# Radiative corrections in atomic physics in the presence of perturbing potentials

S. A. Blundell

CEA/Grenoble, Département de Recherche Fondamentale sur la Matière Condensée, SI2A 17, rue des Martyrs, F-38054 Grenoble Cedex 9, France

K. T. Cheng

University of California, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550

J. Sapirstein

Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556

(Received 1 November 1996)

Energy shifts of radiative corrections in atoms due to perturbing potentials are calculated. The potentials considered are a constant magnetic field, the magnetic field of a nucleus, and the Coulomb interaction from other electrons in many-electron atoms. [S1050-2947(97)05303-1]

PACS number(s): 31.10.+z, 31.30.Gs, 31.30.Jv, 32.60.+i

The calculation of one-loop radiative corrections in atomic physics has played a central role in quantum electrodynamics since the first evaluation of the Lamb shift through the present. In the case of highly charged ions, the Lamb shift is enhanced by a factor of  $Z^4$  and can affect energy shifts at the 1% level. Its evaluation at high Z is complicated by the need for an exact treatment of the electron propagator. Nevertheless, for the point Coulomb problem extremely accurate calculations have been carried out by Mohr and collaborators [1]. These calculations have been confirmed by less precise methods that can, however, also be applied to the non-Coulomb case [2]. In this paper we wish to extend these calculations to include the presence of a perturbing potential. We are particularly interested in the case in which that potential comes from the magnetic field of a nucleus: this bears on recent experiments on the hyperfine splitting of hydrogenlike bismuth [3] and holmium [4], and also has consequences for hydrogen and muonium hyperfine splitting. This problem has been treated in a recent publication [5], and we find fair agreement with that work. We also treat the closely related problem of the evaluation of g factors in hydrogenic ions. This has also been treated by the same group [6], and we find fair agreement with their results at high Z. In addition, the formalism allows one to consider corrections to the nuclear potential arising from other electrons. This approach was used by Indelicato and Mohr [7] to treat the self-energy of n=2 states of lithiumlike uranium as perturbations from the Coulomb potential self-energy. Because of the abovementioned work on the evaluation of the self-energy in non-Coulomb potentials, the self-energy can also be directly evaluated, which provides a useful check on the calculation.

The paper is organized as follows. In the next section the *S*-matrix formalism for the calculation is presented. The following section applies the formalism to the case when the potential arises from other electrons. The case of potentials coming from the nuclear magnetic dipole field and a constant magnetic field are presented in the following two sections, and a summary of results and discussion of directions for future research are given in the conclusion.

#### I. FORMALISM

### A. Perturbation theory

We evaluate energy shifts using Sucher's [8] symmetrized form of the Gell-Mann and Low level-shift formula [9]:

$$\Delta E = \lim_{\epsilon \to 0} \lim_{\lambda \to 1} \frac{i\epsilon}{2} \frac{\partial}{\partial \lambda} \log \langle v | S(\epsilon, \lambda) | v \rangle, \tag{1}$$

where

$$S(\boldsymbol{\epsilon},\boldsymbol{\lambda}) = T \bigg[ \exp \bigg( -i\boldsymbol{\lambda} \int d^4 x e^{-\boldsymbol{\epsilon}|x_0|} H_I(x) \bigg) \bigg].$$
(2)

We work in Furry representation QED with the external field (unless otherwise stated) taken to be a point Coulomb potential of charge Z. The state v represents a single electron, which will usually be in the ground state. For the calculations involving magnetic fields it will be understood to be the 1s state with magnetic quantum number +1/2. The interaction Hamiltonian is  $H_I = H_I^A + H_I^B$ , where

$$H_I^A = e \int d^3x \,\overline{\psi}(x) \,\gamma_\mu A^\mu(x) \,\psi(x) \tag{3}$$

and

$$H_I^B = \int d^3x \,\overline{\psi}(x) V(\mathbf{x}) \,\psi(x). \tag{4}$$

Here  $V(\mathbf{x})$  represents the external perturbing potential. We work with three potentials in this work: the potentials of magnetic fields,

$$V(\mathbf{x}) = -e \,\boldsymbol{\gamma} \cdot \mathbf{A}(\mathbf{x}), \tag{5}$$

with  $\mathbf{A}(\mathbf{x}) = \boldsymbol{\mu} \times \mathbf{x}/(4 \pi |\mathbf{x}|^3)$  for the dipole field of the nucleus and  $\mathbf{A}(\mathbf{x}) = 1/2\mathbf{B} \times \mathbf{x}$  for a constant magnetic field, and the potential

1857

© 1997 The American Physical Society

$$V(\mathbf{x}) = U(|\mathbf{x}|) \gamma_0.$$
 (6)

The first potential is of relevance to hyperfine splitting, the second to the Zeeman effect, and the last to the Lamb shift in ions in which the deviation from the Coulomb potential can be treated as a perturbation.

In the present calculation we will need the first three terms in the expansion of  $S(\epsilon, \lambda)$ ,

$$S^{(1)}(\boldsymbol{\epsilon},\boldsymbol{\lambda}) = (-i\boldsymbol{\lambda}) \int d^4x e^{-\boldsymbol{\epsilon}|x_0|} \langle v|T(:\overline{\psi}(x)V(x)\psi(x):)|v\rangle,$$
(7)
$$S^{(2)}(\boldsymbol{\epsilon},\boldsymbol{\lambda}) = \frac{(-i\boldsymbol{\epsilon}\boldsymbol{\lambda})^2}{2} \int d^4x \int d^4y e^{-\boldsymbol{\epsilon}(|x_0|+|y_0|)} \langle v|$$

$$\times T(:\overline{\psi}(x)A(x)\psi(x)::\overline{\psi}(y)A(y)\psi(y):)|v\rangle,$$
(8)

and

$$S^{(3)}(\boldsymbol{\epsilon},\boldsymbol{\lambda}) = \frac{(-i\boldsymbol{\lambda})^3 e^2}{2!} \int d^4x \int d^4y \int d^4z \\ \times e^{-\boldsymbol{\epsilon}(|x_0| + |y_0| + |z_0|)} \cdot \langle v| \\ \times T(:\overline{\psi}(x)\boldsymbol{A}(x)\psi(x)::\overline{\psi}(y) \\ \times \boldsymbol{A}(y)\psi(y)::\overline{\psi}(z)V(z)\psi(z):)|v\rangle, \quad (9)$$

where only terms linear in  $H_I^B$  are considered in  $S^{(3)}(\epsilon, \lambda)$ . The first two orders of the *S* matrix are readily computed to be

$$S_{\epsilon,\lambda}^{(1)} = \frac{-2i\lambda}{\epsilon} E^{(1)}(v) \tag{10}$$

and

$$S_{\epsilon,\lambda}^{(2)} = -\frac{i\lambda^2}{\epsilon} \Sigma_{vv}(\epsilon_v).$$
(11)

