Title
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Publication Date
1973-09-10

Submitted to
Annals of Physics

LBL-2153
Preprint

c.1

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September 10, 1973

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48

DISCLAIMER

LBL-2153

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* This work was supported in part by the U. S. Atomic Energy Commission and in part by the Air Force Office of Scientific Research, Office of Aerospace Research, United States Air Force, under Grant No. AF-AFOSR-68-1471.

† Based on a dissertation submitted to the University of California at Berkeley as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

SELF-ENERGY RADIATIVE CORRECTIONS

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ABSTRACT

The one-photon self-energy radiative level shift of an electron in a Coulomb field is examined. An expression for the level shift which is suitable for direct numerical evaluation, for Z in the range 10-110, is obtained. It is based on the known Coulomb radial Green's functions and not on a power series expansion in $Z\alpha$. In the following paper, the numerical evaluation of the level shift for the $1S_{\frac{1}{2}}$ state is described.

I. INTRODUCTION

The lowest order radiative corrections to the energy levels in a hydrogen-like system arise from the electron self energy and the vacuum polarization which correspond to the Feynman diagrams in Figs. 1(a) and 1(b), respectively [1]. In these figures, the double line represents propagation of the electron in a static external Coulomb field with nuclear charge number Z. We are concerned here with the evaluation of the bound-state level shift associated with the electron self energy, for Z in the range 10-110. The vacuum polarization term has been considered in detail elsewhere [2].

Theoretical evaluation of the radiative level shifts in hydrogen-like systems with Z not small is of particular interest in view of the recent advances in experiments performed with these systems. Measurements of the Lamb shift in hydrogenic carbon C^{5+} and in hydrogenic oxygen O^{7+} have been made [3], and the feasibility of working with higher Z systems has been demonstrated by the measurement of the lifetime of the $2S_{\frac{1}{2}}$ state in hydrogenic sulphur S^{+15} and in hydrogenic argon Ar^{+17} [4]. The theoretical values of the radiative level shifts in a hydrogen-like system are also useful as an approximation to the radiative level shifts of the innermost electrons in heavy atoms [5]. Values for the radiative level shift due to self energy for a Coulomb potential are not expected to be applicable to the lower levels in heavy muonic atoms, because of the importance of the finite nuclear size in these systems [6].

The self-energy radiative level shift was first calculated nonrelativistically to lowest order in $Z\alpha$ by Bethe [7]. The lowest order term was subsequently calculated relativistically, and evaluation of successively higher order terms followed that. To display the

results of these calculations, we express the level shift in the form

$$\Delta E_n = \frac{\alpha}{\pi}(Z\alpha)^4 F(Z\alpha)\, m_e c^2 , \qquad (1.1)$$

where

$$F(Z\alpha) = A_{40} + A_{41}\, \ell n(Z\alpha)^{-2} + A_{50}(Z\alpha) + A_{60}(Z\alpha)^2$$

$$+ A_{61}(Z\alpha)^2\, \ell n(Z\alpha)^{-2} + A_{62}(Z\alpha)^2\, \ell n^2(Z\alpha)^{-2} + A_{70}(Z\alpha)^3 + \cdots . \qquad (1.2)$$

In Table I, we have listed the values of the coefficients A_{ij} for the $1S_{\frac{1}{2}}$ state and the articles in which these values, or values for other states, are given. Only the self-energy contribution is included in that table. Values for $F(Z\alpha)$ which result from evaluating terms up to a given order in $Z\alpha$ in the series in (1.2) are plotted as functions of Z in Fig. 2. These curves give an indication of the nature of the convergence of the series in (1.2) as a function of Z. The truncated series represent the function poorly for Z near 20, and appear not to be useful approximations for the function for larger Z.

Evaluations of the self-energy level shift for large Z have been made. Brown and Mayers calculated the level shift of the $1S_{\frac{1}{2}}$ state for $Z = 80$ [15] using a method developed by Brown, Langer, and Schaefer [16] which is valid for large Z. Desiderio and Johnson, working with a generalization of that method, evaluated the level shift of the $1S_{\frac{1}{2}}$ state in a Coulomb potential for $Z = 70, 75, 80, 85, 90$ and evaluated the level shift of the $1S_{\frac{1}{2}}$ state in a screened Coulomb potential for $Z = 70, 71, 72, \cdots, 90$ [5]. Erickson has obtained an expression for the radiative level shift which is valid (approximately) for all $Z\alpha$ and agrees, by construction, with the small $Z\alpha$

Table I. Values of the coefficients in Eq. (1.2) for the $1S_{\frac{1}{2}}$ state.

Coefficient		Reference
B	= Bethe logarithm $\simeq$ -2.9841285558(3)	8
A_{40}	$= \frac{4}{3}(B + \frac{11}{24} + \frac{3}{8}) \simeq -2.87$	9
A_{41}	$= \frac{4}{3}$	9
A_{50}	$= 4\pi(1 + \frac{11}{128} - \frac{1}{2}\ell n\, 2) \simeq 9.29$	10
A_{60}	$= -\frac{4}{3}(19.3435 \pm 0.5) \simeq -25.8$	11,12
A_{61}	$= \frac{28}{3}\ell n\, 2 - \frac{21}{20} \simeq 5.42$	13,11
A_{62}	$= -1$	13,14
A_{70}	$\simeq \frac{4}{3}\pi\, 9.56 \simeq 40.0$	12

expansion [12]. The results of these calculations are given, for comparison with the results of our calculation, in the following paper.

In this paper, we obtain an expression for the one-photon self-energy radiative level shift which is suitable for direct numerical evaluation by a computer, for Z in the range 10-110. The standard expression for the level shift is not suitable for direct numerical evaluation for the following reasons. First, there is the difficulty associated with the well-known fact that the expression is formally infinite before mass renormalization. Second, the standard unrenormalized expression is zeroth order in $Z\alpha$ while the net level shift is of order $(Z\alpha)^4 \ln(Z\alpha)^{-2}$. Thus, direct calculation would involve, aside from the problem of dealing with formally infinite expressions, serious loss of numerical significance when the mass renormalization is carried out for $Z\alpha \ll 1$. We note that the latter problem limits the effectiveness of the Brown, Langer, and Schaefer method to the region of large Z [16]. In the subsequent discussion, rearrangement of the expression for the level shift is made in order to overcome these difficulties to the extent that a numerical evaluation, for the range of Z under consideration, is possible. The presentation is arranged as follows. In Sec. II the computational procedure, including the procedure for mass renormalization, is formulated. The energy shift is divided into three parts: a part which we call the low-energy part ΔE_L, a part which we call the high-energy part ΔE_H, and the mass renormalization counterterm ΔE_M. An expression for ΔE_L which is in a form suitable for numerical evaluation is given in Sec. III. In Sec. IV ΔE_H is divided into two parts ΔE_{HA} and ΔE_{HB}, where ΔE_{HA} is relatively easy to evaluate, and ΔE_{HB} is finite and of

order $(Z\alpha)^4$. An expression for ΔE_{HB} suitable for numerical evaluation is given in Sec. V.

In the following paper, we describe the numerical evaluation of the energy shift for the case of the $1S_{\frac{1}{2}}$ state, and give the results of that calculation.

II. FORMULATION OF THE PROBLEM

The energy shift of an electron, in a bound state ψ_n, due to the virtual emission and reabsorption of one photon, is given by the real part of [17,18][1]

$$\Delta E_n = -i\pi\alpha \int d(t_2 - t_1) d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \bar{\psi}_n(x_2)\gamma_\mu S_F^e(x_2,x_1)\gamma^\mu\psi_n(x_1) \times D_F(x_2 - x_1) - \delta m \int d^3\underset{\sim}{x}\bar{\psi}_n(x)\psi_n(x) \qquad (2.1)$$

where $\psi_n(x) = \psi_n(\underset{\sim}{x}) \exp(-iE_n t)$ is the bound-state wave function in coordinate space; $\psi_n(\underset{\sim}{x})$ is a normalized solution of the time-independent Dirac equation

$$[-i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla} + V(\underset{\sim}{x}) + \beta - E_n]\psi_n(\underset{\sim}{x}) = 0 \qquad (2.2)$$

in which $V(\underset{\sim}{x}) = -Z\alpha/|\underset{\sim}{x}|$. The bar over the wave function denotes the adjoint: $\bar{\psi}_n(x) = \psi_n^\dagger(x)\gamma^0$. To keep the terms in the energy shift separately finite, we use the covariant regulator method [19,20] in which the photon propagator in coordinate space is expressed as

$$\frac{1}{2} D_F(x_2 - x_1) = \frac{i}{(2\pi)^4} \int d^4k \exp[-ik(x_2 - x_1)] \times \left[\frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - \Lambda^2 + i\epsilon}\right] . \qquad (2.3)$$

The limit $\Lambda \to \infty$ is to be taken after the integrals in Eq. (2.1) have been evaluated. The free electron mass shift δm, computed using the regulated photon propagator, is [19]

$$\delta m = \frac{\alpha}{\pi}(\tfrac{3}{4} \ell n\, \Lambda^2 + \tfrac{3}{8}) . \tag{2.4}$$

The propagation kernel $S_F^e(x_2,x_1)$ is given by

$$-\tfrac{1}{2} S_F^e(x_2,x_1) = \frac{1}{2\pi i} \int_{C_F} dz\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) \exp[-iz(t_2 - t_1)] . \tag{2.5}$$

The contour C_F, which appears in Fig. 3, extends from $-\infty$ to $+\infty$, passing below the negative real axis and above the positive real axis. The Green's function $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ is the kernel corresponding to the resolvent $G(z) = 1/(H - z)$, where H is the Dirac-Coulomb Hamiltonian. We consider the Green's function in the complex z-plane with cuts in the intervals $(-\infty,-1]$ and $[+1,+\infty)$. The Green's function is an analytic function of z in the cut plane except at the bound state eigenvalues which lie on the real z-axis in the interval $(0,1)$.

