{k} ) \vec{k}  \vec{k}' } \right)$

$$\begin{aligned} \bar{J}_{++} &= \{p^2[E(k) - m][E(k') - m]\bar{A} + k^2\bar{B} - k'^2\bar{B}' - \bar{C}\}\bar{I}_{++}, \\ \bar{J}_{+-} &= \{p^2(k^2 + k'^2)\bar{A} + 4m^2\bar{B} - 4m^2\bar{B}' + 2\bar{C}\}\bar{I}_{+-}, \\ \bar{J}_{--} &= \{p^2[E(k') + m][E(k) + m]\bar{A} \\ &\quad - 4m^2\bar{B} + 4m^2\bar{B}' - \bar{C}\}\bar{I}_{--}, \end{aligned} \quad (78)$$

and the spin averages  $\bar{A}$ ,  $\bar{B}$ ,  $\bar{B}'$ , and  $\bar{C}$  are given in Table IV.

Before combining Eqs. (72) and (77) we note that, since the leading contributions to  $\epsilon$  and  $\bar{\epsilon}$  are of order  $\alpha^6 \ln \alpha^{-1}$ , it is permissible to use the approximation  $E(k') \approx E(k)$ . The error made in doing so is of order  $\alpha^6$ . Moreover, the  $\ln \alpha^{-1}$  dependence arises from the low-momentum region of the integrations, where a neglect of binding would introduce a logarithmic singularity. As discussed in Sec. III, the relevant terms in the expressions for the  $J$ 's ( $\bar{J}$ 's) of Eq. (72) [Eq. (78)] are those which are most singular in the low-momentum region. Examination of Tables I–IV reveals that the most singular term behaves as (momentum) $^{-2}$ , and that the next most singular term has a (momentum) $^{-1}$  behavior. Again, our calculations will show that the most singular term does, indeed, give a  $\alpha^6 \ln \alpha^{-1}$  contribution, and that the next most singular term does not.

Apart from common factors, the most singular term in the integrand of the expression for  $\epsilon + \bar{\epsilon}$  is seen to be

$$\frac{2\pi m i}{k^2 k'^2} \left( -\bar{B} + \bar{B}' + \frac{1}{k^2} C \right)$$

$$= -\frac{8\pi m i}{3k^2 k'^2} \left[ \frac{1}{k^2} + \frac{1}{k'^2} \right] |\vec{k} \times \vec{p}|^2 \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle, \quad (79)$$

while the next most singular term is

$$\begin{aligned} 4m^2 \bar{I}_{--}(\vec{k}, \vec{k}') (B - \bar{B} + \bar{B}') \\ + \bar{I}_{++}(\vec{k}, \vec{k}') (k^2 B + k'^2 \bar{B} - k'^2 \bar{B}' - C - \bar{C}). \end{aligned} \quad (80)$$

The contribution of Eq. (79) to  $\epsilon + \bar{\epsilon}$  is given by

$$\begin{aligned} \frac{4}{3} \frac{m \alpha^3 |\varphi(0)|^2}{(2\pi)^3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3 k}{E^2(k)} \frac{d^3 p}{E(p)(p^2 + \gamma^2)^2} \\ \times \frac{|\vec{k} \times \vec{p}|^2}{k^2 |\vec{k} + \vec{p}|^2} \left[ \frac{1}{k^2} + \frac{1}{|\vec{k} + \vec{p}|^2} \right]. \end{aligned} \quad (81)$$

