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RADIATIVE CORRECTIONS IN HYDROGEN-LIKE SYSTEMS

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(Ph. D. Thesis)

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RADIATIVE CORRECTIONS IN HYDROGEN-LIKE SYSTEMS

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RADIATIVE CORRECTIONS IN HYDROGEN-LIKE SYSTEMS*

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May 14, 1973

ABSTRACT

The one-photon self-energy radiative level shift of the $1S_{\frac{1}{2}}$ state of an electron in a Coulomb field is evaluated numerically for values of the nuclear charge $Z = 10,20,\cdots,110$. The evaluation is based on the known expressions for the Coulomb radial Green's functions and not on a power series expansion in $Z\alpha$. The errors in the values obtained are estimated to be less than 0.1%. The results are compared with the results of previous calculations.

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. 1.1(a) and 1.1(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

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

where

$$F(Z\alpha) = A_{40} + A_{41}\, \ell n(Z\alpha)^{-2} + A_{50}(Z\alpha) + A_{60}(Z\alpha)^2$$
$$+ A_{61}(Z\alpha)^2\, \ell n(Z\alpha)^{-2} + A_{62}(Z\alpha)^2\, \ell n^2(Z\alpha)^{-2} + A_{70}(Z\alpha)^3 + \cdots . \tag{1.2}$$

In Table 1.1, 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. 1.2. These curves give an indication of the nature of the convergence of the series in (1.2) as a function of Z. The series represents the function poorly for Z near 20, and is not a useful approximation 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 for 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 for the $1S_{\frac{1}{2}}$ state in a Coulomb potential for $Z = 70, 75, 80, 85, 90$ and evaluated the level shift for 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 $Z\alpha$ expansion.[12] The results of these calculations appear in Fig. 10.1.

Table 1.1. 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

In the present calculation, we evaluate, to all orders in $Z\alpha$, the self-energy radiative level shift of the $1S_{\frac{1}{2}}$ state of an electron in a Coulomb potential for Z in the range 10-110. The presentation is arranged as follows. In Sec. II, the computational procedure, including the procedure for mass renormalization, is formulated, and some trivial preliminary integrations are performed. The energy shift is divided into three parts which we call the low-energy part ΔE_L, the high-energy part ΔE_H, and the mass renormalization counter term ΔE_M. In Sec. III, some rearrangements are made in the expression for ΔE_L. The integrations over angles in coordinate space in that expression are performed in Sec. IV. The numerical evaluation of ΔE_L is described in Sec. V. In Sec. VI, 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 $\alpha(Z\alpha)^4$. The evaluation of ΔE_{HA}, including the isolation of terms to be cancelled by the mass renormalization counter term, is described in Sec. VII. The integrations over angles in coordinate space in ΔE_{HB} are performed in Sec. VIII. In Sec. IX, the numerical evaluation of ΔE_{HB} is described. The results of the calculation are summarized in Sec. X.

The numerical calculations were done with the CDC 7600 computer at the Lawrence Berkeley Laboratory.

II. PRELIMINARY INTEGRATION

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

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

where $\phi_n(x)$ is the bound-state wave function in coordinate space

$$\phi_n(x) = \psi_n(\underset{\sim}{x}) \exp(-iE_n t) , \tag{2.2}$$

and $\psi_n(\underset{\sim}{x})$ is a normalized solution of the time-independent Dirac equation;

$$[\underset{\sim}{\alpha}\cdot\underset{\sim}{p} + V(\underset{\sim}{x}) + \beta - E_n]\psi_n(\underset{\sim}{x}) = 0 \qquad V(\underset{\sim}{x}) = -\frac{Z\alpha}{|\underset{\sim}{x}|} . \tag{2.3}$$

The bar over the wave function denotes the adjoint: $\bar{\phi}_n(x) = \phi_n{}^\dagger(x)\gamma^0$. To keep the terms in the energy shift separately finite, we use the covariant regulator method,[19,20] where in momentum space the following replacement is made for the photon propagator:

$$\frac{1}{k^2 + i\epsilon} \to \lim_{\Lambda\to\infty}\left[\frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - \Lambda^2 + i\epsilon}\right] . \tag{2.4}$$

The limit is to be taken after the integrals in Eq. (2.1) have been evaluated. The photon propagator in coordinate space can then be expressed as

$$\frac{1}{2} D_F(x_2 - x_1) = \frac{i}{(2\pi)^4} \int d^4k \exp[-ik(x_2 - x_1)]$$

$$\left[\frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - \Lambda^2 + i\epsilon}\right] . \qquad (2.5)$$

The free electron mass shift δm, computed using the regulated photon propagator, is[19]

$$\delta m = \frac{\alpha}{\pi}\left(\frac{3}{4} \ln \Lambda^2 + \frac{3}{8}\right) . \qquad (2.6)$$

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

$$-\frac{1}{2}S_F^{\,e}(x_2,x_1) = \begin{cases} \sum\limits_{\text{pos } E_m} \psi_m(\underset{\sim}{x}_2)\bar{\psi}_m(\underset{\sim}{x}_1) \exp[-iE_m(t_2 - t_1)] & t_2 > t_1 \\ -\sum\limits_{\text{neg } E_m} \psi_m(\underset{\sim}{x}_2)\bar{\psi}_m(\underset{\sim}{x}_1) \exp[-iE_m(t_2 - t_1)] & t_2 < t_1 . \end{cases} \qquad (2.7)$$

An alternative expression for the propagation kernel is

$$-\frac{1}{2} S_F^{\,e}(x_2,x_1) = \frac{1}{2\pi i} \int_{C_F} dz \sum_{E_m} \frac{\psi_m(\underset{\sim}{x}_2)\bar{\psi}_m(\underset{\sim}{x}_1)}{E_m - z} \exp[-iz(t_2 - t_1)] . \qquad (2.8)$$

The contour C_F, which appears in Fig. 2.1, extends from $-\infty$ to $+\infty$, passing below the negative real axis and above the positive real axis. The sum in the integrand in (2.8) is the Green's function for the time-independent Dirac equation

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \sum_{E_m} \frac{\psi_m(\underset{\sim}{x}_2)\, \psi_m^{\dagger}(\underset{\sim}{x}_1)}{E_m - z} \qquad (2.9)$$

$$[\underset{\sim}{\alpha}\cdot\underset{\sim}{p}_2 + V(\underset{\sim}{x}_2) + \beta - z]G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \delta^3(\underset{\sim}{x}_2 - \underset{\sim}{x}_1) .$$

We note that the Green's function $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ is an analytic function of z except possibly for points of the spectrum of the Dirac Hamiltonian. The spectrum consists of the points on the real z-axis in the intervals $(-\infty,-1]$ and $[+1,+\infty)$, and 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

$$\Delta E_n(\Lambda) = \frac{i\alpha}{\pi} \frac{1}{(2\pi)^3} \int d(t_2 - t_1) d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1\, \psi_n^{\dagger}(\underset{\sim}{x}_2)\alpha_\mu \int_{C_F} dz$$

$$\times\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\alpha^\mu\psi_n(\underset{\sim}{x}_1) \int d^4k \exp[i\underset{\sim}{k}\cdot(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)]$$

$$\times \left(\frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - \Lambda^2 + i\epsilon}\right) \exp[-i(k_0 + z - E_n)(t_2 - t_1)]$$

$$- \delta m \int d^3\underset{\sim}{x}\psi_n^{\dagger}(\underset{\sim}{x})\beta\psi_n(\underset{\sim}{x}) . \qquad (2.10)$$

In order to do the integration over $t_2 - t_1$ first, we place in the integrand a convergence factor $\exp(-\delta|t_2 - t_1|)$, where δ temporarily satisfies the condition

$$\delta > |\mathrm{Im}(k_0 + z - E_n)| . \qquad (2.11)$$

We shall eventually let δ tend to zero. We now integrate over $t_2 - t_1$

$$\int_{-\infty}^{\infty} d(t_2 - t_1)\, \exp[-i(k_0 + z - E_n)(t_2 - t_1)]\, \exp(-\delta|t_2 - t_1|)$$

$$= \frac{i}{k_0 + z - E_n + i\delta} - \frac{i}{k_0 + z - E_n - i\delta} \quad . \qquad (2.12)$$

Equation (2.10) can be written

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

$$- \delta m \int d^3\underset{\sim}{x} \psi_n{}^\dagger(\underset{\sim}{x})\beta\psi_n(\underset{\sim}{x}) \qquad (2.13)$$

where

$$I_P = \frac{i}{(2\pi)^3} \int d^4k\, \exp[i\underset{\sim}{k}\cdot(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)] \left(\frac{1}{k^2 + i\epsilon} - \frac{1}{k^2 - \Lambda^2 + i\epsilon} \right)$$

$$\times \left(\frac{1}{k_0 + z - E_n + i\delta} - \frac{1}{k_0 + z - E_n - i\delta} \right) \quad . \qquad (2.14)$$

The integration over k in I_P is done next. It is convenient to integrate over k_0 first

$$\int_{-\infty}^{\infty} dk_0 \left(\frac{1}{k_0{}^2 - \underset{\sim}{k}^2 + i\epsilon} - \frac{1}{k_0{}^2 - \underset{\sim}{k}^2 - \Lambda^2 + i\epsilon} \right) \left(\frac{1}{k_0 + z - E_n + i\delta} - \frac{1}{k_0 + z - E_n - i\delta} \right)$$

$$= -2\pi i \left(\frac{1}{(E_n - z)^2 - \underset{\sim}{k}^2 + i\epsilon} - \frac{1}{(E_n - z)^2 - \underset{\sim}{k}^2 - \Lambda^2 + i\epsilon} \right) . \qquad (2.15)$$

Then we perform the integration over $\underset{\sim}{k}$ in I_P and obtain

$$I_P = -\frac{1}{(2\pi)^2} \int d^3\underset{\sim}{k}\, \exp[i\underset{\sim}{k}\cdot(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)] \left(\frac{1}{\underset{\sim}{k}^2 - (E_n - z)^2 - i\epsilon} - \frac{1}{\underset{\sim}{k}^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon} \right)$$

$$= -\frac{1}{2|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} [\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|) - \exp(-b'|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)] \qquad (2.16)$$

where

$$b = -i[(E_n - z)^2 + i\epsilon]^{\frac{1}{2}} \; ; \quad b' = -i[(E_n - z)^2 - \Lambda^2 + i\epsilon]^{\frac{1}{2}} \quad . \qquad (2.17)$$

The branches of the square roots are determined by the conditions

$$\mathrm{Re}(b) > 0 \; ; \quad \mathrm{Re}(b') > 0 \quad . \qquad (2.18)$$

The energy shift is now expressed as

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

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

$$- \delta m \int d^3\underset{\sim}{x} \psi_n{}^\dagger(\underset{\sim}{x})\beta\psi_n(\underset{\sim}{x}) \quad . \qquad (2.19)$$

In order to facilitate the evaluation of (2.19), we change the contour of integration C_F to a new contour, and divide the integral into two parts which correspond to integrals over separate 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. 2.1. 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 (2.18) 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. 2.2.

We now identify three contributions to 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 (2.19) 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 parts. The first part 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 part 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

$$\Delta E_M = -\delta m \int d^3\underset{\sim}{x}\, \psi_n^\dagger(\underset{\sim}{x})\beta\psi_n(\underset{\sim}{x}) \quad . \tag{2.20}$$

The total energy shift is

$$\Delta E_n = \Delta E_L + \Delta E_H + \Delta E_M \quad . \tag{2.21}$$

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

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

$$\times\ \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\,[\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|) - \exp(-b'|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)]\ . \qquad (3.1)$$

The contour C_L is shown in Fig. 2.2. It extends around the singularity in b from the point z_1 to the point z_2.

We examine the second term in the expression for ΔE_L

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

$$\times\ \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\exp(-b'|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)\ . \qquad (3.2)$$

The singularities of the integrand of the integral over z for this portion of ΔE_L are shown in Fig. 3.1. We now take the limit as $\epsilon \to 0+$ in $S(\Lambda)$. If we require

$$\Lambda > E_n\ , \qquad (3.3)$$

which is permissible since we are interested in the limit where $\Lambda \to \infty$, the singularity at $z = E_n - \Lambda$ lies on the negative real z-axis. Hence, as z_1 and z_2 approach zero, the path of integration C_L becomes a closed contour which contains no singularities, and thus the value of the integral approaches zero;

$$S(\Lambda) = 0 \qquad \text{for } \Lambda > E_n\ . \qquad (3.4)$$

Henceforth we assume that $\Lambda > E_n$. We then have

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

$$\times\ \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)\ . \qquad (3.5)$$

We now consider the limits $\epsilon \to 0+$, and $z_1, z_2 \to 0$ in Eq. (3.5). 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 to z in $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ which, in effect, displaces the singularities of $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ to below the real z-axis,

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) \to \lim_{\delta\to 0+} G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\ . \qquad (3.6)$$

Figure 3.2(a) shows the singularities of the integrand in (3.5) after the replacement indicated in (3.6) has been made. After the limits $\epsilon \to 0+$, $z_1, z_2 \to 0$, have been taken, the contour of integration C_L consists of two parts, as shown in Fig. 3.2(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 (2.18), we have

$$\begin{aligned} b &= -i(E_n - z) \qquad \text{for } z \text{ on } C_B \\ b &= +i(E_n - z) \qquad \text{for } z \text{ on } C_A\ . \end{aligned} \qquad (3.7)$$

Making the appropriate substitutions from (3.7) for b, and deforming the contours C_A and C_B to line segments along the real axis, we obtain

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

$$\times \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.8}$$

We consider the contribution $\Delta E_L^{\,0}$ which corresponds to $\mu = 0$ in (3.8):

$$\Delta E_L^{\,0} = \frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1\, \psi_n^\dagger(\underset{\sim}{x}_2)\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\, \psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.9}$$

The equation

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \frac{1}{E_n - z}\{\delta^3(\underset{\sim}{x}_2 - \underset{\sim}{x}_1) - [H(\underset{\sim}{x}_2) - E_n]\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\} \tag{3.10}$$

follows from the differential equation satisfied by $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$:

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

$$H(\underset{\sim}{x}_2) = -i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla}_2 + V(\underset{\sim}{x}_2) + \beta \quad . \tag{3.11}$$

Substituting the right-hand side of (3.10) for $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ in (3.9), we obtain

$$\Delta E_L^{\,0} = \frac{\alpha}{\pi}\int_0^{E_n} dz\, \frac{E_n - z}{E_n - z - i\delta} \int d^3\underset{\sim}{x}_2\, \psi_n^\dagger(\underset{\sim}{x}_2)\psi_n(\underset{\sim}{x}_2)$$

$$- \frac{\alpha}{\pi}\int_0^{E_n} dz\, \frac{1}{E_n - z - i\delta} \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1\, \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}$$

Equation (3.12) continued next page

Equation (3.12) continued

$$\times\, \psi_n^\dagger(\underset{\sim}{x}_2)[-i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla}_2 + V(\underset{\sim}{x}_2) + \beta - E_n]\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\psi_n(\underset{\sim}{x}_1) \quad . \tag{3.12}$$

Integrating the term containing $\underset{\sim}{\nabla}_2$ by parts, and taking the differential equation satisfied by $\psi^\dagger$ into account, we find

$$\Delta E_L^{\,0} = \frac{\alpha}{\pi} E_n + \frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \psi_n^\dagger(\underset{\sim}{x}_2)\alpha^j\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\psi_n(\underset{\sim}{x}_1)$$

$$\times\, (-i\nabla_2^{\,j})\, \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.13}$$

Note that δ has been set equal to zero wherever doing so introduces no ambiguity. We proceed in a similar manner making the substitution

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \frac{1}{E_n - z}\{\delta^3(\underset{\sim}{x}_2 - \underset{\sim}{x}_1) - G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)[H^\dagger(\underset{\sim}{x}_1) - E_n]\} \tag{3.14}$$

in (3.13). Again integrating by parts and taking the Dirac equation into account, we obtain

$$\Delta E_L^{\,0} = \frac{\alpha}{\pi} E_n + \frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \psi_n^\dagger(\underset{\sim}{x}_2)\alpha^j G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\alpha^\ell\psi_n(\underset{\sim}{x}_1)$$

$$\times\, \nabla_2^{\,j}\nabla_1^{\,\ell}\, \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)^2|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.15}$$

The remainder of ΔE_L is

$$\Delta E_L - \Delta E_L{}^0 = -\frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \psi_n{}^\dagger(\underset{\sim}{x}_2)\alpha^\ell G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\alpha^\ell \psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.16}$$

In view of the equation

$$[\nabla_2{}^2 + (E_n - z)^2] \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} = 0 \quad , \tag{3.17}$$

we can express (3.16) as

$$\Delta E_L - \Delta E_L{}^0 = -\frac{\alpha}{\pi}\int_0^{E_n} dz \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \psi_n{}^\dagger(\underset{\sim}{x}_2)\alpha^j G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\alpha^\ell \psi_n(\underset{\sim}{x}_1)$$

$$\times \delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)^2|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.18}$$

We then have

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

$$\times (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2{}^j\nabla_1{}^\ell) \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)^2|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \quad . \tag{3.19}$$

In order to examine the integral in (3.19), it is useful to make the substitution

$$(\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2{}^j\nabla_1{}^\ell) \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}$$

$$= \frac{1}{4\pi}\int d\Omega_k(\delta_{j\ell}k^2 - k_j k_\ell) \exp[i\underset{\sim}{k}\cdot(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)] \tag{3.20}$$

where $k = |\underset{\sim}{k}| = E_n - z$. We thus obtain

$$\Delta E_L = \frac{\alpha}{\pi} E_n - \frac{\alpha}{4\pi^2}\int_{k< E_n} d^3\underset{\sim}{k}\, \frac{1}{k}\left(\delta_{j\ell} - \frac{k_j k_\ell}{k^2}\right)\int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1$$

$$\times \psi_n{}^\dagger(\underset{\sim}{x}_2)\alpha^j \exp(i\underset{\sim}{k}\cdot\underset{\sim}{x}_2)G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z + i\delta)\alpha^\ell \exp(-i\underset{\sim}{k}\cdot\underset{\sim}{x}_1)\psi_n(\underset{\sim}{x}_1) \quad . \tag{3.21}$$

This equation can be written in the form

$$\Delta E_L = \frac{\alpha}{\pi} E_n - \frac{\alpha}{4\pi^2}\int_{k< E_n} d^3\underset{\sim}{k}\, \frac{1}{k} \sum_{m,\lambda} \frac{\langle n|\underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}|m\rangle\langle m|\underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}|n\rangle}{E_m - E_n + k - i\delta} \tag{3.22}$$

where $\underset{\sim}{\epsilon}_\lambda$ $(\lambda = 1,2)$ are polarization vectors perpendicular to $\underset{\sim}{k}$. 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 $k = E_n$. From the form of ΔE_L given in (3.22), it is apparent that we obtain the real part of ΔE_L by taking the Cauchy principal value of the integral over k.

IV. INTEGRATION OVER ANGLES IN THE EXPRESSION FOR THE LOW-ENERGY PART

We consider the matrix element which appears in the integrand in Eq. (3.19);

$$M = \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \psi_n^\dagger(\underset{\sim}{x}_2)\alpha^j G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\alpha^\ell \psi_n(\underset{\sim}{x}_1)$$

$$\times\ (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})\ \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)^2|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\ . \tag{4.1}$$

The bound-state wave functions can be written as

$$\psi_n(\underset{\sim}{x}) = \begin{bmatrix} f_1(x)\chi_{\kappa_n}^{\mu_n}(\hat{x}) \\ \\ if_2(x)\chi_{-\kappa_n}^{\mu_n}(\hat{x}) \end{bmatrix}\ , \tag{4.2}$$

where $\chi_\kappa^{\mu}(\hat{x})$ is the spin-angular function described in Appendix A, and $f_1(x)$ and $f_2(x)$ are the components of the radial wave function. The Green's function $G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ can be written as a sum over eigenfunctions of the operator K as described in Appendix A;

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$$

$$= \sum_\kappa \begin{bmatrix} G_\kappa^{11}(x_2,x_1,z)\pi_\kappa(\hat{x}_2,\hat{x}_1) & G_\kappa^{12}(x_2,x_1,z)i\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \\ \\ -G_\kappa^{21}(x_2,x_1,z)i\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_\kappa(\hat{x}_2,\hat{x}_1) & G_\kappa^{22}(x_2,x_1,z)\pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \end{bmatrix}. \tag{4.3}$$

We then have

$$M = \int d^3\underset{\sim}{x}_2 d^3\underset{\sim}{x}_1 \sum_\kappa$$

$$\times\ \{f_2(x_2)G_\kappa^{11}(x_2,x_1,z)f_2(x_1)\chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j\pi_\kappa(\hat{x}_2,\hat{x}_1)\sigma^\ell\chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$+\ f_2(x_2)G_\kappa^{12}(x_2,x_1,z)f_1(x_1)\chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell\chi_{\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$+\ f_1(x_2)G_\kappa^{21}(x_2,x_1,z)f_2(x_1)\chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_\kappa(\hat{x}_2,\hat{x}_1)\sigma^\ell\chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$+\ f_1(x_2)G_\kappa^{22}(x_2,x_1,z)f_1(x_1)\chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell\chi_{\kappa_n}^{\mu_n}(\hat{x}_1)\}$$

$$\times\ (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})\ \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)^2|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\ . \tag{4.4}$$

Let

$$T(\rho) = \frac{\sin[(E_n - z)\rho]}{(E_n - z)^2\rho} \tag{4.5}$$

where

$$\rho = |\underset{\sim}{x}_2 - \underset{\sim}{x}_1|\ . \tag{4.6}$$

We consider the integrals

$$A_\kappa^{11}(x_2,x_1) = \int d\Omega_2 d\Omega_1 \chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j\pi_\kappa(\hat{x}_2,\hat{x}_1)\sigma^\ell\chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$\times\ (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})T(\rho)$$

Equation (4.7) continued next page

Equation (4.7) continued

$$A_\kappa^{12}(x_2,x_1) = \int d\Omega_2 d\Omega_1 \chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j \underset{\sim}{\sigma}\cdot\hat{x}_2 \pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell \chi_{\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$\times\ (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})T(\rho)$$

$$A_\kappa^{21}(x_2,x_1) = \int d\Omega_2 d\Omega_1 \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j \underset{\sim}{\sigma}\cdot\hat{x}_2 \pi_{\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell \chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$\times\ (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})T(\rho)$$

$$A_\kappa^{22}(x_2,x_1) = \int d\Omega_2 d\Omega_1 \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\sigma^j \pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell \chi_{\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$\times\ (\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})T(\rho)\ . \qquad (4.7)$$

The derivatives of $T(\rho)$ in (4.7) are

$$\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1\ T(\rho) = \delta_{j\ell}(E_n - z)^2\ T(\rho)\ , \qquad (4.8)$$

and

$$\nabla_2^{\,j}\nabla_1^{\,\ell}\ T(\rho) = -\delta_{j\ell}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho) - (\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^j(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^\ell\frac{1}{\rho}\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho). \qquad (4.9)$$

Therefore, we write the equations

$$\sigma^j\pi_\kappa(\hat{x}_2,\hat{x}_1)\sigma^\ell\delta_{j\ell} = -\pi_\kappa(\hat{x}_2,\hat{x}_1) + \frac{|\kappa|}{\pi}P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)$$

Equation (4.10) continued next page

Equation (4.10) continued

$$\sigma^j\pi_\kappa(\hat{x}_2,\hat{x}_1)\sigma^\ell(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^j(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^\ell = -(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^2\pi_\kappa(\hat{x}_2,\hat{x}_1)$$

$$+ (\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^2\frac{|\kappa|}{2\pi}P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)$$

$$\sigma^j\ \underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell\delta_{j\ell} = -\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)$$

$$\sigma^j\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^j(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^\ell = -(\underset{\sim}{x}_2 - \underset{\sim}{x}_1)^2\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)$$

$$+ (\underset{\sim}{\sigma}\cdot\underset{\sim}{x}_2 - \underset{\sim}{\sigma}\cdot\underset{\sim}{x}_1)\frac{|\kappa|}{2\pi}\{x_2P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\}\ , \qquad (4.10)$$

where $\xi = \hat{x}_2\cdot\hat{x}_1$. The expressions on the right in (4.10) are obtained with the aid of the expression for $\pi_\kappa(\hat{x}_2,\hat{x}_1)$ given in (A.10). In obtaining the last line in (4.10), we took into account the Legendre polynomial identity in (A.15). From (4.8), (4.9), and (4.10), we find

$$\sigma^j\pi_\kappa(\hat{x}_2,\hat{x}_1)\sigma^\ell(\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2^{\,j}\nabla_1^{\,\ell})T(\rho)$$

$$= [-\pi_\kappa(\hat{x}_2,\hat{x}_1) + \frac{|\kappa|}{\pi}P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)]\times[(E_n - z)^2 + \frac{1}{\rho}\frac{\partial}{\partial\rho}]\ T(\rho)$$

$$+ [-\pi_\kappa(\hat{x}_2,\hat{x}_1) + \frac{|\kappa|}{2\pi}P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)]\ \rho\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho)$$

Equation (4.11) continued next page

Equation (4.11) continued

$$\sigma^j \underset{\sim}{\sigma}\cdot\hat{x}_2 \pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell(\delta_{j\ell}\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2{}^j\nabla_1{}^\ell)T(\rho)$$

$$= -\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\left[(E_n - z)^2 + \frac{1}{\rho}\frac{\partial}{\partial\rho}\right]T(\rho)$$

$$- \underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\,\rho\,\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho)$$

$$+ (\underset{\sim}{\sigma}\cdot\underset{\sim}{x}_2 - \underset{\sim}{\sigma}\cdot\underset{\sim}{x}_1)\frac{|\kappa|}{2\pi}\left\{x_2P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\right\}\frac{1}{\rho}\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho)\ . \tag{4.11}$$

Taking the trace of Eq. (4.9), we obtain

$$(E_n - z)^2\,T(\rho) + \rho\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho) = -3\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho)\ . \tag{4.12}$$

Hence

$$\sigma^j\pi_\kappa(\hat{x}_2,\hat{x}_1)\,\sigma^\ell(\delta_{j\ell}\,\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2{}^j\nabla_1{}^\ell)T(\rho)$$

$$= \frac{|\kappa|}{2\pi}P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\,(E_n - z)^2\,T(\rho)$$

$$+\left[\pi_\kappa(\hat{x}_2,\hat{x}_1) - \frac{|\kappa|}{4\pi}P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\right]\frac{2}{\rho}\frac{\partial}{\partial\rho}T(\rho) \tag{4.13}$$

$$\sigma^j\underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\sigma^\ell(\delta_{j\ell}\,\underset{\sim}{\nabla}_2\cdot\underset{\sim}{\nabla}_1 - \nabla_2{}^j\nabla_1{}^\ell)\,T(\rho)$$

$$= \underset{\sim}{\sigma}\cdot\hat{x}_2\pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\frac{2}{\rho}\frac{\partial}{\partial\rho}T(\rho) + (\underset{\sim}{\sigma}\cdot\underset{\sim}{x}_2 - \underset{\sim}{\sigma}\cdot\underset{\sim}{x}_1)$$

$$\times\ \frac{|\kappa|}{2\pi}\left\{x_2P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\right\}\frac{1}{\rho}\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho)\ .$$

In view of Eqs. (A.6), (A.12), and (A.14), we have

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

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

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

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

$$+ \left[x_2P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\right]$$

$$\left.\times\left[x_2P_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1P_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi)\right]\frac{1}{\rho}\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial}{\partial\rho}T(\rho)\right\}\ . \tag{4.14}$$

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

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

$$A^{22}_{\kappa,\kappa_n}(x_2,x_1) = A^{11}_{-\kappa,-\kappa_n}(x_2,x_1)\ . \tag{4.15}$$

We now specialize to the case of an $S_{\frac{1}{2}}$ state. For this case $\kappa_n = -1$, and the expressions for the $A_\kappa(x_2,x_1)$ are

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

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

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

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

$$A_\kappa^{21}(x_2,x_1) = -|\kappa| \int_{-1}^{1} d\xi \left\{ P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, \frac{1}{\rho}\, \frac{\partial}{\partial\rho}\, T(\rho) \right.$$

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

$$A_\kappa^{22}(x_2,x_1) = |\kappa| \int_{-1}^{1} d\xi\, P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)(E_n - z)^2\, T(\rho) \quad . \qquad (4.16)$$

In arriving at the above expression for $A_\kappa^{21}(x_2,x_1)$, we have taken the identity in (A.15) into account. We expand $T(\rho)$, which occurs in (4.16), in a Legendre series in ξ, and then integrate over ξ. We have

$$(E_n - z)\, T(\rho) = \frac{\sin[(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|]}{(E_n - z)|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}$$

$$= \sum_{\ell=0}^{\infty} (2\ell + 1)\, P_\ell(\xi)\, j_\ell(y_2)\, j_\ell(y_1) \qquad (4.17)$$

where j_ℓ is the spherical Bessel function, and

$$y_2 = (E_n - z)x_2 \; ; \qquad y_1 = (E_n - z)x_1 \; . \qquad (4.18)$$

In order to deal with the derivatives of $T(\rho)$ in (4.16), we note that

$$\frac{1}{\rho}\, \frac{\partial}{\partial\rho}\, T(\rho) = -\frac{1}{x_2 x_1}\, \frac{\partial}{\partial\xi}\, T(\rho) \qquad (4.19)$$

and

$$(x_2 - x_1\xi)\, \frac{1}{\rho}\, \frac{\partial}{\partial\rho}\, \frac{1}{\rho}\, \frac{\partial}{\partial\rho}\, T(\rho) = \frac{\partial}{\partial x_2}\, \frac{1}{\rho}\, \frac{\partial}{\partial\rho}\, T(\rho) \; . \qquad (4.20)$$