The energy shift ΔE_n is then the limit as $\Lambda \to \infty$ of

$$\Delta E_n(\Lambda) = -\frac{i\alpha}{2\pi} \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1\, \psi_n^\dagger(\underset{\sim}{x}_2)\alpha_\mu \int_{C_F} dz\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\alpha^\mu \psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} [\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|) - \exp(-b'|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)]$$

$$- \delta m \int d^3\underset{\sim}{x} \psi_n^\dagger(\underset{\sim}{x})\beta\psi_n(\underset{\sim}{x}) \tag{2.6}$$

where

$$b = -i[(E_n - z)^2 + i\epsilon]^{\frac{1}{2}} ; \quad b' = -i[(E_n - z)^2 - \Lambda^2 + i\epsilon]^{\frac{1}{2}} . \tag{2.7}$$

The branches of the square roots are determined by the conditions

$$\mathrm{Re}(b) > 0 ; \quad \mathrm{Re}(b') > 0 . \tag{2.8}$$

In order to facilitate the evaluation of (2.6), we change the contour of integration C_F to a new contour, and divide the integral into two parts which correspond to integrals over different portions C_L and C_H of the new contour. The integrand of the contour integral is an analytic function of z, except for the singularities of $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ and the branch points of b and b'. These features of the integrand are depicted in Fig. 3. In that figure, cuts are drawn from $z = 1$ and $z = -1$ so that $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ is a single-valued analytic function of z in the cut z-plane, except for the bound-state poles. Also, branch cuts are drawn from the singularities of b and b' in such a way that the conditions expressed in (2.8) are satisfied everywhere in the cut z-plane. Because of the analyticity of the integrand, we may deform the contour of integration to the one shown in Fig. 4.

We now identify three parts of the energy shift ΔE_n. The first part ΔE_L, which we shall call the "low-energy part", is the contribution to the integral in (2.6) from the integration along the contour C_L. The contour C_L begins at z_1, passes around the square-root singularity, and ends at z_2. The second part is ΔE_H, the "high-energy part", which comes from the integration along the contour C_H. The contour C_H consists of two disconnected halves. The first half

begins at the point $-R - i0$, extends along a quarter circle centered at the origin to the point $-iR$, and continues up the negative imaginary axis to z_1. The second half begins at z_2, extends up the positive imaginary axis to the point $+iR$, and continues along a quarter circle centered at the origin to the point $+R + i0$. The third part of the energy shift is the mass renormalization term ΔE_M

$$\Delta E_M = -\delta m \int d^3\underset{\sim}{x}\, \psi_n^\dagger(\underset{\sim}{x})\beta\psi_n(\underset{\sim}{x}) \,. \tag{2.9}$$

The total energy shift is

$$\Delta E_n = \Delta E_L + \Delta E_H + \Delta E_M \,. \tag{2.10}$$

For these contributions, we are interested in the limit as $\epsilon \to 0+$, as z_1 and z_2 approach zero from below and above the real axis respectively, and as $R \to \infty$. This limit will be considered first for ΔE_L and then for ΔE_H.

III. THE LOW-ENERGY PART ΔE_L

The low-energy part of the energy shift is

$$\Delta E_L = I_L - I_L' \tag{3.1}$$

where

$$I_L = -\frac{i\alpha}{2\pi}\int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1\, \psi_n^\dagger(\underset{\sim}{x}_2)\,\alpha_\mu \int_{C_L} dz\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$$

$$\times\, \alpha^\mu\, \psi_n(\underset{\sim}{x}_1)\,\frac{e^{-b\rho}}{\rho} \,, \tag{3.2}$$

I_L' is obtained by replacing b by b' in the right-hand side of (3.2),

and $\rho = |\underset{\sim}{x}_2 - \underset{\sim}{x}_1|$. We note that for $\Lambda > E_n$, I_L' vanishes in the limit $\epsilon \to 0+$ and $z_1, z_2 \to 0$, because the integrand of the integral over z is then an analytic function of z on and inside the contour C_L. In (3.2), in the limit $\epsilon \to 0+$, the singularity of b and the pole of $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ at $z = E_n$ coincide. In order to avoid any ambiguity, we temporarily add a small positive imaginary part $i\delta$ to z in $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$. Figure 5(a) shows the singularities of the integrand in (3.2) after the imaginary part has been added. In the limit $\epsilon \to 0+$ and $z_1, z_2 \to 0$, the contour of integration C_L consists of two parts, as shown in Fig. 5(b): C_B below the real axis, and C_A above the real axis. As a result of the condition $\mathrm{Re}(b) > 0$, stated in (2.8), we have

$$b = -i(E_n - z) \qquad \text{for } z \text{ on } C_B \,,$$

$$b = +i(E_n - z) \qquad \text{for } z \text{ on } C_A \,. \tag{3.3}$$

Making the appropriate substitutions from (3.3) in (3.2), and deforming the contours C_A and C_B to line segments along the real axis, we obtain

$$\Delta E_L = \frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1\, \psi_n^\dagger(\underset{\sim}{x}_2)\alpha_\mu\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\alpha^\mu\psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{\sin[(E_n - z)\rho]}{\rho} \,. \tag{3.4}$$

In view of the equation

$$\frac{\sin[(E_n - z)\rho]}{(E_n - z)\rho} = \frac{1}{4\pi}\int d\Omega_k\, \exp[i\underset{\sim}{k}\cdot(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)] \tag{3.5}$$

where $k = |\underset{\sim}{k}| = E_n - z$, we have

$$\Delta E_L = \frac{\alpha}{4\pi^2}\int_{k<E_n} d^3\underset{\sim}{k}\,\frac{1}{k}\left\langle \alpha_\mu\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\frac{1}{H - E_n + k - i\delta}\,\alpha^\mu\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}\right\rangle . \tag{3.6}$$

Henceforth, the brackets $\langle\ \rangle$ denote the expectation value in the bound state ψ_n. In the term corresponding to $\mu = 0$ in (3.6), we employ the relation

$$k^2\left\langle e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\frac{1}{H - E_n + k - i\delta}\,e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}\right\rangle = k + \langle\underset{\sim}{\alpha}\cdot\underset{\sim}{k}\rangle$$

$$+\left\langle \underset{\sim}{\alpha}\cdot\underset{\sim}{k}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\frac{1}{H - E_n + k - i\delta}\,\underset{\sim}{\alpha}\cdot\underset{\sim}{k}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}\right\rangle + \mathcal{O}(\delta) \tag{3.7}$$

to obtain

$$\Delta E_L = \frac{\alpha}{\pi}E_n - \frac{\alpha}{4\pi^2}\int_{k<E_n} d^3\underset{\sim}{k}\,\frac{1}{k}\left(\delta_{j\ell} - \frac{k^j k^\ell}{k^2}\right)$$

$$\times\left\langle \alpha^j\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\frac{1}{H - E_n + k - i\delta}\,\alpha^\ell\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}\right\rangle . \tag{3.8}$$

In (3.8) and in the rest of this section, the limit $\delta \to 0+$ is understood. We note that except for the term $\alpha E_n/\pi$, ΔE_L is exactly what one would obtain using "old-fashioned" perturbation theory to calculate the energy shift due to the interaction of the electron with the transverse electromagnetic field, with the photon momentum cut off at $k = E_n$.

The portion of ΔE_L of order lower than $(Z\alpha)^4\,\ell n(Z\alpha)^{-2}$ is calculated exactly by making the substitution

$$e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\frac{1}{H - E_n + k - i\delta}\,e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}$$

$$= (\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - E_n + k - i\delta)^{-1} \tag{3.9}$$

in (3.8) and retaining only the first few terms in the expansion of the right-hand side of (3.9) in powers of $\underset{\sim}{\alpha}\cdot\underset{\sim}{p}$, V, and $1 - E_n$. The justification for this procedure is discussed by Kroll and Lamb [21]. We find

$$\Delta E_L = \frac{\alpha}{\pi}\left[\frac{3}{2}\langle\beta\rangle + \frac{7}{6}\langle V\rangle + \mathcal{O}\left((Z\alpha)^4\,\ell n(Z\alpha)^{-2}\right)\right] . \tag{3.10}$$

The expression in coordinate space corresponding to (3.8) is

$$\Delta E_L = \frac{\alpha}{\pi}E_n - \frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \psi_n^\dagger(\underset{\sim}{x}_2)\alpha^j G(\underset{\sim}{x}_2,\underset{\sim}{x}_1, z + i\delta)\alpha^\ell\psi_n(\underset{\sim}{x}_1)$$

$$\times(\delta_{j\ell}\nabla_{\underset{\sim}{2}}\cdot\nabla_{\underset{\sim}{1}} - \nabla_2{}^j\nabla_1{}^\ell)\,\frac{\sin[(E_n - z)\rho]}{(E_n - z)^2\rho} . \tag{3.11}$$

The real part of ΔE_L is obtained by taking the Cauchy principal value of the integral over z in (3.11). The bound-state wave function is written as

$$\psi_n(\underset{\sim}{x}) = \begin{bmatrix} f_1(x)\chi_{\kappa_n}^{\mu_n}(\hat{x}) \\ if_2(x)\chi_{-\kappa_n}^{\mu_n}(\hat{x}) \end{bmatrix} \tag{3.12}$$

where $\chi_\kappa^\mu(\hat{x})$ is the spin-angular function described in the appendix, and $f_1(x)$ and $f_2(x)$ are the components of the radial wave function. The Green's function is written as a sum over eigenfunctions of the operator K as described in the appendix:

$$G(\underset{\sim}{x}_2, \underset{\sim}{x}_1, z) = \sum_\kappa \begin{bmatrix} G_\kappa^{11}(x_2,x_1,z)\pi_\kappa(\hat{x}_2,\hat{x}_1) & G_\kappa^{12}(x_2,x_1,z) i\underset{\sim}{\sigma}\cdot\hat{x}_2 \pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \\ -G_\kappa^{21}(x_2,x_1,z) i\underset{\sim}{\sigma}\cdot\hat{x}_2 \pi_\kappa(\hat{x}_2,\hat{x}_1) & G_\kappa^{22}(x_2,x_1,z)\pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \end{bmatrix} . \tag{3.13}$$

We then have

$$\mathrm{Re}(\Delta E_L) = \frac{\alpha}{\pi} E_n - \frac{\alpha}{\pi} P\int_0^{E_n} dz \int_0^\infty dx_2 x_2^2 \int_0^\infty dx_1 x_1^2$$

$$\times \sum_\kappa \sum_{i,j=1}^{2} f_{\bar{i}}(x_2) G_\kappa^{ij}(x_2,x_1,z) f_{\bar{j}}(x_1) A_\kappa^{ij}(x_2,x_1) \tag{3.14}$$

where $\bar{i} = 3 - i$ and $\bar{j} = 3 - j$. Integration over all angles except $\xi = \hat{x}_2\cdot\hat{x}_1$ in $A_\kappa^{ij}(x_2,x_1)$ yields

$$A_\kappa^{11}(x_2,x_1) = |\kappa| \int_{-1}^{1} d\xi \left\{ P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) P_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi) (E_n - z)^2 \, T(\rho) \right.$$

$$\left. - \frac{1}{\kappa\kappa_n}(1-\xi^2) P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) P'_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi) \frac{1}{\rho}\frac{d}{d\rho} T(\rho) \right\} ,$$