The evaluation of the remaining integrals is facilitated by employing the formula

$$\frac{1}{\sqrt{a} b} = \frac{1}{2} \int_0^1 \frac{dv}{(1-v)^{1/2}} \frac{1}{[a + (b-a)v]^{3/2}}, \quad (82)$$

which, when combined with the usual Feynman parameter integrals, can be used to obtain

$$\begin{aligned} \frac{1}{|\vec{p} + \vec{k}|^2 E(p)(p^2 + \gamma^2)^2} = \frac{15}{8} \int_0^1 du (1-u)^{3/2} \\ \times \int_0^1 \frac{dv v}{(1-v)^{1/2}} [(\vec{p} + u\vec{k})^2 + \Lambda]^{-7/2}, \end{aligned} \quad (83)$$

$$\begin{aligned} \frac{1}{|\vec{p} + \vec{k}|^4 E(p)(p^2 + \gamma^2)^2} = \frac{105}{16} \int_0^1 du u(1-u)^{3/2} \\ \times \int_0^1 \frac{dv v}{(1-v)^{1/2}} [(\vec{p} + u\vec{k})^2 + \Lambda]^{-9/2}, \end{aligned}$$

where

$$\Lambda = (1-u)[k^2 u + m^2 + (\gamma^2 - m^2)v] = (1-u)(k^2 u + \Delta) \geq 0. \quad (84)$$

By combining the denominators of the  $d^3 p$  integration with the aid of Eqs. (83), suitably translating the integration variable ( $\vec{p} - \vec{p} - u\vec{k}$ ), and then in-

TABLE II. Spin averages for the uncrossed two-photon term.

	Product of $\alpha$ 's	Coefficient of $\langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle$
A	$\delta_{ij}^T(\hat{k}) \delta_{im}^T(\hat{k}') \langle \alpha_i^{(1)} \alpha_j^{(2)} \alpha_i^{(1)} \alpha_m^{(2)} \rangle$	$-\frac{1}{3} \left( 2 + \frac{ \vec{k} \times \vec{p} ^2}{ \vec{k} ^2  \vec{k}' ^2} \right)$
B	$\delta_{ij}^T(\hat{k}) \delta_{im}^T(\hat{k}') \langle \alpha_i^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(1)} \cdot \vec{k} \alpha_i^{(1)} \alpha_m^{(2)} \vec{\alpha}^{(1)} \cdot \vec{p} + (1 \leftrightarrow 2) \rangle$	$\frac{2}{3} \left( 2(\vec{k} \cdot \vec{p}) + \frac{3 \vec{k} \times \vec{p} ^2}{ \vec{k}' ^2} \right)$
C	$\delta_{ij}^T(\hat{k}) \delta_{im}^T(\hat{k}') \langle \alpha_i^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(1)} \cdot \vec{k} \vec{\alpha}^{(2)} \cdot \vec{k} \alpha_i^{(1)} \alpha_m^{(2)} \vec{\alpha}^{(1)} \cdot \vec{p} \alpha^{(2)} \cdot \vec{p} \rangle$	$-\frac{1}{3} \left( 2k^2 p^2 +  \vec{k} \times \vec{p} ^2 + \frac{ \vec{k} ^2}{ \vec{k}' ^2}  \vec{k} \times \vec{p} ^2 \right)$

TABLE III. Integrals  $\tilde{I}_{\pm\pm}(\vec{k}, \vec{k}')$ .

Signature	Contribution
++	$2\pi i \left( \frac{( \vec{k}' ^2 +  \vec{k}   \vec{k}'  +  \vec{k} ^2)}{2( \vec{k}  +  \vec{k}' )  \vec{k} ^3  \vec{k}' ^3} \right)$
+- & -+	$2\pi i \left( \frac{-1}{4m  \vec{k} ^2  \vec{k}' ^2} \right)$
--	$2\pi i \left( \frac{1}{8m^2 ( \vec{k}'  +  \vec{k} )  \vec{k}   \vec{k}' } \right)$

tegrating symmetrically, we find that Eq. (81) becomes

$$\frac{2m\alpha^3}{3\pi} |\varphi(0)|^2 \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int_0^1 du (1-u)^{3/2} \times \int_0^1 \frac{dv v}{(1-v)^{1/2}} \int_0^\infty \frac{dk}{E^2(k)} \left( \frac{1}{\Lambda} + \frac{uk^2}{\Lambda^2} \right). \quad (85)$$

To our order of accuracy, we may put  $E(k) \approx m$ , and evaluate the remaining integrals to obtain

$$\epsilon + \tilde{\epsilon} = \frac{1}{12} m \alpha^6 \ln \alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle. \quad (86)$$