Here  $E^{(1)}(v) = V_{vv}$ , where

$$V_{mn} \equiv \int d^3x \,\overline{\psi}_m(\mathbf{x}) V(\mathbf{x}) \,\psi_n(\mathbf{x}) \tag{12}$$

and

$$\Sigma_{mn}(\boldsymbol{\epsilon}) \equiv -ie^2 \int d^3x \int d^3y \int \frac{d^4k}{(2\pi)^4} \frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})]}{k^2}$$
$$\times \overline{\psi}_m(\mathbf{x}) \gamma_\mu S_F(\mathbf{x},\mathbf{y};\boldsymbol{\epsilon}-k_0) \gamma^\mu \psi_n(\mathbf{y}). \tag{13}$$

We exclude vacuum polarization effects from the present calculation. Putting these terms into Eq. (1) leads to the energy shift

$$\Delta E(S^{(1)}, S^{(2)}) = E^{(1)}(v) + \Sigma_{vv}(\epsilon_v) + \frac{i}{\epsilon} [E^{(1)}(v) + \Sigma_{vv}(\epsilon_v)] \\ \times [2E^{(1)}(v) + \Sigma_{vv}(\epsilon_v)] + \cdots$$
(14)



FIG. 1. Side left (SL), vertex (V), and side right (SR) diagrams calculated in this work. The double line indicates the electron propagator in the external field, and the wavy line terminated by a cross indicates the additional perturbing potential.

The divergent third term cancels against other  $1/\epsilon$  terms coming from  $S^{(3)}$  and  $S^{(4)}$ . For the present calculation, only the part that is linear in  $H_I^B$ , proportional to the cross term between  $E^{(1)}(v)$  and  $\Sigma_{vv}(\epsilon_v)$ , need be considered.

We now turn to the calculation of the energy shift in third order. Applying Wick's theorem to  $S^{(3)}(\epsilon, \lambda)$  gives three terms associated with the Feynman diagrams of Fig. 1, which we refer to as the *side-left* (SL), *vertex* (V), and *side-right* (SR) diagrams. Because the side-left and side-right diagrams give the same energy shifts, it will be understood from now on that any expression labeled with S represents the sum of SL and SR contributions. For the vertex diagram we have

$$S_{V}^{(3)}(\boldsymbol{\epsilon},\boldsymbol{\lambda}) = -32\pi\alpha\lambda^{3}\boldsymbol{\epsilon}^{3}\int d^{3}x \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}}$$

$$\times \frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{z})]}{k^{2}+i\delta} \int \frac{dE_{1}}{2\pi} \int \frac{dE_{2}}{2\pi}$$

$$\times \overline{\psi}_{v}(\mathbf{x})\gamma_{\mu}S_{F}(\mathbf{x},\mathbf{y};E_{1})V(\mathbf{y})S_{F}(\mathbf{y},\mathbf{z};E_{2})\gamma^{\mu}\psi_{v}(\mathbf{z})$$

$$\times \frac{1}{\boldsymbol{\epsilon}^{2}+(E_{1}-E_{2})^{2}} \frac{1}{\boldsymbol{\epsilon}^{2}+(E_{1}+k_{0}-\boldsymbol{\epsilon}_{v})^{2}}$$

$$\times \frac{1}{\boldsymbol{\epsilon}^{2}+(E_{2}+k_{0}-\boldsymbol{\epsilon}_{v})^{2}}.$$
(15)

The denominators involving  $\epsilon$  act to emphasize the region  $E_1 = E_2 = \epsilon_v - k_0$ , so replacing the arguments of the Dirac-Coulomb propagators with that value and carrying out the  $E_1$  and  $E_2$  integrations, we find a contribution to the energy shift

$$E_{V} = -4\pi i \alpha \int d^{3}x \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}}$$

$$\times \frac{\exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{z})]}{k^{2} + i \delta} \overline{\psi}_{v}(\mathbf{x}) \gamma_{\mu} S_{F}(\mathbf{x}, \mathbf{y}; \boldsymbol{\epsilon}_{v} - k_{0})$$

$$\times V(\mathbf{y}) S_{F}(\mathbf{y}, \mathbf{z}; \boldsymbol{\epsilon}_{v} - k_{0}) \gamma^{\mu} \psi_{v}(\mathbf{z}). \qquad (16)$$

The side diagrams require a little more care because they contain the canceling  $1/\epsilon$  terms mentioned above. These terms are most clearly discussed when a spectral representation is used for the first Dirac-Coulomb propagator in the expression for the side-right diagram,

$$S_{\text{SR}}^{(3)} = -32\alpha \pi \alpha \lambda^{3} \epsilon^{3} \int d^{3}x \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}}$$

$$\times \frac{\exp[i\mathbf{k} \cdot (\mathbf{y} - \mathbf{z})]}{k^{2} + i \delta} \int \frac{dE_{1}}{2\pi} \int \frac{dE_{2}}{2\pi}$$

$$\times \overline{\psi}_{v}(\mathbf{x}) V(\mathbf{x}) S_{F}(\mathbf{x}, \mathbf{y}; E_{1}) \gamma_{\mu} S_{F}(\mathbf{y}, \mathbf{z}; E_{2}) \gamma^{\mu} \psi_{v}(\mathbf{z})$$

$$\times \frac{1}{\epsilon^{2} + (E_{1} - \epsilon_{v})^{2}} \frac{1}{\epsilon^{2} + (E_{1} - E_{2} - k_{0})^{2}}$$

$$\times \frac{1}{\epsilon^{2} + (E_{2} + k_{0} - \epsilon_{v})^{2}}.$$
(17)

We write this spectral representation as

$$S_F(\mathbf{x}, \mathbf{y}; E_1) = \sum_{m_v} \frac{\psi_{v, m_v}(\mathbf{x}) \overline{\psi}_{v, m_v}(\mathbf{y})}{E_1 - \epsilon_v + i\,\delta} + \sum_{n \neq v} \frac{\psi_n(\mathbf{x}) \overline{\psi}_n(\mathbf{y})}{E_1 - \epsilon_n(1 - i\,\delta)},$$
(18)

where we have separated out the contribution from magnetic substates of the state v. The second term in Eq. (18) can be handled in the same manner as the vertex, and yields

$$E_{\rm SR}^{A} = \sum_{n \neq v} \frac{V_{vn} \Sigma_{nv}}{\epsilon_v - \epsilon_n}.$$
 (19)

To analyze the effect of the first term in Eq. (18), we carry out a Taylor expansion of the second Dirac-Coulomb propagator about  $E_2 = \epsilon_v - k_0$ ,

$$S_{F}(\mathbf{x}, \mathbf{y}; E_{2}) = S_{F}(\mathbf{x}, \mathbf{y}; \boldsymbol{\epsilon}_{v} - k_{0}) + (E_{2} - \boldsymbol{\epsilon}_{v} + k_{0})$$
$$\times \frac{\partial}{\partial E} S_{F}(\mathbf{x}, \mathbf{y}; E)|_{E = \boldsymbol{\epsilon}_{v} - k_{0}} + \cdots$$
(20)