Equation (3.15) continued next page

Equation (3.15) continued

$$A_\kappa^{12}(x_2,x_1) = -|\kappa| \int_{-1}^{1} d\xi \left\{ \left[P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) P_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi) \right.\right.$$

$$\left. - \frac{1}{\kappa\kappa_n}(1-\xi^2) P'_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) P'_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi) \right] \frac{1}{\rho}\frac{d}{d\rho} T(\rho)$$

$$+ \left[x_2 P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1 P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) \right]$$

$$\left. \times \left[x_2 P_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1 P_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi) \right] \frac{1}{\rho}\frac{d}{d\rho}\frac{1}{\rho}\frac{d}{d\rho} T(\rho) \right\} \tag{3.15}$$

where P is the Legendre polynomial, P' is the derivative of P with respect to the argument, and $T(\rho) = \sin[(E_n - z)\rho]/[(E_n - z)^2\rho]$. The corresponding expressions for $A_\kappa^{21}(x_2,x_1)$ and $A_\kappa^{22}(x_2,x_1)$ can be obtained by taking advantage of the symmetry

$$A^{21}_{\kappa,\kappa_n}(x_2,x_1) = A^{12}_{-\kappa,-\kappa_n}(x_2,x_1) ,$$

$$A^{22}_{\kappa,\kappa_n}(x_2,x_1) = A^{11}_{-\kappa,-\kappa_n}(x_2,x_1) . \tag{3.16}$$

In the special case of $S_{\frac{1}{2}}$ states ($\kappa_n = -1$), we have

$$A_\kappa^{11}(x_2,x_1) = 2(E_n - z)|\kappa| \left[j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1) + \frac{\kappa^2 - 1}{y_2 y_1}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1) \right] ,$$

$$A_\kappa^{12}(x_2,x_1) = 2(E_n - z)\kappa\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1) , \qquad (3.17)$$

$$A_\kappa^{21}(x_2,x_1) = 2(E_n - z)\kappa\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_2)\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1) ,$$

$$A_\kappa^{22}(x_2,x_1) = 2(E_n - z)|\kappa|\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1)$$

where j is the spherical Bessel function and $y_i = (E_n - z)x_i$, $i = 1,2$.

Values for $\mathrm{Re}(\Delta E_L)$ can be obtained by numerically evaluating the expression in (3.14). Because terms of order lower than $(Z\alpha)^4\, \ell n(Z\alpha)^{-2}$ vanish when all contributions to the energy shift are combined, it is convenient, in view of (3.10), to express the results of the evaluation of $\mathrm{Re}(\Delta E_L)$ in terms of the function $f_L(Z\alpha)$ defined by

$$\mathrm{Re}(\Delta E_L) = \frac{\alpha}{\pi}\left[\frac{3}{2}\langle\beta\rangle + \frac{7}{6}\langle V\rangle + (Z\alpha)^4 f_L(Z\alpha)\right] . \qquad (3.18)$$

In the preceding discussion, we propose evaluating ΔE_L directly, i.e., there is no provision for extracting the terms of order lower than $(Z\alpha)^4\, \ell n(Z\alpha)^{-2}$ before the numerical evaluation is performed. Hence, for Z not large, substantial numerical significance is lost in obtaining values for $f_L(Z\alpha)$ from values of $\mathrm{Re}(\Delta E_L)$. It is possible, with a reasonable amount of computer time, to obtain

highly accurate values for $\mathrm{Re}(\Delta E_L)$ by evaluating (3.14). An important factor in making this possible is the rapid convergence of the sum over κ in that expression. The nature of the convergence is discussed in the following paper. The rapid convergence is, in turn, a consequence of our having symmetrically combined the contributions to $\mathrm{Re}(\Delta E_L)$ from the contours of integration C_A and C_B to obtain (3.4). The sum over κ corresponding to the separate contribution from either C_A or C_B converges so slowly that direct numerical evaluation to high accuracy would involve an excessive amount of computer time.

IV. THE HIGH-ENERGY PART ΔE_H

The high-energy part of the energy shift is given by

$$\Delta E_H = -\frac{i\alpha}{2\pi}\int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1\, \psi_n^\dagger(\underset{\sim}{x}_2)\, \alpha_\mu \int_{C_H} dz\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\alpha^\mu\, \psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{1}{\rho}(e^{-b\rho} - e^{-b'\rho})$$

$$= -\frac{i\alpha}{4\pi^3}\left\langle \int_{C_H} dz \int d^3\underset{\sim}{k} \left(\frac{1}{\underset{\sim}{k}^2 - (E_n - z)^2 - i\epsilon} - \frac{1}{\underset{\sim}{k}^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon} \right) \alpha_\mu \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - z}\, \alpha^\mu \right\rangle . \qquad (4.1)$$

For fixed Λ, the integrand in (4.1) falls off so rapidly as $|z|$ and $|\underset{\sim}{k}| \to \infty$ that the integral over the portions of the contour C_H which are quarter circles of radius R vanishes as $R \to \infty$. Therefore,

in (4.1), we replace the contour C_H by the contour C_H' which is just the portion of C_H along the imaginary z-axis (see Fig. 4).

In order to deal with the part of ΔE_H of order lower than $(Z\alpha)^4$ and the part which becomes infinite as $\Lambda \to \infty$, we isolate in an expression which is relatively easy to evaluate the portion of ΔE_H which has these features. To do this, we take advantage of the identity

$$\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - z} = \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z}$$

$$- \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} V \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z}$$

$$+ \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} V \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - z} V \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} . \tag{4.2}$$

We substitute the right-hand side of (4.2) into (4.1), and consider the contribution of the last term in (4.2) to ΔE_H. That contribution has a finite limit as $\Lambda \to \infty$ which to lowest order in $Z\alpha$ is equal to

$$\frac{\alpha}{\pi}\left(\frac{3}{2}\,\ell n\ 2 - \frac{5}{4}\right)\langle V^2\rangle_{NR} \tag{4.3}$$

where NR means that the expectation value is evaluated in the Pauli-Schrödinger approximation. The expression in (4.3) is of order $(Z\alpha)^4$, and hence the part of ΔE_H which we wish to isolate arises from the first two terms on the right-hand side in (4.2). For the second of those terms, we write

$$\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} V \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} = V \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}$$

$$+ 2z(\beta + z)\, V \frac{1}{[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]^2} + 2z(\beta + z)\left[\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}, V\right] \cdot$$

$$\times \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} + \frac{2z(\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k})}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} V \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}$$

$$- \frac{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + z}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} [\underset{\sim}{\alpha}\cdot\underset{\sim}{p}, V] \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} . \tag{4.4}$$

The contribution of the last three terms in (4.4) to ΔE_H also has a finite limit as $\Lambda \to \infty$; that limit is equal, to lowest order in $Z\alpha$, to

$$\frac{\alpha}{\pi}\left\{(\ell n\ 2 - \tfrac{5}{6})\langle p^2 V\rangle_{NR} + (\tfrac{3}{8} - \tfrac{1}{2}\,\ell n\ 2)\langle[\underset{\sim}{\sigma}\cdot\underset{\sim}{p}, [\underset{\sim}{\sigma}\cdot\underset{\sim}{p}, V]]\rangle_{NR}\right.$$

$$\left. + (\tfrac{1}{3}\,\ell n\ 2 - \tfrac{17}{72})\langle[p^i, [p^i, V]]\rangle_{NR}\right\} . \tag{4.5}$$

This expression is also of order $(Z\alpha)^4$. We therefore write

$$\Delta E_H = \Delta E_{HA} + \Delta E_{HB} + \mathcal{O}(\Lambda^{-1}) \tag{4.6}$$

where

$$\Delta E_{HA} = -\frac{i\alpha}{4\pi^3}\left\langle \int_{C_H'} dz \int d^3\underset{\sim}{k}\left(\frac{1}{\underset{\sim}{k}^2 - (E_n - z)^2 - i\epsilon} \right.\right.$$

$$\left. - \frac{1}{\underset{\sim}{k}^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon}\right) \alpha_\mu \left(\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} \right.$$

$$\left.\left. - V \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} - 2z(\beta + z)\, V \frac{1}{[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]^2} \right) \alpha^\mu \right\rangle \quad . \tag{4.7}$$

The term ΔE_{HA} is just the part of ΔE_H described in the beginning of this paragraph. The evaluation of ΔE_{HB} is discussed in Sec. V. We integrate over $\underset{\sim}{k}$ in (4.7) and express the result as an integral over a parameter η. Taking the equation satisfied by the state vector into account, we then have

$$\Delta E_{HA} = -\frac{i\alpha}{2\pi}\left\langle \int_{C_H'} dz[J(p^2,b) - J(p^2,b')] \right\rangle \tag{4.8}$$

where

$$J(p^2,b) = \int_0^\infty d\eta \left[4E_n - 2z + \left(3 + \frac{b^2 - c^2}{(\eta + b + c)^2} \right)(\beta - E_n) \right.$$

$$\left. + \left(1 + \frac{b^2 - c^2}{(\eta + b + c)^2} \right) V \right] \frac{1}{p^2 + (\eta + b + c)^2} - \frac{2z}{c}(2\beta - z)$$

$$\times\; V \frac{1}{p^2 + (b + c)^2} \tag{4.9}$$

and where

$$c = (1 - z^2)^{\frac{1}{2}}, \qquad \mathrm{Re}(c) > 0 \quad . \tag{4.10}$$

The definition of b and b' is given by Eqs. (2.7) and (2.8). For the terms containing p^2 in (4.9), we make the substitution

$$\frac{1}{p^2 + a^2} = \frac{1}{a^2} - \frac{p^2}{a^2(p^2 + a^2)} \quad . \tag{4.11}$$

In the expression corresponding to the first term on the right side in (4.11), the integral over η is performed easily. In the expression corresponding to the second term on the right side in (4.11), the integrand of the integral over z and η falls off sufficiently rapidly as $|z|$ and $\eta \to \infty$ that the expression has a finite limit as $\Lambda \to \infty$. We thus have

$$\Delta E_{HA} = \Delta E_{HA}{}^1 + \Delta E_{HA}{}^2 + \mathcal{O}(\Lambda^{-1}) \tag{4.12}$$

where

$$\Delta E_{HA}{}^1 = -\frac{i\alpha}{2\pi}\left\langle \int_{C_H'} dz[J(0,b) - J(0,b')] \right\rangle \quad . \tag{4.13}$$