It remains to show that Eq. (80) yields no  $\alpha^6 \ln \alpha^{-1}$  contributions. To see how this can be done, consider the first term in Eq. (80). Using Tables II-IV it leads to a spin-spin contribution given by

$$\frac{\alpha^3 |\varphi(0)|^2}{6(2\pi)^3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3 k}{E^2(k)} \frac{d^3 p}{E(p)(p^2 + \gamma^2)^2} \times \left[ \left( \frac{1}{|\vec{p} + \vec{k}|} - \frac{1}{k} \right) \left( 2 - \frac{3|\vec{k} \times \vec{p}|^2}{k^2 |\vec{k} + \vec{p}|^2} \right) \right]. \quad (87)$$

Let us concentrate on the terms in the square brackets associated with the factor 2, since the remaining expressions can be treated similarly.

The  $d^3 p$  integration can be performed with the aid of Eq. (82), and the remaining  $k$  integration is easily performed, to give

$$-\frac{1}{3} \alpha^2 \frac{|\varphi(0)|^2}{m^2} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \ln(1 + \frac{1}{2} \alpha), \quad (88)$$

which is clearly an  $\alpha^6$  contribution. The remaining term in Eq. (80) is difficult to evaluate exactly, though both its momentum dependence and an approximate evaluation lead us to conclude that it too contributes in order  $\alpha^6$ . Therefore, the  $\alpha^6 \ln \alpha^{-1}$  contribution to  $\epsilon + \tilde{\epsilon}$  is given by Eq. (86).

### C. Calculation of $\epsilon_p$

When computing  $\epsilon_p$ , it must be remembered<sup>3</sup> that the leading term is of order  $\alpha^5$ . Therefore, we must be particularly careful when making approximations, because the error involved could be of order  $\alpha^6 \ln \alpha^{-1}$ . Keeping this in mind, we have found that it is permissible to put  $E(k') = E(k)$  in expressions of the form  $E(k') + m$ , but that this cannot be done in expressions of the form  $E(k') - m$ .

The explicit expression for  $\epsilon_p$  can be obtained<sup>12</sup> from Eqs. (67) and (74) simply by omitting the factor  $[2m(\vec{\alpha}^{(1)} - \vec{\alpha}^{(2)}) \cdot \vec{p} - p^2 - \vec{\alpha}^{(1)} \cdot \vec{p} \vec{\alpha}^{(2)} \cdot \vec{p}] / E(p)$ . The  $k_0$  integration can be performed with the aid of Tables I and III, and the only spin averages encountered are  $A$  and  $\bar{A} = -A$ . Keeping the most singular terms, we find

$$\epsilon_p = \frac{2}{3} \frac{m \alpha^3 |\varphi(0)|^2}{(2\pi)^3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int \frac{d^3 k}{E^2(k)} \times \int \frac{d^3 k}{(p^2 + \gamma^2)} \frac{[E(k) - m]}{k^2 |\vec{k} + \vec{p}|^2} \left( 2 + \frac{|\vec{k} \times \vec{p}|^2}{k^2 |\vec{k} + \vec{p}|^2} \right), \quad (89)$$

where we have omitted terms which can be shown to be of order  $\alpha^6$ . To isolate the  $\alpha^5$  contribution, we note that the integral associated with the factor 2 in the large parentheses is

TABLE IV. Spin averages for the crossed two-photon term.