We thus obtain

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

$$\left. - \frac{1}{\kappa}(1-\xi^2)\, P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\, \frac{1}{x_2 x_1}\, \frac{\partial}{\partial\xi}\, T(\rho) \right\}$$

$$= |\kappa| \int_{-1}^{1} d\xi \left\{ \frac{(E_n - z)^2}{|2\kappa + 1|} \left[(|\kappa + \tfrac{1}{2}| + \tfrac{1}{2})\, P_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(\xi) \right.\right.$$

$$\left.\left. + (|\kappa + \tfrac{1}{2}| - \tfrac{1}{2})\, P_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(\xi) \right] - \frac{\kappa + 1}{x_2 x_1}\, P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) \right\} T(\rho)$$

$$= (E_n - z)|\kappa| \left\{ \frac{1}{|\kappa + \frac{1}{2}|} \left[(|\kappa + \tfrac{1}{2}| + \tfrac{1}{2}) j_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(y_2) \right.\right.$$

$$\times\, j_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(y_1) + (|\kappa + \tfrac{1}{2}| - \tfrac{1}{2}) j_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(y_2)$$

Equation (4.21) continued next page

Equation (4.21) continued

$$\times\ j_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(y_1)\Big] - 2\,\frac{\kappa+1}{y_2 y_1}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)$$

$$= 2(E_n - z)|\kappa|\Big[j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)$$

$$+ \frac{\kappa^2-1}{y_2 y_1}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)\Big] \qquad (4.21)$$

and

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

$$+ \Big[x_2 P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1 P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\Big] \frac{\partial}{\partial x_2}\Big\} \frac{1}{\rho}\frac{\partial}{\partial\rho} T(\rho)$$

$$= -|\kappa| \int_{-1}^{1} d\xi\, \frac{\partial}{\partial x_2}\Big[x_2 P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - x_1 P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\Big] \frac{1}{\rho}\frac{\partial}{\partial\rho} T(\rho)$$

$$= |\kappa| \int_{-1}^{1} d\xi\, \frac{\partial}{\partial x_2}\Big[(x_1 - x_2\xi) P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) - \frac{x_2}{\kappa}(1-\xi^2) P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\Big]$$

$$\times\ \frac{1}{\rho}\frac{\partial}{\partial\rho} T(\rho)$$

$$= |\kappa| \int_{-1}^{1} d\xi\, \frac{\partial}{\partial x_2}\Big[\frac{\partial}{\partial x_1} P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) + \frac{1}{x_1\kappa}(1-\xi^2) P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\frac{\partial}{\partial\xi}\Big] T(\rho)$$

$$= |\kappa| \int_{-1}^{1} d\xi\, \frac{\partial}{\partial x_2}\Big[\frac{\partial}{\partial x_1} P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) + \frac{\kappa+1}{x_1} P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\Big] T(\rho)$$

Equation (4.22) continued next page

Equation (4.22) continued

$$= 2(E_n - z)|\kappa| \frac{\partial}{\partial y_2} j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)$$

$$\times \Big[\frac{\partial}{\partial y_1} j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1) + \frac{\kappa+1}{y_1} j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)\Big]$$

$$= 2(E_n - z)\,\kappa\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1) \quad . \qquad (4.22)$$

The corresponding expression for $A_\kappa^{21}(x_2,x_1)$ is easily obtained by observing that

$$A_\kappa^{21}(x_2,x_1) = A_\kappa^{12}(x_1,x_2) \quad . \qquad (4.23)$$

We also find

$$A_\kappa^{22}(x_2,x_1) = 2(E_n - z)|\kappa|\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1) \ . \qquad (4.24)$$

Hence, for an arbitrary $S_{\frac{1}{2}}$ state, we have

$$M = 2(E_n - z)\int_0^\infty dx_2 x_2^2 \int_0^\infty dx_1 x_1^2 \sum_\kappa$$

$$\Big\{ f_2(x_2) G_\kappa^{11}(x_2,x_1,z) f_2(x_1)|\kappa| \Big[j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)$$

$$+ \frac{\kappa^2-1}{y_2 y_1} j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)\Big]$$

$$+ f_2(x_2) G_\kappa^{12}(x_2,x_1,z)\, f_1(x_1)\,\kappa\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1)$$

Equation (4.25) continued next page

Equation (4.25) continued

$$+ f_1(x_2)\, G_\kappa^{21}(x_2,x_1,z)\, f_2(x_1)\, \kappa\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_2)\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1)$$

$$+ f_1(x_2)\, G_\kappa^{22}(x_2,x_1,z)\, f_1(x_1)\, |\kappa| j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1)\Big\} \quad . \tag{4.25}$$

V. NUMERICAL EVALUATION OF THE LOW-ENERGY PART ΔE_L

The real part of the low-energy part of the energy shift is

$$\mathrm{Re}(\Delta E_L) = \frac{\alpha}{\pi} E_n - \frac{\alpha}{\pi} P \int_0^{E_n} dz\, M\ , \tag{5.1}$$

where M is defined in (4.1), and given for $S_{\frac{1}{2}}$ states in (4.25). We consider only the special case of the $1S_{\frac{1}{2}}$ state. In this case, specification of the principal value of the integral over z is not necessary, because there is no bound-state pole in the integrand in the interval $(0,E_n)$. We have

$$\Delta E_L = \frac{\alpha}{\pi} E_n - \frac{\alpha}{\pi} \int_0^{E_n} dz (E_n - z) \frac{(2\gamma)^{3-2\delta}}{\Gamma(3-2\delta)} \int_0^\infty dx_2 \int_0^\infty dx_1$$

$$\times\ e^{-\gamma(x_2+x_1)} (x_2 x_1)^{2-\delta} \sum_\kappa \Big\{ (1 - E_n)\, G_\kappa^{11}(x_2,x_1,z)\, |\kappa|$$

$$\times \Big[j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1) + \frac{\kappa^2 - 1}{y_2 y_1}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_1) \Big]$$

$$- \gamma\, G_\kappa^{12}(x_2,x_1,z)\, \kappa\, j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1)$$

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

$$+ (1 + E_n)\, G_\kappa^{22}(x_2,x_1,z)\, |\kappa| j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_2)\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(y_1) \Big\} \tag{5.2}$$

where

$$\gamma = Z\alpha \; ; \qquad \delta = 1 - (1 - \gamma^2)^{\frac{1}{2}}$$

$$y_2 = (E_n - z)x_2 \; ; \quad y_1 = (E_n - z)x_1 \quad . \tag{5.3}$$

The expression which appears in (5.2) is in a form suitable for direct numerical evaluation by a computer. We shall first briefly outline the method we use, and then give a detailed description of each step. The triple integral which appears in (5.2) is evaluated, after a change of variables, by Gaussian quadrature. For each value of $Z\alpha$, the multiple integral is evaluated several times. In each successive evaluation, the number of integration points in each dimension is increased. In this way, a convergent sequence of values for the integral is obtained. The integrand is in the form of an infinite sum over κ. This sum is evaluated for each set of values of the integration variables. The most significant contribution to the sum comes from terms for which $|\kappa| \lesssim y$, where y is the smaller of the arguments of the spherical Bessel functions. For $|\kappa| \gtrsim y$, the terms in the sum approach zero rapidly as $|\kappa|$ increases. The spherical Bessel functions and radial Green's functions which appear in the individual terms in the sum are evaluated by algorithms which are described in Appendices B and C.

We introduce new variables of integration in the expression (5.2):

$$t = 1 - \frac{z}{E_n} \; ; \qquad \begin{array}{ll} y = 2\gamma x_1 \; ; & r = \dfrac{x_2}{x_1} \quad \text{for} \quad x_2 < x_1 \\ y = 2\gamma x_2 \; ; & r = \dfrac{x_1}{x_2} \quad \text{for} \quad x_2 > x_1 \quad . \end{array} \tag{5.4}$$

Employing these variables, and noting that the integrand is symmetric under interchange of x_2 and x_1, we have

$$\Delta E_L = \frac{\alpha}{\pi}\left\{E_n + \int_0^1 dt \int_0^\infty dy \int_0^1 dr\; S(r,y,t,\gamma)\right\} \tag{5.5}$$

where

$$\begin{aligned} S(r,y,t,\gamma) = & -\frac{2E_n^{\,2}(2\gamma)^{-3}}{\Gamma(3-2\delta)}\, t r^{2-\delta}\, y^{5-2\delta}\, e^{-y}\, e^{\frac{1}{2}(1-r)y} \\ & \times \sum_\kappa \Bigg\{ (1 - E_n)\, G_\kappa^{11}\left(\frac{ry}{2\gamma}, \frac{y}{2\gamma}, E_n(1-t)\right) |\kappa| \Bigg[j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\left(\frac{ryE_n t}{2\gamma}\right) \\ & \times j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\left(\frac{yE_n t}{2\gamma}\right) + (\kappa^2 - 1)\frac{(2\gamma)^2}{ry^2E_n^{\,2}t^2}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\left(\frac{ryE_n t}{2\gamma}\right) \\ & \times j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\left(\frac{yE_n t}{2\gamma}\right)\Bigg] - \gamma\, G_\kappa^{12}\left(\frac{ry}{2\gamma}, \frac{y}{2\gamma}, E_n(1-t)\right) \kappa j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\left(\frac{ryE_n t}{2\gamma}\right) \\ & \times j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\left(\frac{yE_n t}{2\gamma}\right) - \gamma\, G_\kappa^{21}\left(\frac{ry}{2\gamma}, \frac{y}{2\gamma}, E_n(1-t)\right) \kappa j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\left(\frac{ryE_n t}{2\gamma}\right) \\ & \times j'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\left(\frac{yE_n t}{2\gamma}\right) + (1 + E_n)\, G_\kappa^{22}\left(\frac{ry}{2\gamma}, \frac{y}{2\gamma}, E_n(1-t)\right) \\ & \times |\kappa| j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\left(\frac{ryE_n t}{2\gamma}\right) j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\left(\frac{yE_n t}{2\gamma}\right)\Bigg\} \quad . \end{aligned} \tag{5.6}$$

We next examine the sum over κ to establish the nature of its convergence. Let $T_\kappa(r,y,t,\gamma)$ be the quantity in curly brackets in (5.6) summed over both signs of κ. We then have

$$S(r,y,t,\gamma) = -\frac{2E_n^{\,2}(2\gamma)^{-3}}{\Gamma(3-2\delta)}\, t r^{2-\delta}\, y^{5-2\delta}\, e^{-y}\, e^{\frac{1}{2}(1-r)y} \sum_{\kappa=1}^{\infty} T_\kappa(r,y,t,\gamma). \tag{5.7}$$

The asymptotic behavior of $T_\kappa(r,y,t,\gamma)$ as $\kappa \to \infty$ is found from the asymptotic behavior of the radial Green's functions shown in (A.30) and from the asymptotic behavior of j_ℓ and j'_ℓ when $\ell \to \infty$:

$$j_\ell(x) \sim \frac{\ell!}{(2\ell+1)!}(2x)^\ell; \quad j'_\ell(x) \sim \frac{\ell}{x}\frac{\ell!}{(2\ell+1)!}(2x)^\ell . \tag{5.8}$$

The asymptotic form, when $\kappa \to \infty$, is

$$T_\kappa(r,y,t,\gamma) \sim (1-E_n)\left[\gamma + (1+E_n - E_n t)\frac{y}{2\gamma}\right] r^{-3}\left(\frac{2\gamma}{y}\right)^6$$

$$\times (E_n t)^{-4}\, \kappa^2 \left[\frac{\kappa!}{(2\kappa)!}\right]^2 \left(\frac{E_n try}{\gamma}\right)^{2\kappa} . \tag{5.9}$$

We obtain an indication of the rate of convergence of the sum over κ in (5.7), for κ large, by estimating the remainder

$$R_N = \sum_{\kappa=N+1}^{\infty} A_\kappa , \tag{5.10}$$

where A_κ is the asymptotic form of T_κ given in the right side of (5.9). We have

$$A_{N+1+m} = \left(\frac{N+1+m}{N+1}\right)^2 \left[\frac{(N+1+m)!(2N+2)!}{(N+1)!(2N+2+2m)!}\right]^2 \left(\frac{E_n try}{\gamma}\right)^{2m} A_{N+1} , \tag{5.11}$$

and therefore

$$A_{N+1+m} \le \left(\frac{N+1+m}{N+1}\right)^2 \left[\frac{E_n try}{(2N+3)2\gamma}\right]^{2m} A_{N+1} . \tag{5.12}$$

One can easily show that

$$\sum_{m=0}^{\infty} (N+1+m)^2 x^{2m} < \frac{(N+1)^2}{(1-x^2)^3} \tag{5.13}$$

$$0 < x^2 < 1 ; \quad N \ge 1 .$$

Hence, if N is ≥ 1, and so large that

$$\frac{E_n try}{(2N+3)2\gamma} < 1 , \tag{5.14}$$

we find

$$R_N < \frac{A_{N+1}}{\left[1 - \left(\frac{E_n try}{(2N+3)2\gamma}\right)^2\right]^3} . \tag{5.15}$$

We conclude that for large enough N, R_N approaches zero quite rapidly as N increases. More precisely, we have

$$\lim_{N\to\infty} \frac{R_N}{\left(\frac{e}{2N}\frac{E_n try}{2\gamma}\right)^{2N}} = C \tag{5.16}$$

where C is a constant independent of N.

The above discussion indicates the nature of the convergence of the partial sums

$$S_N = \sum_{\kappa=1}^{N} T_\kappa \tag{5.17}$$

when N is so large that the terms T_κ, $\kappa > N$, are well approximated by the asymptotic forms A_κ. Actually, the partial sums are often

close to the limit before N is sufficiently large for the asymptotic form to be a good approximation. The rapid decrease of T_κ arises as follows. Consider the Bessel function and its derivative which contain the smaller argument in T_κ. For κ greater than the smaller argument, the asymptotic forms in (5.8) are good approximations for these functions. For such κ, it is evident from the asymptotic forms that these functions decrease rapidly as κ increases. On the other hand, the other factors in T_κ are relatively slowly varying as κ increases. Therefore, for κ greater than the smaller of the arguments of the Bessel functions, T_κ decreases rapidly as κ increases, and the partial sums S_N converge rapidly. The behavior of T_κ as a function of κ, for some values of the other parameters, is illustrated in Fig. 5.1. In the numerical computation of $S(r,y,t,\gamma)$, we terminate the sum over κ at $\kappa = N$ when both of the following conditions are met:

$$|T_{N+1}| < 10^{-15}\left|\sum_{\kappa=1}^{N} T_\kappa\right|; \qquad N > \frac{ryE_n t}{2\gamma} . \tag{5.18}$$

We now describe the procedure we use for evaluating $S(r,y,t,\gamma)$. The evaluation is performed by a subroutine which, given a value for each of the arguments r, y, t, and γ, computes the value of $S(r,y,t,\gamma)$. First, a number L

$$L = \frac{ryE_n t}{\gamma} + 25 \tag{5.19}$$

is computed. We find empirically that this number is always larger, and not excessively larger, than the smallest N which satisfies (5.18). The Bessel functions and their derivatives, which appear in

(5.6), with indices in the range 0 to L, are computed with the method described in Appendix B, and stored in arrays. Then, the sum over κ is performed. The radial Green's functions are evaluated as described in Appendix C. The summation over κ is terminated at $\kappa = N$, where N is the smallest number which satisfies the conditions in (5.18). Finally, the sum is multiplied by the remaining factors which appear in (5.7). The evaluation of the gamma function is described in Appendix D.

With values for $S(r,y,t,\gamma)$ available, we numerically evaluate the integrals which appear in (5.5). The integrals are done by repeated one-dimensional Gaussian quadrature with new variables of integration which are defined in subsequent discussion. Integrals evaluated numerically over the interval $(0,1)$ are done, with the appropriate linear mapping to the interval $(-1,1)$, by Gauss-Legendre quadrature; integrals evaluated numerically over the interval $(0,\infty)$ are done by Gauss-Laguerre quadrature.[21] We design the integration scheme to give the result correctly to 11 significant figures when $Z = 10$. The corresponding accuracy in the physically interesting part of the result is much less, for the following reason. The low-energy part ΔE_L is of order α (see Appendix E), while the renormalized self energy is well known to be of order $\alpha(Z\alpha)^4$. Hence, in the worst case that we consider here, i.e., $Z = 10$, the physically interesting part of the number we compute is smaller than the number itself by a factor of order $(10\alpha)^4 \approx 3 \times 10^{-5}$.

In order to motivate the choice of variables used in the r and y integrations, we consider a simple function which exhibits the qualitative features of the dependence of $S(r,y,t,\gamma)$ on its variables. To find such a function, we recall that the main

contribution to the sum $S(r,y,t,\gamma)$ comes from values of κ for which

$$|\kappa| < \frac{ryE_n t}{2\gamma} ,$$

and hence, for $|\kappa| < \frac{ry}{2\gamma}$. Therefore, we expect that the behavior of the sum is qualitatively reproduced by the expression obtained if the radial Green's functions are replaced by their asymptotic forms, for $\frac{ry}{2\gamma} \gg |\kappa|$, which appear in (A.28). Taking the last term in (5.6) as a typical term in the sum, and making the above-mentioned replacement for the radial Green's functions, we obtain

$$S(r,y,t,\gamma) \sim \frac{E_n^{\,2}(1 + E_n)}{\Gamma(3 - 2\delta)} \frac{1 - z}{2\gamma c} t r^{1-\delta-\nu} y^{3-2\delta} e^{-y}$$

$$\times e^{-\frac{1}{2}(\frac{c}{\gamma}-1)(1-r)y} \sum_{\kappa} |\kappa| \, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\left(\frac{ryE_n t}{2\gamma}\right) j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\left(\frac{yE_n t}{2\gamma}\right) , \tag{5.20}$$

where $c = (1 - z^2)^{\frac{1}{2}}$ and $z = E_n(1 - t)$. Here, the symbol $\sim$ means the functions on either side are qualitatively similar in their dependence on the variables. We perform the sum over κ, and replace the relatively slowly varying factors by 1. The result is

$$S(r,y,t,\gamma) \sim e^{-y} e^{-\frac{1}{2}(\frac{c}{\gamma}-1)(1-r)y} \frac{\sin\left[\frac{E_n ty}{2\gamma}(1 - r)\right]}{(1 - r)} . \tag{5.21}$$

The factor $(\frac{c}{\gamma} - 1)$ in the exponent is positive for the range of values of the energy z under consideration.

We now consider the integral

$$S_1(y,t,\gamma) = \int_0^1 dr \, S(r,y,t,\gamma) . \tag{5.22}$$

We note that the qualitative r dependence, from (5.21), of the integrand is

$$e^{-q(1-r)} \frac{\sin[\theta q(1 - r)]}{(1 - r)} \tag{5.23}$$

where

$$q = \frac{1}{2}(\frac{c}{\gamma} - 1)y ; \qquad 0 < q < \infty$$

$$0 < \theta < \left(\frac{1 + \gamma}{1 - \gamma}\right)^{\frac{1}{2}} . \tag{5.24}$$

For $Z \leq 110$, we have $\theta < \pi$. For q large, the sine function in (5.23) oscillates rapidly as r varies, but the oscillations are strongly damped by the exponential. To numerically evaluate the integral in (5.22), we employ the following prescription:

for $0 < q \leq 10$

$$S_1(y,t,\gamma) = \int_0^1 dx \; 2x \, S(x^2,y,t,\gamma) \qquad N = [q] + 9$$

for $10 < q \leq 30$

$$S_1(y,t,\gamma) = \int_0^1 dx \, S(x,y,t,\gamma) \qquad N = \min([0.4q] + 8,18)$$

Equation (5.25) continued next page

Equation (5.25) continued

for $30 < q \leq 100$

$$S_1(y,t,\gamma) = \int_0^1 dx\, \frac{30}{q}\, S\left(1 - \frac{30}{q}\, x,y,t,\gamma\right) + \epsilon \qquad N = 18$$

for $q > 100$

$$S_1(y,t,\gamma) = \int_0^\infty dx\, \frac{1}{q}\, \bar{S}\left(1 - \frac{x}{q},y,t,\gamma\right) \qquad N = 8 \tag{5.25}$$

where N is the number of integration points used to evaluate the integral, $\bar{S}$ is given by

$$\bar{S}(r,y,t,\gamma) = \begin{cases} S(r,y,t,\gamma) & 0 < r < 1 \\ 0 & r \leq 0\,, \end{cases} \tag{5.26}$$

and ϵ is given by

$$\epsilon = \int_1^{\frac{q}{30}} dx\, \frac{30}{q}\, S\left(1 - \frac{30}{q}\, x,y,t,\gamma\right)$$

$$\approx \int_1^{\frac{q}{30}} dx\, e^{-30x}\, e^{-y} \approx 3 \times 10^{-15}\, e^{-y}\,. \tag{5.27}$$

We arrived at the above prescription in the following way. We examined the integral numerically for $\gamma = 10\alpha$ and sample values of y and t which cover the range of values given for these variables when the integrals over y and t are evaluated. For each fixed value of y and t, we tried various variables of integration in the

integral over r, and for each variable of integration, we tried various numbers of points in the integration formula. A choice of integration variable and number of integration points was considered acceptable if the resulting value for the integral was correct to 11 places beyond the decimal point, and the rate of convergence was good. The correctness of the result was judged by varying the number of points in the integration formula and observing the degree of stability of the resulting values for the integral. By good rate of convergence, we mean one for which increasing the number of integration points by two, decreases the error in the result by approximately a factor of 10.

We next consider the integral

$$S_2(t,\gamma) = \int_0^\infty dy\, S_1(y,t,\gamma)\,. \tag{5.28}$$

The dominant y dependence of the integrand is simply

$$e^{-y}\,. \tag{5.29}$$

The method we use to numerically evaluate the integral in (5.28) is as follows:

$$S_2(t,\gamma) = S_{21}(t,\gamma) + S_{22}(t,\gamma) + S_{23}(t,\gamma)$$

$$S_{21}(t,\gamma) = \int_0^1 dx\, S_1(x,t,\gamma) \qquad N = 14$$

$$S_{22}(t,\gamma) = \int_0^1 dx\, 4S_1(1 + 4x,t,\gamma) \qquad N = 12$$

Equation (5.30) continued next page

Equation (5.30) continued

$$S_{23}(t,\gamma) = \int_0^\infty dx\, S_1(5 + x,t,\gamma) \qquad N = 6 . \qquad (5.30)$$

The number N is the number of integration points used to evaluate the integral. We arrived at this method of evaluation by examining the numerical behavior of the integral in (5.28) for $\gamma = 10\alpha$ and sample values for t. For each value of t, we tried various variables of integration and numbers of integration points to evaluate the integral. In choosing a method, we applied the same criterion of acceptability as in the integration over r.

We finally consider the integral over t

$$S_3(\gamma) = \int_0^1 dt\, S_2(t,\gamma) . \qquad (5.31)$$

The most significant feature of the integrand in (5.31) is the presence of the bound-state poles near $t = 0$. This integral is numerically evaluated as follows:

$$S_3(\gamma) = S_{31}(\gamma) + S_{32}(\gamma)$$

$$S_{31}(\gamma) = \int_0^1 dx\, 0.3x^2\, S_2(0.1x^3,\gamma) \qquad N = 14$$

$$S_{32}(\gamma) = \int_0^1 dx\, 2.7x^2\, S_2(0.1 + 0.9x^3,\gamma) \qquad N = 10 . \qquad (5.32)$$

The number N is again the number of integration points used in the numerical evaluation of each integral. We arrived at this method by using the same approach as was used in the preceding integrations.

For $Z = 10, 20, 30, 50, 70, 90$, and 110, we numerically evaluate the integrals in (5.5) three times, employing the variables displayed in Eqs. (5.25), (5.30), and (5.32). In the first evaluation, the number of integration points used to evaluate each integral is two less than the value given for N for that integral. In the second evaluation, the number of integration points used to evaluate each integral is equal to the value given for N for that integral. In the third evaluation, the number of integration points is two greater than the value given for N. For $Z = 40, 60, 80$, and 100, the integrals are evaluated once with the number of integration points equal to the values given for N. The results of these evaluations are listed in Table 5.1.

As we noted earlier, the physically interesting part of the energy shift is of order $\alpha(Z\alpha)^4$. Terms of lower order in $Z\alpha$ cancel when all contributions to the energy shift are combined. The lower order terms in the low-energy part are calculated in Appendix E. Taking into consideration the result of that calculation, we isolate the significant portion of the low-energy part in a function $f_L(Z\alpha)$, defined by

$$\Delta E_L = \frac{\alpha}{\pi}\left[\frac{3}{2}\langle\beta\rangle_n + \frac{7}{6}\langle V\rangle_n + (Z\alpha)^4 f_L(Z\alpha)\right] . \qquad (5.33)$$

The values for $f_L(Z\alpha)$ corresponding to the numbers obtained for $S_3(Z\alpha)$ are listed in Table 5.1.

If, in the sets of three values for $S_3(Z\alpha)$ obtained for $Z = 10, 20, 30, 50, 70, 90$, and 110, the difference between the second and third numbers is taken as an approximate measure of the error in the second number, then the order of magnitude of that error

Table 5.1.

Z	$S_3(Z\alpha)$	$f_L(Z\alpha)$
10	0.492604558261	5.885057461
	0.492604558212	5.885055755
	0.492604558219	5.885055985
20	0.471522661337	4.399376065
	0.471522662028	4.399377589
	0.471522662053	4.399377644
30	0.438918124592	3.635616766
	0.438918122718	3.635615950
	0.438918122834	3.635616000
40	0.397217582472	3.157389794
50	0.348910859260	2.832339685
	0.348910857608	2.832339592
	0.348910857653	2.832339594
60	0.296473044488	2.604438382
70	0.242325295399	2.446696882
	0.242325282906	2.446696699
	0.242325282216	2.446696689
80	0.188809276812	2.346786654
90	0.138167108750	2.302805682
	0.138167073328	2.302805492
	0.138167073750	2.302805494
100	0.092524835161	2.325000983
110	0.053885535012	2.447660167
	0.053885561168	2.447660230
	0.053885562857	2.447660234

is a fairly slowly varying function of Z. In view of this, one can infer the magnitude of error in the values of $S_3(Z\alpha)$ for $Z = 40$, 60, 80, and 100 by interpolation. We note that the errors, as defined above, in the values for $S_3(Z\alpha)$ increase as Z increases. This is to be expected as the integration scheme is designed for $Z = 10$. On the other hand, the errors in the values for $f_L(Z\alpha)$ decrease as Z increases because the effect in $f_L(Z\alpha)$ of the error in $S_3(Z\alpha)$ becomes relatively less important.

As a test against errors in algebra or programming in the evaluation of the low-energy part, we check the behavior of the numbers in Table 5.1 in the limit $Z\alpha \to 0$. From (E.14), we find

$$\lim_{Z\alpha \to 0} S_3(Z\alpha) = \frac{1}{2} . \tag{5.34}$$

This condition, which is not very stringent, appears to be satisfied. The behavior of $f_L(Z\alpha)$ provides a better test. It follows from known results and subsequent work that

$$f_L(Z\alpha) = \frac{4}{3} \ln(Z\alpha)^{-2} - 1.5546\ldots + \mathcal{O}(Z\alpha) . \tag{5.35}$$

[This relation is obtained by combining the known series in (1.2) with Eqs. (10.3), (7.39), and (F.14).] We check for this behavior by plotting values of the function

$$f_L(Z\alpha) - \frac{4}{3} \ln(Z\alpha)^{-2} \tag{5.36}$$

and the limit point in Fig. 5.2. The calculated points in this figure are consistent with the limit point. We note that a deviation of 10^{-5} in the value for $S_3(Z\alpha)$ at $Z = 10$ would produce a deviation of 0.35 in $f_L(Z\alpha)$ which is enough to destroy the consistency in Fig. 5.2.

VI. THE HIGH-ENERGY PART ΔE_H

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

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

$$\times \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\left[\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|) - \exp(-b'|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)\right] . \qquad (6.1)$$

The contour C_H is described in Sec. II, and pictured in Fig. 2.2. In order to display some features of the expression in (6.1), we restore the integral over $\underset{\sim}{k}$ which appears in (2.16). We then have

$$\Delta E_H = -\frac{i\alpha}{4\pi^3}\int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1 \int_{C_H} dz \int d^3\underset{\sim}{k}\left(\frac{1}{\underset{\sim}{k}^2 - (E_n - z)^2 - i\epsilon}\right.$$

$$\left. - \frac{1}{\underset{\sim}{k}^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon}\right)\psi_n^\dagger(\underset{\sim}{x}_2)\, \alpha_\mu\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}_2}\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$$

$$\times\, \alpha^\mu\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}_1}\, \psi_n(\underset{\sim}{x}_1)$$

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

$$\left. - \frac{1}{\underset{\sim}{k}^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon}\right)\alpha_\mu \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - z}\,\alpha^\mu \left|n\right\rangle . \qquad (6.2)$$

For fixed Λ, the integrand in (6.2) 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 (6.2), 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. 2.2).