We integrate over z in (4.13) and arrange the expression so that the part of order lower than $(Z\alpha)^4$ is isolated in terms proportional to the expectation values $\langle\beta\rangle$ and $\langle V\rangle$:

$$\Delta E_{HA}{}^1 = \frac{\alpha}{\pi}\left[\left(\frac{3}{4}\ell n\, \Lambda^2 - \frac{9}{8} \right)\langle\beta\rangle + \left(\frac{1}{2}\ell n\, 2 - \frac{17}{12} \right)\langle V\rangle \right.$$

$$\left. + (Z\alpha)^4\, f_{HA}{}^1(Z\alpha) \right] \tag{4.14}$$

where

$$(Z\alpha)^4 f_{HA}^{\ 1}(Z\alpha) = \left[\frac{(1 - E_n^{\ 2})(3 + 2E_n^{\ 2})}{3E_n^{\ 2}(1 + E_n^{\ 2})} - \frac{1}{2}\ell n\ 2 - \frac{4 - 9E_n^{\ 2} + 3E_n^{\ 4}}{4E_n^{\ 4}}\right.$$

$$\left. \times\ \ell n(1 + E_n^{\ 2})\right] \langle V\rangle + \left[\frac{9}{4} - \frac{9 - 3E_n^{\ 2}}{4E_n^{\ 2}}\ \ell n(1 + E_n^{\ 2})\right] \left\langle\left(1 - \frac{\beta}{E_n}\right) V\right\rangle \quad . \tag{4.15}$$

We then consider

$$\Delta E_{HA}^{\ 2} = -\frac{i\alpha}{2\pi}\left\langle \int_{C_H'} dz[J(p^2,b) - J(0,b)]\right\rangle \quad . \tag{4.16}$$

We substitute the appropriate expressions obtained from the right-hand side of (4.9) into the integrand in (4.16). The result of integration over η and z is then given by

$$\Delta E_{HA}^{\ 2} = \frac{\alpha}{\pi}\left\langle\left[E_n Q_1(p^2) + \beta Q_2(p^2) + VQ_3(p^2) + \frac{\beta}{E_n} VQ_4(p^2)\right] p^2\right\rangle \tag{4.17}$$

where

$$Q_j(p^2) = B_j(p) + B_j(-p) \quad , \qquad j = 1,2,3,4 \tag{4.18}$$

and

$$B_1(p) = \frac{(1 + E_n^{\ 2})^2}{16E_n} A_3(p) + \frac{1 - E_n^{\ 2}}{8E_n} A_1(p) + \frac{1}{16E_n p} A(p) \quad ,$$

$$B_2(p) = -\frac{(1 + E_n^{\ 2})^2}{16E_n} A_3(p) - \frac{5E_n^{\ 4} + 8E_n^{\ 2} - 1}{16E_n^{\ 3}} A_1(p)$$

$$+ \frac{(1 - E_n^{\ 2})(3E_n^{\ 2} - 1)}{8E_n^{\ 4}} A_0(p) - \frac{1}{16E_n^{\ 4}(E_n + p)}\left(\frac{8E_n^{\ 2} - 3}{p} + \frac{1}{E_n + p}\right)$$

$$\times\ A(p) \quad ,$$

$$B_3(p) = -\frac{(1 + E_n^{\ 2})^2}{16E_n} A_3(p) + \frac{3 + E_n^{\ 4}}{16E_n^{\ 3}} A_1(p) - \frac{1}{2E_n^{\ 4}} A_0(p)$$

$$+ \frac{1}{16E_n^{\ 4}(E_n + p)}\left(\frac{15}{p} - \frac{7}{E_n + p}\right) A(p) - \frac{1}{8E_n^{\ 3}(E_n + p)^3}$$

$$\times\ [A(p) - (E_n + p)^2] \quad ,$$

$$B_4(p) = -\frac{1 + E_n^{\ 2}}{2E_n} A_1(p) + \frac{1}{E_n^{\ 2}} A_0(p) - \frac{1}{2E_n^{\ 2}(E_n + p)}\left(\frac{3}{p} - \frac{1}{E_n + p}\right)$$

$$\times\ A(p) \quad ,$$

$$A(p) = \ell n[1 + (E_n + p)^2] \quad ,$$

$$A_j(p) = \frac{1}{p^{j+2}}\left[A(p) - \sum_{\ell=0}^{j} A^{\ell}(0)\ \frac{p^{\ell}}{\ell!}\right] \quad . \tag{4.19}$$

In (4.19), A^{ℓ} denotes the ℓth derivative of A. We note that each function $Q_j(p^2)$, $j = 1,2,3,4$, approaches a constant in the limit $p^2 \to 0$. In order to arrive at a convenient expression for the contribution of each term in (4.17) to the net energy shift, we isolate the contribution of order lower than $(Z\alpha)^4$ in terms proportional to $\langle V \rangle$. The lower order contributions, which come from the terms containing Q_1 and Q_2 in (4.17), are identified by replacing $Q_1(p^2)$ and $Q_2(p^2)$ by the limits

$$\lim_{\substack{p^2\to 0 \\ E_n \to 1}} Q_1(p^2) = \frac{1}{10} \quad \text{and} \quad \lim_{\substack{p^2\to 0 \\ E_n \to 1}} Q_2(p^2) = \frac{1}{2}\,\ell n\, 2 - \frac{7}{20} \,. \tag{4.20}$$

We accordingly define four functions h_j, $j = 1,2,3,4$, by the equations

$$\begin{aligned}
\langle E_n Q_1(p^2) p^2 \rangle &= -\frac{1}{10}\langle V \rangle + (Z\alpha)^4 h_1(Z\alpha) \,, \\
\langle \beta Q_2(p^2) p^2 \rangle &= \left(\frac{7}{20} - \frac{1}{2}\,\ell n\, 2\right) \langle V \rangle + (Z\alpha)^4 h_2(Z\alpha) \,, \\
\langle V Q_3(p^2) p^2 \rangle &= (Z\alpha)^4 h_3(Z\alpha) \,, \\
\left\langle \frac{\beta}{E_n} V Q_4(p^2) p^2 \right\rangle &= (Z\alpha)^4 h_4(Z\alpha) \,.
\end{aligned} \tag{4.21}$$

These functions then have the property that they approach constants as $Z\alpha \to 0$. The constants are given by

$$\begin{aligned}
h_1(0) &= (Z\alpha)^{-4} \left\{ \frac{23}{420} \langle p^4 \rangle_{NR} + \frac{1}{30} \langle p^2 V \rangle_{NR} + \frac{1}{40} \langle [\underset{\sim}{\sigma}\cdot\underset{\sim}{p}, [\underset{\sim}{\sigma}\cdot\underset{\sim}{p}, V]] \rangle_{NR} \right\} \,, \\
h_2(0) &= (Z\alpha)^{-4} \left\{ \left(\frac{103}{420} - \frac{1}{4}\,\ell n\, 2\right) \langle p^4 \rangle_{NR} + \left(\frac{9}{10} - \ell n\, 2\right) \langle p^2 V \rangle_{NR} \right. \\
&\qquad \left. + \left(\frac{1}{8}\,\ell n\, 2 - \frac{7}{80}\right) \langle [\underset{\sim}{\sigma}\cdot\underset{\sim}{p}, [\underset{\sim}{\sigma}\cdot\underset{\sim}{p}, V]] \rangle_{NR} \right\} \,, \\
h_3(0) &= (Z\alpha)^{-4} \left(\frac{31}{15} - 3\,\ell n\, 2\right) \langle p^2 V \rangle_{NR} \,, \\
h_4(0) &= (Z\alpha)^{-4} \left(4\,\ell n\, 2 - \frac{8}{3}\right) \langle p^2 V \rangle_{NR} \,.
\end{aligned} \tag{4.22}$$

To facilitate evaluation of the h's, we employ the expression for the momentum space wave function given in (A.9) and the expression for the function given in (A.11) to arrive at the following equations:

$$\begin{aligned}
(Z\alpha)^4 h_1(Z\alpha) &= \frac{1}{10}\langle V \rangle + E_n \int_0^\infty dp\, p^4 [|g_1(p)|^2 + |g_2(p)|^2]\, Q_1(p^2) \,, \\
(Z\alpha)^4 h_2(Z\alpha) &= \left(\frac{1}{2}\,\ell n\, 2 - \frac{7}{20}\right) \langle V \rangle + \int_0^\infty dp\, p^4 [|g_1(p)|^2 - |g_2(p)|^2] \\
&\qquad \times Q_2(p^2) \,, \\
(Z\alpha)^4 h_3(Z\alpha) &= \int_0^\infty dp\, p^4 [g_1^*(p)(Vg)_1(p) + g_2^*(p)(Vg)_2(p)] Q_3(p^2) \,, \\
(Z\alpha)^4 h_4(Z\alpha) &= E_n^{-1} \int_0^\infty dp\, p^4 [g_1^*(p)(Vg)_1(p) - g_2^*(p)(Vg)_2(p)] Q_4(p^2)
\end{aligned} \tag{4.23}$$

The functions h_j can readily be evaluated, for relevant values of $Z\alpha$, by numerical integration over p in (4.23).

The total value of ΔE_{HA} is then given by

$$\Delta E_{HA} = \frac{\alpha}{\pi}[(\tfrac{3}{4}\ell n\,\Lambda^2 - \tfrac{9}{8})\langle\beta\rangle - \tfrac{7}{6}\langle V\rangle + (Z\alpha)^4 f_{HA}(Z\alpha)] \qquad (4.24)$$

where

$$f_{HA}(Z\alpha) = f_{HA}^{1}(Z\alpha) + \sum_{i=1}^{4} h_i(Z\alpha) . \qquad (4.25)$$

V. THE HIGH-ENERGY REMAINDER ΔE_{HB}

The remainder of the high-energy part ΔE_{HB} is evaluated in coordinate space. The separation of ΔE_H given by (4.6) and (4.7) corresponds to the separation of the resolvent $G(z)$ into two parts $G_A(z)$ and $G_B(z)$ where

$$G(z) = G_A(z) + G_B(z) , \qquad (5.1)$$

and

$$G_A(z) = \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} + \beta - z} - \frac{1}{2}\left\{V, \frac{1}{p^2 + 1 - z^2}\right\} - z(\beta + z) \times \left\{V, \frac{1}{[p^2 + 1 - z^2]^2}\right\} . \qquad (5.2)$$

The curly brackets in (5.2) denote the symmetric product: $\{X,Y\} = XY + YX$. The symmetrization is introduced merely for convenience, and does not affect the result.