The leading term in this expansion gives

$$E_{\rm SR}(1/\epsilon) = -\frac{3i}{2\epsilon} E^{(1)} \Sigma_{vv}(\epsilon_v), \qquad (21)$$

which when combined with the identical SL term cancels the  $1/\epsilon$  terms discussed above. The next term in the expansion (20) gives the energy shift, which we will in the following refer to as the *derivative* term,

$$E_{S}^{B} = 4i \pi \alpha \sum_{m_{v}} \int d^{3}x \int d^{3}y \int d^{3}z \int d^{3}w \int \frac{d^{4}k}{(2\pi)^{4}} \\ \times \frac{\exp[i\mathbf{k}\cdot(\mathbf{y}-\mathbf{z})]}{k^{2}+i\delta} \overline{\psi}_{v}(\mathbf{x}) V(\mathbf{x}) \psi_{vm_{v}}(\mathbf{x}) \overline{\psi}_{vm_{v}}(\mathbf{y}) \\ \times \gamma_{\mu} S_{F}(\mathbf{y},\mathbf{w};\epsilon_{v}-k_{0}) \gamma_{0} S_{F}(\mathbf{w},\mathbf{z};\epsilon_{v}-k_{0}) \gamma^{\mu} \psi_{v}(\mathbf{z}).$$

$$(22)$$

This can be rewritten if we recognize the integration over *x* as giving  $V_{vvm_v}$  and use the fact that the remaining integral is diagonal in magnetic quantum number, so

$$E_{S}^{B} = 4i \pi \alpha E^{(1)}(v) \int d^{3}y \int d^{3}z \int d^{3}w \int \frac{d^{4}k}{(2\pi)^{4}} \\ \times \frac{\exp[i\mathbf{k} \cdot (\mathbf{y} - \mathbf{z})]}{k^{2} + i \delta} \overline{\psi}_{v}(\mathbf{y}) \gamma_{\mu} S_{F}(\mathbf{y}, \mathbf{w}; \boldsymbol{\epsilon}_{v} - k_{0}) \\ \times \gamma_{0} S_{F}(\mathbf{w}, \mathbf{z}; \boldsymbol{\epsilon}_{v} - k_{0}) \gamma^{\mu} \psi_{v}(\mathbf{z}).$$
(23)

The three terms we have derived using the *S*-matrix formalism can also be derived by directly modifying the self-energy expression [7]. The vertex term corresponds to modifying the Dirac-Coulomb propagator to account for the external potential, the derivative term to modifying the energy flowing through that line, and  $E_S^A$  to modifying the external wave functions.

#### **B.** Treatment of ultraviolet divergences

The expressions  $E_V$  and  $E_S$  are both ultraviolet divergent. However, their sum is ultraviolet finite, so that in principle one might attempt to evaluate that sum directly in coordinate space. We choose instead to use coordinate space only for ultraviolet finite quantities defined as the difference of these expressions with terms in which the two Dirac-Coulomb propagators are replaced by free propagators. Thus, considering first  $E_V$ , we rearrange its calculation as  $E_V = (E_V - E_V(0,0))_x + E_V(0,0)_p \equiv E_V^s + E_V^p$ , where  $E_V(0,0)$ is  $E_V$  with both propagators replaced by free propagators, and the subscript x (p) indicates that the calculation is to be carried out in coordinate (momentum) space. The term  $E_V^s$ does not require regularization, but  $E_V(0,0)_p$  does, and we make this expression finite by working in  $n=4-\epsilon$  dimensions. Then the explicit forms for the breakup of  $E_V$  are

$$E_{V}^{s} = -4\pi i\alpha \int d^{3}x \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}}$$

$$\times \frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{z})]}{k^{2}+i\delta} [\overline{\psi}_{v}(\mathbf{x})\gamma_{\mu}S_{F}(\mathbf{x},\mathbf{y};\boldsymbol{\epsilon}_{v}-k_{0})V(\mathbf{y})$$

$$\times S_{F}(\mathbf{y},\mathbf{z};\boldsymbol{\epsilon}_{v}-k_{0})$$

$$\times \gamma^{\mu}\psi_{v}(\mathbf{z}) - \overline{\psi}_{v}(\mathbf{x})\gamma_{\mu}S_{0}(\mathbf{x},\mathbf{y};\boldsymbol{\epsilon}_{v}-k_{0})V(\mathbf{y})$$

$$\times S_{0}(\mathbf{y},\mathbf{z};\boldsymbol{\epsilon}_{v}-k_{0})\gamma^{\mu}\psi_{v}(\mathbf{z})], \qquad (24)$$

and

$$E_V^p = -4\pi i\alpha \int d^3 p_1 \int d^3 p_2 \int \frac{d^n k}{(2\pi)^n} \frac{1}{k^2 + i\delta} \overline{\psi}_v(\mathbf{p}_2) \gamma_\mu$$

$$\times \frac{1}{p_2 - k_1 - m} V(\mathbf{p}_2 - \mathbf{p}_1) \frac{1}{p_1 - k_1 - m}$$

$$\times \gamma^\mu \psi_v(\mathbf{p}_1), \qquad (25)$$

where

$$V(\mathbf{q}) \equiv \int \frac{d^3 y}{(2\pi)^3} e^{-i\mathbf{y}\cdot\mathbf{q}} V(\mathbf{y}).$$
(26)

The integration over k can be carried out after introducing Feynman parameters, and we have

$$E_{V}^{p} = \frac{\alpha}{2\pi} \left( \frac{C}{\epsilon} - 1 \right) \int d^{3}p_{1} \int d^{3}p_{2} \overline{\psi}_{v}(\mathbf{p}_{2}) V(\mathbf{p}_{2} - \mathbf{p}_{1}) \psi_{v}(\mathbf{p}_{1})$$
$$- \frac{\alpha}{4\pi} \int \rho d\rho \int dx \int d^{3}p_{1} \int d^{3}p_{2} \frac{\overline{\psi}_{v}(\mathbf{p}_{2}) N_{0} \psi_{v}(\mathbf{p}_{1})}{D}$$
$$- \frac{\alpha}{2\pi} \int \rho d\rho \int dx \int d^{3}p_{1} \int d^{3}p_{2} \log \left( \frac{D}{m^{2}} \right) \overline{\psi}_{v}(\mathbf{p}_{2})$$
$$\times V(\mathbf{p}_{2} - \mathbf{p}_{1}) \psi_{v}(\mathbf{p}_{1}). \tag{27}$$

In the above expression  $C = (4\pi)^{\epsilon/2} \Gamma(1 + \epsilon/2), Q_{\mu} \equiv \rho [xp_1 + (1-x)p_2]_{\mu}, \quad D \equiv Q^2 + \rho x (m^2 - p_1^2) + \rho (1-x)(m^2 - p_2^2),$ and  $N_0 \equiv \gamma_{\mu} (\not p_2 - \not Q + m) V(\mathbf{p}_2 - \mathbf{p}_1) (\not p_1 - \not Q + m) \gamma^{\mu}$ . We note that to derive the above expression we performed manipulations on the Dirac gamma matrices that relied on the potentials considered in this paper being components of a four-vector.