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

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

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

$$+ \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z}\, V\, \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - z}\, V\, \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} . \qquad (6.3)$$

We substitute (6.3) into (6.2), and consider the contribution of the last term in (6.3) to ΔE_H:

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

$$\left. - \frac{1}{\underset{\sim}{k}^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon}\right)$$

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

$$\times\, V\, \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z}\,\alpha^\mu \left|n\right\rangle . \qquad (6.4)$$

A count of powers in the integrand shows that the convergence of the integrals over z and $\underset{\sim}{k}$ is uniform in Λ. Hence the term containing Λ gives no contribution in the limit $\Lambda \to \infty$. Furthermore, the

expression in (6.4) is of order $\alpha(Z\alpha)^4$ (see Appendix F). Hence, the part of ΔE_H which we wish to isolate arises from the terms

$$\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} - \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} V \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} \tag{6.5}$$

in (6.3). For the second term in (6.5), we write

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

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

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

$$- \frac{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + z}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} [\underset{\sim}{\alpha}\cdot\underset{\sim}{p}, V] \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} \quad . \tag{6.6}$$

The contribution of the last three terms in (6.6) to ΔE_H is

$$\frac{i\alpha}{4\pi^3}\left\langle n \middle| \int_{C_H'} dz \int d^3\underset{\sim}{k}\left(\frac{1}{\underset{\sim}{k}^2 - (E_n - z)^2 - i\epsilon} - \frac{1}{k^2 + \Lambda^2 - (E_n - z)^2 - i\epsilon}\right)\right.$$

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

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

Equation (6.7) continued next page

Equation (6.7) continued

$$\left.\left. - \frac{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + z}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} [\underset{\sim}{\alpha}\cdot\underset{\sim}{p}, V] \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}\right)\alpha^\mu \middle| n \right\rangle \quad . \tag{6.7}$$

Again, a count of powers in the integrand of the integrals over z and $\underset{\sim}{k}$ shows that we may ignore the term which contains Λ. This is more easily seen, in the case of the first of the three terms, with the aid of the identity

$$\left[\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}, V\right] = \frac{1}{\underset{\sim}{k}^2 + 1 - z^2}\left[\frac{2\underset{\sim}{p}\cdot\underset{\sim}{k} - \underset{\sim}{p}^2}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}, V\right] \quad . \tag{6.8}$$

The expression in (6.7) is of order $\alpha(Z\alpha)^4$. This is shown explicitly in Appendix F.

We now write

$$\Delta E_H = \Delta E_{HA} + \Delta E_{HB} \tag{6.9}$$

where

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

$$\alpha_\mu\left(\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z} - V \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} - 2z(\beta + z)\, V \frac{1}{[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]^2}\right) \alpha^\mu \left| n \right\rangle \quad , \tag{6.10}$$

and ΔE_{HB} is equal to the sum of the expressions in (6.4) and (6.7). The term ΔE_{HA} is just the part of ΔE_H described in the beginning of the preceding paragraph. It is evaluated in Sec. VII.

The remainder of the high-energy part ΔE_{HB} is evaluated in coordinate space. The separation of ΔE_H given by (6.9) and (6.10) corresponds to the separation of the (abstract) Green's function $G(z)$ into two parts $G_A(z)$ and $G_B(z)$ where

$$G(z) = G_A(z) + G_B(z) , \tag{6.11}$$

and

$$G_A(z) = \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} + \beta - z} - \frac{1}{2}\left\{V, \frac{1}{p^2 + 1 - z^2}\right\} - z(\beta + z) \times \left\{V, \frac{1}{[p^2 + 1 - z^2]^2}\right\} . \tag{6.12}$$

The curly brackets in (6.12) denote the symmetric product: $\{A,B\} = AB + BA$. The symmetrization is introduced merely for convenience, and does not affect the result. This is easily seen by considering a typical term in (6.10):

$$\left\langle n \middle| \alpha_\mu V \int d\Omega_k \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} \alpha^\mu \middle| n \right\rangle = \left\langle n \middle| (\alpha^\mu)^\dagger \left(\int d\Omega_k \times \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} \right)^\dagger V^\dagger (\alpha_\mu)^\dagger \middle| n \right\rangle = \left\langle n \middle| \alpha_\mu \int d\Omega_k \times \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} V \alpha^\mu \middle| n \right\rangle . \tag{6.13}$$

The first equality in (6.13) holds because the expectation value is real. The coordinate-space representation of $G_A(z)$ is

$$G_A(\underset{\sim}{x}_2, \underset{\sim}{x}_1, z) = \left[-i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla}_2 + \beta + z + \frac{1}{2}\left(\frac{\gamma}{x_2} + \frac{\gamma}{x_1}\right) \times \left(1 - \frac{z(\beta + z)}{c}\frac{\partial}{\partial c}\right)\right] \frac{e^{-c|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}}{4\pi|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \tag{6.14}$$

where $\gamma = Z\alpha$ and $c = (1 - z^2)^{\frac{1}{2}}$, $\mathrm{Re}(c) > 0$. With the aid of the expansion

$$\frac{e^{-c|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}}{4\pi|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} = -c \sum_\kappa j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_>)\, \pi_\kappa(\hat{x}_2, \hat{x}_1) \tag{6.15}$$

in which $x_< = \min(x_2, x_1)$, $x_> = \max(x_2, x_1)$, j_ℓ is the spherical Bessel function, and $h^{(1)}_\ell$ is the spherical Hankel function of the first kind [π_κ appears in (A.11)], and with the aid of the identities

$$-i\underset{\sim}{\alpha}\cdot\underset{\sim}{\nabla}_2 = -i\underset{\sim}{\alpha}\cdot\hat{x}_2 \frac{1}{x_2}\frac{\partial}{\partial x_2} x_2 + i\underset{\sim}{\alpha}\cdot\hat{x}_2 \frac{\underset{\sim}{\sigma}\cdot\underset{\sim}{L}_2 + 1}{x_2}$$

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{L}_2 + 1)\pi_\kappa(\hat{x}_2, \hat{x}_1) = -\kappa\, \pi_\kappa(\hat{x}_2, \hat{x}_1) , \tag{6.16}$$

we obtain

$$G_A(\underset{\sim}{x}_2, \underset{\sim}{x}_1, z) = \sum_\kappa \begin{bmatrix} G^{11}_{A,\kappa}(x_2, x_1, z)\pi_\kappa(\hat{x}_2, \hat{x}_1) & G^{12}_{A,\kappa}(x_2, x_1, z) i\underset{\sim}{\sigma}\cdot\hat{x}_2 \pi_{-\kappa}(\hat{x}_2, \hat{x}_1) \\ -G^{21}_{A,\kappa}(x_2, x_1, z)\, i\underset{\sim}{\sigma}\cdot\hat{x}_2\, \pi_\kappa(\hat{x}_2, \hat{x}_1) & G^{22}_{A,\kappa}(x_2, x_1, z)\pi_{-\kappa}(\hat{x}_2, \hat{x}_1) \end{bmatrix} \tag{6.17}$$

where

$$G^{11}_{A,\kappa}(x_2,x_1,z) = F_\kappa^{11}(x_2,x_1,z) + \frac{\gamma}{2}\frac{x_2+x_1}{x_2x_1c^2}\{(1+2\kappa z)F_\kappa^{11}(x_2,x_1,z)$$

$$- z(z+1)[x_2F_\kappa^{21}(x_2,x_1,z) + x_1F_\kappa^{12}(x_2,x_1,z)]\}$$

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

$$G^{21}_{A,\kappa}(x_2,x_1,z) = F_\kappa^{21}(x_2,x_1,z) \qquad (6.18)$$

$$G^{22}_{A,\kappa}(x_2,x_1,z) = F_\kappa^{22}(x_2,x_1,z) - \frac{\gamma}{2}\frac{x_2+x_1}{x_2x_1c^2}\{(1+2\kappa z)F_\kappa^{22}(x_2,x_1,z)$$

$$- z(z-1)[x_2F_\kappa^{12}(x_2,x_1,z) + x_1F_\kappa^{21}(x_2,x_1,z)]\} \ .$$

The F's in (6.18) are elements of the free radial Green's functions, and are given explicitly in (A.32). The expression in (6.17) is the analog of the expression in (A.25) 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

$$G^{ij}_{B,\kappa}(x_2,x_1,z) = G_\kappa^{ij}(x_2,x_1,z) - G^{ij}_{A,\kappa}(x_2,x_1,z) \qquad i,j = 1,2 \ . \qquad (6.19)$$

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

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

$$\times \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|}\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|) \ . \qquad (6.20)$$

VII. NUMERICAL EVALUATION OF ΔE_{HA}

Upon rationalizing the denominator and summing over μ in (6.10), we obtain

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

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

$$\left.\left. + V\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} - 2z(2\beta - z)\,V\frac{1}{[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]^2}\right)\right|n\right\rangle \ . \qquad (7.1)$$

The integrals over $\underset{\sim}{k}$ are performed with the aid of the following identities, valid for $\mathrm{Re}(b) > 0$ and $\mathrm{Re}(c) > 0$:

$$\int d^3\underset{\sim}{k}\,\frac{1}{\underset{\sim}{k}^2 + b^2}\,\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + c^2} = 2\pi^2\int_0^\infty d\eta\,\frac{1}{p^2 + (\eta + b + c)^2}$$

$$\int d^3\underset{\sim}{k}\,\frac{1}{\underset{\sim}{k}^2 + b^2}\,\frac{k^j}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + c^2} = \pi^2\int_0^\infty d\eta\left[1 + \frac{b^2 - c^2}{(\eta + b + c)^2}\right]$$

$$\frac{p^j}{p^2 + (\eta + b + c)^2}$$

$$\int d^3\underset{\sim}{k}\,\frac{1}{\underset{\sim}{k}^2 + b^2}\,\frac{1}{[(\underset{\sim}{p} - \underset{\sim}{k})^2 + c^2]^2} = \frac{\pi^2}{c}\,\frac{1}{p^2 + (b + c)^2} \ . \qquad (7.2)$$

Taking these identities and the equation satisfied by $\langle n|$ into account, we have

$$\Delta E_{HA} = -\frac{i\alpha}{2\pi}\left\langle n\left|\int_{C'_H} dz[J(p^2,b) - J(p^2,b')]\right|n\right\rangle \tag{7.3}$$

where

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

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

$$\times\ V\frac{1}{p^2 + (b + c)^2} \tag{7.4}$$

and where

$$\begin{aligned} b &= -i[(E_n - z)^2 + i\epsilon]^{\frac{1}{2}} && \mathrm{Re}(b) > 0 \\ b' &= -i[(E_n - z)^2 - \Lambda^2 + i\epsilon]^{\frac{1}{2}} && \mathrm{Re}(b') > 0 \\ c &= (1 - z^2)^{\frac{1}{2}} && \mathrm{Re}(c) > 0 \ . \end{aligned} \tag{7.5}$$

For the terms containing p^2, we make the substitution

$$\frac{1}{p^2 + a^2} = \frac{1}{a^2} - \frac{p^2}{a^2(p^2 + a^2)} \ . \tag{7.6}$$

In the resulting expression, the integral over η can be performed easily in the terms corresponding to the first term on the right side in (7.6). In the terms corresponding to the second term on the right in (7.6), the integrands in the integrals over z and η fall off

sufficiently rapidly as $|z|$ and $\eta \to \infty$ that there is no contribution from the terms containing Λ when $\Lambda \to \infty$. We thus have

$$\Delta E_{HA} = \Delta E_{HA}{}^1 + \Delta E_{HA}{}^2 + \mathcal{O}(\Lambda^{-1}) \tag{7.7}$$

where

$$\Delta E_{HA}{}^1 = -\frac{i\alpha}{2\pi}\left\langle n\left|\int_{C'_H} dz[J(0,b) - J(0,b')]\right|n\right\rangle \tag{7.8}$$

and where

$$J(0,b) = \frac{4E_n - 2z}{b + c} + \left[\frac{4}{3}\frac{1}{b + c} - \frac{8}{3}\frac{c}{(b + c)^2} + \frac{2}{c(b + c)^2}\right]V$$

$$- \frac{4z}{c(b + c)^2}\beta V \ . \tag{7.9}$$

We consider $\Delta E_{HA}{}^2$ subsequently.

We now consider the integral over z in (7.8). We shall evaluate one of the terms in detail to display the method used, and just list the values for the remaining terms. The term we examine is

$$I = \frac{1}{i}\int_{C'_H} dz\ z\left(\frac{1}{b + c} - \frac{1}{b' + c}\right) \ . \tag{7.10}$$

The integral is written as the sum of two terms corresponding to z on the negative imaginary axis and z on the positive imaginary axis. The limits $\epsilon \to 0$ and $z_1, z_2 \to 0$, prescribed at the end of Sec. II, are taken in each integral. The appropriate branches of the functions b and b' are taken in each case. In terms of the variable $y = -iz$, we have

$$I = i\int_{-\infty}^{0} dy\, y\left(\frac{1}{(1+y^2)^{\frac{1}{2}} - y - iE_n} - \frac{1}{(1+y^2)^{\frac{1}{2}} + (\Lambda^2 + y^2 + 2iyE_n - E_n^{\,2})^{\frac{1}{2}}}\right)$$

$$+ i\int_{0}^{\infty} dy\, y\left(\frac{1}{(1+y^2)^{\frac{1}{2}} + y + iE_n} - \frac{1}{(1+y^2)^{\frac{1}{2}} + (\Lambda^2 + y^2 + 2iyE_n - E_n^{\,2})^{\frac{1}{2}}}\right)$$

$$= 2\,\mathrm{Im}\int_{0}^{\infty} dy\, y\left(\frac{1}{(1+y^2)^{\frac{1}{2}} + y - iE_n} - \frac{1}{(1+y^2)^{\frac{1}{2}} + (\Lambda^2 + y^2 - 2iyE_n - E_n^{\,2})^{\frac{1}{2}}}\right) . \qquad (7.11)$$

Introducing a new variable of integration $t = (1+y^2)^{\frac{1}{2}} - y$ into the integral in (7.11) gives

$$I = \frac{1}{2}\,\mathrm{Im}\int_{0}^{1} dt\, \frac{1-t^4}{t^2}\left[\frac{1}{1 - iE_n t} - \frac{1}{\frac{1}{2}(1+t^2) + (t^2\Lambda^2 + \frac{1}{4} - \frac{1}{2}t^2 + \frac{1}{4}t^4 - iE_n(t - t^3) - t^2E_n^{\,2})^{\frac{1}{2}}}\right]. \qquad (7.12)$$

For fixed Λ, the integral in (7.12) is well defined. The first term in the integrand is infinite at $t = 0$, and behaves like $t^{-2} + iE_n t^{-1}$. Subtracting this function from the first term in the integrand and

adding it to the second leads to two well-defined integrals. The first of these is easily evaluated:

$$\frac{1}{2}\,\mathrm{Im}\int_{0}^{1} dt\left[\frac{1-t^4}{t^2}\,\frac{1}{1 - iE_n t} - \left(\frac{1}{t^2} + \frac{iE_n}{t}\right)\right]$$

$$= -\frac{E_n}{4}\left[1 + \frac{1 - E_n^{\,2}}{E_n^{\,2}} - \frac{1 - E_n^{\,4}}{E_n^{\,4}}\,\ell n(1 + E_n^{\,2})\right] . \qquad (7.13)$$

To order Λ^{-1}, the second integral is equal to

$$\frac{1}{2}\,\mathrm{Im}\int_{0}^{1} dt\,\frac{1}{t^2}\left[1 + iE_n t - \frac{1}{\frac{1}{2} + (t^2\Lambda^2 + \frac{1}{4} - iE_n t)^{\frac{1}{2}}}\right] . \qquad (7.14)$$

The terms which have been ignored in arriving at the integral in (7.14) give no contribution in the limit $\Lambda \to \infty$. A typical correction is of the form

$$\left|\int_{0}^{1} dt\,\frac{1}{\left[\frac{1}{2} + (t^2\Lambda^2 + \frac{1}{4} - iE_n t)^{\frac{1}{2}}\right]^2}\right| < \int_{0}^{1} dt\,\frac{1}{(\Lambda^2 t^2 + \frac{1}{4})}$$

$$= \frac{1}{\Lambda}\int_{0}^{\Lambda} dx\,\frac{1}{(x^2 + \frac{1}{4})} = \mathcal{O}(\Lambda^{-1}) . \qquad (7.15)$$

The integral in (7.14) is evaluated with the aid of the expansion

$$\frac{1}{\frac{1}{2} + (t^2\Lambda^2 + \frac{1}{4} - iE_n t)^{\frac{1}{2}}} = \frac{1}{\frac{1}{2} + (t^2\Lambda^2 + \frac{1}{4})^{\frac{1}{2}}}$$

$$+ \frac{\frac{1}{2}\,iE_n t}{\left[\frac{1}{2} + (t^2\Lambda^2 + \frac{1}{4})^{\frac{1}{2}}\right]^2 (t^2\Lambda^2 + \frac{1}{4})^{\frac{1}{2}}} + \cdots . \qquad (7.16)$$

Terms beyond the second in this expansion give no contribution to the integral in the limit $\Lambda \to \infty$. Substituting (7.16) into (7.14) and introducing the new variable of integration $u = (\Lambda^2 t^2 + \frac{1}{4})^{\frac{1}{2}} - \frac{1}{2}$, we obtain to order Λ^{-1}

$$\frac{E_n}{2}\int_0^1 dt\,\frac{1}{t}\left[1 - \frac{1}{2\left[\frac{1}{2} + (t^2\Lambda^2 + \frac{1}{4})^{\frac{1}{2}}\right]^2 (t^2\Lambda^2 + \frac{1}{4})^{\frac{1}{2}}}\right]$$

$$= \frac{E_n}{4}\int_0^\Lambda du\,\frac{4 + 5u + 2u^2}{(1+u)^3} = \frac{E_n}{4}\left[\ln \Lambda^2 + \frac{3}{2}\right] . \tag{7.17}$$

In this way, we obtain the following integrals:

$$\frac{1}{i}\int_{C_H'} dz\left[\frac{1}{b+c} - \frac{1}{b'+c}\right] = \frac{1}{2}\left[\ln \Lambda^2 - 1 + \frac{1 - E_n^2}{E_n^2}\ln(1 + E_n^2)\right] + \mathcal{O}(\Lambda^{-1})$$

$$\frac{1}{i}\int_{C_H'} dz\, z\left[\frac{1}{b+c} - \frac{1}{b'+c}\right] = \frac{E_n}{4}\left[\ln \Lambda^2 + \frac{1}{2} - \frac{1 - E_n^2}{E_n^2} + \frac{1 - E_n^4}{E_n^4}\ln(1 + E_n^2)\right] + \mathcal{O}(\Lambda^{-1})$$

$$\frac{1}{i}\int_{C_H'} dz\left[\frac{c}{(b+c)^2} - \frac{c}{(b'+c)^2}\right] = \frac{1}{4}\left[\ln \Lambda^2 - \frac{1}{2} - \frac{(3 - E_n^2)(1 - E_n^2)}{E_n^2(1 + E_n^2)} + \frac{(3 + E_n^2)(1 - E_n^2)}{E_n^4}\ln(1 + E_n^2)\right] + \mathcal{O}(\Lambda^{-1})$$

Equation (7.18) continued next page

Equation (7.18) continued

$$\frac{1}{i}\int_{C_H'} dz\,\frac{1}{c(b+c)^2} = \left[1 + \frac{1 - E_n^2}{1 + E_n^2} - \frac{1}{E_n^2}\ln(1 + E_n^2)\right]$$

$$\frac{1}{i}\int_{C_H'} dz\,\frac{z}{c(b+c)^2} = \frac{1}{E_n}\left[1 - \frac{1}{E_n^2}\ln(1 + E_n^2)\right] . \tag{7.18}$$

In order to express the part of $\Delta E_{HA}{}^1$ of order lower than $\alpha(Z\alpha)^4$ in terms of the expectation values $\langle\beta\rangle_n = \langle n|\beta|n\rangle$ and $\langle V\rangle_n = \langle n|V|n\rangle$, we take into account the relations

$$\langle E_n - \beta\rangle_n = 0$$

$$\langle (E_n - \beta)V\rangle_n = \mathcal{O}\left((Z\alpha)^4\right)$$

$$1 - E_n^2 = -\langle\beta V\rangle_n . \tag{7.19}$$

We then find

$$\Delta E_{HA}{}^1 = \frac{\alpha}{\pi}\left[\left(\frac{3}{4}\ln \Lambda^2 - \frac{9}{8}\right)\langle\beta\rangle_n + \left(\frac{1}{2}\ln 2 - \frac{17}{12}\right)\langle V\rangle_n + (Z\alpha)^4 f_{HA}{}^1(Z\alpha)\right] \tag{7.20}$$

where

$$(Z\alpha)^4 f_{HA}{}^1(Z\alpha) = \left[\frac{(1 - E_n^2)(3 + 2E_n^2)}{3E_n^2(1 + E_n^2)} - \frac{1}{2}\ln 2 - \frac{4 - 9E_n^2 + 3E_n^4}{4E_n^4}\times \ln(1 + E_n^2)\right]\langle V\rangle_n + \left[\frac{9}{4} - \frac{9 - 3E_n^2}{4E_n^2}\ln(1 + E_n^2)\right]\left\langle\left(1 - \frac{\beta}{E_n}\right)V\right\rangle_n . \tag{7.21}$$

The above formula is valid for any bound state. For the $1S_{\frac{1}{2}}$ state, we have

$$E_{1S}^{\;2} = 1 - (Z\alpha)^2$$

$$\langle V\rangle_{1S} = \frac{-(Z\alpha)^2}{[1 - (Z\alpha)^2]^{\frac{1}{2}}} \tag{7.22}$$

$$\left\langle\left(1 - \frac{\beta}{E_{1S}}\right)V\right\rangle_{1S} = 0 \ .$$

Numerical values for $f_{HA}^{\;1}(Z\alpha)$ are listed in Table 7.1. We note that

$$\lim_{Z\alpha\to 0} f_{HA}^{\;1}(Z\alpha) = -\frac{7}{12} - \frac{1}{4}\,\ell n\, 2 \ . \tag{7.23}$$

We now consider $\Delta E_{HA}^{\;2}$ given by

$$\Delta E_{HA}^{\;2} = \frac{i\alpha}{2\pi}\left\langle n\left|\int_{C_H'} dz\left\{\int_0^\infty d\eta\left[4E_n - 2z + \left(3 + \frac{b^2 - c^2}{(\eta + b + c)^2}\right)\right.\right.\right.\right.$$

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

$$\left.\left.\times\ \frac{p^2}{p^2 + (\eta + b + c)^2} - \frac{2z}{c}\,\frac{2\beta - z}{(b + c)^2}\,V\,\frac{p^2}{p^2 + (b + c)^2}\right\}\right|n\right\rangle \ . \tag{7.24}$$

In the integral over z, we introduce the variable of integration $y = -iz$. We then have

$$\frac{1}{i}\int_{C_H'} dz\, A(z,b,c) = \int_{-\infty}^{0} dy\, A\left(iy, -y - iE_n, (1 + y^2)^{\frac{1}{2}}\right)$$

$$+ \int_0^\infty dy\, A\left(iy, y + iE_n, (1 + y^2)^{\frac{1}{2}}\right)$$

$$= 2\,\mathrm{Re}\int_0^\infty dy\, A\left(-iy, y - iE_n, (1 + y^2)^{\frac{1}{2}}\right) \ , \tag{7.25}$$

valid for $A^*(z,b,c) = A(z^*,b^*,c)$ which is the case in (7.24). We next introduce the variable of integration $s = (1 + y^2)^{\frac{1}{2}} + y$, and then shift the variable of integration η by an amount $-s$: $\eta \to \eta - s$. The resulting expression is

$$\Delta E_{HA}^{\;2} = -\frac{\alpha}{2\pi}\left\langle n\left|\mathrm{Re}\int_1^\infty ds\left\{(1 + s^{-2})\int_s^\infty d\eta\left[4E_n + i(s - s^{-1})\right.\right.\right.\right.$$

$$+ \left(3 - \frac{1 + E_n^{\;2} + iE_n(s - s^{-1})}{(\eta - iE_n)^2}\right)(\beta - E_n)$$

$$\left. + \left(1 - \frac{1 + E_n^{\;2} + iE_n(s - s^{-1})}{(\eta - iE_n)^2}\right)V\right]\frac{1}{(\eta - iE_n)^2}\,\frac{p^2}{p^2 + (\eta - iE_n)^2}$$

$$\left.\left. + i(1 - s^{-2})\,\frac{4\beta + i(s - s^{-1})}{(s - iE_n)^2}\,V\,\frac{p^2}{p^2 + (s - iE_n)^2}\right\}\right|n\right\rangle \ . \tag{7.26}$$

The form of the double integral over η and s, which appears in (7.26), is modified with the replacement

$$\int_1^\infty ds \int_s^\infty d\eta\, B(s,\eta) \rightarrow \int_1^\infty ds \int_1^s d\eta\, B(\eta,s) \; . \tag{7.27}$$

The integration over η is easily performed. We obtain

$$\Delta E_{HA}^{\;2} = -\frac{\alpha}{2\pi} \left\langle n \middle| \mathrm{Re} \int_1^\infty ds(s - s^{-1}) \left\{ 4E_n + \tfrac{i}{2}(s - s^{-1}) \right.\right.$$

$$+ \left(3 - \frac{1 + E_n^{\;2} + \frac{i}{2} E_n(s - s^{-1})}{(s - iE_n)^2} \right) (\beta - E_n)$$

$$\left. + \left(s^{-2} - \frac{1 + E_n^{\;2} + \frac{i}{2} E_n(s - s^{-1})}{(s - iE_n)^2} \right) V + 4is^{-1}\beta V \right\}$$

$$\left. \times \frac{1}{(s - iE_n)^2} \frac{p^2}{p^2 + (s - iE_n)^2} \middle| n \right\rangle \; . \tag{7.28}$$

The integration over s is elementary (the algebra is somewhat lengthy). The result is expressed as

$$\Delta E_{HA}^{\;2} = \frac{\alpha}{\pi} \left\langle n \middle| \{ E_n Q_1(p^2) + \beta Q_2(p^2)\right.$$

$$\left. + VQ_3(p^2) + \frac{\beta}{E_n} VQ_4(p^2) \} p^2 \middle| n \right\rangle \tag{7.29}$$

where

$$Q_j(p^2) = B_j(p) + B_j(-p) \qquad j = 1,2,3,4 \tag{7.30}$$

and where

$$B_1(p) = \frac{(1 + E_n^{\;2})^2}{16E_n p^5} \left\{ \ln[1 + (E_n + p)^2] - \frac{2E_n p}{1 + E_n^{\;2}} + \frac{(3 - E_n^{\;2})2E_n p^3}{3(1 + E_n^{\;2})^3} \right\}$$

$$+ \frac{1 - E_n^{\;2}}{8E_n p^3} \left\{ \ln[1 + (E_n + p)^2] - \frac{2E_n p}{1 + E_n^{\;2}} \right\} + \frac{1}{16E_n p} \ln[1 + (E_n + p)^2]$$

$$B_2(p) = -\frac{(1 + E_n^{\;2})^2}{16E_n p^5} \left\{ \ln[1 + (E_n + p)^2] - \frac{2E_n p}{1 + E_n^{\;2}} + \frac{(3 - E_n^{\;2})2E_n p^3}{3(1 + E_n^{\;2})^3} \right\}$$

$$- \frac{5E_n^{\;4} + 8E_n^{\;2} - 1}{16E_n^{\;3} p^3} \left\{ \ln[1 + (E_n + p)^2] - \frac{2E_n p}{1 + E_n^{\;2}} \right\}$$

$$+ \frac{(1 - E_n^{\;2})(3E_n^{\;2} - 1)}{8E_n^{\;4} p^2} \ln \left[\frac{1 + (E_n + p)^2}{1 + E_n^{\;2}} \right]$$

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

$$B_3(p) = -\frac{(1 + E_n^{\;2})^2}{16E_n p^5} \left\{ \ln[1 + (E_n + p)^2] - \frac{2E_n p}{1 + E_n^{\;2}} \right.$$

$$\left. + \frac{(3 - E_n^{\;2})2E_n p^3}{3(1 + E_n^{\;2})^3} \right\} + \frac{3 + E_n^{\;4}}{16E_n^{\;3} p^3} \left\{ \ln[1 + (E_n + p)^2] - \frac{2E_n p}{1 + E_n^{\;2}} \right\}$$

$$- \frac{1}{2E_n^{\;4} p^2} \ln \left[\frac{1 + (E_n + p)^2}{1 + E_n^{\;2}} \right] + \frac{1}{16E_n^{\;4}(E_n + p)} \left[\frac{15}{p} - \frac{7}{E_n + p} \right]$$

$$\times \ln[1 + (E_n + p)^2] - \frac{1}{8E_n^{\;3}(E_n + p)^3} \left\{ \ln[1 + (E_n + p)^2] - (E_n + p)^2 \right\}$$

Equation (7.31) continued next page

Equation (7.31) continued

$$B_4(p) = -\frac{1+E_n^2}{2E_n p^3}\left\{\ln[1+(E_n+p)^2] - \frac{2E_n p}{1+E_n^2}\right\}$$

$$+\frac{1}{E_n^2 p^2}\ln\left[\frac{1+(E_n+p)^2}{1+E_n^2}\right]$$

$$-\frac{1}{2E_n^2(E_n+p)}\left[\frac{3}{p}-\frac{1}{E_n+p}\right]\ln[1+(E_n+p)^2] \quad . \qquad (7.31)$$

We note that each Q_j, $j = 1,2,3,$ and 4, approaches a constant in the limit $p^2 \to 0$. In order to obtain a convenient way of expressing the contribution of each term in (7.29) to the net energy shift, we isolate the contribution of order lower than $\alpha(Z\alpha)^4$ in terms proportional to $\langle V\rangle_n$. The lower order contributions, which come from the terms containing Q_1 and Q_2 in (7.29), are identified by replacing $Q_1(p^2)$ and $Q_2(p^2)$ by the limits

$$\lim_{\substack{p^2\to 0\\ E_n\to 1}} Q_1(p^2) = \frac{1}{10} \quad \text{and} \quad \lim_{\substack{p^2\to 0\\ E_n\to 1}} Q_2(p^2) = \frac{1}{2}\ln 2 - \frac{7}{20} \quad . \qquad (7.32)$$

We obtain

$$\langle n|E_n Q_1(p^2)p^2|n\rangle \sim \frac{1}{10}\langle n|p^2|n\rangle \sim -\frac{1}{10}\langle n|V|n\rangle$$

$$\langle n|\beta Q_2(p^2)p^2|n\rangle \sim (\tfrac{1}{2}\ln 2 - \tfrac{7}{20})\langle n|\beta p^2|n\rangle$$

$$\sim -(\tfrac{1}{2}\ln 2 - \tfrac{7}{20})\langle n|V|n\rangle \quad . \qquad (7.33)$$

In (7.33), the symbol $\sim$ means equal to order $(Z\alpha)^2$. We then define four functions h_j, $j = 1,2,3,$ and 4, by the equations

$$\langle n|E_n Q_1(p^2)p^2|n\rangle = -\frac{1}{10}\langle V\rangle_n + (Z\alpha)^4 h_1(Z\alpha)$$

$$\langle n|\beta Q_2(p^2)p^2|n\rangle = (\tfrac{7}{20} - \tfrac{1}{2}\ln 2)\langle V\rangle_n + (Z\alpha)^4 h_2(Z\alpha)$$

$$\langle n|VQ_3(p^2)p^2|n\rangle = (Z\alpha)^4 h_3(Z\alpha)$$

$$\langle n|\frac{\beta}{E_n}VQ_4(p^2)p^2|n\rangle = (Z\alpha)^4 h_4(Z\alpha) \quad . \qquad (7.34)$$

The h's are evaluated by evaluating the corresponding matrix elements in (7.34). To do this, we take into account the form of the momentum-space wave function given in (G.1) and the form of the function given in (G.6), and arrive at the following expressions:

$$(Z\alpha)^4 h_1(Z\alpha) = \frac{1}{10}\langle V\rangle_n + E_n\int_0^\infty dp\, p^4[g_1(p)^2 + g_2(p)^2]\, Q_1(p^2)$$

$$(Z\alpha)^4 h_2(Z\alpha) = (\tfrac{1}{2}\ln 2 - \tfrac{7}{20})\langle V\rangle_n + \int_0^\infty dp\, p^4[g_1(p)^2 - g_2(p)^2] \times Q_2(p^2)$$

$$(Z\alpha)^4 h_3(Z\alpha) = \int_0^\infty dp\, p^4[g_1(p)Vg_1(p) + g_2(p)Vg_2(p)]Q_3(p^2)$$

$$(Z\alpha)^4 h_4(Z\alpha) = E_n^{-1}\int_0^\infty dp\, p^4[g_1(p)Vg_1(p) - g_2(p)Vg_2(p)]Q_4(p^2)$$

(7.35)

where, for the $1S_{\frac{1}{2}}$ state, the g's and Vg's are given explicitly in (G.5) and (G.7). The integrals which appear in (7.35) are evaluated by Gaussian quadrature with new variables of integration x given by

$$p = (Z\alpha)\frac{1 - x^2}{x^2} \qquad \text{in } h_1, h_2$$

$$p = (Z\alpha)\frac{1 - x^3}{x^3} \qquad \text{in } h_3, h_4 \quad . \tag{7.36}$$

We use a 60-point Gauss-Legendre formula. The numerical error in the h's with this method of evaluation, as determined by observing the convergence in the values for the integrals as the number of integration points is increased, is of the order of 10^{-12} or less for $10 \leq Z \leq 110$. The results of this evaluation are listed in Table 7.1.