The coordinate-space representation of $G_A(z)$ is

$$G_A(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \left[-i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla}_2 + \beta + z + \frac{Z\alpha}{2}\left(\frac{1}{x_2} + \frac{1}{x_1}\right) \times \left(1 - \frac{z(\beta + z)}{c}\frac{d}{dc}\right)\right] \frac{e^{-c\rho}}{4\pi\rho}$$

$$= \sum_{\kappa} \begin{bmatrix} G^{11}_{A,\kappa}(x_2,x_1,z)\pi_{\kappa}(\hat{x}_2,\hat{x}_1) & G^{12}_{A,\kappa}(x_2,x_1,z)i\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \\ -G^{21}_{A,\kappa}(x_2,x_1,z)i\underset{\sim}{\sigma}\cdot\hat{x}_2\,\pi_{\kappa}(\hat{x}_2,\hat{x}_1) & G^{22}_{A,\kappa}(x_2,x_1,z)\pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \end{bmatrix} \qquad (5.3)$$

where

$$G^{11}_{A,\kappa}(x_2,x_1,z) = F_{\kappa}^{11}(x_2,x_1,z) + \frac{Z\alpha}{2}\frac{x_2 + x_1}{x_2x_1c^2}\{(1 + 2\kappa z)F_{\kappa}^{11}(x_2,x_1,z) - z(z + 1)[x_2F_{\kappa}^{21}(x_2,x_1,z) + x_1F_{\kappa}^{12}(x_2,x_1,z)]\} ,$$

$$G^{12}_{A,\kappa}(x_2,x_1,z) = F_{\kappa}^{12}(x_2,x_1,z) ,$$

$$G^{21}_{A,\kappa}(x_2,x_1,z) = F_{\kappa}^{21}(x_2,x_1,z) ,$$

$$G^{22}_{A,\kappa}(x_2,x_1,z) = F_{\kappa}^{22}(x_2,x_1,z) - \frac{Z\alpha}{2}\frac{x_2 + x_1}{x_2x_1c^2}\{(1 + 2\kappa z)F_{\kappa}^{22}(x_2,x_1,z) - z(z - 1)[x_2F_{\kappa}^{12}(x_2,x_1,z) + x_1F_{\kappa}^{21}(x_2,x_1,z)]\} , \qquad (5.4)$$

and where c is defined in (4.10). The F's in (5.4) are elements of the free radial Green's functions, and are given explicitly in (A.20). The expression in (5.3) is the analog of the expression in (3.13) for the Coulomb Green's function, and there exists a corresponding expression for $G_B(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ in which

$$G^{ij}_{B,\kappa}(x_2,x_1,z) = G_\kappa{}^{ij}(x_2,x_1,z) - G^{ij}_{A,\kappa}(x_2,x_1,z) \; ; \quad i,j = 1,2 \; . \tag{5.5}$$

That expression for $G_B(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ is the basis for our numerical evaluation of ΔE_{HB} for which we employ the formula

$$\Delta E_{HB} = -\frac{i\alpha}{2\pi}\int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1 \, \psi_n{}^\dagger(\underset{\sim}{x}_2)\,\alpha_\mu \int_{C'_H} dz \; G_B(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\alpha^\mu\psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{e^{-b\rho}}{\rho} \; . \tag{5.6}$$

Substituting the expression for the wave function given in (3.12) and the expression for $G_B(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ described above into (5.6) yields

$$\Delta E_{HB} = -\frac{i\alpha}{2\pi}\int_{C'_H} dz \int_0^\infty dx_2 x_2{}^2 \int_0^\infty dx_1 x_1{}^2$$

$$\times \sum_\kappa \sum_{i,j=1}^{2} [f_i(x_2)G^{ij}_{B,\kappa}(x_2,x_1,z)f_j(x_1)A_\kappa(x_2,x_1)$$

$$- f_{\bar{i}}(x_2)G^{ij}_{B,\kappa}(x_2,x_1,z)f_{\bar{j}}(x_1)A_\kappa{}^{ij}(x_2,x_1)] \tag{5.7}$$

where $\bar{i} = 3 - i$ and $\bar{j} = 3 - j$. Integrating over all angles except $\xi = \hat{x}_2\cdot\hat{x}_1$ in $A_\kappa(x_2,x_1)$ and $A_\kappa{}^{ij}(x_2,x_1)$, we obtain

$$A_\kappa(x_2,x_1) = \frac{|\kappa|}{2}\int_{-1}^{1} d\xi [P_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi)\, P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)$$

$$+ \frac{1}{\kappa\kappa_n}(1-\xi^2)\, P'_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi)\, P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)] \frac{e^{-b\rho}}{\rho} \; ,$$

$$A_\kappa{}^{11}(x_2,x_1) = \frac{|\kappa|}{2}\int_{-1}^{1} d\xi [3P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\, P_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi)$$

$$+ \frac{1}{\kappa\kappa_n}(1-\xi^2)\, P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\, P'_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi)] \frac{e^{-b\rho}}{\rho} \; ,$$

$$A_\kappa{}^{12}(x_2,x_1) = \frac{|\kappa|}{2}\int_{-1}^{1} d\xi [P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) P_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi)$$

$$- \frac{1}{\kappa\kappa_n}(1-\xi^2)\, P'_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, P'_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi)] \frac{e^{-b\rho}}{\rho} \; . \tag{5.8}$$

The corresponding expressions for $A_\kappa{}^{21}(x_2,x_1)$ and $A_\kappa{}^{22}(x_2,x_1)$ are obtained by taking advantage of the symmetry expressed in (3.16). For $S_{\frac{1}{2}}$ states, integration over ξ gives

$$A_\kappa(x_2,x_1) = -|\kappa|\, bj_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(ibx_>) ,$$

$$A_\kappa^{11}(x_2,x_1) = -3\,|\kappa|\, bj_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_>)$$

$$+ \frac{4\kappa(\kappa+1)}{2\kappa+1}\, b\Big[j_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(ibx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(ibx_>)$$

$$- j_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(ibx_>)\Big] ,$$

$$A_\kappa^{12}(x_2,x_1) = -|\kappa|\, bj_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_>) ,$$

$$A_\kappa^{21}(x_2,x_1) = -|\kappa|\, bj_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_>) ,$$

$$A_\kappa^{22}(x_2,x_1) = -3\,|\kappa|\, bj_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_>) , \tag{5.9}$$

in which $x_< = \min(x_2,x_1)$, $x_> = \max(x_2,x_1)$, j is the spherical Bessel function, and $h^{(1)}$ is the spherical Hankel function of the first kind.

It is convenient to express ΔE_{HB} in terms of the function $f_{HB}(Z\alpha)$ defined by

$$\Delta E_{HB} = \frac{\alpha}{\pi}(Z\alpha)^4 f_{HB}(Z\alpha) . \tag{5.10}$$

The function $f_{HB}(Z\alpha)$ approaches a constant as $Z\alpha \to 0$. In view of (4.3) and (4.5), the value of the constant is given by

$$f_{HB}(0) = (Z\alpha)^{-4}\left\{(\tfrac{3}{2}\ln 2 - \tfrac{5}{4})\langle V^2\rangle_{NR} + (\ln 2 - \tfrac{5}{6})\langle p^2 V\rangle_{NR}\right.$$

$$\left. + (\tfrac{3}{8} - \tfrac{1}{2}\ln 2)\langle[\sigma\cdot p,[\sigma\cdot p,V]]\rangle_{NR} + (\tfrac{1}{3}\ln 2 - \tfrac{17}{72})\langle[p^i,[p^i,V]]\rangle_{NR}\right\} . \tag{5.11}$$

The remainder ΔE_{HB} can be evaluated numerically with the aid of (5.7). The numerical cancellations, which correspond to the removal of ΔE_{HA} from ΔE_H, occur in forming the difference in Eq. (5.5). The individual terms in that difference can be calculated with sufficient accuracy that the numerical cancellation does not cause trouble. The separation shown in (5.1) and (5.2) leads to a function $G^{ij}_{A,\kappa}(x_2,x_1,z)$ which approximates $G_\kappa{}^{ij}(x_2,x_1,z)$ in the critical region (κ, x_2, x_1 large, $x_2 \approx x_1$) sufficiently well that the expression for ΔE_{HB} in (5.7) is a convergent integral over z of a function which is of order $(Z\alpha)^4$. We note that the removal of ΔE_{HA} from ΔE_H before the sum over κ or any integrals have been performed numerically is an essential feature of this calculation. If ΔE_{HA} were subtracted at a later stage of the computation, possibly after the sum over κ and the integrals over x_2 and x_1 in (5.7) were performed, then for Z not large there would be a substantial loss of numerical significance. This would necessitate a highly accurate evaluation of the sum and integrals, which, in turn, would require an excessive amount of computer time due to the slow convergence of the sum over κ. That sum is examined in the following paper.

VI. CONCLUSION

The total value for the self-energy radiative level shift is obtained by adding the constituent parts:

$$\mathrm{Re}(\Delta E_n) = \mathrm{Re}(\Delta E_L) + \Delta E_{HA} + \Delta E_{HB} + \Delta E_M \ . \tag{6.1}$$

The terms on the right in (6.1) appear in Eqs. (3.18), (4.24), (5.10), and (2.9) respectively. The last three terms in (6.1) are real-valued quantities. We note that in each of the expressions listed above for the terms on the right in (6.1), the part of order lower than $(Z\alpha)^4 \, \ell n(Z\alpha)^{-2}$ is expressed analytically in terms of the expectation values $\langle \beta \rangle$ and $\langle V \rangle$. The sum of the lower order parts is zero. We thus have

$$\Delta E_n = \frac{\alpha}{\pi}(Z\alpha)^4 \, F(Z\alpha) \, m_e c^2 \tag{6.2}$$

where

$$F(Z\alpha) = f_L(Z\alpha) + f_{HA}(Z\alpha) + f_{HB}(Z\alpha) \ . \tag{6.3}$$

In (6.2) it is understood that we mean the real part of the energy shift. Expressions suitable for the direct numerical evaluation of the functions on the right in (6.3) are given in the preceding sections.

The contour of integration for the integral over z in (2.6) used in this calculation was chosen to be a convenient one with regard to the numerical work. The final contour consists of the real z-axis from zero to the bound-state energy and the imaginary z-axis. On both these portions of the contour, the quantity c, defined in (A.17), is real. This is convenient for the numerical evaluation of the

radial Green's functions. Another attractive feature of the contour of integration used here is the fact that it leads to the rapid convergence of the sum over κ in (3.14) discussed at the end of Sec. III.