The treatment of  $E_S^B$  follows along the lines of the vertex calculation: the coordinate space part of the calculation is carried out only after the free propagator term is subtracted, and the latter is evaluated in momentum space with dimensional regularization. The former term is

$$E_{S}^{s} = 4 \pi i \alpha E^{(1)}(v) \int d^{3}x \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}} \\ \times \frac{\exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{z})]}{k^{2} + i \delta} [\overline{\psi}_{v}(\mathbf{x}) \gamma_{\mu} S_{F}(\mathbf{x}, \mathbf{y}; \boldsymbol{\epsilon}_{v} - k_{0}) \\ \times \gamma_{0} S_{F}(\mathbf{y}, \mathbf{z}; \boldsymbol{\epsilon}_{v} - k_{0}) \gamma^{\mu} \psi_{v}(\mathbf{z}) - \overline{\psi}_{v}(\mathbf{x}) \\ \times \gamma_{\mu} S_{0}(\mathbf{x}, \mathbf{y}; \boldsymbol{\epsilon}_{v} - k_{0}) \gamma_{0} S_{0}(\mathbf{y}, \mathbf{z}; \boldsymbol{\epsilon}_{v} - k_{0}) \gamma^{\mu} \psi_{v}(\mathbf{z})]$$

$$(28)$$

and the latter

$$E_{S}^{p} = 4i\pi\alpha E^{(1)}(v) \int d^{3}p \int \frac{d^{n}k}{(2\pi)^{n}} \frac{1}{k^{2} + i\delta} \overline{\psi}_{v}(\mathbf{p}) \gamma_{\mu}$$
$$\times \frac{1}{p - k - m} \gamma_{0} \frac{1}{p - k - m} \gamma^{\mu} \psi_{v}(\mathbf{p}). \tag{29}$$

The divergent momentum space term can be treated in the same way as the vertex, and there results

$$E_{S}^{p} = -E^{(1)}(v) \frac{\alpha}{2\pi} \left(\frac{C}{\epsilon} - 1\right) \int d^{3}p \,\overline{\psi}_{v}(\mathbf{p}) \gamma_{0}\psi_{v}(\mathbf{p})$$
$$+ \frac{\alpha}{4\pi} E^{(1)} \int \rho d\rho \int d^{3}p \frac{\overline{\psi}_{v}(\mathbf{p})N_{1}\psi_{v}(\mathbf{p})}{D_{1}}$$
$$+ \frac{\alpha}{2\pi} E^{(1)} \int \rho d\rho \int d^{3}p \log\left(\frac{D_{1}}{m^{2}}\right) \overline{\psi}_{v}(\mathbf{p}) \gamma_{0}\psi_{v}(\mathbf{p}),$$
(30)

where now  $D_1 \equiv \rho^2 p^2 + \rho (m^2 - p^2)$ , and  $N_1 \equiv \gamma_{\mu} [p(1 - \rho) + m] \gamma_0 [p(1 - \rho) + m] \gamma^{\mu}$ .

At this point we observe that the ultraviolet divergent terms cancel, since the coefficient of the  $(C/\epsilon-1)$  term in the vertex is the momentum space representation of

 $E^{(1)}(v)$  and the corresponding coefficient in the side-left and side-right graphs is a normalization integral. Thus we are left with a completely ultraviolet-finite calculation. It would of course be possible to make the graphs individually finite by including the usual renormalization counterterms associated with vertex and wave function renormalization. However, these counterterms also cancel by Ward's identity [10], so as long as we consider the graphs together the final answer does not require their explicit introduction. While the remaining integrals are all ultraviolet finite, there is one more source of possible singularities, to which we now turn.

#### C. Reference-state contributions

Reference-state (RS) contributions can occur when one of the states in the spectral representation of an electron propagator coincides with the external state v. We have already encountered one kind of reference-state contribution in the analysis of the side graphs, where the term involving v in the spectral decomposition of a certain electron propagator led to canceling the  $1/\epsilon$  term and the finite residue  $E_S^B$  [see Eq. (18) and the subsequent discussion]. The contributions we now wish to discuss are contained within  $E_S^B$  itself and  $E_V$ , and arise when both the electron propagators inside the photon loop involve the external state v. These contributions are then obtained by replacing the electron propagators in Eqs. (16) and (23) with the terms in their spectral decomposition involving v. For  $E_V$  this gives

$$E_{V}^{\text{RS}} = -4\pi i \alpha \sum_{m_{v}m_{w}} \int d^{3}x \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}}$$
$$\times \frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{z})]}{k^{2}+i\delta} \frac{1}{(-k_{0}+i\delta)^{2}} \overline{\psi}_{v}(\mathbf{x}) \gamma_{\mu}\psi_{vm_{v}}(\mathbf{x})$$
$$\times \overline{\psi}_{vm_{v}}(\mathbf{y}) V(\mathbf{y}) \psi_{vm_{w}}(\mathbf{y}) \overline{\psi}_{vm_{w}}(\mathbf{z}) \gamma^{\mu}\psi_{v}(\mathbf{z}), \qquad (31)$$

and for  $E_S^B$ 

$$E_{\delta}^{\text{RS}} = 4 \pi i \alpha E^{(1)}(v) \sum_{m_{v}} \int d^{3}y \int d^{3}z \int \frac{d^{4}k}{(2\pi)^{4}} \\ \times \frac{\exp[i\mathbf{k} \cdot (\mathbf{y} - \mathbf{z})]}{k^{2} + i \delta} \\ \times \frac{1}{(-k_{0} + i \delta)^{2}} \overline{\psi}_{v}(\mathbf{y}) \gamma_{\mu} \psi_{vm_{v}}(\mathbf{y}) \overline{\psi}_{vm_{v}}(\mathbf{z}) \gamma^{\mu} \psi_{v}(\mathbf{z}).$$
(32)

Now, if  $V(\mathbf{x}) = U(|\mathbf{x}|) \gamma_0$ , the *y* integration in  $E_V^{\text{RS}}$  gives  $E^{(1)}(v) \delta_{m_v m_w}$ , and  $E_V^{\text{RS}}$  and  $E_S^{\text{RS}}$  then cancel each other identically. Thus in this case there is no reference-state contribution. However, the cancellation is incomplete when magnetic fields are present, as will be shown in the next section. This lack of cancellation requires particular care, since (in the Feynman gauge used here) the  $k_0$  integrals in  $E_V^{\text{RS}}$  and  $E_S^{\text{RS}}$  are separately divergent as  $k_0 \rightarrow 0$ , while the  $k_0$  integral of the sum of the integrands of  $E_V^{\text{RS}}$  and  $E_S^{\text{RS}}$  is finite. Thus the sum  $E_V^{\text{RS}} + E_S^{\text{RS}}$  is finite and well-defined, but its evaluation

requires special treatment. Other combinations of states in the propagators of  $E_V$  and  $E_S^B$  give finite  $k_0$  integrals and can be handled straightforwardly.