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

$$\Delta E_{HA} = \frac{\alpha}{\pi}[(\tfrac{3}{4}\,\ell n\,\Lambda^2 - \tfrac{9}{8})\langle\beta\rangle_n - \tfrac{7}{6}\langle V\rangle_n + (Z\alpha)^4 f_{HA}(Z\alpha)] \tag{7.37}$$

where

$$f_{HA}(Z\alpha) = f_{HA}{}^{1}(Z\alpha) + \sum_{i=1}^{4} h_i(Z\alpha) \quad . \tag{7.38}$$

Values for $f_{HA}(Z\alpha)$ are listed in Table 7.1. From (7.23) and the results in (F.20), we have

$$\lim_{Z\alpha \to 0} f_{HA}(Z\alpha) = \frac{1}{6} - 2\,\ell n\,2 \quad . \tag{7.39}$$

Table 7.1. The results of numerical evaluation of $f_{HA}{}^{1}$, h_1, h_2, h_3, h_4, and the total f_{HA}. All figures shown are correct.

Z	$f_{HA}{}^{1}(Z\alpha)$	$h_1(Z\alpha)$	$h_2(Z\alpha)$	$h_3(Z\alpha)$	$h_4(Z\alpha)$	$f_{HA}(Z\alpha)$
10	-0.759762	0.061029	-0.235254	0.041051	-0.308422	-1.201358
20	-0.769348	0.047569	-0.219782	0.045286	-0.303368	-1.199643
30	-0.785874	0.033259	-0.208071	0.050676	-0.301391	-1.211401
40	-0.810250	0.017768	-0.198607	0.057061	-0.301606	-1.235634
50	-0.843934	0.000742	-0.190326	0.064314	-0.303269	-1.272473
60	-0.889193	-0.018187	-0.182321	0.072286	-0.305666	-1.323081
70	-0.949575	-0.039426	-0.173684	0.080762	-0.308012	-1.389936
80	-1.030831	-0.063471	-0.163350	0.089399	-0.309339	-1.477591
90	-1.142851	-0.091023	-0.149890	0.097638	-0.308314	-1.594440
100	-1.304309	-0.123305	-0.131106	0.104522	-0.302901	-1.757100
110	-1.555971	-0.163032	-0.103036	0.108286	-0.289584	-2.003337

VIII. INTEGRATION OVER ANGLES IN THE EXPRESSION FOR ΔE_{HB}

We now perform the integration over angles in the matrix element which appears in Eq. (6.20):

$$M = \int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1 \, \psi_n^{\dagger}(\underset{\sim}{x}_2) \, \alpha_\mu \, G_B(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) \, \alpha^\mu \, \psi_n(\underset{\sim}{x}_1)$$

$$\times \frac{1}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} \exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|) \quad . \tag{8.1}$$

The integration is similar to the integration in Sec. IV. We draw on results obtained in that section. For convenience, we omit the subscript B from $G_B(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)$ in the rest of this section.

We consider separately two portions M_1 and M_2 of M corresponding respectively to $\mu = 0$ and $\mu = 1,2,$ and 3 in (8.1). We have

$$M_1 = \int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1 \, \psi_n^{\dagger}(\underset{\sim}{x}_2) \, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) \, \psi_n(\underset{\sim}{x}_1) \, \frac{e^{-b\rho}}{\rho} \tag{8.2}$$

where

$$\rho = |\underset{\sim}{x}_2 - \underset{\sim}{x}_1| \, . \tag{8.3}$$

Employing the forms given in (4.2) and (4.3), we obtain

$$M_1 = \int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1 \sum_{\kappa}$$

$$\{f_1(x_2) \, G_\kappa^{11}(x_2,x_1,z) \, f_1(x_1) \, \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2) \, \pi_\kappa(\hat{x}_2,\hat{x}_1) \, \chi_{\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$- f_1(x_2) \, G_\kappa^{12}(x_2,x_1,z) \, f_2(x_1) \, \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2) \, \underset{\sim}{\sigma}\cdot\hat{x}_2 \, \pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \, \chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)$$

Equation (8.4) continued next page

Equation (8.4) continued

$$- f_2(x_2) \, G_\kappa^{21}(x_2,x_1,z) \, f_1(x_1) \, \chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2) \, \underset{\sim}{\sigma}\cdot\hat{x}_2 \, \pi_\kappa(\hat{x}_2,\hat{x}_1) \, \chi_{\kappa_n}^{\mu_n}(\hat{x}_1)$$

$$+ f_2(x_2) \, G_\kappa^{22}(x_2,x_1,z) \, f_2(x_1) \, \chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2) \, \pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \, \chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)\} \, \frac{e^{-b\rho}}{\rho} \quad . \tag{8.4}$$

All of the integrals over angles in (8.4) are of the form

$$A_\kappa(x_2,x_1) = \int d\Omega_2 \int d\Omega_1 \, \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2) \, \pi_\kappa(\hat{x}_2,\hat{x}_1) \, \chi_{\kappa_n}^{\mu_n}(\hat{x}_1) \, \frac{e^{-b\rho}}{\rho} \, . \tag{8.5}$$

In view of Eq. (A.14), we have

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

$$+ \frac{1}{\kappa\kappa_n}(1 - \xi^2) \, P'_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi) \, P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)] \, \frac{e^{-b\rho}}{\rho} \quad , \tag{8.6}$$

and in the special case of $S_{\frac{1}{2}}$ states

$$A_\kappa(x_2,x_1) = \frac{|\kappa|}{2} \int_{-1}^{1} d\xi \, P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) \, \frac{e^{-b\rho}}{\rho} \tag{8.7}$$

where $\xi = \hat{x}_2\cdot\hat{x}_1$ in both formulas. With the aid of the Legendre series expansion

$$\frac{\exp(-b|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|)}{|\underset{\sim}{x}_2 - \underset{\sim}{x}_1|} = - b \sum_{\ell=0}^{\infty} (2\ell + 1) \, P_\ell(\xi) \, j_\ell(ibx_<) \, h_\ell^{(1)}(ibx_>) \tag{8.8}$$

in which $x_< = \min(x_2,x_1)$, $x_> = \max(x_2,x_1)$, j_ℓ is the spherical Bessel function, and $h_\ell^{(1)}$ is the spherical Hankel function of the first kind, we obtain

$$A_\kappa(x_2,x_1) = -|\kappa|\, b j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(ibx_>) \tag{8.9}$$

for $S_{\frac{1}{2}}$ states. Hence

$$\begin{aligned} M_1 = -b\int_0^\infty dx_2 x_2^2 \int_0^\infty dx_1 x_1^2 \sum_\kappa |\kappa| \{ & f_1(x_2)\, G_\kappa^{11}(x_2,x_1,z)\, f_1(x_1) \\ & + f_1(x_2)\, G_\kappa^{12}(x_2,x_1,z)\, f_2(x_1) + f_2(x_2)\, G_\kappa^{21}(x_2,x_1,z)\, f_1(x_1) \\ & + f_2(x_2)\, G_\kappa^{22}(x_2,x_1,z)\, f_2(x_1)\}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(ibx_>) \,. \end{aligned} \tag{8.10}$$

The portion M_2 of M is given by

$$\begin{aligned} M_2 &= -\int d^3\underset{\sim}{x}_2 \int d^3\underset{\sim}{x}_1\, \psi_n^\dagger(\underset{\sim}{x}_2)\, \alpha^i\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z)\, \alpha^i\, \psi_n(\underset{\sim}{x}_1)\, \frac{e^{-b\rho}}{\rho} \\ &= -\int_0^\infty dx_2 x_2^2 \int_0^\infty dx_1 x_1^2 \sum_\kappa \{ f_2(x_2)\, G_\kappa^{11}(x_2,x_1,z)\, f_2(x_1) \\ &\quad \times A_\kappa^{11}(x_2,x_1) + f_2(x_2)\, G_\kappa^{12}(x_2,x_1,z)\, f_1(x_1)\, A_\kappa^{12}(x_2,x_1) \\ &\quad + f_1(x_2)\, G_\kappa^{21}(x_2,x_1,z)\, f_2(x_1)\, A_\kappa^{21}(x_2,x_1) + f_1(x_2)\, G_\kappa^{22}(x_2,x_1,z) \\ &\quad \times f_1(x_1)\, A_\kappa^{22}(x_2,x_1)\} \end{aligned} \tag{8.11}$$

where

$$A_\kappa^{11}(x_2,x_1) = \int d\Omega_2 \int d\Omega_1\, \chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\, \sigma^i\, \pi_\kappa(\hat{x}_2,\hat{x}_1)\, \sigma^i\, \chi_{-\kappa_n}^{\mu_n}(\hat{x}_1)\, \frac{e^{-b\rho}}{\rho}$$

$$A_\kappa^{12}(x_2,x_1) = \int d\Omega_2 \int d\Omega_1\, \chi_{-\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\, \sigma^i\, \underset{\sim}{\sigma}\cdot\hat{x}_2\, \pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\, \sigma^i\, \chi_{\kappa_n}^{\mu_n}(\hat{x}_1) \times \frac{e^{-b\rho}}{\rho}$$

$$A_\kappa^{21}(x_2,x_1) = \int d\Omega_2 \int d\Omega_1\, \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\, \sigma^i\, \underset{\sim}{\sigma}\cdot\hat{x}_2\, \pi_\kappa(\hat{x}_2,\hat{x}_1)\, \sigma^i\, \chi_{-\kappa_n}^{\mu_n}(\hat{x}_1) \times \frac{e^{-b\rho}}{\rho}$$

$$A_\kappa^{22}(x_2,x_1) = \int d\Omega_2 \int d\Omega_1\, \chi_{\kappa_n}^{\mu_n\dagger}(\hat{x}_2)\, \sigma^i\, \pi_{-\kappa}(\hat{x}_2,\hat{x}_1)\, \sigma^i\, \chi_{\kappa_n}^{\mu_n}(\hat{x}_1)\, \frac{e^{-b\rho}}{\rho} \,. \tag{8.12}$$

With the aid of the appropriate relations in (4.10), (A.12), and (A.14), we obtain

$$\begin{aligned} A_\kappa^{11}(x_2,x_1) = \frac{|\kappa|}{2}\int_{-1}^{1} d\xi\, [& 3P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\, P_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi) \\ & + \frac{1}{\kappa\kappa_n}(1-\xi^2)\, P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\, P'_{|\kappa_n-\frac{1}{2}|-\frac{1}{2}}(\xi)]\, \frac{e^{-b\rho}}{\rho} \end{aligned} \tag{8.13}$$

and

$$\begin{aligned} A_\kappa^{12}(x_2,x_1) = \frac{|\kappa|}{2}\int_{-1}^{1} d\xi\, [& P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, P_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi) \\ & - \frac{1}{\kappa\kappa_n}(1-\xi^2)\, P'_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, P'_{|\kappa_n+\frac{1}{2}|-\frac{1}{2}}(\xi)]\, \frac{e^{-b\rho}}{\rho} \,. \end{aligned} \tag{8.14}$$

In the special case of $S_{\frac{1}{2}}$ states, we have

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

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

$$A_\kappa^{12}(x_2,x_1) = \frac{1}{2}|\kappa| \int_{-1}^{1} d\xi\, P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, \frac{e^{-b\rho}}{\rho}$$

$$A_\kappa^{21}(x_2,x_1) = \frac{1}{2}|\kappa| \int_{-1}^{1} d\xi\, P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, \frac{e^{-b\rho}}{\rho}$$

$$A_\kappa^{22}(x_2,x_1) = \frac{3}{2}|\kappa| \int_{-1}^{1} d\xi\, P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi)\, \frac{e^{-b\rho}}{\rho} \quad . \tag{8.15}$$

The last two relations in (8.15) follow from Eqs. (8.13) and (8.14) and the fact that

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

$$A^{22}_{\kappa,\kappa_n}(x_2,x_1) = A^{11}_{-\kappa,-\kappa_n}(x_2,x_1) \quad . \tag{8.16}$$

Integration over ξ in (8.15) yields

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

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

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

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

$$A_\kappa^{21}(x_2,x_1) = A_\kappa^{12}(x_2,x_1)$$

$$A_\kappa^{22}(x_2,x_1) = -\,3\,|\kappa|\, b j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_>) \quad . \tag{8.17}$$

We thus have

$$M_2 = b\int_0^\infty dx_2 x_2^2 \int_0^\infty dx_1 x_1^2 \sum_\kappa |\kappa| \Big\{ [3 f_2(x_2)\, G_\kappa^{11}(x_2,x_1,z)\, f_2(x_1)$$

$$+ f_2(x_2)\, G_\kappa^{12}(x_2,x_1,z)\, f_1(x_1) + f_1(x_2)\, G_\kappa^{21}(x_2,x_1,z)\, f_2(x_1)$$

$$+ 3 f_1(x_2)\, G_\kappa^{22}(x_2,x_1,z)\, f_1(x_1)]\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(ibx_>)$$

$$- f_2(x_2)\, G_\kappa^{11}(x_2,x_1,z)\, f_2(x_1)\, 4\,\frac{\kappa+1}{|2\kappa+1|}\Big[j_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(ibx_<)$$

$$\times\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{3}{2}}(ibx_>) - j_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(ibx_<)\, h^{(1)}_{|\kappa+\frac{1}{2}|+\frac{1}{2}}(ibx_>)\Big]\Big\} \quad . \tag{8.18}$$

IX. NUMERICAL EVALUATION OF ΔE_{HB}

The quantity ΔE_{HB} is given by

$$\Delta E_{HB} = -\frac{i\alpha}{2\pi}\int_{C'_H} dz\, M(z,b) \tag{9.1}$$

where M is defined in (8.1). Introducing the variable of integration u into (9.1), where $z = iu$ on the positive imaginary z-axis and $z = -iu$ on the negative imaginary z-axis, and choosing the appropriate branch of b in each case, we obtain

$$\Delta E_{HB} = \frac{\alpha}{2\pi}\int_0^\infty du[M(iu,u + iE_n) + M(-iu,u - iE_n)]$$

$$= \frac{\alpha}{\pi}\int_0^\infty du\, \mathrm{Re}\left(M(iu,u + iE_n)\right) \quad . \tag{9.2}$$

Because ΔE_{HB} is of order $(Z\alpha)^4$, it is convenient to introduce the function $f_{HB}(Z\alpha)$ defined by

$$\Delta E_{HB} = \frac{\alpha}{\pi}(Z\alpha)^4 f_{HB}(Z\alpha) \ . \tag{9.3}$$

In terms of the new variable of integration t, where $u = \frac{1}{2}(t^{-1} - t)$, we have

$$f_{HB}(\gamma) = \frac{1}{2}\gamma^{-4}\int_0^1 dt(t^{-2} + 1)\, \mathrm{Re}\left(M\left(\tfrac{i}{2}(t^{-1} - t), \tfrac{1}{2}(t^{-1} - t) + iE_n\right)\right). \tag{9.4}$$

In the expression for M which is the sum of M_1 and M_2 in (8.10) and (8.18), we introduce new variables of integration:

$$y = 2\gamma x_1 \ ; \qquad r = \frac{x_2}{x_1} \qquad \text{for } x_2 < x_1$$

$$y = 2\gamma x_2 \ ; \qquad r = \frac{x_1}{x_2} \qquad \text{for } x_2 > x_1 \ . \tag{9.5}$$

Taking into account the fact that the integrand in that expression is symmetric under interchange of x_2 and x_1, specializing to $1S_{\frac{1}{2}}$-state wave functions, and substituting the expression for M into (9.4), we obtain

$$f_{HB}(\gamma) = \int_0^1 dt \int_0^\infty dy \int_0^1 dr\, S(r,y,t,\gamma) \tag{9.6}$$

where

$$S(r,y,t,\gamma) = \frac{8(2\gamma)^{-7}}{\Gamma(3 - 2\delta)}(t^{-2} + 1)\, r^{2-\delta}\, y^{5-2\delta}\, e^{-y}\, e^{\frac{1}{2}(1-r)y}$$

$$\times \sum_{\kappa=1}^{\infty} T_\kappa(r,y,t,\gamma) \tag{9.7}$$

and where

$$T_\kappa(r,y,t,\gamma) = -\sum_{\substack{\text{signs}\\ \text{of } \kappa}} |\kappa|\, \mathrm{Re}\Big([u + iE_n]\{[(1 + E_n)\, G^{11}_{B,\kappa} - \gamma G^{12}_{B,\kappa}$$

$$- \gamma G^{21}_{B,\kappa} + (1 - E_n)G^{22}_{B,\kappa}]\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}} - [3(1 - E_n)\, G^{11}_{B,\kappa} - \gamma G^{12}_{B,\kappa}$$

$$- \gamma G^{21}_{B,\kappa} + 3(1 + E_n)G^{22}_{B,\kappa}]\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}} + (1 - E_n)\, G^{11}_{B,\kappa}$$

$$\times 4\,\frac{\kappa + 1}{|2\kappa + 1|}\,[j_{|\kappa+\frac{1}{2}|-\frac{3}{2}}\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{3}{2}} - j_{|\kappa+\frac{1}{2}|+\frac{1}{2}}\, h^{(1)}_{|\kappa+\frac{1}{2}|+\frac{1}{2}}]\}\Big) \quad . \tag{9.8}$$

The functions G_B are defined in (6.19). The arguments of the functions G_B, j, and $h^{(1)}$ are given by

$$G^{ij}_{B,\kappa} = G^{ij}_{B,\kappa}\left(\frac{ry}{2\gamma}, \frac{y}{2\gamma}, iu\right)$$

$$j_\kappa = j_\kappa\left((iu - E_n)\frac{ry}{2\gamma}\right)$$

$$h^{(1)}_\kappa = h^{(1)}_\kappa\left((iu - E_n)\frac{y}{2\gamma}\right) \tag{9.9}$$

$$u = \frac{1}{2}(t^{-1} - t) .$$

The numerical evaluation of ΔE_{HB} is similar to the evaluation of ΔE_L. The integrations in (9.6) are performed by Gaussian quadrature. The function $S(r,y,t\ \gamma)$ is computed with the aid of (9.7); the truncation of the sum over κ is discussed below. The numerical evaluation of the spherical Bessel functions and radial Green's functions which appear in (9.8) is described in Appendices H and I.

We now examine the convergence of the sum over κ in (9.7). For $\kappa \to +\infty$, we have

$$G^{11}_{B,\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\frac{1}{2}\gamma(1 - r) + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G^{12}_{B,\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G^{21}_{B,\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[2\gamma z(1 - r)y - \gamma^2 \ln r + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

Equation (9.10) continued next page

Equation (9.10) continued

$$G^{22}_{B,\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\frac{1}{2}\gamma(1 - \frac{1}{r}) + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G^{11}_{B,-\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\frac{1}{2}\gamma(1 - \frac{1}{r}) + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G^{12}_{B,-\kappa}(ry,y,z) = -\frac{r^{\kappa-1}}{2\kappa y^2}\left[2\gamma z(1 - r)y - \gamma^2 \ln r + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G^{21}_{B,-\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G^{22}_{B,-\kappa}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\frac{1}{2}\gamma(1 - r) + \mathcal{O}(\tfrac{1}{\kappa})\right] \tag{9.10}$$

and

$$j_\kappa(ry)\, h^{(1)}_\kappa(y) = \frac{r^\kappa}{2\kappa i y}\left[1 + \mathcal{O}(\tfrac{1}{\kappa})\right] . \tag{9.11}$$

Hence, for fixed r, y, t, and γ,

$$T_\kappa(r,y,t,\gamma) = 2\gamma^4 \frac{r^{2\kappa-2}}{\kappa y^3}(1 - r)$$

$$\times \left[(1 + E_n)\frac{1 - r^2}{r} + (1 - E_n)\frac{1 - r^4}{r^2} - 2\gamma^2 \ln r + \mathcal{O}(\tfrac{1}{\kappa})\right] \tag{9.12}$$

as $\kappa \to \infty$. We define a function $P_\kappa(r,y,t,\gamma)$ by writing

$$T_\kappa(r,y,t,\gamma) = \frac{r^{2\kappa}}{\kappa} P_\kappa(r,y,t,\gamma) . \tag{9.13}$$

In order to obtain an approximation for the remainder R_N which is left if the sum over κ in (9.7) is truncated at $\kappa = N$, we assume that for $\kappa \geq 1.5 \frac{cy}{2\gamma}$, where $c = (1 + u^2)^{\frac{1}{2}}$ and $\mathrm{Re}(c) > 0$, the function P_κ, as a function of κ, is sufficiently slowly varying compared to $(r^{2\kappa})/\kappa$ that the following approximation is justified:

$$R_N = \sum_{\kappa=N+1}^{\infty} T_\kappa \simeq P_{N+1} \sum_{\kappa=N+1}^{\infty} \frac{r^{2\kappa}}{\kappa} \quad . \tag{9.14}$$

This assumption is suggested by the form of the expression in (9.12) together with a numerical examination of the terms in the sum in (9.7) for various values of the parameters. From (9.14), we obtain

$$|R_N| \lesssim \frac{1}{1 - r^2} |T_{N+1}| \quad . \tag{9.15}$$

The sum over κ in (9.7) is thus truncated at $\kappa = N$, where N is the smallest number which is greater than 3, greater than or equal to $1.5\ cy/2\gamma$, and large enough that the magnitude of the absolute contribution of the remainder, as estimated by (9.15), to the sum S is less than 10^{-4}. The validity of this error approximation was tested by evaluating the sum S with the cutoff described above, and then re-evaluating the sum with the error bound of 10^{-4} replaced by an error bound of 10^{-6}. The two values for the sum were then compared. The evaluation and comparison was made for all combinations of the values $r = 0.1, 0.5, 0.9$, $y = 0.1, 1, 10$, $t = 0.1, 0.5, 0.9$, and $\gamma = 10/137, 110/137$, and for the values $(r,y,t,\gamma) = (0.99, 10, 0.1, 110/137)$, $(0.999, 10, 0.1, 110/137)$, $(0.99, 1, 0.1, 10/137)$, $(0.999, 1, 0.1, 10/137)$, $(0.99, 10, 0.9, 10/137)$, and $(0.999, 10, 0.9, 10/137)$. In all cases, the magnitude

of the difference between the two values for S was less than 10^{-4}. The validity of the error approximation is further tested by reducing the error bound in some of the final evaluations of ΔE_{HB}.

In the evaluation of the sum S, the products of Bessel functions which appear in (9.8) are evaluated recursively, as described in Appendix H, before the sum over κ in (9.7) is performed. Therefore, we need a preliminary moderate over-estimate N_0 for the number of Bessel functions which are needed to evaluate the sum to the desired accuracy. The value we employ for this purpose, for specified values of r, y, t, and γ, is given by

$$N_0 = \max(N_1, N_2, 3) + 1 \tag{9.16}$$

where

$$N_1 = [1.5 \frac{cy}{2\gamma}] \tag{9.17}$$

and

$$N_2 = \left[0.5 \frac{\ln\left(\frac{1 - r^2}{10^4\ B\ P_\infty}\right)}{\ln r} \right] + 3 \tag{9.18}$$

where B is the coefficient of the sum over κ in (9.7). If it is found, in a particular evaluation of S, that N_0 is too small, then the value of N_0 is increased by 10 and the evaluation of S is begun again.

A crude approximation for the function $S(r,y,t,\gamma)$, which serves to motivate our choice of variables of integration in the numerical evaluation of the integrals in (9.6), is obtained by replacing the radial Green's functions in (9.8) by their asymptotic

forms for large argument which appear in (A.28). Taking the first term in the curly brackets in (9.8) as a typical term, replacing the radial Green's functions in that term by the first terms in the corresponding asymptotic expansions, and performing the sum over κ, we obtain

$$S(r,y,t,\gamma) \sim e^{-y}\, e^{-\frac{1}{2}(\frac{1}{\gamma t}-1)(1-r)y} \quad . \tag{9.19}$$

In arriving at the expression in (9.19), we have set relatively slowly varying factors equal to 1. Two singular factors t^{-2} and $(1 - r)^{-1}$ which have been set equal to 1 in arriving at (9.19) are the result of the crude nature of the approximation. The behavior of S near $t = 0$ corresponds to the behavior of the integrand in (9.1) for large $|z|$. The considerations of Sec. VI show that S is integrable in this region. That S is integrable near $r = 1$ is seen by inspection of (9.12).

We next give the method that we use to numerically evaluate the integrals in (9.6). The Gaussian integration formulas mentioned in Sec. V are used here. We employ the notation

$$S_1(y,t,\gamma) = \int_0^1 dr\, S(r,y,t,\gamma)$$

$$S_{21}(t,\gamma) = \int_0^2 dy\, S_1(y,t,\gamma)$$

$$S_{22}(t,\gamma) = \int_2^\infty dy\, S_1(y,t,\gamma)$$

Equation (9.20) continued next page

Equation (9.20) continued

$$s_{3i}(\gamma) = \int_0^1 dt\, S_{2i}(t,\gamma) \qquad i = 1,2$$

$$q = \frac{1}{2}\left(\frac{1}{\gamma t} - 1\right)y \quad . \tag{9.20}$$

Four regions, A, B, C, and D, in the space of the parameters r, y, t, and γ are defined by

$$\begin{aligned} &A: \ y < 2, \quad Z < 60 \\ &B: \ y < 2, \quad Z \geq 60 \\ &C: \ y > 2, \quad Z < 60 \\ &D: \ y > 2, \quad Z \geq 60 \quad . \end{aligned} \tag{9.21}$$

In the following, N_A, N_B, N_C, and N_D are the number of integration points used in the evaluation of the integrals with which they appear when the parameters are in the corresponding regions. The integral over r in (9.6) is evaluated as follows:

$$S_1(y,t,\gamma) = \int_0^1 dx\, 2x\, S(x^2,y,t,\gamma) \qquad 0 < q \leq 1$$

$$S_1(y,t,\gamma) = \int_0^1 dx\, S(x,y,t,\gamma) \qquad 1 < q \leq 12$$

$$S_1(y,t,\gamma) = \int_0^1 dx\, \frac{12}{q}\, S\left(1 - \frac{12}{q}x,y,t,\gamma\right) + \epsilon \qquad q > 12$$

(9.22)

where for all three integrals

$$N_A = N_C = N_D = 5 , \qquad N_B = \begin{cases} 6 & \text{for } t \geq 0.2 \\ 8 & \text{for } t < 0.2 \end{cases} \tag{9.23}$$

and where

$$\epsilon = \int_1^{\frac{q}{12}} dx \, \frac{12}{q} \, S(1 - \frac{12}{q}x, y, t, \gamma) \quad . \tag{9.24}$$

The contribution of ϵ to the value of the integral is neglected. In view of (9.19), an approximate over estimate for ϵ is given by

$$\epsilon \approx A(1 - \frac{12}{q}, y, t, \gamma) \int_1^{\frac{q}{12}} dx \, e^{-12x} \, e^{-y}$$

$$\gtrsim \frac{1}{12} S(1 - \frac{12}{q} x_0, y, t, \gamma) \tag{9.25}$$

where $A(r,y,t,\gamma)$ is the ratio of $S(r,y,t,\gamma)$ to the term on the right side in (9.19), and x_0 is the largest value assigned to x in the numerical evaluation represented by the third equation in (9.22). We examined the corresponding values for S which occurred in the numerical integrations and found, based on the estimate in (9.25), that the magnitude of ϵ was always less than 4×10^{-4}, and in most cases it was much less than that value. We evaluate the integral over y in (9.6) in the following way:

$$S_{21}(t,\gamma) = \int_0^1 dx \, 4x \, S_1(2x^2, t, \gamma)$$

$$N_A = \begin{cases} 10 & \text{for } t \geq 0.5 \\ 12 & \text{for } t < 0.5 \end{cases} \qquad N_B = \begin{cases} 8 & \text{for } t \geq 0.4 \\ 10 & \text{for } 0.1 \leq t < 0.4 \\ 12 & \text{for } t < 0.1 \end{cases}$$

$$S_{22}(t,\gamma) = \int_0^\infty dx \, S_1(2 + x, t, \gamma)$$

$$N_C = N_D = \begin{cases} 4 & \text{for } t > 0.5 \\ 3 & \text{for } t \leq 0.5 \end{cases} \quad . \tag{9.26}$$

The integral over t in (9.6) is evaluated as follows:

$$S_{31}(\gamma) = \int_0^1 dx \, 2x \, S_{21}(1 - x^2, \gamma) \qquad N_A = 6$$

$$S_{3i}(\gamma) = \int_0^1 dx \, S_{2i}(x, \gamma) \qquad \begin{array}{l} i = 1; \; N_B = 6 \\ i = 2; \; N_C = 4, \\ \qquad N_D = 5 \quad . \end{array} \tag{9.27}$$

The choices of variables of integration and numbers of integration points in the preceding discussion are the results of an effort to obtain a numerical value for the integrals in (9.6) with an error less than 5×10^{-4} in magnitude and with the use of a minimum amount of computer time. We arrived at the above scheme with an approach

analogous to the one used in the numerical evaluation of the low-energy part. The values for N_A, N_B, N_C, and N_D were determined by an examination of the integrals at the values $Z = 30$, 110, 50, and 110 respectively.