The numerical evaluation of the level shift of the $1S_{\frac{1}{2}}$ state is described in the following paper. We expect that the method of calculating the self-energy radiative level shift which is presented here and in the following paper could easily be extended to calculate the level shifts of the bound states with principal quantum number $n = 2$.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor Eyvind H. Wichmann for his guidance and continued interest during the course of this work. Helpful conversations with Dr. Ira W. Herbst and Professor Charles Schwartz are gratefully acknowledged.

APPENDIX

In this appendix, we discuss some relevant properties of the Dirac wave functions and Green's function for the case of a Coulomb potential. The Dirac Hamiltonian is given by

$$H(\underset{\sim}{x}) = \underset{\sim}{\alpha}\cdot\hat{x}\, p_x + i\underset{\sim}{\alpha}\cdot\hat{x}\,\beta\,\frac{K}{x} + V(x) + \beta\ , \tag{A.1}$$

where

$$p_x = -i\,\frac{1}{x}\,\frac{d}{dx}\,x \tag{A.2}$$

and

$$K = \beta(\underset{\sim}{\sigma}\cdot\underset{\sim}{L} + 1)\ . \tag{A.3}$$

The spectrum of K consists of all nonzero integers. A wave function which is a simultaneous eigenstate of H, of K (with eigenvalue $-\kappa$), and of the third component of angular momentum J_z (with eigenvalue μ), is written as [22]

$$\psi_n(\underset{\sim}{x}) = \begin{bmatrix} f_1(x)\,\chi_\kappa^{\ \mu}(\hat{x}) \\ \\ if_2(x)\,\chi_{-\kappa}^{\ \mu}(\hat{x}) \end{bmatrix}\ , \tag{A.4}$$

where f_1 and f_2 are the components of the radial wave function (corresponding to g and f in Ref. 22), and $\chi_\kappa^{\ \mu}$ is a two-component spin-angular function explicitly given by

$$\chi_\kappa^{\ \mu}(\hat{x}) = \begin{bmatrix} -\frac{\kappa}{|\kappa|}\left[\frac{\kappa+\frac{1}{2}-\mu}{2\kappa+1}\right]^{\frac{1}{2}} Y^{\mu-\frac{1}{2}}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\hat{x}) \\ \\ \left[\frac{\kappa+\frac{1}{2}+\mu}{2\kappa+1}\right]^{\frac{1}{2}} Y^{\mu+\frac{1}{2}}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\hat{x}) \end{bmatrix}\ . \tag{A.5}$$

We use the notation

$$\pi_\kappa(\hat{x}_2,\hat{x}_1) = \sum_\mu \chi_\kappa^{\ \mu}(\hat{x}_2)\,\chi_\kappa^{\ \mu\dagger}(\hat{x}_1)$$

$$= \frac{|\kappa|}{4\pi}\left\{IP_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) + \frac{1}{\kappa}\,i\underset{\sim}{\sigma}\cdot(\hat{x}_2\times\hat{x}_1)\right. \tag{A.6}$$

$$\left.\times\ P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\right\}\ ,$$

where $\xi = \hat{x}_2\cdot\hat{x}_1$, P is the Legendre polynomial, and P' is the derivative of P with respect to the argument; I is the 2×2 identity matrix.

The components f_1 and f_2 of the radial wave function, which appear in (A.4), satisfy the radial differential equation

$$\begin{bmatrix} 1 + V(x) - E_n & -\frac{1}{x}\,\frac{d}{dx}\,x + \frac{\kappa}{x} \\ \\ \frac{1}{x}\,\frac{d}{dx}\,x + \frac{\kappa}{x} & -1 + V(x) - E_n \end{bmatrix} \begin{bmatrix} f_1(x) \\ \\ f_2(x) \end{bmatrix} = 0\ , \tag{A.7}$$

where E_n is the energy. We are interested in the case where the potential is the Coulomb potential: $V(x) = -Z\alpha/x$. For the $1S_{\frac{1}{2}}$ ($\kappa = -1$) state, the normalized solution is given by

$$f_1(x) = N^{\frac{1}{2}}(1 + E_n)^{\frac{1}{2}} x^{-\delta} e^{-\gamma x} ,$$

$$f_2(x) = -N^{\frac{1}{2}}(1 - E_n)^{\frac{1}{2}} x^{-\delta} e^{-\gamma x} , \qquad (A.8)$$

$$\gamma = Z\alpha; \quad E_n = (1 - \gamma^2)^{\frac{1}{2}}; \quad \delta = 1 - E_n; \quad N = \frac{(2\gamma)^{3-2\delta}}{2\Gamma(3 - 2\delta)} .$$

The momentum-space wave function is written in the form

$$\phi_n(\underset{\sim}{p}) = (2\pi)^{-3/2} \int d^3\underset{\sim}{x}\, e^{-i\underset{\sim}{p}\cdot\underset{\sim}{x}} \psi_n(\underset{\sim}{x}) = \begin{bmatrix} g_1(p)\, \chi_\kappa^{\mu}(\hat{p}) \\ \\ g_2(p)\, \chi_{-\kappa}^{\mu}(\hat{p}) \end{bmatrix} \qquad (A.9)$$

For the $1S_{\frac{1}{2}}$ state, we have

$$g_1(p) = M^{\frac{1}{2}}(1 + E_n)^{\frac{1}{2}} \frac{\sin[(2 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2 + p^2]^{\frac{1}{2}(2-\delta)}} ,$$

$$g_2(p) = -M^{\frac{1}{2}}(1 - E_n)^{\frac{1}{2}} \left\{ \frac{\sin[(1 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{(1 - \delta)\, p^2[\gamma^2 + p^2]^{\frac{1}{2}(1-\delta)}} - \frac{\cos[(2 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2 + p^2]^{\frac{1}{2}(2-\delta)}} \right\} ,$$

$$M = \Gamma(2 - \delta)^2 \frac{(2\gamma)^{3-2\delta}}{\pi\Gamma(3 - 2\delta)} . \qquad (A.10)$$

The result of the action of the Coulomb potential on the state vector in momentum space is denoted by $(V\phi_n)(\underset{\sim}{p})$. It is obtained by taking the Fourier transform of $V(x)\psi_n(\underset{\sim}{x})$. We have

$$(V\phi_n)(\underset{\sim}{p}) = \begin{bmatrix} (Vg)_1(p)\, \chi_\kappa^{\mu}(\hat{p}) \\ \\ (Vg)_2(p)\, \chi_{-\kappa}^{\mu}(\hat{p}) \end{bmatrix} \qquad (A.11)$$

where

$$(Vg)_1(p) = -\frac{\gamma M^{\frac{1}{2}}}{E_n}(1 + E_n)^{\frac{1}{2}} \frac{\sin[(1 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2 + p^2]^{\frac{1}{2}(1-\delta)}} ,$$

$$(Vg)_2(p) = \frac{\gamma M^{\frac{1}{2}}}{E_n}(1 - E_n)^{\frac{1}{2}} \left\{ \frac{\sin[\delta\tan^{-1}(\frac{p}{\gamma})]}{\delta p^2[\gamma^2 + p^2]^{-\frac{1}{2}\delta}} - \frac{\cos[(1 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2 + p^2]^{\frac{1}{2}(1-\delta)}} \right\} \qquad (A.12)$$

The Dirac Green's function $G(\underset{\sim}{x}_2, \underset{\sim}{x}_1, z)$, which satisfies the equation

$$[H(\underset{\sim}{x}_2) - z]\, G(\underset{\sim}{x}_2, \underset{\sim}{x}_1, z) = \delta^3(\underset{\sim}{x}_2 - \underset{\sim}{x}_1) , \qquad (A.13)$$

can be written as an expansion in eigenfunctions of K [2,23]:

$$G(\underset{\sim}{x}_2, \underset{\sim}{x}_1, z) = \sum_\kappa \begin{bmatrix} G_\kappa^{11}(x_2, x_1, z)\, \pi_\kappa(\hat{x}_2, \hat{x}_1) & G_\kappa^{12}(x_2, x_1, z)\, i\underset{\sim}{\sigma}\cdot\hat{x}_2\, \pi_{-\kappa}(\hat{x}_2, \hat{x}_1) \\ \\ -G_\kappa^{21}(x_2, x_1, z)\, i\underset{\sim}{\sigma}\cdot\hat{x}_2\, \pi_\kappa(\hat{x}_2, \hat{x}_1) & G_\kappa^{22}(x_2, x_1, z)\, \pi_{-\kappa}(\hat{x}_2, \hat{x}_1) \end{bmatrix} , \qquad (A.14)$$

where the summation extends over all possible values of κ.

The $G_\kappa^{ij}(x_2,x_1,z)$ are the elements of the radial Green's functions, and they satisfy the equation

$$\begin{bmatrix} 1 + V(x_2) - z & -\frac{1}{x_2}\frac{d}{dx_2}x_2 + \frac{\kappa}{x_2} \\ \frac{1}{x_2}\frac{d}{dx_2}x_2 + \frac{\kappa}{x_2} & -1 + V(x_2) - z \end{bmatrix} \begin{bmatrix} G_\kappa^{11}(x_2,x_1,z) & G_\kappa^{12}(x_2,x_1,z) \\ G_\kappa^{21}(x_2,x_1,z) & G_\kappa^{22}(x_2,x_1,z) \end{bmatrix}$$

$$= I\frac{1}{x_2x_1}\delta(x_2 - x_1) \quad . \qquad (A.15)$$

For $x_1 > x_2$, the radial Green's functions for the Coulomb potential are given by the following expressions:

$$G_\kappa^{11}(x_2,x_1,z) = (1 + z)\, Q[(\lambda - \nu)\, M_{\nu-\frac{1}{2},\lambda}(2cx_2) - (\kappa - \tfrac{\gamma}{c})$$

$$\times M_{\nu+\frac{1}{2},\lambda}(2cx_2)][(\kappa + \tfrac{\gamma}{c})W_{\nu-\frac{1}{2},\lambda}(2cx_1) + W_{\nu+\frac{1}{2},\lambda}(2cx_1)] \ ,$$

$$G_\kappa^{12}(x_2,x_1,z) = cQ[(\lambda - \nu)\, M_{\nu-\frac{1}{2},\lambda}(2cx_2) - (\kappa - \tfrac{\gamma}{c})\, M_{\nu+\frac{1}{2},\lambda}(2cx_2)]$$

$$\times [(\kappa + \tfrac{\gamma}{c})\, W_{\nu-\frac{1}{2},\lambda}(2cx_1) - W_{\nu+\frac{1}{2},\lambda}(2cx_1)] \ ,$$

$$G_\kappa^{21}(x_2,x_1,z) = cQ[(\lambda - \nu)\, M_{\nu-\frac{1}{2},\lambda}(2cx_2) + (\kappa - \tfrac{\gamma}{c})\, M_{\nu+\frac{1}{2},\lambda}(2cx_2)]$$

$$\times [(\kappa + \tfrac{\gamma}{c})\, W_{\nu-\frac{1}{2},\lambda}(2cx_1) + W_{\nu+\frac{1}{2},\lambda}(2cx_1)] \ ,$$