As explained in the next section, we evaluate the integral over the spatial components of k analytically, and the integral over the time component  $k_0$  numerically after a Wick rotation,  $k_0 \rightarrow i\omega$ . For the reference-state terms, that procedure would lead to a divergent integral  $\int d\omega/\omega^2$ . To regulate this divergence, we replace  $k_0 \rightarrow k_0 + \Delta$ , where  $\Delta$  is a regulator to be taken to 0 at the end of the calculation. Thus, for example, we would treat the integral

$$-i \int_{-\infty}^{\infty} \frac{dk_0}{(k_0 - i\,\delta)^2} f(k_0), \tag{33}$$

by introducing the regulator (which then allows taking  $\delta \rightarrow 0$ ), and then carrying out the Wick rotation, which leads to

$$2 \operatorname{Re} \int_{0}^{\infty} d\omega \frac{f(i\omega)}{(i\omega + \Delta)^{2}},$$
(34)

where we have assumed that  $f(i\omega) = f(-i\omega)$ . Note that for constant f both integrals vanish, the first by reason of Cauchy's theorem, and the second identically. It is noteworthy that although no linear reference state singularity is present, logarithmically divergent terms proportional to  $log(\Delta)$  are present in  $E_V^{RS}$  and  $E_S^{RS}$  separately, but cancel when one forms the sum of these two terms. In practice we calculate the sum  $E_V^{RS} + E_S^{RS}$  for several values of  $\Delta$ , and take the limit  $\Delta \rightarrow 0$  by polynomial extrapolation.

### **D.** Angular reduction

The coordinate-space part of the calculation involves carrying out a partial-wave expansion of the photon propagator. If a spectral decomposition of the electron propagators is made, and we make the Wick rotation  $k_0 \rightarrow i\omega$ , the angle integrations can then be done for the vertex term. In the case

$$V(\mathbf{x}) = U(|\mathbf{x}|) \gamma_0, \qquad (35)$$

there results

$$E_{V} = -\frac{\alpha}{\pi} \sum_{[ij]l}^{\infty} (2l+1) \frac{1}{2j_{v}+1} \int_{0}^{\infty} \omega d\omega$$

$$\times \frac{(\epsilon_{v}-\epsilon_{i})(\epsilon_{v}-\epsilon_{j})-\omega^{2}}{[(\epsilon_{v}-\epsilon_{i})^{2}+\omega^{2}][(\epsilon_{v}-\epsilon_{j})^{2}+\omega^{2}]} \int_{0}^{\infty} dy R_{ij}(y) U(y)$$

$$\times \int_{0}^{\infty} dx \int_{0}^{\infty} dz [C_{l}^{2}(\kappa_{v}\kappa_{i})R_{vi}(x)R_{jv}(z)i_{l}(\omega r_{<})k_{l}(\omega r_{>})$$

$$+ C_{l}^{2}(\kappa_{v}\kappa_{i})P_{vi}^{l}(x)P_{jv}^{l}(z)i_{l+1}(\omega r_{<})k_{l+1}(\omega r_{>})$$

$$- C_{l}^{2}(-\kappa_{v}\kappa_{i})V_{vi}^{l}(x)V_{jv}^{l}(z)i_{l}(\omega r_{<})k_{l}(\omega r_{>})$$

$$+ C_{l}^{2}(\kappa_{v}\kappa_{i})Q_{vi}^{l}(x)Q_{jv}^{l}(z)i_{l-1}(\omega r_{<})k_{l-1}(\omega r_{>})]. \quad (36)$$

We have introduced here the following functions:

$$R_{ij}(r) = g_i(r)g_j(r) + f_i(r)f_j(r), \qquad (37)$$

$$P_{ij}^{J}(r) = \sqrt{\frac{J+1}{2J+1}} \left( g_i(r)f_j(r) - f_i(r)g_j(r) + \frac{\kappa_i - \kappa_j}{J+1} [g_i(r)f_j(r) + f_i(r)g_j(r)] \right), \quad (38)$$

$$V_{ij}^{J}(r) = \frac{\kappa_i + \kappa_j}{\sqrt{J(J+1)}} [g_i(r)f_j(r) + f_i(r)g_j(r)], \quad (39)$$

and

$$Q_{ij}^{J}(r) = \sqrt{\frac{J}{2J+1}} \bigg( g_{j}(r)f_{i}(r) - f_{j}(r)g_{i}(r) + \frac{\kappa_{i} - \kappa_{j}}{J} [g_{i}(r)f_{j}(r) + f_{i}(r)g_{j}(r)] \bigg), \quad (40)$$

where g(r) and f(r) are the upper and lower radial components of the Dirac wave function,

$$\psi(r) = \frac{1}{r} \begin{pmatrix} ig(r) & \chi_{\kappa\mu}(\Omega) \\ f(r) & \chi_{-\kappa\mu}(\Omega) \end{pmatrix}.$$
 (41)

In the above

$$C_{l}(ij) \equiv (-1)^{j_{i}+1/2} \sqrt{(2j_{i}+1)(2j_{j}+1)} \\ \times \begin{pmatrix} j_{i} & j_{j} & l \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \Pi(l_{i}, l_{j}, l),$$
(42)

where  $\Pi(l_i, l_j, l)$  is unity if the sum  $l_i + l_j + l$  is even, and otherwise vanishes. The side graphs can be treated similarly, and become

$$E_{S} = \frac{\alpha}{\pi} E^{(1)}(v) \sum_{[i]l} (2l+1) \frac{1}{2j_{v}+1} \int_{0}^{\infty} \omega d\omega$$

$$\times \frac{(\epsilon_{v} - \epsilon_{i})^{2} - \omega^{2}}{[(\epsilon_{v} - \epsilon_{i})^{2} + \omega^{2}]^{2}} \int_{0}^{\infty} dx \int_{0}^{\infty} dz$$

$$\times [C_{l}^{2}(\kappa_{v}\kappa_{i})R_{vi}(x)R_{iv}(z)i_{l}(\omega r_{<})k_{l}(\omega r_{>})$$

$$+ C_{l}^{2}(\kappa_{v}\kappa_{i})P_{vi}^{l}(x)P_{iv}^{l}(z)i_{l+1}(\omega r_{<})k_{l+1}(\omega r_{>})$$

$$- C_{l}^{2}(-\kappa_{v}\kappa_{i})V_{vi}^{l}(x)V_{iv}^{l}(z)i_{l}(\omega r_{<})k_{l}(\omega r_{>})$$

$$+ C_{l}^{2}(\kappa_{i}\kappa_{v})Q_{vi}^{l}(x)Q_{iv}^{l}(z)i_{l-1}(\omega r_{<})k_{l-1}(\omega r_{>})].$$
(43)

We note that the reference state singularities i=j=v for the vertex and i=v for the side graphs can be seen to cancel identically once it is noted that  $E^{(1)}(v) = \int dy R_{vv}(y) U(y)$ . In the calculation the sum over l was usually carried out up to l=12.