The results of the numerical integrations are given in Table 9.1. In that table, where three values are given for a single point, the middle value is the result obtained with the above described method of integration; the upper value is the result of evaluating the integrals with a number of integration points in each integral which is one less than the number of integration points specified for that integral in the above method; the lower value is the result obtained with one extra integration point in each integral. The single values in that table are the results of evaluating the integrals with the method of integration described above, except that the value for S_{32} at $Z = 40$ is obtained with one extra integration point in each integral. Values for f_{HB}, obtained by adding the corresponding values for S_{31} and S_{32}, are also listed in Table 9.1. We have given error limits with each value for f_{HB}. These are subjective estimates of the maximum uncertainty in the values, based on an examination of the behavior of the numbers within the groups of three values obtained for S_{31} and S_{32} for a given Z. For values of Z for which only one evaluation was made, the error limit was obtained by interpolating between the error limits for neighboring values of Z. The numbers marked with an asterisk in Table 9.1 are the values obtained by evaluating the integrals with the integration method described above, and with the error bound employed in truncating the sum over κ reduced to 10^{-5}. Comparison of these values with the corresponding unstarred values in

Table 9.1

Z	$S_{31}(Z\alpha)$	$S_{32}(Z\alpha)$	$f_{HB}(Z\alpha)$
10	-0.007094	-0.027008	
	-0.007685	-0.020876	
	-0.007650	-0.022085	-0.030(2)
20	0.070451	-0.024465	0.046(1)
30	0.155291	-0.025616	
	0.154183	-0.026785	
	0.154438	-0.026712	0.1277(5)
40	0.252596	-0.039257	0.2133(7)
50	0.359596	-0.052991	
	0.358150	-0.054137	
	0.357949	-0.053430	0.3045(8)
60	0.458330	-0.055898	0.4024(4)
70	0.552628	-0.041619	
	0.552438	-0.041645	
	0.552314	-0.041598	0.5107(4)
80	0.646615	-0.012562	0.6341(6)
90	0.752997	0.026850	
	0.752544	0.027536	
	0.752223	0.027442	0.7797(7)
100	0.888973	0.074809	0.9638(8)
110	1.092590	0.124257	
	1.091980	0.125498	
	1.091547	0.125506	1.2171(8)
30	0.154205*	-0.026737*	
110	1.092001*	0.125555*	

the table indicates that the method used to attain the desired accuracy in the sum over κ is effective.

As a check against errors in algebra or programming in the numerical evaluation of f_{HB}, we plot, in Fig. 9.1, the calculated values for $f_{HB}(Z\alpha)$ for $Z = 10, 20, 30, 40$, and 50 and the limit point $f_{HB}(0) = -0.093457$ given in (F.14). The calculated points appear to be consistent with the limit point.

X. CONCLUSION

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

$$\Delta E_n = \Delta E_L + \Delta E_{HA} + \Delta E_{HB} + \Delta E_M \,. \tag{10.1}$$

The terms on the right in (10.1) appear in Eqs. (5.33), (7.37), (9.3), and (2.20) respectively. The terms of order lower than $\alpha(Z\alpha)^4$ add up to zero, as they should, and we are left with

$$\Delta E_n = \frac{\alpha}{\pi} (Z\alpha)^4 F(Z\alpha)\, m_e c^2 \tag{10.2}$$

where

$$F(Z\alpha) = f_L(Z\alpha) + f_{HA}(Z\alpha) + f_{HB}(Z\alpha) \,. \tag{10.3}$$

Values for $F(Z\alpha)$ for the $1S_{\frac{1}{2}}$ state are given in Table 10.1. The numbers in parentheses in that table are error limits associated with f_{HB}, and are discussed at the end of Sec. IX. The calculated values for $F(Z\alpha)$ along with values for $F(Z\alpha)$ obtained from the results of previous calculations are shown in Fig. 10.1.

For Z in the range 70-90, we compare the results of this calculation with the results, for a Coulomb potential, of Desiderio and Johnson.[5] In Table 10.2, we list the values they give (in Rydbergs), the corresponding values for $F(Z\alpha)$, and the values that we obtain for $F(Z\alpha)$. The agreement is good.

To compare our calculated values for $F(Z\alpha)$ to the coefficients in Table 1.1, we consider the function

Table 10.1. Values for $F(Z\alpha)$ obtained in this calculation.

Z	$F(Z\alpha)$
10	4.654(2)
20	3.246(1)
30	2.5519(5)
40	2.1351(7)
50	1.8644(8)
60	1.6838(4)
70	1.5675(4)
80	1.5032(6)
90	1.4880(7)
100	1.5317(8)
110	1.6614(8)

Table 10.2. The results of the Desiderio and Johnson calculation for a Coulomb potential and the results of this calculation. The numbers in the third column are the Desiderio and Johnson results converted to our units and rounded to three figures. The numbers in the fourth column are our results rounded to three figures.

Z	Desiderio and Johnson[5] ΔE_n(Ry)	Desiderio and Johnson $F(Z\alpha)$	This calculation $F(Z\alpha)$
70	9.1	1.53	1.57
75	11.9	1.52	
80	15.0	1.48	1.50
85	19.1	1.48	
90	23.5	1.45	1.49

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

$$- A_{61}(Z\alpha)^2\,\ell n(Z\alpha)^{-2} - A_{62}(Z\alpha)^2\,\ell n^2(Z\alpha)^{-2}] \,. \qquad (10.4)$$

In view of Eq. (1.2), we have

$$\lim_{Z\alpha\to 0} G(Z\alpha) = A_{60} \,. \qquad (10.5)$$

If there were a significant inconsistency between the values for $F(Z\alpha)$ and the coefficients which appear in (10.4), except possibly for A_{61}, then $G(Z\alpha)$ would increase rapidly in magnitude as $Z\alpha \to 0$. We have plotted the values of $G(Z\alpha)$, corresponding to the calculated values of $F(Z\alpha)$, in Fig. 10.2. Inspection of the points in that figure suggests that $G(Z\alpha)$ approaches a constant as $Z\alpha \to 0$. In fact, the value of the constant is approximately the value of A_{60} which appears in Table 1.1.

It is of interest to estimate the value of A_{60} which corresponds to the points in Fig. 10.2. In order to do this, it is necessary to make some assumption concerning the behavior of $G(Z\alpha)$ as $Z\alpha \to 0$. We make an estimate based on the assumption that $G(Z\alpha)$ is of the form

$$G(Z\alpha) = A_{60} + A_{70}(Z\alpha) + A_{71}(Z\alpha)\,\ell n(Z\alpha)^{-2} + \mathcal{O}\left((Z\alpha)^2\right) \qquad (10.6)$$

where $\mathcal{O}\left((Z\alpha)^2\right)$ is meant to include terms of the form $(Z\alpha)^2\,\ell n^n(Z\alpha)^{-2}$. There is some theoretical motivation for making this assumption. We fit the function

$$G_A(Z\alpha) = \bar{A}_{60} + \bar{A}_{70}(Z\alpha) + \bar{A}_{71}(Z\alpha)\,\ell n(Z\alpha)^{-2} \qquad (10.7)$$

to the calculated values for $G(Z\alpha)$ at the points $Z = 10$, 20, and 30. The resulting values for $\bar{A}_{60}$, $\bar{A}_{70}$, and $\bar{A}_{71}$ are

$$\bar{A}_{60} = -31. \pm 1.$$

$$\bar{A}_{70} = 25. \pm 2. \qquad (10.8)$$

$$\bar{A}_{71} = 6.7 \pm 0.8 \,.$$

We also fit the function $G_A(Z\alpha)$ to the calculated values for $G(Z\alpha)$ at the points $Z = 20$, 30, and 40, and at the points $Z = 30$, 40, and 50. The difference between the values for the $\bar{A}$'s corresponding to the different fits is less than the uncertainties listed in (10.8). The uncertainties in (10.8) are based on the stability of the $\bar{A}$'s with respect to varying the set of points used in making the fit rather than on the maximum uncertainties of the individual points. Erickson and Yennie[11] and Erickson[12] have given the following estimates for A_{60}:

$$A_{60} = -\frac{4}{3}\,(19.08 \pm 5) \simeq -25.4 \pm 6.7 \qquad \text{Ref. 11}$$

$$(10.9)$$

$$A_{60} = -\frac{4}{3}\,(19.3435 \pm 0.5) \simeq -25.79 \pm 0.67 \qquad \text{Ref. 12} \,.$$

Our value for $\bar{A}_{60}$ is consistent with the value for A_{60} given by Erickson and Yennie.

In conclusion, we wish to say that we see no reason why the method of calculating the self-energy radiative level shift which has been presented here could not easily be extended to calculate the level shifts for the bound states with principal quantum number $n = 2$.

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APPENDIX A

In this appendix, we discuss some relevant properties of the Dirac wave functions and Green's functions 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

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

and

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

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

$$\psi_n(\underset{\sim}{x}) = \begin{bmatrix} f_1(x)\ \chi_\kappa^{\ \mu}(\hat{x}) \\ \\ i f_2(x)\ \chi_{-\kappa}^{\ \mu}(\hat{x}) \end{bmatrix}\ , \tag{A.4}$$

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

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

The spin-angular functions have the property

$$\underset{\sim}{\sigma}\cdot\hat{x}\ \chi_\kappa^{\ \mu}(\hat{x}) \ = \ -\chi_{-\kappa}^{\ \mu}(\hat{x}) \ . \tag{A.6}$$

The functions are orthonormal

$$\int d\Omega\ \chi_{\kappa_2}^{\mu_2\dagger}(\hat{x})\ \chi_{\kappa_1}^{\mu_1}(\hat{x}) \ = \ \delta_{\kappa_2,\kappa_1}\ \delta_{\mu_2,\mu_1} \ , \tag{A.7}$$

and they are complete

$$\sum_{\kappa,\mu} \chi_\kappa^{\ \mu}(\hat{x}_2)\ \chi_\kappa^{\ \mu\dagger}(\hat{x}_1) \ = I\ \delta(\phi_2 - \phi_1)\ \delta(\cos\theta_2 - \cos\theta_1) \ . \tag{A.8}$$

The summation in (A.8) extends over values of μ and κ given by

$$\mu \ = \ -j,-j+1,\cdots,j-1,j \qquad j = |\kappa| - \tfrac{1}{2}$$
$$\kappa \ = \ \pm 1,\pm 2,\pm 3,\cdots,\pm\infty \ , \tag{A.9}$$

and θ and ϕ are the polar and azimuthal angles associated with $\hat{x}$; I is the 2×2 identity matrix. The addition theorem for the spin-angular functions is

$$\sum_\mu \chi_\kappa^{\ \mu}(\hat{x}_2)\ \chi_\kappa^{\ \mu\dagger}(\hat{x}_1) \ = \ \frac{|\kappa|}{4\pi}\ \{IP_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) + \frac{1}{\kappa}\ i\underset{\sim}{\sigma}\cdot(\hat{x}_2\times\hat{x}_1)$$
$$\times\ P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)\} \ , \tag{A.10}$$

where P_ℓ is the ℓth Legendre polynomial, $\xi = \hat{x}_2\cdot\hat{x}_1$, and P'_ℓ is the derivative of P_ℓ with respect to its argument. We shall use the notation

$$\pi_\kappa(\hat{x}_2,\hat{x}_1) \ = \ \sum_\mu \chi_\kappa^{\ \mu}(\hat{x}_2)\ \chi_\kappa^{\ \mu\dagger}(\hat{x}_1) \ . \tag{A.11}$$

For any integrable function h, we have

$$\int d\Omega_2 \int d\Omega_1\ h(\xi)\ \chi_{\kappa_2}^{\mu_2\dagger}(\hat{x}_2)\ \chi_{\kappa_1}^{\mu_1}(\hat{x}_1)$$
$$= \ 2\pi\ \delta_{\kappa_2,\kappa_1}\ \delta_{\mu_2,\mu_1} \int_{-1}^{1} d\xi\ h(\xi)\ P_{|\kappa_2+\frac{1}{2}|-\frac{1}{2}}(\xi) \ . \tag{A.12}$$

This formula is easily derived if $h(\xi)$ can be expanded in a Legendre series. In that case, we express the Legendre polynomials in that series in terms of the spin-angular functions by observing that

$$P_\ell(\xi) \ = \ \frac{4\pi}{2\ell+1}[\pi_\ell(\hat{x}_2,\hat{x}_1) + \pi_{-\ell-1}(\hat{x}_2,\hat{x}_1)] \ , \tag{A.13}$$

and then perform the integrations over angles in (A.12) with the aid of the equation in (A.7). We also have

$$\int d\Omega_2 \int d\Omega_1\ h(\xi)\ \chi_{\kappa_2}^{\mu_2\dagger}(\hat{x}_2)\ \pi_\kappa(\hat{x}_2,\hat{x}_1)\ \chi_{\kappa_1}^{\mu_1}(\hat{x}_1)$$
$$= \ \delta_{\kappa_2,\kappa_1}\ \delta_{\mu_2,\mu_1}\ \frac{|\kappa|}{2} \int_{-1}^{1} d\xi\ h(\xi)[P_{|\kappa_2+\frac{1}{2}|-\frac{1}{2}}(\xi)\ P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)$$
$$+ \frac{1}{\kappa\kappa_2}\ (1-\xi^2)\ P'_{|\kappa_2+\frac{1}{2}|-\frac{1}{2}}(\xi)\ P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi)] \ . \tag{A.14}$$

Equation (A.14) is obtained from (A.12), (A.6), and the Legendre polynomial identity

$$P_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(\xi) - \xi P_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) - \frac{1}{\kappa}(1-\xi^2)\ P'_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(\xi) \ = \ 0 \ . \tag{A.15}$$

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

$$\begin{bmatrix} 1 + V(x) - E_n & -\frac{1}{x}\frac{\partial}{\partial x} x + \frac{\kappa}{x} \\ \frac{1}{x}\frac{\partial}{\partial x} x + \frac{\kappa}{x} & -1 + V(x) - E_n \end{bmatrix} \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix} = 0 \quad , \qquad (A.16)$$

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

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

$$f_2(x) = -N^{\frac{1}{2}}(1 - E_n)^{\frac{1}{2}} x^{-\delta} e^{-\gamma x} \qquad (A.17)$$

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

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

$$[H(\underset{\sim}{x}_2) - z]\, G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \delta^3(\underset{\sim}{x}_2 - \underset{\sim}{x}_1) \quad , \qquad (A.18)$$

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

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \sum_{\kappa,\mu} \begin{bmatrix} G_\kappa^{11}(x_2,x_1,z)\, \chi_\kappa^{\mu}(\hat{x}_2)\, \chi_\kappa^{\mu\dagger}(\hat{x}_1) & -iG_\kappa^{12}(x_2,x_1,z)\, \chi_\kappa^{\mu}(\hat{x}_2)\, \chi_{-\kappa}^{\mu\dagger}(\hat{x}_1) \\ iG_\kappa^{21}(x_2,x_1,z)\, \chi_{-\kappa}^{\mu}(\hat{x}_2)\, \chi_\kappa^{\mu\dagger}(\hat{x}_1) & G_\kappa^{22}(x_2,x_1,z)\, \chi_{-\kappa}^{\mu}(\hat{x}_2)\, \chi_{-\kappa}^{\mu\dagger}(\hat{x}_1) \end{bmatrix} , \qquad (A.19)$$

where the summation extends over all possible values of κ and μ. The $G_\kappa^{ij}(x_2,x_1,z)$ are the elements of the radial Green's functions, and they satisfy the equation

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

$$= I \frac{1}{x_2 x_1} \delta(x_2 - x_1) \quad . \qquad (A.20)$$

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.21) continued next page

Equation (A.21) continued

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

$$\times\ M_{\nu+\frac{1}{2},\lambda}(2cx_2)]\ [(\kappa + \tfrac{\gamma}{c})\, W_{\nu-\frac{1}{2},\lambda}(2cx_1) - W_{\nu+\frac{1}{2},\lambda}(2cx_1)]\ , \qquad (A.21)$$

where

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

$$Q = \frac{1}{(x_1x_2)^{\frac{1}{2}}(4c^2x_1x_2)}\,\frac{\Gamma(\lambda - \nu)}{\Gamma(1 + 2\lambda)}\ , \qquad (A.22)$$

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.21) and the symmetry conditions

$$\begin{aligned} G_\kappa^{11}(x_1,x_2,z) &= G_\kappa^{11}(x_2,x_1,z) \\ G_\kappa^{12}(x_1,x_2,z) &= G_\kappa^{21}(x_2,x_1,z) \\ G_\kappa^{21}(x_1,x_2,z) &= G_\kappa^{12}(x_2,x_1,z) \\ G_\kappa^{22}(x_1,x_2,z) &= G_\kappa^{22}(x_2,x_1,z)\ . \end{aligned} \qquad (A.23)$$

The radial Green's functions are described extensively in Ref. 2. Properties of the radial Green's functions can readily be established with the aid of the identities

$$\frac{d}{dx}\, x^{-\frac{1}{2}}\, M_{\nu+\frac{1}{2},\lambda}(x) = \left(\frac{\nu}{x} - \frac{1}{2}\right)x^{-\frac{1}{2}}\, M_{\nu+\frac{1}{2},\lambda}(x) + \frac{\lambda - \nu}{x}\, x^{-\frac{1}{2}}\, M_{\nu-\frac{1}{2},\lambda}(x)$$

$$\frac{d}{dx}\, x^{-\frac{1}{2}}\, M_{\nu-\frac{1}{2},\lambda}(x) = \left(\frac{1}{2} - \frac{\nu}{x}\right)x^{-\frac{1}{2}}\, M_{\nu-\frac{1}{2},\lambda}(x) + \frac{\lambda + \nu}{x}\, x^{-\frac{1}{2}}\, M_{\nu+\frac{1}{2},\lambda}(x)$$

$$\frac{d}{dx}\, x^{-\frac{1}{2}}\, W_{\nu+\frac{1}{2},\lambda}(x) = \left(\frac{\nu}{x} - \frac{1}{2}\right)x^{-\frac{1}{2}}\, W_{\nu+\frac{1}{2},\lambda}(x) + \frac{\nu^2 - \lambda^2}{x}\, x^{-\frac{1}{2}}\, W_{\nu-\frac{1}{2},\lambda}(x)$$

$$\frac{d}{dx}\, x^{-\frac{1}{2}}\, W_{\nu-\frac{1}{2},\lambda}(x) = \left(\frac{1}{2} - \frac{\nu}{x}\right)x^{-\frac{1}{2}}\, W_{\nu-\frac{1}{2},\lambda}(x) - \frac{1}{x}\, x^{-\frac{1}{2}}\, W_{\nu+\frac{1}{2},\lambda}(x)\ . \qquad (A.24)$$

Because the radial Green's functions are independent of the quantum number μ, we can write

$$G(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \sum_\kappa \begin{bmatrix} G_\kappa^{11}(x_2,x_1,z)\ \pi_\kappa(\hat{x}_2,\hat{x}_1) & G_\kappa^{12}(x_2,x_1,z)\ i\underset{\sim}{\sigma}\cdot\hat{x}_2\ \pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \\ -G_\kappa^{21}(x_2,x_1,z)\ i\underset{\sim}{\sigma}\cdot\hat{x}_2\ \pi_\kappa(\hat{x}_2,\hat{x}_1) & G_\kappa^{22}(x_2,x_1,z)\ \pi_{-\kappa}(\hat{x}_2,\hat{x}_1) \end{bmatrix}\ . \qquad (A.25)$$

We next give asymptotic forms for the radial Green's functions. We shall restrict our attention to the case in which $x_2 < x_1$ in $G_\kappa^{ij}(x_2,x_1,z)$. We give the asymptotic behavior in terms of new variables defined by

$$y = x_1 \; ; \qquad r = \frac{x_2}{x_1} \, . \tag{A.26}$$

The first limit of interest is for x_2 and $x_1 \gg |\kappa|$. The Whittaker functions have the following asymptotic forms, for α,β fixed, $\beta > 0$, $x > 0$,[25]

$$M_{\alpha,\beta}(x) = \frac{\Gamma(1+2\beta)}{\Gamma(\beta+\frac{1}{2}-\alpha)} e^{\frac{x}{2}} x^{-\alpha} \left[1 - \frac{(\beta+\frac{1}{2}+\alpha)(\beta-\frac{1}{2}-\alpha)}{x} + \mathcal{O}\left(\frac{1}{x^2}\right) \right]$$

$$W_{\alpha,\beta}(x) = e^{-\frac{x}{2}} x^{\alpha} \left[1 + \frac{(\beta+\frac{1}{2}-\alpha)(\beta-\frac{1}{2}+\alpha)}{x} + \mathcal{O}\left(\frac{1}{x^2}\right) \right] \tag{A.27}$$

as $x \to \infty$. By $x^{\pm\alpha}$, we mean $e^{\pm\alpha \ln x}$, $\ln x$ real. From these expressions, we find

$$G_\kappa^{11}(ry,y,z) = (z+1)\, S \left\{ 1 + \frac{1+r}{2cry}\frac{\gamma}{c} - \frac{1-r}{2cry}\left[\kappa(\kappa+1) - \frac{\gamma^2}{c^2}\right] + \mathcal{O}\left(\frac{1}{y^2}\right) \right\}$$

$$G_\kappa^{12}(ry,y,z) = -cS \left\{ 1 - \frac{1+r}{2cry}\kappa - \frac{1-r}{2cry}\left[\kappa^2 - \frac{\gamma}{c}\left(1+\frac{\gamma}{c}\right)\right] + \mathcal{O}\left(\frac{1}{y^2}\right) \right\}$$

$$G_\kappa^{21}(ry,y,z) = cS \left\{ 1 + \frac{1+r}{2cry}\kappa - \frac{1-r}{2cry}\left[\kappa^2 + \frac{\gamma}{c}\left(1-\frac{\gamma}{c}\right)\right] + \mathcal{O}\left(\frac{1}{y^2}\right) \right\}$$

Equation (A.28) continued next page

Equation (A.28) continued

$$G_\kappa^{22}(ry,y,z) = (z-1)\, S \left\{ 1 - \frac{1+r}{2cry}\frac{\gamma}{c} - \frac{1-r}{2cry}\left[\kappa(\kappa-1) - \frac{\gamma^2}{c^2}\right] + \mathcal{O}\left(\frac{1}{y^2}\right) \right\}$$

$$S = \frac{r^{-\nu}}{2cry^2} e^{-(1-r)cy} \, . \tag{A.28}$$

The symbols ν, γ, and c are defined in (A.22).

The second limit of interest is for $|\kappa| \gg x_1 > x_2$. For α,x fixed, $x > 0$, the Whittaker functions have the following asymptotic forms[26]

$$M_{\alpha,\beta}(x) = x^{\beta+\frac{1}{2}} \left[1 + \frac{\frac{1}{4}(\frac{x}{2})^2 - \alpha\frac{x}{2}}{\beta} + \mathcal{O}\left(\frac{1}{\beta^2}\right) \right]$$

$$W_{\alpha,\beta}(x) = \frac{\Gamma(2\beta)}{\Gamma(\beta+\frac{1}{2}-\alpha)} x^{-\beta+\frac{1}{2}} \left[1 - \frac{\frac{1}{4}(\frac{x}{2})^2 - \alpha\frac{x}{2}}{\beta} + \mathcal{O}\left(\frac{1}{\beta^2}\right) \right] \tag{A.29}$$

as $\beta \to \infty$. From these expressions, we obtain the asymptotic forms of the Green's functions for $|\kappa| \to \infty$. We list the cases for positive and negative subscripts separately.

<u>$\kappa > 0$</u>

$$G_\kappa^{11}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\gamma + (z+1)ry + \mathcal{O}\left(\frac{1}{\kappa}\right)\right]$$

$$G_\kappa^{12}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\mathcal{O}\left(\frac{1}{\kappa}\right)\right]$$

Equation (A.30) continued next page

Equation (A.30) continued

$$G_\kappa^{21}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[2\kappa - \gamma^2 \ln r + 2\gamma z(1-r)y - \tfrac{1}{2}(1-r^2)c^2y^2 + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G_\kappa^{22}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\gamma + (z-1)y + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G_{-\kappa}^{11}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\gamma + (z+1)y + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G_{-\kappa}^{12}(ry,y,z) = -\frac{r^{\kappa-1}}{2\kappa y^2}\left[2\kappa - \gamma^2 \ln r + 2\gamma z(1-r)y - \tfrac{1}{2}(1-r^2)c^2y^2 + \mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G_{-\kappa}^{21}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\mathcal{O}(\tfrac{1}{\kappa})\right]$$

$$G_{-\kappa}^{22}(ry,y,z) = \frac{r^{\kappa-1}}{2\kappa y^2}\left[\gamma + (z-1)ry + \mathcal{O}(\tfrac{1}{\kappa})\right] . \qquad \text{(A.30)}$$

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.25) with the G's replaced by F's, where

$$F_\kappa^{ij}(x_2,x_1,z) = \lim_{\gamma\to 0} G_\kappa^{ij}(x_2,x_1,z) \qquad i,j = 1,2 . \qquad \text{(A.31)}$$

For $x_1 > x_2$:

$$F_\kappa^{11}(x_2,x_1,z) = -(z+1)\, c j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_1)$$

$$F_\kappa^{12}(x_2,x_1,z) = -ic^2 \frac{\kappa}{|\kappa|} j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_1)$$

$$F_\kappa^{21}(x_2,x_1,z) = -ic^2 \frac{\kappa}{|\kappa|} j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(icx_1) \qquad \text{(A.32)}$$

$$F_\kappa^{22}(x_2,x_1,z) = -(z-1)\, c j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_2)\, h^{(1)}_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(icx_1) .$$

In (A.32), j_ℓ is the spherical Bessel function, and $h_\ell^{(1)}$ is the spherical Hankel function of the first kind. For this case, the sum over κ is known, and is just

$$F(\underset{\sim}{x}_2,\underset{\sim}{x}_1,z) = \left[\left(\frac{c}{x} + \frac{1}{x^2}\right) i\underset{\sim}{\alpha}\cdot\underset{\sim}{x} + \beta + z\right]\frac{e^{-cx}}{4\pi x} \qquad \text{(A.33)}$$

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

APPENDIX B

For the computation of the low-energy part, we give a method by which, for a given value of x, $0 < x < 500$, and a given value of L, we can evaluate $j_\ell(x)$ and $j'_\ell(x)$ for $0 \le \ell \le L$. If the values of the $j_\ell(x)$ are known, the values of the $j'_\ell(x)$ are easily obtained from

$$j'_0(x) = -j_1(x)$$
$$j'_\ell(x) = j_{\ell-1}(x) - \frac{\ell+1}{x} j_\ell(x) \qquad \ell \neq 0 . \tag{B.1}$$

To evaluate the Bessel functions, it is convenient to first compute the values of the function

$$r_\ell(x) = \frac{2\ell+3}{x} \frac{j_{\ell+1}(x)}{j_\ell(x)} \tag{B.2}$$

at the point x for ℓ in the range $0 \le \ell < L$. From the recurrence relation

$$(2\ell+1)\, j_\ell(x) = x[j_{\ell-1}(x) + j_{\ell+1}(x)] , \tag{B.3}$$

we find

$$r_{\ell-1}(x) = \frac{1}{1 - \frac{x^2}{(2\ell+1)(2\ell+3)} r_\ell(x)} . \tag{B.4}$$

In view of the asymptotic form of $j_\ell(x)$, we have

$$\lim_{\ell\to\infty} r_\ell(x) = 1 . \tag{B.5}$$

The recursion relation in (B.4) is numerically unstable for increasing ℓ, and stable for decreasing ℓ. We compute the $r_\ell(x)$ recursively, with the aid of (B.4), in the direction of decreasing ℓ. To obtain the initial value $r_L(x)$, we use a variation of the method of J. C. P. Miller.[27] We begin the computation with the approximation $r_N(x) = 1$, for some $N > L$. The actual value of $r_N(x)$ is

$$r_N(x) = 1 + \epsilon , \tag{B.6}$$

where $|\epsilon| \ll 1$, if N is sufficiently large. Substituting $r_N(x) = 1$ into (B.4), we obtain the following approximate value for $r_{N-1}(x)$:

$$\frac{1}{1 - \frac{x^2}{(2N+1)(2N+3)}}$$
$$= \frac{1}{1 - \frac{x^2}{(2N+1)(2N+3)}(1+\epsilon) + \frac{\epsilon x^2}{(2N+1)(2N+3)}}$$
$$= r_{N-1}(x) - \frac{\epsilon x^2}{(2N+1)(2N+3)} [r_{N-1}(x)]^2 + \mathcal{O}\left(\frac{\epsilon^2 x^4}{N^4}\right) . \tag{B.7}$$

The error in the value for $r_{N-1}(x)$ is much less than the error in the value for $r_N(x)$, for large enough N. We next compute, with the aid of (B.4), an approximate value for $r_{N-2}(x)$ from the approximate value for $r_{N-1}(x)$, and so on until we obtain a value for $r_L(x)$. By starting with a large enough N, we obtain a value for $r_L(x)$ which is correct to approximately 12 significant figures. The value we use for N is given by

$$N = \max(L, L_0) + [15 + 0.1x] \tag{B.8}$$

where $L_0 = [x]$.[28] The function $[15 + 0.1x]$ was determined empirically by examining the convergence in the sequence of values for $r_{L_0}(x)$ corresponding to a sequence of increasing values of N. From the value for $r_L(x)$, values for the $r_\ell(x)$, $0 \leq \ell < L$, are calculated. The $j_\ell(x)$ are then computed with the aid of

$$\begin{aligned} j_0(x) &= \frac{\sin x}{x} \\ j_{\ell+1}(x) &= \frac{x}{2\ell + 3}\, r_\ell(x)\, j_\ell(x) \quad . \end{aligned} \tag{B.9}$$

Values for $j_\ell(x)$ and $j'_\ell(x)$ obtained by using the above method were tested by numerically evaluating the following sums:

$$\sum_{\ell=0}^{\infty} (2\ell + 1)\, j_\ell(ry)\, j_\ell(y) = \frac{\sin[(1 - r)y]}{(1 - r)y}$$

$$\sum_{\ell=0}^{\infty} (2\ell + 1)\, \ell(\ell + 1)\, j_\ell(ry)\, j_\ell(y)$$

$$= 2ry^2 \left\{ \frac{\sin[(1 - r)y]}{(1 - r)^3\, y^3} - \frac{\cos[(1 - r)y]}{(1 - r)^2\, y^2} \right\}$$

$$\sum_{\ell=0}^{\infty} (2\ell + 1)\, j'_\ell(ry)\, j_\ell(y) = \frac{\sin[(1 - r)y]}{(1 - r)^2\, y^2} - \frac{\cos[(1 - r)y]}{(1 - r)y}$$

$$\sum_{\ell=0}^{\infty} (2\ell + 1)\, j_\ell(ry)\, j'_\ell(y) = \frac{\cos[(1 - r)y]}{(1 - r)y} - \frac{\sin[(1 - r)y]}{(1 - r)^2\, y^2} \quad . \tag{B.10}$$

These sums were evaluated for all combinations of the values $r = 0.2, 0.4, \cdots, 1.0$ and $y = 0.001, 0.005, 0.01, 0.05, \cdots, 500$. In each case, the sum was truncated at $\ell = N$, where N is the smallest number for which the magnitude of the ratio of the Nth term to the sum of the first N terms is less than 10^{-12}. The results are consistent with 12 significant figures being correct in the values for the spherical Bessel functions.