	Product of $\alpha$ 's	Coefficient of $\langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle$
$\bar{A}$	$\delta_{ij}^T(\hat{k}') \delta_{im}^T(\hat{k}) \langle \alpha_i^{(1)} \alpha_j^{(2)} \alpha_m^{(1)} \alpha_j^{(2)} \rangle$	$\frac{1}{3} \left( 2 + \frac{ \vec{k} \times \vec{p} ^2}{ \vec{k} ^2  \vec{k}' ^2} \right)$
$\bar{B}$	$\delta_{ij}^T(\hat{k}') \delta_{im}^T(\hat{k}) \langle \alpha_i^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(1)} \cdot \vec{k}' \alpha_m^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(1)} \cdot \vec{p} \rangle$	$\frac{1}{3} \left( -2\vec{k}' \cdot \vec{p} + \frac{3 \vec{k} \times \vec{p} ^2}{ \vec{k} ^2} \right)$
$\bar{B}'$	$\delta_{ij}^T(\hat{k}') \delta_{im}^T(\hat{k}) \langle \alpha_i^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(2)} \cdot \vec{k} \alpha_m^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(2)} \cdot \vec{p} \rangle$	$-\frac{1}{3} \left( 2\vec{k} \cdot \vec{p} + \frac{3 \vec{k} \times \vec{p} ^2}{ \vec{k}' ^2} \right)$
$\bar{C}$	$\delta_{ij}^T(\hat{k}') \delta_{im}^T(\hat{k}) \langle \alpha_i^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(1)} \cdot \vec{k}' \vec{\alpha}^{(2)} \cdot \vec{k} \alpha_m^{(1)} \alpha_j^{(2)} \vec{\alpha}^{(1)} \cdot \vec{p} \vec{\alpha}^{(2)} \cdot \vec{p} \rangle$	$\frac{2}{3} [ \vec{p} ^2 (\vec{k} \cdot \vec{k}') -  \vec{k} \times \vec{p} ^2]$

$$\frac{4}{3} \alpha^2 |\varphi(0)|^2 \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int_0^\infty \frac{dk [E(k) - m]}{(k^2 + \gamma^2) E^2(k)}, \quad (90)$$

which has a leading  $\alpha^5$  contribution and no  $\ln \alpha^{-1}$  dependence. Thus, the  $\alpha^6 \ln \alpha^{-1}$  dependence of  $\epsilon_P$  is contained in the remaining term in Eq. (89), which may be integrated over  $d^3p$  with the aid of the formula

$$\frac{|\vec{k} \times \vec{p}|^2}{(p^2 + \gamma^2)^2 |\vec{k} + \vec{p}|^4} = 6 \int_0^1 \frac{du u(1-u) |\vec{k} \times \vec{p}|^2}{[(\vec{p} + u\vec{k})^2 + (1-u)(u\vec{k}^2 + \gamma^2)]^4}, \quad (91)$$

to give

$$\epsilon_P = \frac{m \alpha^3 |\varphi(0)|^2}{3} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \times \int_0^\infty \frac{dk [E(k) - m]}{E^2(k)} \left( \frac{1}{k^3} \tan^{-1} \frac{k}{\gamma} - \frac{\gamma}{k^2(k^2 + \gamma^2)} \right). \quad (92)$$

The last term in the large parentheses is of order  $\alpha^7$ , while the first term, after using

$$[E(k) - m]/E^2(k) \approx k^2/2m^2 E(k),$$

can be integrated to give

$$\epsilon_P = \frac{1}{96} m \alpha^6 \ln \alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle. \quad (93)$$

Finally, by adding Eqs. (86) and (93) we have

$$\Delta E_2(\alpha^6 \ln \alpha^{-1}) = \frac{3}{32} m \alpha^6 \ln \alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle. \quad (94)$$

#### V. NONCONTRIBUTING DIAGRAMS

In this section, we briefly summarize<sup>13</sup> our arguments for the absence of  $\alpha^6 \ln \alpha^{-1}$  contributions from the other diagrams which are known to contribute in order  $\alpha^5$ . For the most part, the proof that a particular term does not contain an  $\alpha^6 \ln \alpha^{-1}$  contribution consists of actually evaluating the relevant integrals and thereby showing that this is the case. Since a successive repetition of this procedure, though necessary, is not particularly illuminating, we will confine our attention to the terms which would appear most likely to yield an  $\alpha^6 \ln \alpha^{-1}$  contribution. The results for the remainder of the terms investigated will then be stated, with details available in Ref. 13.