For the magnetic potentials a more complicated expression for the vertex arises. For the nuclear dipole potential,

$$E_{V} = -\frac{\sqrt{3}\alpha}{4\pi I} E_{F} \sum_{[ij]l} (2l+1)(-1)^{l} C_{1}(-\kappa_{j}\kappa_{i}) \begin{cases} j_{i} & j_{j} & 1 \\ j_{v} & j_{v} & l \end{cases}$$

$$\times \int_{0}^{\infty} \omega d\omega \frac{(\epsilon_{v} - \epsilon_{i})(\epsilon_{v} - \epsilon_{j}) - \omega^{2}}{[(\epsilon_{v} - \epsilon_{i})^{2} + \omega^{2}][(\epsilon_{v} - \epsilon_{j})^{2} + \omega^{2}]}$$

$$\times \int_{0}^{\infty} dy \frac{1}{y^{2}} V_{ij}^{1}(y) \int_{0}^{\infty} dx \int_{0}^{\infty} dz [C_{l}(\kappa_{v}\kappa_{i})C_{l}(\kappa_{j}\kappa_{v})$$

$$\times R_{vi}(x)R_{jv}(z)i_{l}(\omega r_{<})k_{l}(\omega r_{>}) + C_{l}(\kappa_{v}\kappa_{i})C_{l}(\kappa_{j}\kappa_{v})$$

$$\times P_{vi}^{l}(x)P_{jv}^{l}(z)i_{l+1}(\omega r_{<})k_{l+1}(\omega r_{>}) - C_{l}(-\kappa_{v}\kappa_{i})$$

$$\times C_{l}(-\kappa_{j}\kappa_{v})V_{vi}^{l}(x)V_{jv}^{l}(z)i_{l}(\omega r_{<})k_{l}(\omega r_{>})$$

$$+ C_{l}(k_{v}k_{i})C_{l}(k_{j}k_{v})Q_{vi}^{l}(x)Q_{jv}^{l}(z)i_{l-1}(\omega r_{<})k_{l-1}(\omega r_{>})]$$

$$(44)$$

In the above

$$I \equiv \int_0^\infty \frac{dr}{r^2} g_v(r) f_v(r). \tag{45}$$

The reference state singularity cancellation is incomplete in this case. It does cancel for the l=0 partial wave, as can be seen upon noting that

$$C_{1}(1,-1) \begin{cases} j_{v} & j_{v} & 1 \\ j_{v} & j_{v} & 0 \end{cases} = -\frac{1}{\sqrt{6}},$$
(46)

but the cancellation does not occur when l=1. We treat this situation as discussed above, by altering the valence energy with a regulator  $\Delta$  that is extrapolated to zero. The treatment of the Zeeman effect is similar to the above, basically consisting of replacing  $1/r^2$  with r.

#### E. Breakup of calculation

We divide the calculation of the vertex and side diagrams into five parts. The most straightforward term to evaluate is  $E_S^A$ , because it is closely related to the evaluation of the self-energy. Specifically, if we define a perturbed wave function  $\tilde{v}$  by

$$\langle \tilde{v} | = \sum_{n \neq v} \frac{V_{vn} \langle n |}{\epsilon_v - \epsilon_n}, \tag{47}$$

then  $E_{\text{SR}}^A = \sum_{\tilde{v}v} (\epsilon_v)$ . One needs only to form the perturbed orbital  $\tilde{v}$  on the same grid as the original orbital, and modify the self-energy code appropriately.

The second two parts of the calculation are the momentum-space subtraction terms for the vertex and side terms,  $E_V^p$  and  $E_S^p$ , with the understanding that the canceling divergent terms are dropped. These terms are evaluated with the Monte-Carlo integration program VEGAS [11]. The next part of the calculation is carried out in coordinate space, and consists of the sum of  $E_V^s$  and  $E_S^s$ . Finally there is a pole term which arises from the Wick rotation  $k_0 \rightarrow i\omega$  in the evaluation of the vertex term. A pole on the imaginary axis must be avoided with a semicircle, which gives rise to this term. While the spectral representation of one propagator collapses

TABLE I. Contributions to the 1s self-energy at Z = 80 from the perturbing potential  $\alpha/r$ : units are a.u.

$E_S^A$	0.2769	
$E_V^s + E_S^s  onumber \\ E_V^P$	-0.1181	
	0.0440	
$E_S^P$	-0.0113	
E (pole)	0.1685	
Total	0.3600	

to the ground state, the other propagator can be shown to produce the same kind of perturbed state described in connection with  $E_S^A$ , and one finds the expression

$$E(\text{pole}) = \operatorname{Re}\alpha \sum_{m_v} \int d^3x \int d^3y \frac{1}{|\mathbf{x} - \mathbf{y}|} \\ \times [\overline{\psi}_v(\mathbf{x}) \gamma_\mu \widetilde{\psi}_{vm_v}(\mathbf{x}) \overline{\psi}_{vm_v}(\mathbf{y}) \gamma^\mu \psi_v(\mathbf{y}) \\ + \overline{\psi}_v(\mathbf{x}) \gamma_\mu \overline{\psi}_{vm_v}(\mathbf{x}) \widetilde{\overline{\psi}}_{vm_v}(\mathbf{y}) \gamma^\mu \psi_v(\mathbf{y})].$$
(48)

This term is related to the pole term part of  $E_S^A$ , in which the perturbation acts on the outer wave functions, and in this case just doubles that term. The situation is somewhat more complicated when excited states are considered, as will be discussed below. The total result for the sum of the vertex and side graphs is then written

$$E(V+SL+SR) = E_S^A + (E_V^s + E_S^s) + E_V^p + E_S^p + E(\text{pole}).$$
(49)

# II. CALCULATIONS FOR POTENTIALS ARISING FROM OTHER ELECTRONS

As a first example we consider the self-energy of a ground-state electron in a point Coulomb potential of charge Z as a perturbation of charge  $Z_0$ . In this case

$$U(\mathbf{x}) = \frac{(Z_0 - Z)\,\alpha}{|\mathbf{x}|}.\tag{50}$$

If we carry out a Taylor expansion of the self-energy in the form

$$\Delta E_{\rm SE}(Z) = \Delta E_{\rm SE}(Z_0) + (Z - Z_0)R(Z_0) + O((Z - Z_0)^2),$$
(51)

we can use the very accurate 1s self-energies presented by Mohr [1] to determine  $R(Z_0)$ . To test the method we work at  $Z_0=80$ , where R(80)=0.3599 a.u. As discussed above, the calculation breaks into five parts, which are shown in Table I. We observe the dominance of  $\Sigma_s^A$ , arguments for which were presented in [12]. However, to get the four digit agreement found, it is clear that the smaller terms coming from the vertex and remaining parts of the side graphs are necessary.

We next turn to a discussion of the self-energy of n=2 states of lithiumlike uranium. In this case we include finite nuclear size, using a Fermi distribution with c=7.137 35 fm

TABLE II. Contributions to the  $2s_{1/2}$ ,  $2p_{1/2}$ , and  $2p_{3/2}$  selfenergy at Z=92 from the perturbing potential  $2Y_0(1s,1s;r)$ : units are a.u.