APPENDIX C

The method given here for numerically evaluating the radial Green's functions $G_\kappa(x_2,x_1,z)$ is valid for the range of parameters involved in the computation of the low-energy part:

$$|\kappa| < 500$$

$$x_2, x_1 \text{ real}; \quad 0 < x_2 < x_1 < 250$$

$$z \text{ real}; \quad 0 < z < E_1 \ , \tag{C.1}$$

where E_1 is the $1S_{\frac{1}{2}}$ bound-state energy. We refer to Eq. (A.21) in which the radial Green's functions are given in terms of Whittaker functions and gamma functions.

We first evaluate

$$M_{\nu\pm\frac{1}{2},\lambda}(2cx_2) \ . \tag{C.2}$$

The following series expansion is used:[29]

$$M_{\alpha,\beta}(x) = x^{\beta+\frac{1}{2}} e^{-\frac{1}{2}x} \sum_{n=0}^{\infty} \frac{\Gamma(n+\beta+\frac{1}{2}-\alpha)\,\Gamma(2\beta+1)}{\Gamma(\beta+\frac{1}{2}-\alpha)\,\Gamma(n+2\beta+1)} \frac{x^n}{n!} \ . \tag{C.3}$$

In our case, the parameters in (C.3) obey the restrictions

$$\alpha \text{ real}; \quad -\frac{1}{2} < \alpha < \frac{3}{2}$$

$$\beta \text{ real}; \quad 0 < \beta < 500$$

$$x \text{ real}; \quad 0 < x < 500$$

$$\beta + \frac{1}{2} - \alpha > 0 \ . \tag{C.4}$$

We consider the sum which appears in (C.3)

$$S = \sum_{n=0}^{\infty} T(n) \ , \tag{C.5}$$

where

$$T(n) = \frac{\Gamma(n+\beta+\frac{1}{2}-\alpha)\,\Gamma(2\beta+1)}{\Gamma(\beta+\frac{1}{2}-\alpha)\,\Gamma(n+2\beta+1)} \frac{x^n}{\Gamma(n+1)} \ . \tag{C.6}$$

We have

$$T(0) = 1$$

$$T(n+1) = \frac{(n+\beta+\frac{1}{2}-\alpha)x}{(n+2\beta+1)(n+1)} T(n) \ . \tag{C.7}$$

The terms in the sum in (C.5), which are all non-negative, are easily computed numerically with the aid of (C.7). If the first N terms are used to approximate the sum, the error E is

$$E = \sum_{n=N+1}^{\infty} T(n) \ . \tag{C.8}$$

A simple estimate for E can be given. We find

$$\frac{\Gamma(n+1+\beta+\frac{1}{2}-\alpha)}{\Gamma(n+1+2\beta+1)} = \frac{(n+\beta+\frac{1}{2}-\alpha)}{(n+2\beta+1)} \frac{\Gamma(n+\beta+\frac{1}{2}-\alpha)}{\Gamma(n+2\beta+1)}$$

$$< \frac{\Gamma(n+\beta+\frac{1}{2}-\alpha)}{\Gamma(n+2\beta+1)} \ , \tag{C.9}$$

which gives

$$E < \frac{\Gamma(N + 1 + \beta + \frac{1}{2} - \alpha)\,\Gamma(2\beta + 1)}{\Gamma(\beta + \frac{1}{2} - \alpha)\,\Gamma(N + 1 + 2\beta + 1)} \sum_{n=N+1}^{\infty} \frac{x^n}{\Gamma(n + 1)} \quad . \qquad (C.10)$$

We also find

$$\sum_{n=N+1}^{\infty} \frac{x^n}{\Gamma(n + 1)} < \frac{x^{N+1}}{\Gamma(N + 2)} \sum_{n=0}^{\infty} \left(\frac{x}{N + 2}\right)^n$$

$$= \frac{x^{N+1}}{\Gamma(N + 2)} \frac{N + 2}{N + 2 - x} \quad \text{for} \quad N + 2 > x \; . \qquad (C.11)$$

The resulting estimate is

$$E < \frac{N + 2}{N + 2 - x} T(N + 1) \quad \text{for} \quad N + 2 > x \quad . \qquad (C.12)$$

With the aid of (C.12), the sum in (C.5) can be calculated to a preassigned accuracy. The number of terms necessary is not excessive, because for $N > x$, $T(N)$ approaches zero rapidly as N increases. Our goal is to obtain 12 significant figure accuracy in the evaluation of the radial Green's functions.

We next evaluate $W_{\alpha,\beta}(x)$. The range of the variables is given in (C.4). Two methods of evaluation are used. The choice of method depends on the magnitude of x.

For $x > 30$, we use the large-x asymptotic expansion. This asymptotic expansion can be obtained from the integral representation[30]

$$W_{\alpha,\beta}(x) = \frac{x^{\alpha}\, e^{-\frac{1}{2}x}}{\Gamma(\beta + \frac{1}{2} - \alpha)} \int_0^{\infty} dt\; t^{\beta-\frac{1}{2}-\alpha}(1 + \tfrac{t}{x})^{\beta-\frac{1}{2}+\alpha}\, e^{-t} \qquad (C.13)$$

$$|\arg x| < \pi \; ; \qquad \mathrm{Re}(\beta + \tfrac{1}{2} - \alpha) > 0$$

with the expansion

$$(1 + \tfrac{t}{x})^{\beta-\frac{1}{2}+\alpha} = \sum_{n=0}^{N} \frac{\Gamma(\beta + \frac{1}{2} + \alpha)}{\Gamma(\beta + \frac{1}{2} + \alpha - n)} \frac{1}{n!} (\tfrac{t}{x})^n + R_N \quad . \qquad (C.14)$$

Integrating term by term, we find

$$W_{\alpha,\beta}(x) = x^{\alpha}\, e^{-\frac{1}{2}x}\, S'$$

$$S' = \sum_{n=0}^{N} T'(n) + E' \quad , \qquad (C.15)$$

where

$$T'(n) = \frac{\Gamma(n + \beta + \frac{1}{2} - \alpha)\,\Gamma(\beta + \frac{1}{2} + \alpha)}{\Gamma(\beta + \frac{1}{2} - \alpha)\,\Gamma(\beta + \frac{1}{2} + \alpha - n)} \frac{1}{\Gamma(n + 1)\, x^n} \quad . \qquad (C.16)$$

The $T'(n)$ satisfy

$$T'(0) = 1$$

$$T'(n + 1) = \frac{(n + \beta + \frac{1}{2} - \alpha)(\beta - \frac{1}{2} + \alpha - n)}{(n + 1)x} T'(n) \quad . \qquad (C.17)$$

In order to obtain an estimate for the error E' in (C.15), we employ Lagrange's form for the remainder in (C.14)[31]

$$R_N = \frac{\Gamma(\beta + \frac{1}{2} + \alpha)}{\Gamma(\beta + \frac{1}{2} + \alpha - N - 1)} \frac{1}{(N+1)!} \left(\frac{t}{x}\right)^{N+1} \left(1 + \theta \frac{t}{x}\right)^{\beta - \frac{1}{2} + \alpha - N - 1}$$

$$0 \leq \theta \leq 1 \ . \qquad (C.18)$$

We note

$$\left|\left(1 + \theta \frac{t}{x}\right)^{\beta - \frac{1}{2} + \alpha - N - 1}\right| \leq 1 \quad \text{for} \quad N + 1 > \beta - \tfrac{1}{2} + \alpha \ . \qquad (C.19)$$

Combining (C.18) and (C.19) in the bound for E'

$$|E'| \leq \frac{1}{\Gamma(\beta + \frac{1}{2} - \alpha)} \int_0^\infty dt \, t^{\beta - \frac{1}{2} - \alpha} |R_N| e^{-t} \qquad (C.20)$$

yields

$$|E'| \leq |T'(N+1)| \quad \text{for} \quad N + 1 > \beta - \tfrac{1}{2} + \alpha \ . \qquad (C.21)$$

The value of $W_{\alpha,\beta}(x)$ is then obtained by performing the sum in (C.15). The value for N is determined by requiring that $N + 1 > \beta - \frac{1}{2} + \alpha$, and that the ratio of the error, as given by (C.21), to the value of the sum be less than 10^{-12} in magnitude. For $x > 30$, we find empirically that such an accuracy can always be achieved.

For $x \leq 30$, $W_{\alpha,\beta}(x)$ is computed with the aid of[32]

$$W_{\alpha,\beta}(x) = \frac{\Gamma(2\beta)}{\Gamma(\beta + \frac{1}{2} - \alpha)} M_{\alpha,-\beta}(x) + \frac{\Gamma(-2\beta)}{\Gamma(-\beta + \frac{1}{2} - \alpha)} M_{\alpha,\beta}(x) \qquad (C.22)$$

$$|\arg x| < \tfrac{3}{2}\pi \ ; \qquad 2\beta \neq \text{integer}.$$

This can be written

$$W_{\alpha,\beta}(x) = \frac{\Gamma(2\beta)}{\Gamma(\beta + \frac{1}{2} - \alpha)} x^{\frac{1}{2} - \beta} e^{-\frac{1}{2}x} (U + \eta S) \ , \qquad (C.23)$$

where

$$\eta = x^{2\beta} \frac{\Gamma(\beta + \frac{1}{2} - \alpha)\, \Gamma(-2\beta)}{\Gamma(2\beta)\, \Gamma(-\beta + \frac{1}{2} - \alpha)}$$

$$= -x^{2\beta} \frac{\sin[\pi(\beta + \frac{1}{2} + \alpha)]}{\sin(\pi 2\beta)} \frac{\Gamma(\beta + \frac{1}{2} - \alpha)\, \Gamma(\beta + \frac{1}{2} + \alpha)}{\Gamma(2\beta)\, \Gamma(2\beta + 1)} \ ; \qquad (C.24)$$

the term S is the same as in (C.5), and the term U is given by

$$U = \sum_{n=0}^{\infty} V(n) \ , \qquad (C.25)$$

where

$$V(n) = \frac{\Gamma(n - \beta + \frac{1}{2} - \alpha)\, \Gamma(-2\beta + 1)}{\Gamma(-\beta + \frac{1}{2} - \alpha)\, \Gamma(n - 2\beta + 1)} \frac{x^n}{\Gamma(n+1)} \ . \qquad (C.26)$$

The $V(n)$ are computed from

$$V(0) = 1$$

$$V(n+1) = \frac{(n - \beta + \frac{1}{2} - \alpha)x}{(n - 2\beta + 1)(n+1)} V(n) \ . \qquad (C.27)$$

The error which results from truncating the sum in (C.25) after N terms is

$$E'' = \sum_{n=N+1}^{\infty} V(n) \ . \qquad (C.28)$$

An estimate for E'' can be made by considering

$$\frac{\Gamma(n+1-\beta+\frac{1}{2}-\alpha)}{\Gamma(n+1-2\beta+1)} = \frac{(n-\beta+\frac{1}{2}-\alpha)}{(n-2\beta+1)}\,\frac{\Gamma(n-\beta+\frac{1}{2}-\alpha)}{\Gamma(n-2\beta+1)}$$

$$\leq \frac{(N+1-\beta+\frac{1}{2}-\alpha)}{(N+1-2\beta+1)}\,\frac{\Gamma(n-\beta+\frac{1}{2}-\alpha)}{\Gamma(n-2\beta+1)} \tag{C.29}$$

$$\text{for} \quad n > N > 2\beta - 2 \; ; \qquad \beta - \tfrac{1}{2} - \alpha > 0 \; ,$$

and

$$\frac{\Gamma(n+1-\beta+\frac{1}{2}-\alpha)}{\Gamma(n+1-2\beta+1)} \leq \frac{\Gamma(n-\beta+\frac{1}{2}-\alpha)}{\Gamma(n-2\beta+1)} \tag{C.30}$$

$$\text{for} \quad n > 2\beta \; ; \qquad \beta - \tfrac{1}{2} - \alpha \leq 0 \; .$$

If we let

$$\theta = \max\left\{\frac{(N+1-\beta+\frac{1}{2}-\alpha)}{(N+1-2\beta+1)} \, , \, 1\right\} \; , \tag{C.31}$$

then it follows from (C.29) and (C.30) that

$$|E''| \leq \left|\frac{\Gamma(N+1-\beta+\frac{1}{2}-\alpha)\,\Gamma(-2\beta+1)}{\Gamma(-\beta+\frac{1}{2}-\alpha)\,\Gamma(N+1-2\beta+1)}\right| \sum_{n=N+1}^{\infty} \frac{x^n\,\theta^{n-N-1}}{\Gamma(n+1)} \tag{C.32}$$

$$\text{for} \quad N > 2\beta - 1 \; .$$

With the aid of the bound in (C.11), we find

$$|E''| < \frac{N+2}{N+2-\theta x}\,|V(N+1)| \tag{C.33}$$

$$\text{for} \quad N > 2\beta - 1; \qquad N + 2 > \theta x \; .$$

Guided by the estimates in (C.33) and (C.12), one can evaluate the individual terms U and S numerically to any preassigned precision. However, the expression in (C.23) is numerically unsafe when x is large and β is small. This can be seen by considering the large-x asymptotic forms for $M_{\alpha,\beta}(x)$ and $W_{\alpha,\beta}(x)$ given in Eq. (A.27). We find that for $x \to \infty$

$$U \sim \frac{\Gamma(1-2\beta)}{\Gamma(-\beta+\frac{1}{2}-\alpha)}\, x^{\beta-\frac{1}{2}-\alpha}\, e^{x} \tag{C.34}$$

$$\eta S \sim -U \tag{C.35}$$

and

$$U + \eta S \sim \frac{\Gamma(\beta+\frac{1}{2}-\alpha)}{\Gamma(2\beta)}\, x^{\beta-\frac{1}{2}+\alpha} \; . \tag{C.36}$$

Hence in the worst case, which occurs when $x = 30$, the sum is roughly e^{-30} times the individual terms, which corresponds to a loss of approximately 13 significant figures. We have studied this cancellation numerically, and find that by using double precision arithmetic, which gives approximately 27 significant figure accuracy, we can achieve better than 12 significant figure accuracy in the evaluation of the sum $U + \eta S$.

For $x = 30$, we compared the two values obtained for $W_{\alpha,\beta}(x)$ using the two methods described above. The comparison was made for various combinations of the remaining parameters. In all cases, the two values agreed to approximately 12 significant figures.

The method that we use for evaluating the gamma function is given in Appendix D.

We note that care is required in handling potentially very large or very small quantities in the evaluation of the radial Green's functions. Quantities such as x^{β} or $\Gamma(2\beta)$ can be greater than 10^{1000} for the range of values of x and β under consideration. Such magnitudes are out of the range for real constants in the computer. The allowed range is given by

$$10^{-294} < |R| < 10^{322} . \tag{C.37}$$

In order to avoid this problem, we compute the logarithm of quantities with extreme magnitudes. We find that when all such factors have been combined, the result is of moderate magnitude and can be safely exponentiated. For the parameters which occur in the low-energy evaluation of the radial Green's functions, the range of magnitude of the terms in the sums in (C.5), (C.15), and (C.25) is within the allowed limits.

An additional consideration which we should mention is the roundoff error which occurs for values of z near E_1. In computing ΔE_L, we evaluate $G_\kappa(x_2,x_1,z)$ for values of E_1-z which are quite small. This results in the loss of significant figures in the evaluation of $G_\kappa(x_2,x_1,z)$, through error in the computation of $\lambda-\nu$, when $|\kappa| = 1$:

$$\lim_{z\to E_1^-} (\lambda - \nu) \sim \frac{E_1 - z}{\gamma^2} \qquad \text{for } |\kappa| = 1 . \tag{C.38}$$

The quantities λ and ν appear in (C.2). However, this error is not serious in the context of this calculation. We are interested in the integral over z of an expression which contains $G_\kappa(x_2,x_1,z)$ as

a factor. The integrand is proportional to E_1-z for z near E_1, which effectively suppresses the effect of the roundoff error.

As a check that the numerical evaluation of the radial Green's functions was programmed correctly, we computed the expectation value of the Dirac Green's function in various bound states. From the representation

$$G(z) = \frac{1}{H - z} = \sum_m |m\rangle \frac{1}{E_m - z} \langle m| \tag{C.39}$$

and the orthogonality of the state vectors, we have

$$\langle n|G(z)|n\rangle = \frac{1}{E_n - z} . \tag{C.40}$$

This is equivalent to the identity

$$(E_n - z)\int_0^\infty dx_2 \int_0^\infty dx_1\, x_2^{\,2}\, x_1^{\,2} \{ f_1(x_2)\, G^{11}_{\kappa_n}(x_2,x_1,z)\, f_1(x_1)$$

$$+ f_1(x_2)\, G^{12}_{\kappa_n}(x_2,x_1,z)\, f_2(x_1) + f_2(x_2)\, G^{21}_{\kappa_n}(x_2,x_1,z)\, f_1(x_1)$$

$$+ f_2(x_2)\, G^{22}_{\kappa_n}(x_2,x_1,z)\, f_2(x_1)\} = 1 , \tag{C.41}$$

where κ_n is the angular quantum number of the bound state $|n\rangle$. The integrals in (C.41) were done numerically with essentially the same techniques as those described in the section on numerical evaluation of the low-energy part. The evaluation was made for all states with principal quantum number 1 or 2, for nuclear charges of 10 and 110, and for energies $z = 0.1E_1, 0.2E_1, \cdots, 0.9E_1$. In all cases, the error in the result is less than 10^{-11}.

APPENDIX D

Our numerical evaluation of the gamma function is based on Stirling's asymptotic series[33]

$$\ln \Gamma(y) = (y - \tfrac{1}{2}) \ln y - y + \tfrac{1}{2} \ln(2\pi) + \frac{1}{12y} - \frac{1}{360y^3}$$

$$+ \frac{1}{1260y^5} - \frac{1}{1680y^7} + \frac{1}{1188y^9} - \frac{691}{360360y^{11}}$$

$$+ \frac{1}{156y^{13}} - \frac{3617}{122400y^{15}} + R \qquad \text{(D.1)}$$

for $|\arg y| \leq \frac{\pi}{2} - \delta$.

The relation between the remainder R and the value of the argument y is particularly simple if y is positive real. In this case, the remainder R has a value between zero and the first omitted term in Stirling's series[33]

$$0 < R < \frac{43867}{244188} \frac{1}{y^{17}} . \qquad \text{(D.2)}$$

Two sets of values which we consider are

$$\begin{aligned} 0 < R < 10^{-14} \quad & \text{for } y > 7 \\ 0 < R < 10^{-28} \quad & \text{for } y > 46 . \end{aligned} \qquad \text{(D.3)}$$

The second set of values is relevant to double precision evaluation of the gamma function. From the relations in (D.3), it follows that for sufficiently large y, we obtain an accurate value for the gamma function by evaluating the series in (D.1). To evaluate the gamma

function of argument x, where x is too small to satisfy the appropriate condition in (D.3), we take advantage of the relation

$$\Gamma(x) = \left\{ \prod_{i=0}^{n-1} \frac{1}{(x+i)} \right\} \Gamma(x+n) . \qquad \text{(D.4)}$$

In (D.4), we choose n large enough that $y = x + n$ is greater than the appropriate number in (D.3). We then evaluate $\Gamma(y)$ with the series in (D.1), and obtain $\Gamma(x)$ with the aid of (D.4). The relative error in this value for $\Gamma(x)$ is then just R.

In the case where y is complex and satisfies the condition $|\arg y| \leq \frac{1}{4}\pi$, we have the slightly weaker bound on the remainder R in (D.1):[33]

$$|E| < \frac{43867}{244188} \frac{1}{|y|^{17}} . \qquad \text{(D.5)}$$

Thus, for $\max(7, \mathrm{Re}(x)) \geq |\mathrm{Im}(x)|$, we employ the preceding method to evaluate $\Gamma(x)$, choosing n in (D.4) large enough that $\mathrm{Re}(x + n) > 7$.

APPENDIX E

In this section, we compute the contributions to the low-energy part of order 1 and $(Z\alpha)^2$. The low-energy part is

$$\Delta E_L = \frac{\alpha}{\pi} E_n - \frac{\alpha}{4\pi^2} \int_{k< E_n} d^3\underset{\sim}{k}\, \frac{1}{k} \sum_\lambda \langle n | \underset{\sim}{\epsilon}_\lambda \cdot \underset{\sim}{\alpha}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} \frac{1}{H - E_n + k - i\delta}$$

$$\times\ \underset{\sim}{\epsilon}_\lambda \cdot \underset{\sim}{\alpha}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}} | n \rangle \quad . \qquad (E.1)$$

The exponentials are eliminated by writing

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

$$= \left\{ e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} [\underset{\sim}{\alpha}\cdot\underset{\sim}{p} + V + \beta - E_n + k - i\delta] e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}} \right\}^{-1}$$

$$= [\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - E_n + k - i\delta]^{-1} \quad . \qquad (E.2)$$

We note that for a bound state n

$$\langle p \rangle_n = \mathcal{O}(Z\alpha); \quad \langle V \rangle_n = \mathcal{O}((Z\alpha)^2);$$

$$1 - E_n = \mathcal{O}((Z\alpha)^2) \quad . \qquad (E.3)$$

Therefore, we might expect to find the leading behavior of ΔE_L, for small $Z\alpha$, by expanding the expression in (E.2) in powers of p, V, and $1 - E_n$.[34] To second order in $Z\alpha$, such an expansion is, in fact, valid. However, if we were to try to carry the expansion farther, two difficulties would arise. The first difficulty is that the expectation values of operators such as V^3 and p^6 are infinite for S states. The second difficulty is that the integral over k would diverge for

k near 0 in some of the higher order terms.

We first note the identity

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

$$- \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - E_n + k - i\delta} V \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - E_n + k - i\delta} \quad . \qquad (E.4)$$

In the first term on the right side in (E.4), we rationalize the denominator and find

$$\sum_\lambda \underset{\sim}{\epsilon}_\lambda \cdot \underset{\sim}{\alpha} \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - E_n + k - i\delta} \underset{\sim}{\epsilon}_\lambda \cdot \underset{\sim}{\alpha}$$

$$= 2\, \frac{\underset{\sim}{\alpha}\cdot\underset{\sim}{k} - k^{-2}\, \underset{\sim}{p}\cdot\underset{\sim}{k}\, \underset{\sim}{\alpha}\cdot\underset{\sim}{k} - \beta + E_n - k}{p^2 - 2\underset{\sim}{p}\cdot\underset{\sim}{k} + 1 - E_n^2 + 2E_n k - i\delta} \quad . \qquad (E.5)$$

We now expand the denominator in (E.5) in powers of $Z\alpha$, guided by the behavior indicated in (E.3). We drop terms which have an expectation value of order higher than $(Z\alpha)^2$. Terms odd in $\underset{\sim}{k}$, which vanish on integration over angles of $\underset{\sim}{k}$, are also dropped. We obtain

$$\sum_\lambda \underset{\sim}{\epsilon}_\lambda \cdot \underset{\sim}{\alpha} \frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - E_n + k - i\delta} \underset{\sim}{\epsilon}_\lambda \cdot \underset{\sim}{\alpha}$$

$$\sim k^{-2}\, \underset{\sim}{\alpha}\cdot\underset{\sim}{k}\, \underset{\sim}{p}\cdot\underset{\sim}{k} - k^{-3}\, \underset{\sim}{\alpha}\cdot\underset{\sim}{k}\, \underset{\sim}{p}\cdot\underset{\sim}{k} + (E_n - \beta - k)$$

$$\times \left[\frac{1}{kE_n} - \frac{p^2 + 1 - E_n^2}{2k^2} + k^{-3} (\underset{\sim}{p}\cdot\underset{\sim}{k})^2 \right] \quad . \qquad (E.6)$$

The contribution from the term proportional to $E_n-\beta$ is of order $(Z\alpha)^4$ because

$$\langle n|(E_n - \beta)|n\rangle = 0$$

$$\langle n|(E_n - \beta)p^2|n\rangle = \mathcal{O}\left((Z\alpha)^4\right) . \tag{E.7}$$

We then have

$$\int_{k<E_n} d^3\underset{\sim}{k}\,\frac{1}{k}\sum_\lambda \underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}\,\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - E_n + k - i\delta}\,\underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}$$

$$\sim 4\pi\int_0^{E_n} dk\, k\{\tfrac{1}{3}\,\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \tfrac{1}{3}\,k^{-1}\,\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - E_n^{-1} + \tfrac{1}{2}\,k^{-1}(p^2 + 1 - E_n^2) - \tfrac{1}{3}\,p^2\}$$

$$\sim -4\pi\{\tfrac{1}{6}\,\underset{\sim}{\alpha}\cdot\underset{\sim}{p} + \tfrac{1}{2}\,E_n - \tfrac{1}{3}\,p^2 - \tfrac{1}{2}(1 - E_n^2)\} . \tag{E.8}$$

This expression can be simplified by noting that to order $(Z\alpha)^2$ the expectation values of $\underset{\sim}{\alpha}\cdot\underset{\sim}{p}$, p^2, $1 - E_n^2$, and $-V$ are equal. Hence, to the desired order, the contribution from (E.8) is the same as that from

$$-4\pi\{\tfrac{1}{2}\,E_n + \tfrac{2}{3}\,V\} . \tag{E.9}$$

The second term on the right side in (E.4) is already of order $(Z\alpha)^2$ due to the factor V, so we drop the terms V and $\underset{\sim}{\alpha}\cdot\underset{\sim}{p}$ in the denominators. We find

$$-\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - E_n + k - i\delta}\,V\,\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - E_n + k - i\delta}$$

$$\sim -\left[\frac{-\underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + E_n - k}{1 - E_n^2 + 2E_nk}\right]^2 V , \tag{E.10}$$

and

$$-\sum_\lambda \underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}\left[\frac{-\underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + E_n - k}{1 - E_n^2 + 2E_nk}\right]^2 V\,\underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}$$

$$= -2\left[\frac{\underset{\sim}{\alpha}\cdot\underset{\sim}{k} - \beta + E_n - k}{1 - E_n^2 + 2E_nk}\right]^2 V \sim -V . \tag{E.11}$$

In obtaining the second relation in (E.11), we dropped terms odd in $\underset{\sim}{k}$, and took into account the fact that

$$\langle n|V(\beta - E_n)|n\rangle = \mathcal{O}\left((Z\alpha)^4\right) . \tag{E.12}$$

Thus,

$$-\int_{k<E_n} d^3\underset{\sim}{k}\,\frac{1}{k}\sum_\lambda \underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}\,\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - E_n + k - i\delta}$$

$$\times\; V\,\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - E_n + k - i\delta}\,\underset{\sim}{\epsilon}_\lambda\cdot\underset{\sim}{\alpha}$$

$$\sim -4\pi\int_0^{E_n} dk\, kV \sim -4\pi\,\tfrac{1}{2}\,V . \tag{E.13}$$

Combining the results in (E.9) and (E.13), we obtain

$$\Delta E_L = \frac{\alpha}{\pi}\left(\frac{3}{2}\langle\beta\rangle_n + \frac{7}{6}\langle V\rangle_n + R\right) \quad . \tag{E.14}$$

The remainder R can be written by collecting the exact remainders in the above expansions. For example, one contribution comes from the term

$$2\int_0^{E_n} dk\, k\left\langle n\left|\frac{E_n - \beta}{p^2 + 1 - E_n^2 + 2E_n k}\right|n\right\rangle$$

$$= 2\int_0^{E_n} dk\, k\left\langle n\left|(E_n - \beta)\left[\frac{1}{2E_n k} - \frac{p^2 + 1 - E_n^2}{2E_n k(p^2 + 1 - E_n^2 + 2E_n k)}\right]\right|n\right\rangle$$

$$= \langle n|(E_n - \beta)|n\rangle - \left\langle n\left|(E_n - \beta)\frac{p^2 + 1 - E_n^2}{2E_n^2}\,\ell n\left[\frac{p^2 + 1 + E_n^2}{p^2 + 1 - E_n^2}\right]\right|n\right\rangle$$

$$= 0 + \mathcal{O}\left((Z\alpha)^4\,\ell n(Z\alpha)^2\right) \quad . \tag{E.15}$$

There are many terms in R. Rather than listing them, we describe their relevant features. The terms are all in the form of an integral over the vector $\underset{\sim}{k}$. For fixed k, after integration over angles of $\underset{\sim}{k}$, the integrands are all of order $(Z\alpha)^4$. In some cases, as in (E.15), dropping higher order terms which appear with k in the denominator leads to a divergent integral over k. In these cases, the higher order terms must be retained and one obtains a contribution of order $(Z\alpha)^4\,\ell n(Z\alpha)^2$. In the rest of the terms, dropping the higher order terms leaves a convergent integral over k. These terms are of order $(Z\alpha)^4$.