Equation (A.16) continued next page

Equation (A.16) continued

$$G_\kappa^{22}(x_2,x_1,z) = (1 - z)\, Q[(\lambda - \nu)\, M_{\nu-\frac{1}{2},\lambda}(2cx_2) + (\kappa - \tfrac{\gamma}{c})$$

$$\times M_{\nu+\frac{1}{2},\lambda}(2cx_2)]\,[(\kappa + \tfrac{\gamma}{c})\, W_{\nu-\frac{1}{2},\lambda}(2cx_1) - W_{\nu+\frac{1}{2},\lambda}(2cx_1)] \ , \qquad (A.16)$$

where

$$c = (1 - z^2)^{\frac{1}{2}}, \quad \mathrm{Re}(c) > 0; \quad \lambda = (\kappa^2 - \gamma^2)^{\frac{1}{2}}; \quad \nu = \frac{\gamma z}{c}; \quad \gamma = Z\alpha \ ; \qquad (A.17)$$

$$Q = \frac{1}{(x_1x_2)^{\frac{1}{2}}(4c^2x_1x_2)}\frac{\Gamma(\lambda - \nu)}{\Gamma(1 + 2\lambda)} \ ,$$

and $M_{\alpha,\beta}(x)$ and $W_{\alpha,\beta}(x)$ are the Whittaker functions [24]. For $x_2 > x_1$, the radial Green's functions can be obtained from (A.16) together with the symmetry conditions

$$\begin{aligned} G_\kappa^{11}(x_1,x_2,z) &= G_\kappa^{11}(x_2,x_1,z) \ , \\ G_\kappa^{12}(x_1,x_2,z) &= G_\kappa^{21}(x_2,x_1,z) \ , \\ G_\kappa^{21}(x_1,x_2,z) &= G_\kappa^{12}(x_2,x_1,z) \ , \\ G_\kappa^{22}(x_1,x_2,z) &= G_\kappa^{22}(x_2,x_1,z) \ . \end{aligned} \qquad (A.18)$$

The radial Green's functions are described extensively in Ref. 2.

The free electron Dirac Green's function $F(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ can also be written in the form given in (A.14) with the G's replaced by F's, where

$$F_\kappa^{ij}(x_2,x_1,z) = \lim_{\gamma\to 0} G_\kappa^{ij}(x_2,x_1,z) \; ; \quad i,j = 1,2 \; . \qquad (A.19)$$

For $x_1 > x_2$:

$$\begin{aligned}
F_\kappa^{11}(x_2,x_1,z) &= -(z+1)\, cj_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_1) \; , \\
F_\kappa^{12}(x_2,x_1,z) &= -ic^2 \frac{\kappa}{|\kappa|}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_1) \; , \\
F_\kappa^{21}(x_2,x_1,z) &= -ic^2 \frac{\kappa}{|\kappa|}\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_1) \; , \\
F_\kappa^{22}(x_2,x_1,z) &= -(z-1)\, cj_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_1) \; .
\end{aligned} \qquad (A.20)$$

For this case, the sum over κ is known, and is just

$$F(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \left[\left(\frac{c}{x}+\frac{1}{x^2}\right) i\underset{\sim}{\alpha}\cdot\underset{\sim}{x} + \beta + z\right] \frac{e^{-cx}}{4\pi x} \; , \qquad (A.21)$$

$$\underset{\sim}{x} = \underset{\sim}{x}_2 - \underset{\sim}{x}_1 \; ; \qquad x = |\underset{\sim}{x}| \; .$$

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FOOTNOTE

1. We employ units in which $c = \hbar = m_e = 1$. Four vectors have the form $a = (a^0, a)$. The scalar product of two four vectors a and b is $ab = a^0 b^0 - \underset{\sim}{a}\cdot\underset{\sim}{a}$. We use the standard gamma matrices

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}; \quad \alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}; \quad \gamma^0 = \beta; \quad \gamma^i = \beta\alpha^i,$$

$i = 1,2,3$. The σ^i are the usual Pauli matrices. For repeated Greek indices, summation over $0,1,2,3$ is implied; for repeated Latin indices summation over $1,2,3$ is implied. We use the notation $\gamma_\mu A \gamma^\mu = \gamma^0 A \gamma^0 - \gamma^i A \gamma^i$; $\alpha_\mu A \alpha^\mu = A - \alpha^i A \alpha^i$.

FIGURE CAPTIONS

Fig. 1. The Feynman diagrams corresponding to the lowest order radiative corrections to the energy levels in a hydrogen-like system. The diagrams in (a) and (b) correspond to the electron self energy and the vacuum polarization respectively.

Fig. 2. The curves labeled (4), (5), (6), and (7) are the successive approximations to $F(Z\alpha)$ which result from evaluating known terms of order up to 4th, 5th, 6th, and 7th in the series in Eq. (1.2).

Fig. 3. The contour C_F and the singularities of the integrand in the complex z-plane. The points to the left of $z = +1$ represent the bound-state poles; E_n is the ground-state energy in this diagram.

Fig. 4. The new contour in the complex z-plane.

Fig. 5. The complex z-plane with the singularities of the integrand in Eq. (3.2). In the upper diagram, the branch points of b are at $E_n \pm (-i\epsilon)^{\frac{1}{2}}$. As $\epsilon \to 0+$, the branch points meet at E_n. In the lower diagram, the cuts, which are drawn to insure $\mathrm{Re}(b) > 0$, meet at E_n and extend along the real z-axis. In this diagram $z_1 = z_2 = 0$.