State	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
$E_S^A$	-0.0777	-0.0243	-0.0137
$E_V^s + E_S^s$	0.0530	0.0823	0.0972
$E_V^P$ $E_S^P$	-0.0611	-0.0581	-0.0591
$E_{S}^{P}$	0.0811	0.0718	0.0708
E (pole)	-0.0873	-0.0958	-0.0978
$E(P^2)$	-0.0101	-0.0131	-0.0236
Total	-0.1021	-0.0372	-0.0262
СН	-0.1009	-0.0358	-0.0260

and t=2.3 fm. Following Indelicato and Mohr [7], we first account for the presence of the core 1s electrons by introducing the potential

$$U(r) = 2Y_0(1s, 1s; r) \equiv 2\alpha \int_0^\infty dx [g_{1s}^2(x) + f_{1s}^2(x)] \frac{1}{r_>},$$
(52)

where  $r_{>} \equiv \max(r, x)$ . In this case, however, because we are dealing with excited states, a new contribution enters that we call the double-pole term. This term was discussed in a paper on helium decay rates [13], where a more complete discussion can be found. Here we simply note that when the state v is of higher energy than other bound states, there are terms in both the vertex and side graphs in which double poles are present in the complex plane that are encircled when the Wick rotation  $k_0 \rightarrow i\omega$  is carried out. By Cauchy's theorem these give rise to derivatives, and the following energy shift results:

$$E(P^{2}) = \operatorname{Re}\alpha \sum_{a < v} \left[ E^{(1)}(v) - E^{(1)}(a) \right] \frac{\partial}{\partial k_{0}} \int d^{3}x \int d^{3}y \\ \times \frac{\exp[ik_{0}|\mathbf{x} - \mathbf{z}|]}{|\mathbf{x} - \mathbf{y}|} \overline{\psi}_{v}(\mathbf{x}) \gamma_{\mu} \psi_{a}(\mathbf{x}) \overline{\psi}_{a}(\mathbf{y}) \\ \times \gamma^{\mu} \psi_{v}(\mathbf{y})|_{k_{0} = \epsilon_{u} - \epsilon_{u}}.$$
(53)

The imaginary part of this equation plays a role in shifting the energy difference entering into the equations for decay rates from its lowest order value to the more accurate firstorder value [13]. We include this term in Table II. We note that the pole term E(pole) is also modified to include a sum over all states *a* with energy less than or equal to the valence state, with a factor of 2 if a complete pole is encircled.

In this case, while  $E_s^A$  is still an important contribution, the other parts of the calculation play a significant role, in particular for the  $2p_{3/2}$  state, where the double-pole term almost completely accounts for the effect.

Because it is possible to evaluate the self-energy directly in non-Coulomb potentials, a check on the calculation is afforded by working with the potential formed from the combination of the perturbing potential with the Coulomb potential. This potential, when made self-consistent by iterating

TABLE III. Contributions to hfs in units of  $(\alpha/\pi)E_F$ .

Ζ	$E_S^A$	$E_S^p$	$E_V^p$	$E_V^s + E_S^s$	Total
5	-0.1046	4.5904	-2.2957	-2.0154	0.1747
10	-0.2609	3.2482	-1.3657	-1.7812	-0.1596
15	-0.4340	2.4930	-0.9464	-1.6007	-0.4881
20	-0.6150	1.9802	-0.7169	-1.4583	-0.8100
30	-0.9910	1.3056	-0.5008	-1.2525	-1.4387
40	-1.3857	0.8729	-0.4311	-1.1171	-2.0610
50	-1.8067	0.5703	-0.4300	-1.0281	-2.6945
60	-2.2686	0.3479	-0.4693	-0.9712	-3.3612
67	-2.6232	0.2254	-0.5124	-0.9460	-3.8562
70	-2.7873	0.1795	-0.5351	-0.9381	-4.0810
80	-3.3869	0.0498	-0.6225	-0.9227	-4.8823
83	-3.5866	0.0169	-0.6525	-0.9210	-5.1432
90	-4.0910	-0.0505	-0.7275	-0.9214	-5.7904
100	-4.9300	-0.1267	-0.8487	-0.9305	- 6.8359

until the 1*s* orbital satisfies the Dirac equation with that potential, we call a core-Hartree potential; it was used to calculate the Lamb shift in lithiumlike uranium [14]. At this high Z, the effect of iteration is very small, and we can compare with the above calculation. This is done in the last row of Table II, and it is seen that good agreement is found. The results for the 2*s* and  $2p_{1/2}$  states are also consistent with new calculations of Indelicato and Mohr [15].

#### **III. HYPERFINE SPLITTING CALCULATIONS**

It is convenient to work with a stretched state  $(m_e = +1/2, m_N = +1/2)$ , which has an energy 1/4 of the full hyperfine splitting (hfs),

$$E^{(1)}(v) = \frac{\alpha}{3} \frac{g_N}{m_N} \int_0^\infty \frac{dr}{r^2} g_v(r) f_v(r) = \frac{1}{4} E_F^{(1)}.$$
 (54)

There are numerical difficulties associated with the almost singular small-r behavior that we avoid by using a finite nucleus in solving the Dirac equation. Note, however, that we do not use a distribution for magnetism. While this distribution is an important effect for the overall hfs, its contribution to radiative corrections is of higher order, and we do not include it in the present calculation. Note that our definition of  $E_F$  includes both the effect of finite nuclear size and also the Breit correction, since we use relativistic wave functions. Care should be taken in comparing with other calculations that may use different definitions.

We present the results for hyperfine splitting as a multiple of  $(\alpha/\pi)E_F$  in Table III. Note that the pole term is not present in this case. This is because when the regulator that is used to handle reference-state singularities is employed, the pole term is moved into the  $E_V^s + E_S^s$  term. This part of the calculation required particular care, because as the regulator is taken to zero, structure of the integrand at low values of  $\omega$  must be taken account of, which requires a very large number of Gaussian points.

A particularly interesting aspect of this calculation is its connection with the known low-Z behavior of the self-

energy correction to hfs in hydrogenic systems, which has been studied in terms of a power series. At present, the first few terms of the power series are known to be [16,17]

$$E_{F} = \frac{\alpha}{\pi} E_{F}^{(1)} \Biggl\{ \frac{1}{2} + \left( \log 2 - \frac{13}{4} \right) \pi(Z\alpha) + \Biggl[ -\frac{2}{3} \log^{2}(Z\alpha)^{-2} + \left( \frac{37}{72} - \frac{8}{3} \log 2 \right) \log(Z\alpha)^{-2} + 17.1 \Biggr] (Z\alpha)^{2} + \left( \frac{5}{2} \log 2 - \frac{191}{32} \right) \pi(Z\alpha)^{3} \log(Z\alpha)^{-2} + O((Z\alpha)^{3}) \Biggr\}.$$
(55)

Note that the constant term 17.1 supersedes an earlier calculation [18], which included some, but not all, terms of order  $\alpha(Z\alpha)^3 E_F$  and higher. Unfortunately, our present accuracy is not sufficient to provide a check on the higher-order terms.

The present calculation is in fair agreement with an earlier work [5]. For example, at Z=83 that work found the result -5.098, about 1% smaller than our result. While it is unlikely that experiment could distinguish the two numbers at high Z, discrepancies at low Z will have consequences for muonium and hydrogen hyperfine splitting, and will have to be resolved. At Z=10, Ref. [5] finds -0.1627, and the difference with the present result is much greater than our estimated error, which is 3 in the last digit.