Of all the terms to be considered, the one most similar in structure to the crossed transverse photon kernel and the Coulomb-transverse kernel is the crossed Coulomb kernel. This similarity to contributing diagrams suggests that the crossed Coulomb diagram may yield an  $\alpha^6 \ln \alpha^{-1}$ , and for this reason we investigate it in some detail.

#### Crossed Coulomb Contribution

The crossed Coulomb kernel  $I_{CC}(x, x')$  is

$$I_{CC}(x, x') = -[(4\pi\alpha)^2/(2\pi)^8] \times \int d^4k d^4k' \gamma_4^{(1)} \gamma_4^{(2)} G_{\vec{k}}(x, x') \gamma_4^{(1)} \gamma_4^{(2)} (1/\vec{k}^2)(1/\vec{k}'^2)$$

$$\times e^{i(\mathbf{k}-\mathbf{k}') \cdot (\mathbf{x}+\mathbf{x}')/2}, \quad (95)$$

and the corresponding energy shift  $\Delta E_{CC}$  is given by

$$\Delta E_{CC} = -2i \int d^4x d^4x' \bar{\varphi}_P(0) I_{CC}(x, x') \varphi_c'(\vec{x}'). \quad (96)$$

Using Eqs. (66) and (95) and proceeding as in the earlier two photon calculations, we obtain

$$\Delta E_{CC} = -\frac{\alpha^3 |\varphi(0)|^2}{12m\pi^2} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle \int d^3k \times \int \frac{d^3p |\vec{k} \times \vec{p}|^2}{k^2 |\vec{k} + \vec{p}|^2 (p^2 + \gamma^2)^2 E^3(k)}. \quad (97)$$

The remaining integrals can be evaluated with the aid of Eq. (82) to give

$$\Delta E_{CC} = -\frac{1}{48} m \alpha^6 \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle, \quad (98)$$

which is clearly of order  $\alpha^6$ . It should be noted that for small values of the momenta  $k$  and  $p$ , the integrand of Eq. (97) behaves as (momentum)<sup>0</sup>, compared to the (momentum)<sup>-2</sup> behavior of the integrands in Eqs. (81) and (89), which led to a  $\ln \alpha^{-1}$  contribution. This further supports our contention that anything less than a (momentum)<sup>-2</sup> behavior will not give rise to a logarithmic dependence on  $\alpha$ .

We have carried out similar calculations for the one and two photon annihilation terms and for the radiative corrections to the one transverse photon exchange and one photon annihilation terms.<sup>13</sup> In none of these terms do we find an  $\alpha^6 \ln \alpha^{-1}$  contribution. We have checked that the replacement of  $G_K^c(x, x')$  by  $G_K(x, x')$  in Eq. (63) does not affect the  $\alpha^6 \ln \alpha^{-1}$  dependence of the corresponding energy  $\epsilon$ .

Since terms involving three photons are at least of order  $\alpha^6$ , we conclude that the  $\alpha^6 \ln \alpha^{-1}$  terms arise from the one and two virtual transverse photon contributions, which have been evaluated in Secs. III and IV.

TABLE V. Theoretical contributions to positronium frequencies.

Order	$\Delta\nu$ 10 <sup>5</sup> MHz	% of contribution or last order		
		Actual	Expected	
Schrödinger level (ionization frequency)	$\alpha^2$	16 449.2	•••	•••
Triplet-singlet	$\alpha^4$	2.043 86	0.012	0.005
ground-state	$\alpha^5$	-0.010 05	0.49	0.73
splitting	$\alpha^6 \ln \alpha^{-1}$	0.000 34	3.4	3.6
	$\alpha^6$ (est)	±0.000 07	•••	20

## VI. SUMMARY AND DISCUSSION

Combining Eqs. (52), (61), and (94), we obtain

$$\Delta E_1 + \Delta E_{CT} + \Delta E_2 = \frac{3}{32} m \alpha^6 \ln \alpha^{-1} \langle \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} \rangle, \quad (99)$$

which leads to a triplet-singlet energy separation of

$$\Delta E(\alpha^6 \ln \alpha^{-1}) = \frac{3}{8} m \alpha^6 \ln \alpha^{-1}. \quad (100)$$