APPENDIX F

In this appendix, we first calculate ΔE_{HB} to lowest order in $Z\alpha$. The quantity ΔE_{HB} is the sum of the expressions in (6.4) and (6.7).

We seek the lowest order contribution of

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

$$\left.\left.\times\, V\,\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + V + \beta - z}\,V\,\frac{1}{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta - z}\,\alpha^\mu\right|n\right\rangle \tag{F.1}$$

to ΔE_{HB}. To obtain that contribution, we replace the potential V which appears in the denominator in (F.1) by zero. This is done because V is of order $(Z\alpha)^2$, in the sense that $\langle V\rangle_n = \mathcal{O}\left((Z\alpha)^2\right)$. There is no danger of introducing a small denominator in making this replacement, because the new rationalized denominator is bounded below:

$$\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} < 1 \qquad \text{for } z \text{ on } C_H' \quad . \tag{F.2}$$

We also replace $\underset{\sim}{p}$ everywhere by zero, because $\langle|\underset{\sim}{p}|\rangle_n = \mathcal{O}(Z\alpha)$. In the new expression, we rationalize the denominators, perform the sum over μ

$$\alpha_\mu[-\underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + z]^3\,\alpha^\mu = (4\beta - 2\underset{\sim}{\alpha}\cdot\underset{\sim}{k})(k^2 + 1 + 3z^2)$$

$$- 6z(k^2 + 1) - 2z^3 \quad , \tag{F.3}$$

and integrate over angles of $\underset{\sim}{k}$. We take into account the fact that to lowest order in $Z\alpha$, the expectation values of βV^2 and V^2 are equal. We thus find that the lowest order contribution of the quantity in (F.1) is equal to the lowest order part of

$$-\frac{i\alpha}{\pi^2}\int_{C_H'} dz \int_0^\infty dk\, k^2 \frac{1}{k^2 - (E_n - z)^2 - i\epsilon}$$

$$\times \left(\frac{4 - 6z}{[k^2 + 1 - z^2]^2} + \frac{16z^2 - 8z^3}{[k^2 + 1 - z^2]^3}\right) \langle V^2\rangle_n \quad . \qquad \text{(F.4)}$$

Integrating over k, we obtain

$$-\frac{i\alpha}{2\pi}\int_{C_H'} dz \left[\frac{2 - 3z}{c(b + c)^2} + \frac{(2z^2 - z^3)(b + 3c)}{c^3(b + c)^3}\right] \langle V^2\rangle_n \qquad \text{(F.5)}$$

$$b = -i[(E_n - z)^2 + i\epsilon]^{\frac{1}{2}} , \qquad \mathrm{Re}(b) > 0$$

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

Finally, the integration over z is performed as described in Sec. VII. Retaining only the lowest order part $(E_n \cong 1)$, we have

$$\frac{\alpha}{\pi}\left(\frac{3}{2}\,\ell n\, 2 - \frac{5}{4}\right) \langle V^2\rangle_{NR} \qquad \text{(F.6)}$$

where NR denotes the non-relativistic limit of the expectation value in the state n.

We now find the lowest order contribution of

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

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

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

$$\left.\left. - \frac{\underset{\sim}{\alpha}\cdot\underset{\sim}{p} - \underset{\sim}{\alpha}\cdot\underset{\sim}{k} + \beta + z}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}\,[\underset{\sim}{\alpha}\cdot\underset{\sim}{p}, V]\,\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}\right)\alpha^\mu\left|n\right.\right\rangle \quad . \qquad \text{(F.7)}$$

The following identities are relevant here:

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

$$= \frac{4z(2\beta - z)}{\underset{\sim}{k}^2 + 1 - z^2}\left\{\left[\frac{2\underset{\sim}{p}\cdot\underset{\sim}{k}}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2}, V\right]\frac{1}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2}\right.$$

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

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

$$\left. - \left[\frac{\underset{\sim}{p}^2}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}, V\right]\frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}\right\} ; \qquad \text{(F.8a)}$$

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

$$= \frac{4z\underset{\sim}{\alpha}\cdot\underset{\sim}{p}}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} V \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} - \frac{4z\underset{\sim}{\alpha}\cdot\underset{\sim}{k}}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2}$$

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

$$- \frac{4z\underset{\sim}{\alpha}\cdot\underset{\sim}{k}}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2} \frac{2\underset{\sim}{p}\cdot\underset{\sim}{k}}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} V \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}$$

$$- \frac{4z\underset{\sim}{\alpha}\cdot\underset{\sim}{k}}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2} V \frac{2\underset{\sim}{p}\cdot\underset{\sim}{k}}{(\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2)[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]} \quad ; \text{(F.8b)}$$

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

$$= \frac{(4\delta_{ij} - 2\alpha^i\alpha^j)p^i}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} [p^j, V] \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}$$

$$- \frac{(4\delta_{ij} - 2\alpha^i\alpha^j)k^i}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2} [p^j, V] \frac{1}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2}$$

$$- \frac{(4\delta_{ij} - 2\alpha^i\alpha^j)k^i\ 2\underset{\sim}{p}\cdot\underset{\sim}{k}}{(\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2)[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]} [p^j, V] \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2}$$

Equation (F.8c) continued next page

Equation (F.8c) continued

$$- \frac{(4\delta_{ij} - 2\alpha^i\alpha^j)k^i}{\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2} [p^j, V] \frac{2\underset{\sim}{p}\cdot\underset{\sim}{k}}{(\underset{\sim}{p}^2 + \underset{\sim}{k}^2 + 1 - z^2)[(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2]}$$

$$- \frac{2z}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} [\underset{\sim}{\alpha}\cdot\underset{\sim}{p}, V] \frac{1}{(\underset{\sim}{p} - \underset{\sim}{k})^2 + 1 - z^2} \quad . \qquad \text{(F.8c)}$$

We substitute Eqs. (F.8) into (F.7), and consider the non-relativistic limit of the expectation value. In this limit, the large (upper) component of the wave function is replaced by $|n\rangle_S$, the two-component Pauli-Schrödinger wave function, and the small (lower) component is replaced by $\frac{1}{2}\underset{\sim}{\sigma}\cdot\underset{\sim}{p}|n\rangle_S$. For terms which connect large components to large components and small components to small components, only the contribution of the large components is retained. We then replace $\underset{\sim}{p}$ by zero wherever it appears in a denominator. All the terms which survive the integration over angles of $\underset{\sim}{k}$ are separately of order $(Z\alpha)^4$, i.e., they have one factor V and either two factors of $\underset{\sim}{p}$, or one factor of $\underset{\sim}{p}$ and one factor of $\underset{\sim}{\alpha}$. The expectation value of each such combination is of order $(Z\alpha)^4$. The lowest order contribution of (F.7) is then given, after integration over angles of $\underset{\sim}{k}$, by

$$\frac{i\alpha}{\pi^2} \int_{C_H'} dz \int_0^\infty dk \frac{k^2}{k^2 - (E_n - z)^2 - i\epsilon} \left\{ - \frac{8}{3} \frac{z(2 - z)k^2}{(k^2 + 1 - z^2)^4} \right.$$

$$\left. \times \langle [p^i, [p^i, V]] \rangle_{NR} + \left[\frac{4z}{(k^2 + 1 - z^2)^2} - \frac{16}{3} \frac{zk^2}{(k^2 + 1 - z^2)^3} \right] \right.$$

Equation (F.9) continued next page

Equation (F.9) continued

$$\times \langle p^2 V - \tfrac{1}{4}[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR}$$

$$+ \frac{1}{(k^2+1-z^2)^2}\ \langle 2[p^i,[p^i,V]] - [\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR}$$

$$\left. + \frac{4}{3}\,\frac{k^2}{(k^2+1-z^2)^3}\ \langle [\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]] - [p^i,[p^i,V]]\rangle_{NR}\right\} \quad . \qquad (F.9)$$

Integration over k yields

$$\frac{i\alpha}{\pi}\int_{C_H'} dz\left\{\frac{2z}{3(b+c)^3}\ \langle p^2 V\rangle_{NR} - \frac{1+z}{6(b+c)^3}\ \langle [\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR}\right.$$

$$\left. + \left[\frac{2c^2+2cb+b^2}{6c(c+b)^4} + (1-2z)\,\frac{c^2+4cb+b^2}{12c^3(c+b)^4}\right]\langle [p^i,[p^i,V]]\rangle_{NR}\right\} \quad , \qquad (F.10)$$

where b and c are defined in (F.5). We integrate over z in (F.10), keeping only the terms of lowest order in $Z\alpha$, and obtain

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

$$\left. + (\tfrac{1}{3}\ \ell n\ 2 - \tfrac{17}{72})\langle [p^i,[p^i,V]]\rangle_{NR}\right\} . \qquad (F.11)$$

Combining the results in (F.6) and (F.11), we have

$$\Delta E_{HB} = \frac{\alpha}{\pi}\left\{(\tfrac{3}{2}\ \ell n\ 2 - \tfrac{5}{4})\langle V^2\rangle_{NR} + (\ell n\ 2 - \tfrac{5}{6})\langle p^2 V\rangle_{NR}\right.$$

$$+ (\tfrac{3}{8} - \tfrac{1}{2}\ \ell n\ 2)\langle [\underset{\sim}{\sigma}\cdot\underset{\sim}{p}[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR} + (\tfrac{1}{3}\ \ell n\ 2 - \tfrac{17}{72})$$

$$\left. \times \langle [p^i,[p^i,V]]\rangle_{NR} + \mathcal{O}\big((Z\alpha)^5\big)\right\} \quad . \qquad (F.12)$$

For the $1S_{\frac{1}{2}}$ state

$$\langle V^2\rangle_{NR} = 2(Z\alpha)^4$$

$$\langle p^2 V\rangle_{NR} = -3(Z\alpha)^4$$

$$\langle [\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR} = -4(Z\alpha)^4$$

$$\langle [p^i,[p^i,V]]\rangle_{NR} = -4(Z\alpha)^4 \quad , \qquad (F.13)$$

and hence

$$\Delta E_{HB}(1S_{\frac{1}{2}}) = \frac{\alpha}{\pi}\left[(\tfrac{2}{3}\ \ell n\ 2 - \tfrac{5}{9})(Z\alpha)^4 + \mathcal{O}\big((Z\alpha)^5\big)\right] \quad . \qquad (F.14)$$

The limits as $Z\alpha \to 0$ of the functions h_1, h_2, h_3, and h_4, which are defined in (7.34), are now considered. To obtain these limits, we examine the behavior of Q_1, Q_2, Q_3, and Q_4, defined in (7.30), near $p^2 = 0$ and $E_n = 1$:

$$Q_1(p^2) = \frac{1}{10} + \frac{1}{15}(1 - E_n) - \frac{1}{84}p^2 + \mathcal{O}\left((1 - E_n)^2\right) + \mathcal{O}\left((1 - E_n)p^2\right) + \mathcal{O}(p^4)$$

$$Q_2(p^2) = \frac{1}{2}\ln 2 - \frac{7}{20} + (\ln 2 - \frac{9}{10})(1 - E_n) + (\frac{1}{4}\ln 2 - \frac{43}{210})p^2 + \mathcal{O}\left((1 - E_n)^2\right) + \mathcal{O}\left((1 - E_n)p^2\right) + \mathcal{O}(p^4)$$

$$Q_3(p^2) = \frac{31}{15} - 3\ln 2 + \mathcal{O}(1 - E_n) + \mathcal{O}(p^2)$$

$$Q_4(p^2) = 4\ln 2 - \frac{8}{3} + \mathcal{O}(1 - E_n) + \mathcal{O}(p^2) \quad . \tag{F.15}$$

We also note the identities

$$\begin{aligned} \langle p^2 + E_n V + \underset{\sim}{\alpha}\cdot\underset{\sim}{p}\, V\rangle_n &= 0 \\ \langle \beta p^2 + V + \beta\, \underset{\sim}{\alpha}\cdot\underset{\sim}{p}\, V\rangle_n &= 0 \end{aligned} \tag{F.16}$$

which combined with the first two equations in (7.34) yield

$$\begin{aligned} h_1(Z\alpha) &= (Z\alpha)^{-4}\left\{\frac{1}{10}(1 - E_n{}^2)\langle V\rangle_n - \frac{1}{10}E_n\langle\underset{\sim}{\alpha}\cdot\underset{\sim}{p}\, V\rangle_n + \langle E_n[Q_1(p^2) - \frac{1}{10}]p^2\rangle_n\right\} \\ h_2(Z\alpha) &= (Z\alpha)^{-4}\left\{(\frac{7}{20} - \frac{1}{2}\ln 2)\langle\beta\, \underset{\sim}{\alpha}\cdot\underset{\sim}{p}\, V\rangle_n + \langle\beta[Q_2(p^2) - (\frac{1}{2}\ln 2 - \frac{7}{20})]p^2\rangle_n\right\} \quad . \end{aligned} \tag{F.17}$$

We take the non-relativistic limit of the expectation values in (F.17), and then replace Q_1 and Q_2 by the first three terms in the corresponding expansion which appears in (F.15). We obtain

$$\begin{aligned} h_1(0) &= (Z\alpha)^{-4}\left\{\frac{23}{420}\langle p^4\rangle_{NR} + \frac{1}{30}\langle p^2 V\rangle_{NR} + \frac{1}{40}\langle[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR}\right\} \\ h_2(0) &= (Z\alpha)^{-4}\left\{(\frac{103}{420} - \frac{1}{4}\ln 2)\langle p^4\rangle_{NR} + (\frac{9}{10} - \ln 2)\langle p^2 V\rangle_{NR} + (\frac{1}{8}\ln 2 - \frac{7}{80})\langle[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},[\underset{\sim}{\sigma}\cdot\underset{\sim}{p},V]]\rangle_{NR}\right\} \quad . \end{aligned} \tag{F.18}$$

The limits as $Z\alpha \to 0$ of h_3 and h_4 are obtained by taking the non-relativistic limit of the corresponding expectation values in (7.34) and then replacing Q_3 and Q_4 by the leading term in the corresponding expansion which appears in (F.15). We have

$$\begin{aligned} h_3(0) &= (Z\alpha)^{-4}(\frac{31}{15} - 3\ln 2)\langle p^2 V\rangle_{NR} \\ h_4(0) &= (Z\alpha)^{-4}(4\ln 2 - \frac{8}{3})\langle p^2 V\rangle_{NR} \quad . \end{aligned} \tag{F.19}$$

In the case of the $1S_{\frac{1}{2}}$ state, the limits are

$$\begin{aligned} h_1(0) &= \frac{31}{420} \\ h_2(0) &= \frac{5}{4}\ln 2 - \frac{118}{105} \\ h_3(0) &= 9\ln 2 - \frac{31}{5} \\ h_4(0) &= 8 - 12\ln 2 \quad . \end{aligned} \tag{F.20}$$

APPENDIX G

In this section, we list some formulas related to the Fourier transforms of the Dirac wave functions for a Coulomb field. The momentum-space wave function is written in the form

$$\phi_n(\underset{\sim}{p}) = \begin{bmatrix} g_1(p) & \chi_\kappa^{\ \mu}(\hat{p}) \\ g_2(p) & \chi_{-\kappa}^{\ \mu}(\hat{p}) \end{bmatrix} \tag{G.1}$$

where $\chi_\kappa^{\ \mu}$ is the two-component spin-angular function described in Appendix A. The ϕ_n are defined by

$$\phi_n(\underset{\sim}{p}) = (2\pi)^{-\frac{3}{2}} \int d^3\underset{\sim}{x}\, e^{-i\underset{\sim}{p}\cdot\underset{\sim}{x}}\, \psi_n(\underset{\sim}{x}) \ . \tag{G.2}$$

From the expansion

$$e^{-i\underset{\sim}{p}\cdot\underset{\sim}{x}} = 4\pi \sum_{\kappa,\mu} (-i)^{|\kappa+\frac{1}{2}|-\frac{1}{2}}\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(px)\, \chi_\kappa^{\ \mu}(\hat{p})\, \chi_\kappa^{\ \mu}(\hat{x}) \tag{G.3}$$

and the orthogonality of the $\chi_\kappa^{\ \mu}$'s, we obtain

$$\begin{aligned} g_1(p) &= (-i)^{|\kappa+\frac{1}{2}|-\frac{1}{2}} \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty dx\, x^2\, j_{|\kappa+\frac{1}{2}|-\frac{1}{2}}(px)\, f_1(x) \\ g_2(p) &= -(-i)^{|\kappa-\frac{1}{2}|+\frac{1}{2}} \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^\infty dx\, x^2\, j_{|\kappa-\frac{1}{2}|-\frac{1}{2}}(px)\, f_2(x) \end{aligned} \tag{G.4}$$

where f_1 and f_2 are the components of the coordinate-space radial wave functions, and j_ℓ is the spherical Bessel function. For the $1S_{\frac{1}{2}}$ state, we have

$$\begin{aligned} g_1(p) &= N^{\frac{1}{2}}(1 + E_n)^{\frac{1}{2}} \frac{\sin[(2 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2 + p^2]^{\frac{1}{2}(2-\delta)}} \\ g_2(p) &= -N^{\frac{1}{2}}(1 - E_n)^{\frac{1}{2}} \left\{ \frac{\sin[(1 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{(1 - \delta)p^2[\gamma^2 + p^2]^{\frac{1}{2}(1-\delta)}} - \frac{\cos[(2 - \delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2 + p^2]^{\frac{1}{2}(2-\delta)}} \right\} \end{aligned} \tag{G.5}$$

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

We also give the expression for the Coulomb potential acting on the wave function in momentum space $V\phi_n(\underset{\sim}{p})$. It is obtained by taking the Fourier transform of $V(\underset{\sim}{x})\, \psi_n(\underset{\sim}{x})$. Because of the spherical symmetry of the potential, the calculation is similar to that for the wave function, the only difference being the presence of a factor $V(x)$ in the integrand in Eq. (G.4). We find

$$V\phi_n(\underset{\sim}{p}) = \begin{bmatrix} Vg_1(p) & \chi_\kappa^{\ \mu}(\hat{p}) \\ Vg_2(p) & \chi_{-\kappa}^{\ \mu}(\hat{p}) \end{bmatrix} \tag{G.6}$$

where

$$Vg_1(p) = -\frac{\gamma N^{\frac{1}{2}}}{E_n}(1+E_n)^{\frac{1}{2}}\frac{\sin[(1-\delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2+p^2]^{\frac{1}{2}(1-\delta)}}$$

$$Vg_2(p) = \frac{\gamma N^{\frac{1}{2}}}{E_n}(1-E_n)^{\frac{1}{2}}\left\{\frac{\sin[\delta\tan^{-1}(\frac{p}{\gamma})]}{\delta p^2[\gamma^2+p^2]^{-\frac{1}{2}\delta}} - \frac{\cos[(1-\delta)\tan^{-1}(\frac{p}{\gamma})]}{p[\gamma^2+p^2]^{\frac{1}{2}(1-\delta)}}\right\} . \tag{G.7}$$

APPENDIX H

We describe here the method used to evaluate the products of spherical Bessel and Hankel functions $j_\ell(x)\, h_\ell^{(1)}(y)$ which arise in the numerical evaluation of ΔE_{HB}. The relevant ranges for the parameters x, y, and ℓ are given by

$$0 < \frac{x}{y} < 1$$

$$0 < \mathrm{Re}(y) < 200 \; ; \qquad 0 < \mathrm{Im}(y) < 20{,}000 \tag{H.1}$$

$$0 \le \ell \le 20{,}000 \; .$$

The evaluation is done by a subroutine in which for a given value of x, y, and L, $1 \le L \le 20{,}000$, the set of values $j_\ell(x)\, h_\ell^{(1)}(y)$, $0 \le \ell \le L$, is computed.

It is convenient to first compute the set of values $r_\ell(x)$ defined in Eq. (B.2). We use the method described in Appendix B to compute these values, except that here we replace the number N defined in (B.8) by the number N'

$$N' = \max(L, L_0') + [15 + 0.1\,\mathrm{Re}(x)] \; , \tag{H.2}$$

where $L_0' = [|x|]$. This expression for N' was arrived at with the method analogous to the one described in Appendix B for finding N.

We also compute the set of values $t_\ell(y)$, where

$$t_\ell(y) = \frac{2\ell+1}{y}\frac{h_\ell^{(1)}(y)}{h_{\ell+1}^{(1)}(y)} \; , \tag{H.3}$$

at the point y for ℓ in the range $0 \le \ell < L$. Because the function $h_\ell^{(1)}(y)$ satisfies the recurrence relation

$$(2\ell + 1)\, h_\ell^{(1)}(y) = y[h_{\ell-1}^{(1)}(y) + h_{\ell+1}^{(1)}(y)] \,, \tag{H.4}$$

we have

$$t_{\ell+1}(y) = \frac{1}{1 - \frac{y^2}{(2\ell + 1)(2\ell + 3)}\, t_\ell(y)} \,. \tag{H.5}$$

We also have

$$\lim_{\ell \to \infty} t_\ell(y) = 1 \,. \tag{H.6}$$

The values $t_\ell(y)$, $0 < \ell < L$, are computed recursively, with (H.5), in the direction of increasing ℓ. The initial value is given by

$$t_0(y) = \frac{1}{1 - iy} \,. \tag{H.7}$$

The products $j_\ell(x)\, h_\ell^{(1)}(y)$, $0 \le \ell \le L$, are then computed recursively with the aid of

$$j_0(x)\, h_0^{(1)}(y) = \frac{\sin x}{x} \frac{e^{iy}}{iy} \tag{H.8}$$

and

$$j_{\ell+1}(x)\, h_{\ell+1}^{(1)}(y) = \frac{2\ell + 1}{2\ell + 3} \frac{x}{y} \frac{r_\ell(x)}{t_\ell(y)}\, j_\ell(x)\, h_\ell^{(1)}(y) \,. \tag{H.9}$$

We tested the subroutine which computes the products $j_\ell(x)\, h_\ell^{(1)}(y)$ by numerically evaluating the following sums:

$$\sum_{\ell=0}^{\infty} (2\ell + 1)\, j_\ell(ry)\, h_\ell^{(1)}(y) = \frac{e^{iy(1-r)}}{iy(1 - r)}$$

$$\sum_{\ell=0}^{\infty} (2\ell + 1)\, \ell(\ell + 1)\, j_\ell(ry)\, h_\ell^{(1)}(y) \tag{H.10}$$

$$= 2r(iy)^2 \left\{ \frac{1}{[iy(1 - r)]^3} - \frac{1}{[iy(1 - r)]^2} \right\} e^{iy(1-r)} \,.$$

The evaluation was made for all combinations of the values $\mathrm{Re}(y) = 0.01, 0.02, 0.1, 0.2, \cdots, 100, 200$, $\mathrm{Im}(y) = 0.01, 0.02, 0.1, 0.2, \cdots, 100, 200$, $r = 0.2, 0.4, 0.6, 0.8$, and for all combinations of the values $\mathrm{Re}(y) = 0.01, 0.02, 0.1, 0.2, \cdots, 100, 200$, $\mathrm{Im}(y) = 1000, 2000, 10000, 20000$, and $r = 0.99$. In each case, the sum over ℓ in (H.10) was terminated when the ratio of the last term in the partial sum to the partial sum was less than 10^{-15} in magnitude. The values of the sums agree with the corresponding expressions on the right side in (H.10) to more than 11 significant figures.

APPENDIX I

In this appendix, we give the method used to evaluate the Coulomb radial Green's functions $G_\kappa(x_2,x_1,z)$ for the range of parameters encountered in the numerical evaluation of ΔE_{HB}. The range is given by

$$|\kappa| < 20{,}000$$

$$x_2, x_1 \text{ real} ; \qquad 0 < x_2 < x_1 < 200 \tag{I.1}$$

$$\mathrm{Re}(z) = 0 ; \qquad 0 < \mathrm{Im}(z) < 100 .$$

We first consider the evaluation of $M_{\alpha,\beta}(x)$ for the following range of variables:

$$\mathrm{Re}(\alpha) = \pm\tfrac{1}{2} ; \qquad 0 < \mathrm{Im}(\alpha) < 1$$

$$0 < \beta < 20{,}000 \tag{I.2}$$

$$0 < x < 40{,}000 .$$

Two methods of evaluation are used. The choice of method depends on the relative magnitude of x and β. For $x < 20\,\beta^{\frac{1}{2}}$, we employ the power series for $M_{\alpha,\beta}(x)$ obtained by expanding the exponential function in the integral representation

$$M_{\alpha,\beta}(x) = \frac{\Gamma(1+2\beta)}{\Gamma(\beta+\frac{1}{2}-\alpha)\,\Gamma(\beta+\frac{1}{2}+\alpha)}\, x^{\beta+\frac{1}{2}} \int_0^1 dt\; t^{\beta-\frac{1}{2}-\alpha}(1-t)^{\beta-\frac{1}{2}+\alpha} \times e^{(t-\frac{1}{2})x} \tag{I.3}$$

$$\mathrm{Re}(\beta+\tfrac{1}{2}\pm\alpha) > 0 \qquad |\arg x| < \pi$$

in powers of x. The resulting series is

$$M_{\alpha,\beta}(x) = x^{\beta+\frac{1}{2}} \sum_{n=0}^{\infty} I(n)\, \frac{(\frac{x}{2})^n}{n!} \tag{I.4}$$

where

$$I(n) = \frac{\Gamma(1+2\beta)}{\Gamma(\beta+\frac{1}{2}-\alpha)\,\Gamma(\beta+\frac{1}{2}+\alpha)} \int_0^1 dt\; t^{\beta-\frac{1}{2}-\alpha}(1-t)^{\beta-\frac{1}{2}+\alpha} \times (2t-1)^n . \tag{I.5}$$

It is convenient to consider the corresponding expansions

$$M_{\nu-\frac{1}{2},\lambda}(2cx_2) \pm M_{\nu+\frac{1}{2},\lambda}(2cx_2) = (2cx_2)^{\lambda+\frac{1}{2}} \sum_{n=0}^{N} I_\pm(n)\, \frac{(cx_2)^n}{n!} + E_\pm(N) \tag{I.6}$$

where $E_\pm(N)$ are the remainders. The functions $I_\pm$ satisfy the equations

$$I_+(n+1) = I_-(n) - \frac{2\nu}{n+1+2\lambda}\, I_+(n)$$

$$I_-(n+1) = \frac{n+1}{n+1+2\lambda}\, I_+(n) . \tag{I.7}$$

These relations together with the initial values $I_+(0) = 2$ and $I_-(0) = 0$ provide a simple (and safe) method for numerically evaluating the series in (I.6). We obtain approximate values for the errors $E_\pm$ in (I.6), which arise from truncating the sum over n at $n = N$, by estimating these errors to lowest order in ν. Let

$$\lim_{\nu\to 0} I_{\pm}(n) = I_{\pm}^{0}(n)$$

$$\lim_{\nu\to 0} E_{\pm}(N) = E_{\pm}^{0}(N) \; . \tag{I.8}$$

Then

$$I_{+}^{0}(n) = \begin{cases} 2\,\dfrac{\Gamma(\lambda+\frac{1}{2})\,\Gamma(\frac{1}{2}n+\frac{1}{2})}{\Gamma(\frac{1}{2})\,\Gamma(\lambda+\frac{1}{2}n+\frac{1}{2})} & n \text{ even} \\ 0 & n \text{ odd} \end{cases} \tag{I.9}$$

and

$$E_{+}^{0}(N) = 2(2cx_2)^{\lambda+\frac{1}{2}} \sum_{m=\frac{N+1}{2}}^{\infty} \frac{\Gamma(\lambda+\frac{1}{2})\,\Gamma(m+\frac{1}{2})}{\Gamma(\frac{1}{2})\,\Gamma(\lambda+m+\frac{1}{2})}\,\frac{(cx_2)^{2m}}{(2m)!} \qquad N \text{ odd} \; . \tag{I.10}$$

Because

$$\frac{\Gamma(m+\frac{1}{2})(cx_2)^{2m}}{\Gamma(\lambda+m+\frac{1}{2})(2m)!} \le \left[\frac{(cx_2)^2}{(2\lambda+N+2)(N+3)}\right]^{m-\frac{1}{2}(N+1)} \times \frac{\Gamma(\frac{1}{2}N+1)(cx_2)^{N+1}}{\Gamma(\lambda+\frac{1}{2}N+1)(N+1)!} \tag{I.11}$$

for $m \ge \frac{1}{2}(N+1)$, we have

$$E_{+}^{0}(N) < 2(2cx_2)^{\lambda+\frac{1}{2}}\,\frac{\Gamma(\lambda+\frac{1}{2})\,\Gamma(\frac{1}{2}N+1)}{\Gamma(\frac{1}{2})\,\Gamma(\lambda+\frac{1}{2}N+1)}\,\frac{(cx_2)^{N+1}}{(N+1)!} \times \frac{(2\lambda+N+2)(N+3)}{(2\lambda+N+2)(N+3)-(cx_2)^2} \tag{I.12}$$

for

$$(2\lambda+N+2)(N+3) > (cx_2)^2 \; , \tag{I.13}$$

where N is odd. We then have

$$|E_{+}(N)| < (2cx_2)^{\lambda+\frac{1}{2}}|I_{+}(N+1)|\frac{(cx_2)^{N+1}}{(N+1)!}\,\frac{(2\lambda+N+2)(N+3)}{(2\lambda+N+2)(N+3)-(cx_2)^2} \times [1+\mathcal{O}(|\nu|)] \; , \tag{I.14}$$

valid when N is odd and satisfies (I.13). The corresponding expression for E_{-} is

$$|E_{-}(N)| < (2cx_2)^{\lambda+\frac{1}{2}}|I_{-}(N+1)|\frac{(cx_2)^{N+1}}{(N+1)!}\,\frac{(2\lambda+N+3)(N+2)}{(2\lambda+N+3)(N+2)-(cx_2)^2} \times [1+\mathcal{O}(|\nu|)] \; , \tag{I.15}$$

valid when N is even and satisfies

$$(2\lambda+N+3)(N+2) > (cx_2)^2 \; . \tag{I.16}$$

In the numerical evaluation of (I.6), the value of N is taken to be the smallest value for which both (I.16) is satisfied and the errors $E_{\pm}$ corresponding to N and $N-1$, as estimated in (I.14) and

(I.15), are less than 10^{-12} times the corresponding partial sums in magnitude.