## **IV. ZEEMAN EFFECT CALCULATIONS**

The treatment of the last potential considered here, that of a constant magnetic field, is for the most part identical to the treatment of hyperfine splitting, amounting simply to the replacement of  $1/r^2$  with r. This replacement strongly suppresses the effect of the finite size of the nucleus, and we therefore deal with the point nucleus case for these calculations. The only part of the calculation that requires a different treatment is the evaluation of  $E_V^p$ . Because the Fourier transform of the potential is

$$V(\mathbf{q}) = -\frac{ie}{2} \boldsymbol{\gamma} \cdot (\mathbf{B} \times \nabla_{\mathbf{q}}) \,\delta^{3}(\mathbf{q}), \qquad (56)$$

 $E_V^p$  is evaluated using integration by parts, which involves several terms, as the derivative can act on either the numerator, denominator, or wave function. The overall  $\delta$  function, however, considerably simplifies the numerical evaluation of the resulting integral.

The energy shift of a ground state electron with magnetic quantum number m in a magnetic field is, with the neglect of recoil corrections,

$$E_{\text{Zeeman}} = \frac{|e|B}{2m} g_e m. \tag{57}$$

We write the g factor as

$$g_{e} = 2 \left[ \frac{2\gamma + 1}{3} + \frac{\alpha}{\pi} C^{(2)}(Z\alpha) + \left(\frac{\alpha}{\pi}\right)^{2} C^{(4)}(Z\alpha) + \cdots \right],$$
(58)

TABLE IV. Contributions to the function  $C^{(2)}(Z\alpha)$ .

Ζ	$E_S^A$	$E_S^p$	$E_V^p$	$E_V^s + E_S^s$	Total
5	0.00541	4.58838	-4.09514	0.00148(1)	0.50013(1)
10	0.01695	3.24241	-2.76245	0.00362	0.50053
15	0.03234	2.48297	-2.01926	0.00545	0.50150
20	0.05064	1.96608	-1.52015	0.00659	0.50316
25	0.07131	1.58291	-1.15542	0.00699	0.50579
30	0.09415	1.28453	-0.87567	0.00645	0.50946
40	0.14565	0.84754	-0.47525	0.00286	0.52080
50	0.20493	0.54403	-0.20623	-0.00371	0.53902
60	0.27347	0.32442	-0.01826	-0.01253	0.56710
70	0.35261	0.16256	0.11518	-0.02260	0.60775
80	0.44614	0.04328	0.20952	-0.03265	0.66629
90	0.56008	-0.04258	0.27415	-0.04099	0.75066
100	0.70590	-0.10043	0.31472	-0.04528	0.87491

where  $\gamma = \sqrt{1 - (Z\alpha)^2}$  and the functions  $C^{2i}(Z\alpha)$  are generalizations of the loop expansion of the electron g-2 to include the effects of atomic binding [19]. The first two terms in the expansion of  $C^{(2)}(Z\alpha)$  are known to be [20]

$$C^{(2)}(Z\alpha) = \frac{1}{2} + \frac{(Z\alpha)^2}{12} + \cdots$$
 (59)

We tabulate  $C^{(2)}(Z\alpha)$  in Table IV. We note that at low Z the momentum space terms  $E_V^p$  and  $E_S^p$  account for the bulk of the Schwinger correction, unlike the case with hyperfine splitting. Again unlike that case, where there is very strong dependence on the nuclear charge, in this case  $C^{(2)}$  varies smoothly as Z is increased, and has changed only by a factor of less than 2 at Z=100. A feature of note is the difficulty of controlling the partial-wave expansion at low Z. At the lowest Z treated here, Z=5, the partial wave expansion changes sign at l=31, and it was difficult to reliably extrapolate the sum to infinity. The turnover occurs for lower l at higher Z, and better control was possible there. We performed a fit of the function to the form

$$C^{(2)}(Z\alpha) = \frac{1}{2} + A(Z\alpha)^2 + B(Z\alpha)^4,$$
 (60)

and found A to be consistent with 1/12 and  $B \approx 3.5$ .

# V. CONCLUSIONS

We have developed in this paper a calculational scheme that allows the calculation of potential corrections to oneloop self-energy graphs valid to all orders in  $Z\alpha$ . An important feature of the calculation is the isolation of ultraviolet divergent terms via the subtraction of terms in which the external-field propagators are replaced with free propagators, which significantly improves the numerical evaluation. Perhaps the most important application is to hyperfine splitting at low Z, since there are indications that a perturbative expansion is inadequate even at Z=1 unless carried out to very high orders. Our present precision, however, is not great enough to bear on muonium hyperfine splitting, and the improvement of this precision is the most important extension of the present work.

## ACKNOWLEDGMENTS

This work was partially supported by NSF Grant No. PHY-95-13179. The workf of K.T.C. was performed under the auspices of the U.S. Department of Energy by Lawrence

Livermore National Laboratory under Contract No. W-7405-Eng-48. We would like to thank Barry Taylor and Peter Mohr for valuable conversations and W. R. Johnson for providing code. J.S. would like to acknowledge the hospitality shown by LLNL.

- P.J. Mohr, Phys. Rev. A 46, 4421 (1992); P.J. Mohr and Y.-K. Kim, *ibid.* 45, 2727 (1992).
- [2] S.A. Blundell and N. Snyderman, Phys. Rev. A 44, R1427 (1991); K.T. Cheng, W.R. Johnson, and J. Sapirstein, *ibid.* 47, 1817 (1993); I. Lindgren, H. Persson, S. Salomonson, and A. Ynnermann, *ibid.* 47, 4555 (1993).
- [3] I. Klaft et al., Phys. Rev. Lett. 73, 2425 (1994).
- [4] Jose R. Crespo Lopez-Urrutia, P. Beiersdorfer, Daniel Savin, and Klaus Widmann, Phys. Rev. Lett. (to be published).
- [5] H. Persson *et al.*, Phys. Rev. Lett. **76**, 1433 (1996); Per Sunnergren, Ph.D. thesis, University of Goteborg (1996).
- [6] H. Persson et al. (unpublished).
- [7] P. Indelicato and P.J. Mohr, Theor. Chem. Acta 80, 207 (1991).
- [8] J. Sucher, Phys. Rev. 107, 1448 (1957).
- [9] M. Gell-Mann and F. Low, Phys. Rev. 84, 350 (1951).
- [10] J.C. Ward, Phys. Rev. 78, 1824 (1950).
- [11] G.P. Lepage, J. Comput. Phys. 27, 192 (1978).

- [12] S.A. Blundell, Phys. Rev. A 47, 1790 (1993).
- [13] W.R. Johnson, D. Plante, and J. Sapirstein, in Advances in Atomic and Molecular Physics, edited by B. Bederson (Academic, New York, 1995).
- [14] K.T. Cheng, W.R. Johnson, and J. Sapirstein, Phys. Rev. Lett. 66, 2960 (1991).
- [15] P. Mohr (private communication).
- [16] K. Pachucki, Phys. Rev. A 54, 1994 (1996). This result is consistent with an independent calculation of Kinoshita and Nio [T. Kinoshita (private communication)].
- [17] S. Karshenboim, Z. Phys. D 36, 11 (1996).
- [18] J.R. Sapirstein, Phys. Rev. Lett. 51, 985 (1983).
- [19] This notation is chosen to be consistent with conventions being used in the preparation of the revised set of recommended values of fundamental constants [P. Mohr and B. Taylor (private communication)].
- [20] H. Grotch, Phys. Rev. Lett. 24, 39 (1970).