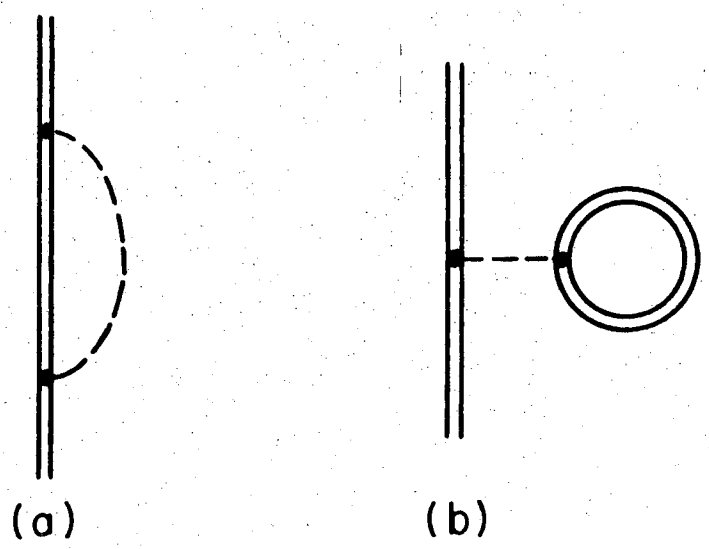

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Fig. 1

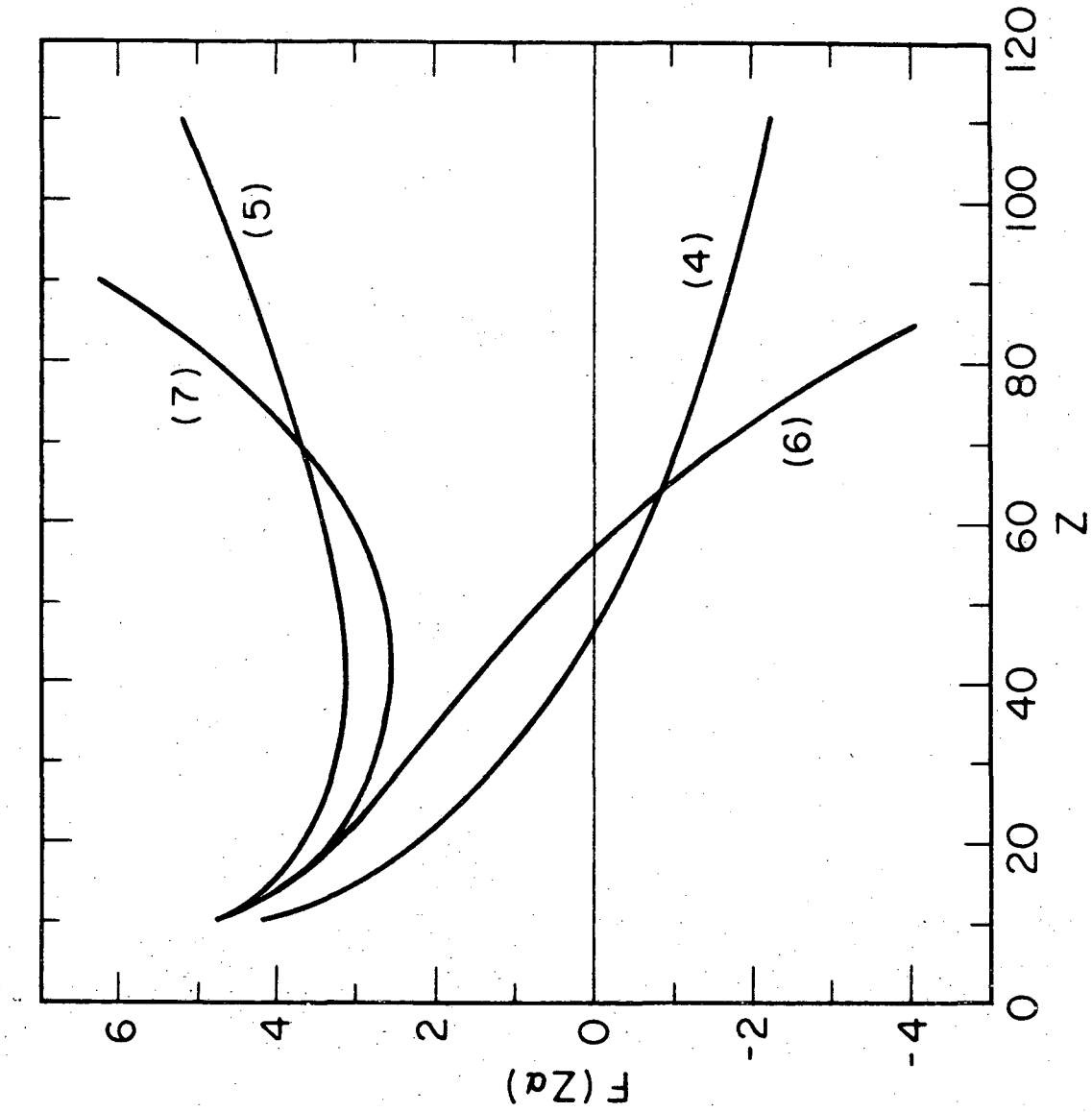

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Fig. 2

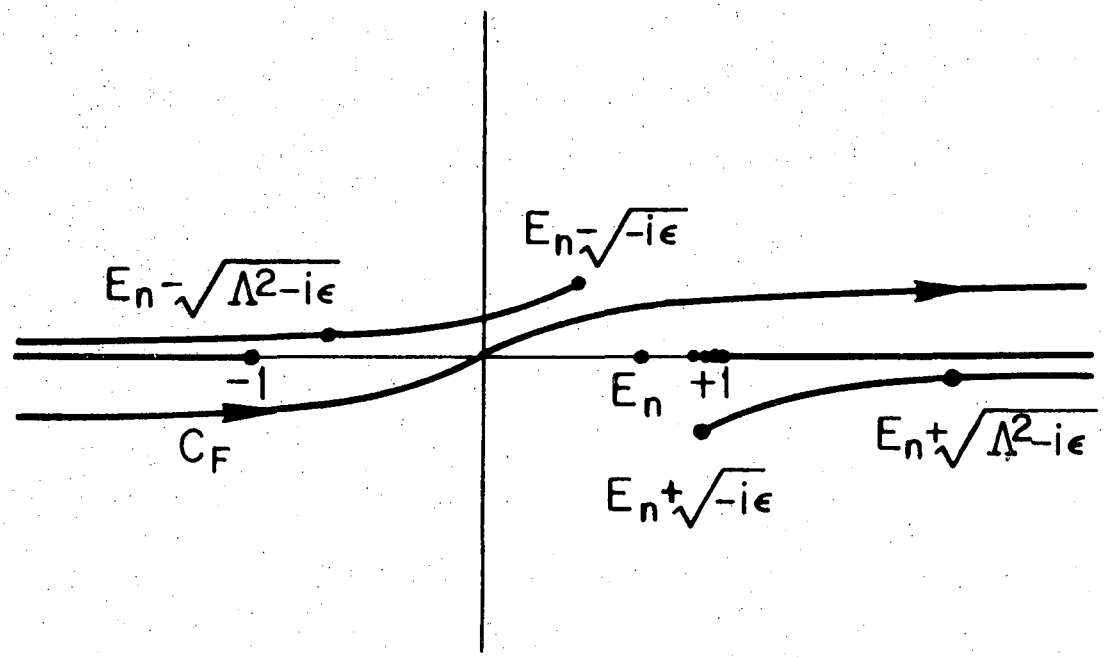

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Fig. 3

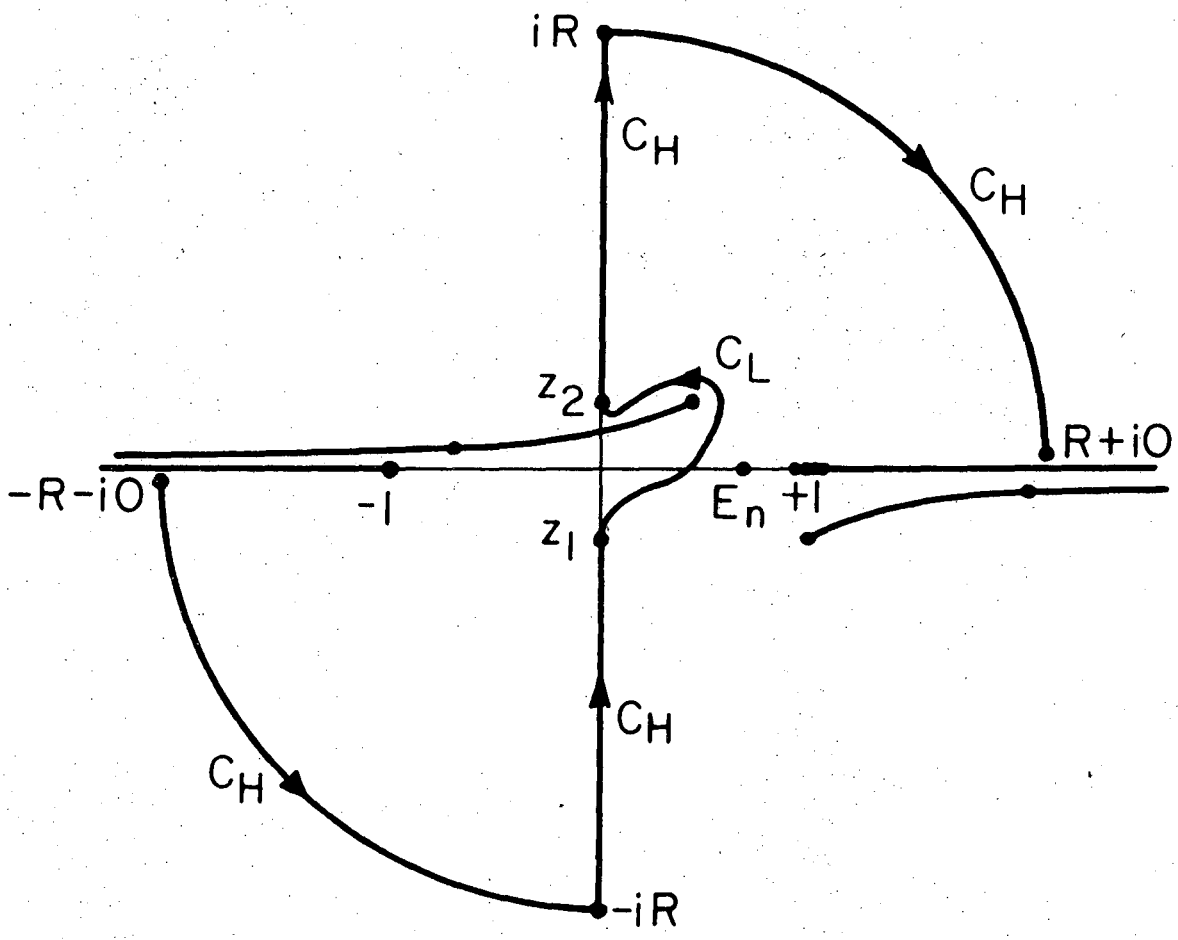

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Fig. 4

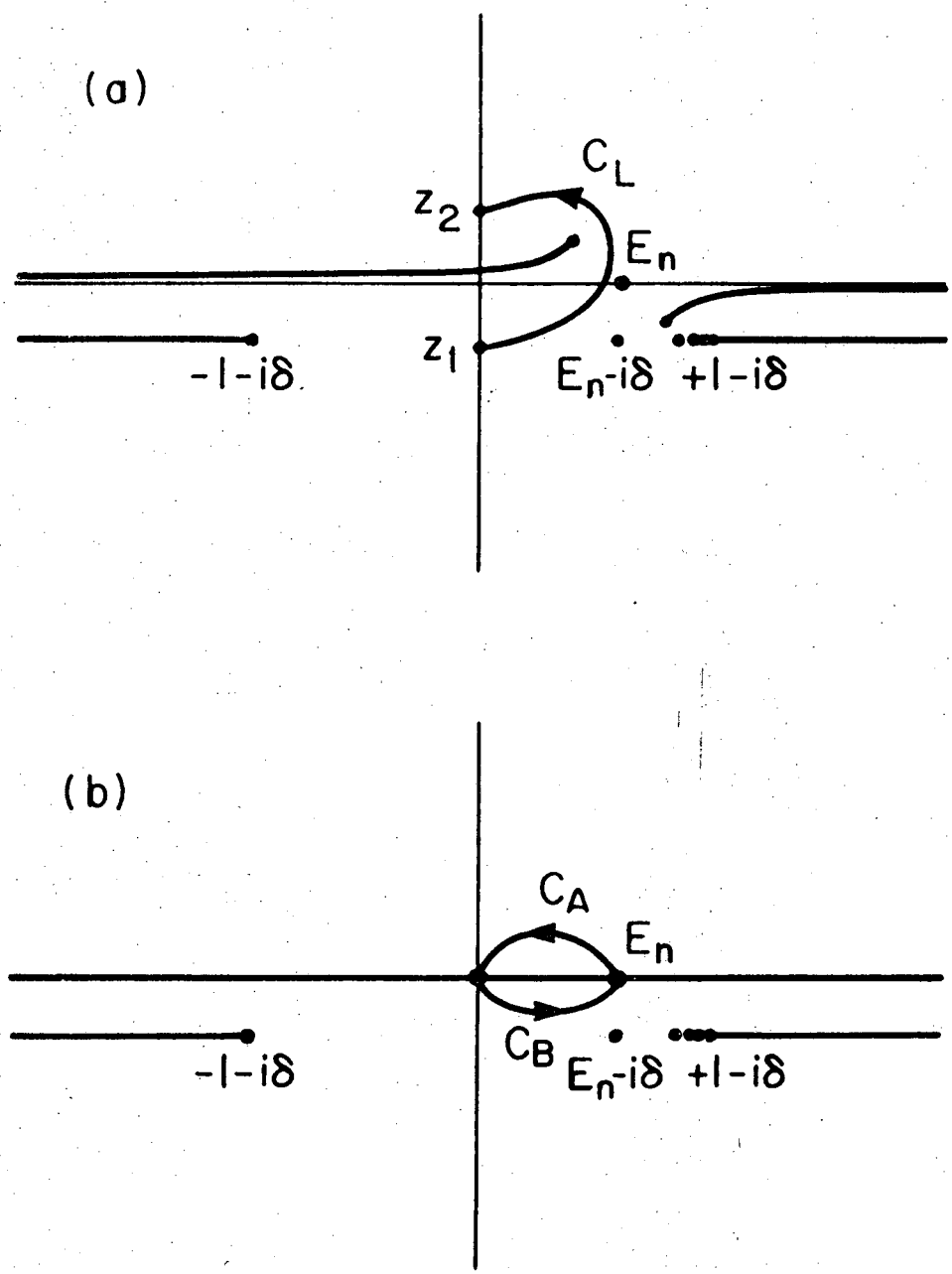

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Fig. 5

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