Taking the value of  $\alpha^{-1}$  to be<sup>14</sup>

$$\alpha^{-1} = 137.03608, \quad (101)$$

Eq. (100) leads to a frequency shift  $\Delta\nu$  given by

$$\Delta\nu(\alpha^6 \ln \alpha^{-1}) = 34 \text{ MHz}. \quad (102)$$

When this correction is added to the previous result of Karplus and Klein (KK),<sup>3</sup> we obtain

$$\nu^{\text{th}}(\text{KK}) = 2.03381 \times 10^5 \text{ MHz}, \quad (103)$$

$$\nu^{\text{th}}(\text{this paper}) = 2.03415 \times 10^5 \text{ MHz},$$

which are to be compared with the experimental value<sup>4</sup>

$$\nu^{\text{exp}}(1970) = 2.03403(12) \times 10^5 \text{ MHz} \quad (104)$$

One observes that, while the previous theoretical value was about two standard deviations below the experimental result, the contributions we obtain raise the theoretical value to one standard deviation above experiment. Considering the estimated  $m\alpha^6$  contributions given in Table V, the agreement between theory and experiment seems quite reasonable.<sup>15</sup>

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## APPENDIX

Introducing the Fourier transform of  $\varphi_{Kc}(x)$  by

$$\varphi_{Kc}(x) = (2\pi)^{-3/2} \int d^3p \varphi_{Kc}(\vec{p}, t) e^{i\vec{p}\cdot\vec{x}}, \quad (A1)$$

the various terms in Eq. (39) are given by

$$\varphi_c(\vec{p}, t) = 2\alpha(2\pi)^{-1/2} \frac{m}{E} \left(1 + \frac{\vec{\alpha}^{(1)} \cdot \vec{p}}{2m}\right) \left(1 - \frac{\vec{\alpha}^{(2)} \cdot \vec{p}}{2m}\right) \times [m f_+(t) + E f_-(t)] \frac{\varphi_P(0)}{(p^2 + \gamma^2)^2}, \quad (A2)$$

$$\delta\varphi_c(\vec{p}, t) = \frac{1}{2} \alpha(2\pi)^{-1/2} p^2 \frac{[m f_+(t) - E f_-(t)]}{mE} \frac{\varphi_P(0)}{(p^2 + \gamma^2)^2}, \quad (A3)$$

$$\delta\varphi'_c(\vec{p}, t) = -\frac{1}{2} \alpha(2\pi)^{-1/2} p^2 (\vec{\alpha}^{(1)} + \vec{\alpha}^{(2)}) \cdot \vec{p} \epsilon(t) \frac{f_-(t)}{mE} \times \frac{\varphi_P(0)}{(p^2 + \gamma^2)^2}, \quad (A4)$$

where

$$E = (p^2 + m^2)^{1/2}, \quad \gamma = \frac{1}{2} m \alpha, \quad (A5)$$

$$f_{\pm}(t) = \frac{1}{2} (e^{-i(E-m)|t|} \pm e^{-i(E+m)|t|}).$$

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†Permanent address: Department of Physics, The Johns Hopkins University, Baltimore, Md. 21218.

‡Present address: Department of Physics, University of Surrey, Guildford, Surrey, England.

§Present address: Department of Physics, Michigan State University, East Lansing, Mich. 48823.

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<sup>8</sup>Equation (26) follows since  $\delta(x_0) \Lambda_K(x, y) \delta(y_0)$  is independent of  $K$ .

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<sup>11</sup>In computing  $I_{\pm\pm}(\vec{k}, \vec{k}')$ , the poles are defined by replacing  $E(k)$  by  $E(k) - i\epsilon$ . Further, we have kept only the most singular terms in each integral for reasons explained in the text.

<sup>12</sup>The term  $-\varphi_P(0)[U_K(x, x') + \bar{I}_K(x, x')]\varphi_P(0)$  in  $\epsilon_P$  is known to be of order  $\alpha^5$  (Ref. 3), and will not be computed.

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