The numerical evaluation of $M_{\alpha,\beta}(x)$ for $x \geq 20\beta^{\frac{1}{2}}$ is done with the aid of the expansion in (C.3). In this case, the summation is begun at $n = n_0$, where n_0 is approximately the value n for which the magnitude of $T(n)$, defined in (C.6), has its maximum value. In view of (C.7), it is apparent that we obtain an approximate value for n_0 by solving for u in

$$\left|\frac{(u + \beta)x}{(u + 2\beta)u}\right| = 1 . \tag{I.17}$$

The relevant solution is

$$u = \left(\beta^2 + \frac{x^2}{4}\right)^{\frac{1}{2}} + \frac{x}{2} - \beta , \tag{I.18}$$

and we let

$$n_0 = [u] . \tag{I.19}$$

We then evaluate $\bar{S}$, where

$$\bar{S} = \sum_{n=0}^{\infty} \bar{T}(n) = \sum_{n=n_0}^{N_1} \bar{T}(n) + \sum_{n=N_2}^{n_0-1} \bar{T}(n) + E_1 + E_2 \tag{I.20}$$

and

$$\begin{aligned} \bar{T}(n_0) &= 1 \\ \bar{T}(n + 1) &= \frac{(n + \beta + \frac{1}{2} - \alpha)x}{(n + 2\beta + 1)(n + 1)} \bar{T}(n) . \end{aligned} \tag{I.21}$$

The value that we use for N_1 is determined by making an estimate of the error E_1, where

$$E_1 = \sum_{n=N_1+1}^{\infty} \bar{T}(n) . \tag{I.22}$$

For $N_1 \geq 0$,

$$|\bar{T}(N_1 + 1 + m)| \leq \theta^m |\bar{T}(N_1 + 1)| \tag{I.23}$$

$$\theta = \left|\frac{(N_1 + \frac{3}{2} + \beta - \alpha)x}{(N_1 + 2 + 2\beta)(N_1 + 2)}\right| ,$$

and hence for N_1 large enough that $\theta < 1$, we have

$$|E_1| < \frac{1}{1 - \theta} |\bar{T}(N_1 + 1)| . \tag{I.24}$$

We perform the first sum over n on the right in (I.20), testing the value of the error as each term is added, and terminating the sum when the magnitude of the ratio of the error, as given in (I.24), to the partial sum is less than 10^{-11}. The second sum on the right in (I.20) is then performed in the direction of decreasing n. This sum is terminated when the same condition on the error is satisfied. In this case, the estimate for the error is given by

$$|E_2| = \left|\sum_{n=0}^{N_2-1} \bar{T}(n)\right| < N_2 |\bar{T}(N_2 - 1)| \tag{I.25}$$

for N_2 smaller than the value of n for which $|\bar{T}(n)|$ is at the maximum. The value of the Whittaker function is then

$$M_{\alpha,\beta}(x) = x^{\beta+\frac{1}{2}} e^{-\frac{1}{2}x} T(n_0) \bar{S} . \tag{I.26}$$

From the coefficient of $\bar{S}$ in (I.26), we store separately the complex logarithm of

$$\frac{\Gamma(n_0 + \beta + \frac{1}{2} - \alpha)}{\Gamma\left(n_0 + \beta + \frac{1}{2} - \mathrm{Re}(\alpha)\right)} \frac{\Gamma\left(\beta + \frac{1}{2} - \mathrm{Re}(\alpha)\right)}{\Gamma(\beta + \frac{1}{2} - \alpha)} . \tag{I.27}$$

and the double precision logarithm of

$$\frac{\Gamma\left(n_0 + \beta + \frac{1}{2} - \mathrm{Re}(\alpha)\right) \Gamma(2\beta + 1) x^{n_0+\beta+\frac{1}{2}}}{\Gamma\left(\beta + \frac{1}{2} - \mathrm{Re}(\alpha)\right) \Gamma(n_0 + 2\beta + 1) \Gamma(n_0 + 1)} e^{-\frac{1}{2}x} . \tag{I.28}$$

Storing the double precision logarithm of (I.28) is necessary because of the loss of significant figures which occurs when the logarithm of a quantity with a very large magnitude is added to the logarithm of a quantity with a very small magnitude.

As a test of the programming of the two methods of evaluation of $M_{\alpha,\beta}(x)$ given above, we compared the two values obtained for this function with these methods for $x = 20\beta^{\frac{1}{2}}$ and α and β given a large number of sample values which cover the range for these parameters relevant to the evaluation of ΔE_{HB}. In all cases, the relative magnitude of the difference of the two values was less than 10^{-11}.

In the numerical evaluation of $W_{\alpha,\beta}(x)$, the choice of method of evaluation depends, as in Appendix C, on whether x is less than or greater than 30. The two methods used here are basically the same as those described in Appendix C, except for some modifications necessary to accommodate the large range of parameters and complex numbers which occur here.

For $x > 30$, we evaluate $W_{\alpha,\beta}(x)$ with the aid of the asymptotic expansion given by Eqs. (C.15) and (C.16). The summation over n in (C.15) is begun at $n = n_0'$, where n_0' is approximately the value of n for which the magnitude of $T'(n)$ is at its first relative maximum encountered as the value of n increases from zero. An approximate value for n_0' is obtained by solving for u in

$$\left|\frac{(\beta + u)(\beta - u)}{ux}\right| = 1 . \tag{I.29}$$

The solution of interest is

$$u = \left(\beta^2 + \frac{x^2}{4}\right)^{\frac{1}{2}} - \frac{x}{2} \tag{I.30}$$

and we set

$$n_0' = [u] . \tag{I.31}$$

The sum $\bar{S}'$ is then formed where

$$\bar{S}' = \frac{S'}{T'(n_0')} = \sum_{n=N_1'}^{n_0} \bar{T}'(n) + \sum_{n=n_0+1}^{N_2'} \bar{T}'(n) + E_1' + E_2' , \tag{I.32}$$

and

$$\bar{T}'(n) = \frac{T'(n)}{T'(n_0')} . \tag{I.33}$$

The first sum on the right in (I.32) is performed in the direction of decreasing n. The error which results from truncating this portion of the sum at $n = N_1'$ is estimated by

$$|E_1'| = \left|\sum_{n=0}^{N_1'-1} \bar{T}'(n)\right| \leq N_1'|\bar{T}'(N_1' - 1)| \qquad (I.34)$$

for N_1' smaller than the value n for which $|\bar{T}'(n)|$ is at its first maximum. The second sum on the right in (I.32) is then performed in the direction of increasing n. An estimate for the error which results from truncating the sum at $n = N_2'$ is made by considering the exact expression for the remainder R_N in (C.14)

$$R_N = \frac{\Gamma(\beta + \frac{1}{2} + \alpha)}{\Gamma(\beta - \frac{1}{2} + \alpha - N)} \frac{1}{N!} \left(\frac{t}{x}\right)^{N+1} \int_0^1 dv(1 - v)^N \left(1 + \frac{t}{x} v\right)^{\beta - \frac{3}{2} + \alpha - N} \qquad (I.35)$$

which leads to

$$|R_N| \leq \left|\frac{\Gamma(\beta + \frac{1}{2} + \alpha)}{\Gamma(\beta - \frac{1}{2} + \alpha - N)}\right| \frac{1}{(N+1)!} \left(\frac{t}{x}\right)^{N+1} \qquad (I.36)$$

$$\text{for } N + 1 \geq \mathrm{Re}(\beta - \tfrac{1}{2} + \alpha) .$$

Then from

$$|E_2'| = \left|\bar{S}' - \sum_{n=0}^{N_2'} \bar{T}'(n)\right| \leq \frac{1}{|T'(n_0') \, \Gamma(\beta + \frac{1}{2} - \alpha)|} \int_0^\infty dt$$

$$\times \; t^{\mathrm{Re}(\beta - \frac{1}{2} - \alpha)} |R_{N_2'}| e^{-t} , \qquad (I.37)$$

we obtain

$$|E_2'| \leq \left|\frac{\Gamma\left(\mathrm{Re}(N_2' + \beta + \frac{3}{2} - \alpha)\right)}{\Gamma(N_2' + \beta + \frac{3}{2} - \alpha)}\right| |\bar{T}'(N_2' + 1)| \qquad (I.38)$$

$$\text{for } N_2' + 1 \geq \mathrm{Re}(\beta - \tfrac{1}{2} + \alpha) .$$

And because

$$\left|\frac{\Gamma(\mathrm{Re}(w))}{\Gamma(w)}\right| = \frac{\mathrm{Re}(w) - 1}{|\Gamma(i \, \mathrm{Im}(w) + 1)|} \left|\int_0^1 ds \; s^{\mathrm{Re}(w)-2}(1 - s)^{i\mathrm{Im}(w)}\right|$$

$$\leq \left|\frac{1}{\Gamma(i \, \mathrm{Im}(w) + 1)}\right| \qquad (I.39)$$

$$\text{for } \mathrm{Re}(w) > 1 ,$$

we have

$$|E_2'| \leq \frac{1}{|\Gamma(1 - \nu)|} |\bar{T}'(N_2' + 1)| \qquad (I.40)$$

$$\text{for } N_2' + 1 \geq \mathrm{Re}(\beta - \tfrac{1}{2} + \alpha) .$$

We also have

$$|E_2'| \leq \left[M + \frac{1}{|\Gamma(1 - \nu)|}\right] |\bar{T}'(N_2' + 1)| \qquad (I.41)$$

$$\text{for } N_2' + 1 < \mathrm{Re}(\beta - \tfrac{1}{2} + \alpha) ,$$

where $M = [\mathrm{Re}(\beta - \frac{1}{2} + \alpha - N_2')]$. The relation in (I.41) follows from the fact that $|\bar{T}'(n)|$ decreases as n increases for $N_2' + 1 \leq n \leq \mathrm{Re}(\beta + \frac{1}{2} + \alpha)$, where N_2' is large enough to take

into account the approximate nature of the choice of n_0'. The sums on the right in (I.32) are truncated at values of N_1' and N_2' for which the magnitude of the ratio of the error, as given by the appropriate estimate (I.34), (I.40), or (I.41), to the partial sum is less than 10^{-11}. The value of the Whittaker function is then just

$$W_{\alpha,\beta}(x) = x^{\alpha} e^{-\frac{1}{2}x} T'(n_0) \bar{S}' . \tag{I.42}$$

The coefficient of $\bar{S}'$ in (I.42) is factorized into a complex factor with a magnitude of order 1 whose complex logarithm is stored, and a real factor whose double precision logarithm is stored, in analogy with the separation shown in (I.27) and (I.28).

For $x \leq 30$, we employ the method described in Appendix C, beginning with Eq. (C.22), to evaluate $W_{\alpha,\beta}(x)$. It is necessary to have double precision accuracy in that method. This is accomplished here by explicitly programming the complex arithmetic operations in terms of separate double precision real and imaginary parts for the variables involved. The term S, which appears in (C.23), is evaluated with the aid of (C.5) and (C.7). An estimate for the error which results from truncating the sum over n at a finite value N is easily obtained with the appropriate modification of the discussion leading to (I.24). The term U, which appears in (C.23), is evaluated with the aid of (C.25) and (C.27). The error which results from truncating the sum over n in (C.25) at $n = N$ is estimated by observing that

$$\left| \frac{(n - \beta + \frac{1}{2} - \alpha)x}{(n - 2\beta + 1)(n + 1)} \right| \tag{I.43}$$

is < 1 and decreases as n increases for $n \geq \left[\beta + \frac{x}{2} + \left(\beta^2 + \frac{x^2}{4} + x\right)^{\frac{1}{2}}\right]$ and $n \geq 2$, which implies

$$|E''| = \left| \sum_{n=N+1}^{\infty} V(n) \right| < \frac{1}{1 - \theta} |V(N + 1)| \tag{I.44}$$

$$\text{for } N + 1 \geq \left[\beta + \frac{x}{2} + \left(\beta^2 + \frac{x^2}{4} + x\right)^{\frac{1}{2}}\right] \quad \text{and} \quad N \geq 1$$

where

$$\theta = \left| \frac{(N - \beta + \frac{3}{2} - \alpha)x}{(N - 2\beta + 2)(N + 2)} \right| . \tag{I.45}$$

In evaluating $W_{\alpha,\beta}(x)$, we first evaluate U, truncating the sum over n in (C.25) when the magnitude of the ratio of the remainder of the sum to the partial sum is less than 10^{-26}. We then form the sum S and truncate the sum over n in (C.5) at the value $n = N$ when the magnitude of the ratio of the remainder of the sum to the combined partial sum

$$U + \eta \sum_{n=0}^{N} T(n) \tag{I.46}$$

is less than 10^{-11}.

In evaluating $W_{\alpha,\beta}(x)$ with the preceding method, we need the full double precision accuracy for certain combinations of the parameters in W. The worst case, where the full accuracy is required, is for $|\kappa| = 1$ and x near 30. We explored other regions in the parameter space by examining the numerical behavior of the series for sample values of the parameters. On the basis of this study, we found

that some time-saving modifications in the method of evaluation could be made in certain regions of the parameter space. For $\beta < 40$ and $x \leq \frac{3}{2}(\beta - 6)$, single precision arithmetic is used. For $\beta \geq 40$, the contribution of the term ηS in (C.23) is negligible and the term U is evaluated with single precision arithmetic; in this case, the contribution to the sum in (C.25) from terms with $n > \beta$ is negligible.

To check the programming of the two methods of evaluation of $W_{\alpha,\beta}(x)$ described above, we compared the two values obtained with the two methods for $x = 30$ and sample values for the remaining parameters. This was done for a large number of sample values, and in all cases, the agreement between the two values for $W_{\alpha,\beta}(x)$ was satisfactory.

We now briefly describe the method used to evaluate the free radial Green's functions $F_\kappa(x_2,x_1,z)$ for the range of parameters given in (I.1). The free Green's functions are given in terms of spherical Bessel and Hankel functions of imaginary argument in (A.32).

We first consider the evaluation of $j_\ell(ix)$. We employ the power series

$$j_\ell(ix) = \left(\frac{ix}{2}\right)^\ell \sum_{n=0}^{\infty} \frac{\Gamma(\frac{3}{2})}{\Gamma(n + \ell + \frac{3}{2})} \frac{1}{n!}\left(\frac{x}{2}\right)^{2n} . \qquad (I.47)$$

The summation over n in (I.47) is begun at $n = n_0$, where $n_0 = \left[\frac{1}{2}(\ell^2 + x^2)^{\frac{1}{2}} - \frac{1}{2}\ell\right]$, which is near the value of n for which the magnitude of the terms in the sum is a maximum. The summation is performed first in the direction of decreasing n, and then in the direction of increasing n from n_0. In each case, we terminate the sum when the magnitude of the ratio of the remainder to the partial sum is less than 10^{-11}. Estimates for the remainders are easily

obtained as in the Coulomb case. The sum over n is normalized by extracting the $\underline{n_0}$th term as an overall factor.

To evaluate $h_\ell^{(1)}(ix)$, we employ the series

$$h_\ell^{(1)}(ix) = -(2ix)^{-\ell}\frac{e^{-x}}{x}\sum_{n=0}^{\ell}\frac{\Gamma(2\ell + 1 - n)(2x)^n}{\Gamma(\ell - n + 1)\,\Gamma(n + 1)} . \qquad (I.48)$$

The method we use for evaluating the sum is the analog of that used in the evaluation of $j_\ell(ix)$; in this case we have $n_0 = [\ell + x - (\ell^2 + x^2)^{\frac{1}{2}}]$.

As a check on the programming of the Coulomb radial Green's function algorithm, we numerically evaluated expectation values of the Green's function. The relevant formulas appear in (C.39), (C.40), and (C.41). The evaluation was made for the state with $n = 2$, $\kappa = -2$, with $Z = 110$, and for the state with $n = 2$, $\kappa = -1$, with $Z = 10$. In both cases, evaluations were made for values of the energy given by $z = iu$, where $u = 1,51,101,151$, and 201. In all cases, the result was correct to at least 11 significant figures. As a check on the programming of the free radial Green's function algorithm, we numerically performed the sum over κ in the 1,1 element of the free Green's function, in the form given in (A.25), for the case $\hat{x}_2 = \hat{x}_1$. The sum over κ was terminated at $|\kappa| = N$ when the magnitude of the ratio of the $\underline{N}$th term of the sum to the partial sum was less than 10^{-15}. The result was compared numerically to the value for the sum obtained from the expression in (A.33). The comparison was made for all combinations of the values $x_2/x_1 = 0.2,0.8$, $x_1 = 0.1,1,10$, and $z = 0.79i$, and for the values $x_2/x_1 = 0.95$, $x_1 = 0.1,1,10$, and $z = 197i$. In all cases, there was agreement to at least 12 significant

figures. Further checks were performed on both the Coulomb and free radial Green's function programs. We checked numerically that the functions satisfied the appropriate differential equation. We also examined numerically the asymptotic behavior of the functions in the limit $|\kappa| \to \infty$, with the remaining parameters fixed, and in the limit $x_1 \to \infty$, with x_2/x_1 and the remaining parameters fixed. The asymptotic values were compared with the values obtained from Eqs. (A.28) and (A.30). The results were in satisfactory agreement.

FOOTNOTES AND REFERENCES

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1. H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Academic Press, New York, 1957). Recent reviews of quantum electrodynamics are: N. M. Kroll, "Status of Quantum Electrodynamics Theory," Atomic Physics 3, Proceedings of the Third International Conference on Atomic Physics (Plenum Press, New York, 1973); B. E. Lauthrup, A. Peterman, and E. de Rafael, Physics Reports 3, No. 4 (1972); S. J. Brodsky, "Radiative Problems and Quantum Electrodynamics," Proceedings of the 1971 International Symposium on Electron and Photon Interactions at High Energies, Laboratory of Nuclear Studies, Cornell University, 1972.
2. E. H. Wichmann and N. M. Kroll, Phys. Rev. 101, 843 (1956).
3. M. Leventhal and D. E. Murnick, Phys. Rev. Letters 25, 1237 (1970); D. E. Murnick, M. Leventhal, and H. W. Kugel, Phys. Rev. Letters 27, 1625 (1971); H. W. Kugel, M. Leventhal, and D. E. Murnick, Phys. Rev. A6, 1306 (1972); M. Leventhal, D. E. Murnick, and H. W. Kugel, Phys. Rev. Letters 28, 1609 (1972); G. P. Lawrence, C. Y. Fan, and S. Bashkin, Phys. Rev. Letters 28, 1612 (1972), and Erratum Phys. Rev. Letters 29, 320 (1972).
4. R. Marrus and R. W. Schmieder, Phys. Rev. A5, 1160 (1972).
5. A. M. Desiderio and W. R. Johnson, Phys. Rev. A3, 1267 (1971); in this work, it is found that the inclusion of finite nuclear size and screening reduces the $1S_{\frac{1}{2}}$ state self-energy shift by approximately 2% for Z in the range 70-90.

6. R. C. Barrett, S. J. Brodsky, G. W. Erickson, and M. H. Goldhaber, Phys. Rev. 166, 1589 (1968).

7. H. A. Bethe, Phys. Rev. 72, 339 (1947).

8. H. A. Bethe, L. M. Brown, and J. R. Stehn, Phys. Rev. 77, 370 (1950); J. M. Harriman, Phys. Rev. 101, 594 (1956); C. Schwartz and J. J. Tiemann, Ann. Phys. (N.Y.) 6, 178 (1959); M. Lieber, Phys. Rev. 174, 2037 (1968); R. W. Huff, Phys. Rev. 186, 1367 (1969); S. Klarsfeld and A. Marquet, Phys. Letters 43B, 201 (1973).

9. R. P. Feynman, Phys. Rev. 74, 1430 (1948), and Phys. Rev. 76, 769 (1949); H. Fukuda, Y. Miyamoto, and S. Tomonaga, Progr. Theoret. Phys. (Kyoto) 4, 47, 121 (1949); N. M. Kroll and W. E. Lamb, Jr., Phys. Rev. 75, 388 (1949); J. Schwinger, Phys. Rev. 75, 898 (1949); J. B. French and V. F. Weisskopf, Phys. Rev. 75, 1240 (1949).

10. M. Baranger, Phys. Rev. 84, 866 (1951); R. Karplus, A. Klein, and J. Schwinger, Phys. Rev 86, 288 (1952); M. Baranger, H. A. Bethe, and R. P. Feynman, Phys. Rev. 92, 482 (1953).

11. G. W. Erickson and D. R. Yennie, Ann. Phys. (N.Y.) 35, 271, 447 (1965).

12. G. W. Erickson, Phys. Rev. Letters 27, 780 (1971).

13. A. J. Layzer, Phys. Rev. Letters 4, 580 (1960); A. J. Layzer, J. Math. Phys. 2, 292, 308 (1961).

14. H. M. Fried and D. R. Yennie, Phys. Rev. Letters 4, 583 (1960); Phys. Rev 112, 1391 (1958).

15. G. E. Brown and D. F. Mayers, Proc. Roy. Soc. (London) A251, 105 (1959).

16. G. E. Brown, J. S. Langer, and G. W. Schaefer, Proc. Roy. Soc. (London) A251, 92 (1959).

17. M. Baranger, H. A. Bethe, and R. P. Feynman, Phys. Rev. 92, 482 (1953). The correspondence between the notation used there and the notation used here is

$$K_+^V(x_2,x_1) = -\frac{1}{2} S_F^e(x_2,x_1)$$

$$\delta_+[(x_2 - x_1)^2] = 2\pi i\, D_F(x_2 - x_1) \quad .$$

18. We employ units in which $c = \hbar = m_e = 1$. The value assigned to α^{-1} is 137.03602. Four vectors have the form $a = (a^0, \underset{\sim}{a})$. 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:

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

$$\gamma^0 = \beta \; ; \qquad \gamma^i = \beta\alpha^i \, , \qquad i = 1,2,3.$$

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

$$\gamma_\mu \mathcal{O} \gamma^\mu = \gamma^0 \mathcal{O} \gamma^0 - \gamma^i \mathcal{O} \gamma^i$$

$$\alpha_\mu \mathcal{O} \alpha^\mu = \mathcal{O} - \alpha^i \mathcal{O} \alpha^i \quad .$$

19. R. P. Feynman, Phys. Rev. 76, 769 (1949).

20. W. Pauli and F. Villars, Rev. Mod. Phys. 21, 434 (1949).

21. A. H. Stroud and Don Secrest, Gaussian Quadrature Formulas (Prentice-Hall, Englewood Cliffs, 1966).

22. M. E. Rose, Relativistic Electron Theory (John Wiley and Sons, New York, 1961).

23. G. E. Brown and G. W. Schaefer, Proc. Roy. Soc. (London) A233, 527 (1956).

24. E. T. Whittaker and G. N. Watson, A Course of Modern Analysis (Cambridge University Press, Cambridge, 1927).

25. W. Magnus, F. Oberhettinger, and R. P. Soni, Formulas and Theorems for the Special Functions of Mathematical Physics, third edition (Springer-Verlag, New York, 1966, p. 317).

26. Ibid., p. 318.

27. Miller's method is described in M. Abramowitz and I. A. Stegun, editors, Handbook of Mathematical Functions, National Bureau of Standards Applied Mathematics Series, 1964, p. 452.

28. By the notation $[x]$, we mean the largest integer $\leq x$.

29. E. T. Whittaker and G. N. Watson, op. cit., p. 337.

30. Ibid., p. 340.

31. Ibid., p. 96.

32. Ibid., p. 346.

33. Ibid., pp. 252-3.

34. This method of expansion is suggested by the method used by Kroll and Lamb to calculate the fourth order part of the Lamb shift; N. M. Kroll and W. E. Lamb, Jr., Phys. Rev. 75, 388 (1949).

FIGURE CAPTIONS

Fig. 1.1. 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. 1.2. 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. 2.1. 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. 2.2. The new contour in the complex z-plane.

Fig. 3.1. The complex z-plane with the singularities of the integrand in Eq. (3.2).

Fig. 3.2. The complex z-plane with the singularities of the integrand in Eq. (3.5). 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 $z_1 = z_2 = 0$.

Fig. 5.1. In this graph, we have plotted $\log_{10}|T_\kappa(r,y,t,\gamma)|$ as a function of κ, for various values of r, y, t, and γ. The vertical line on each curve gives the value, on the same scale as κ, of the smaller argument of the Bessel functions.

Fig. 5.2. The points in this graph are the calculated values of $f_L(Z\alpha) - \frac{4}{3}\ln(Z\alpha)^{-2}$ for $Z = 10, 20, 30, 40$, and 50. The point at $Z = 0$ is the limit as $Z\alpha \to 0$, of the same function and is obtained by an independent method.

Fig. 9.1. Numerically calculated values for $f_{HB}(Z\alpha)$ for $Z = 10, 20, 30, 40$, and 50 and the value of the limit point $f_{HB}(0)$ which is calculated in Appendix F.

Fig. 10.1. Values for the function $F(Z\alpha)$ obtained in this calculation and values for $F(Z\alpha)$ based on the results of previous calculations. The curve with the error estimates is based on the graph given in Ref. 12. According to Desiderio and Johnson, there is an error in algebra in the work leading to the result of Brown and Mayers.

Fig. 10.2. Calculated values for $G(Z\alpha)$. The error limits on the point at $Z = 10$ correspond to the error limits of $F(Z\alpha)$ at $Z = 10$. The dashed line shows the function $G_A(Z\alpha)$ fitted to $G(Z\alpha)$ at $Z = 10, 20$, and 30.

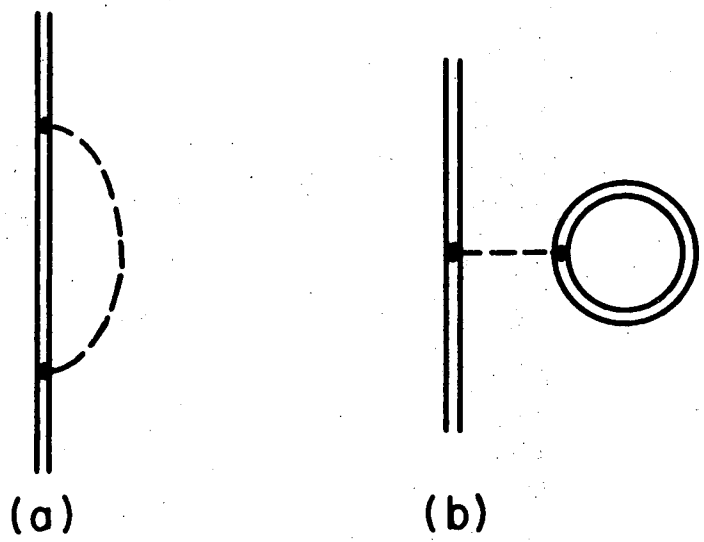

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Fig. 1.1

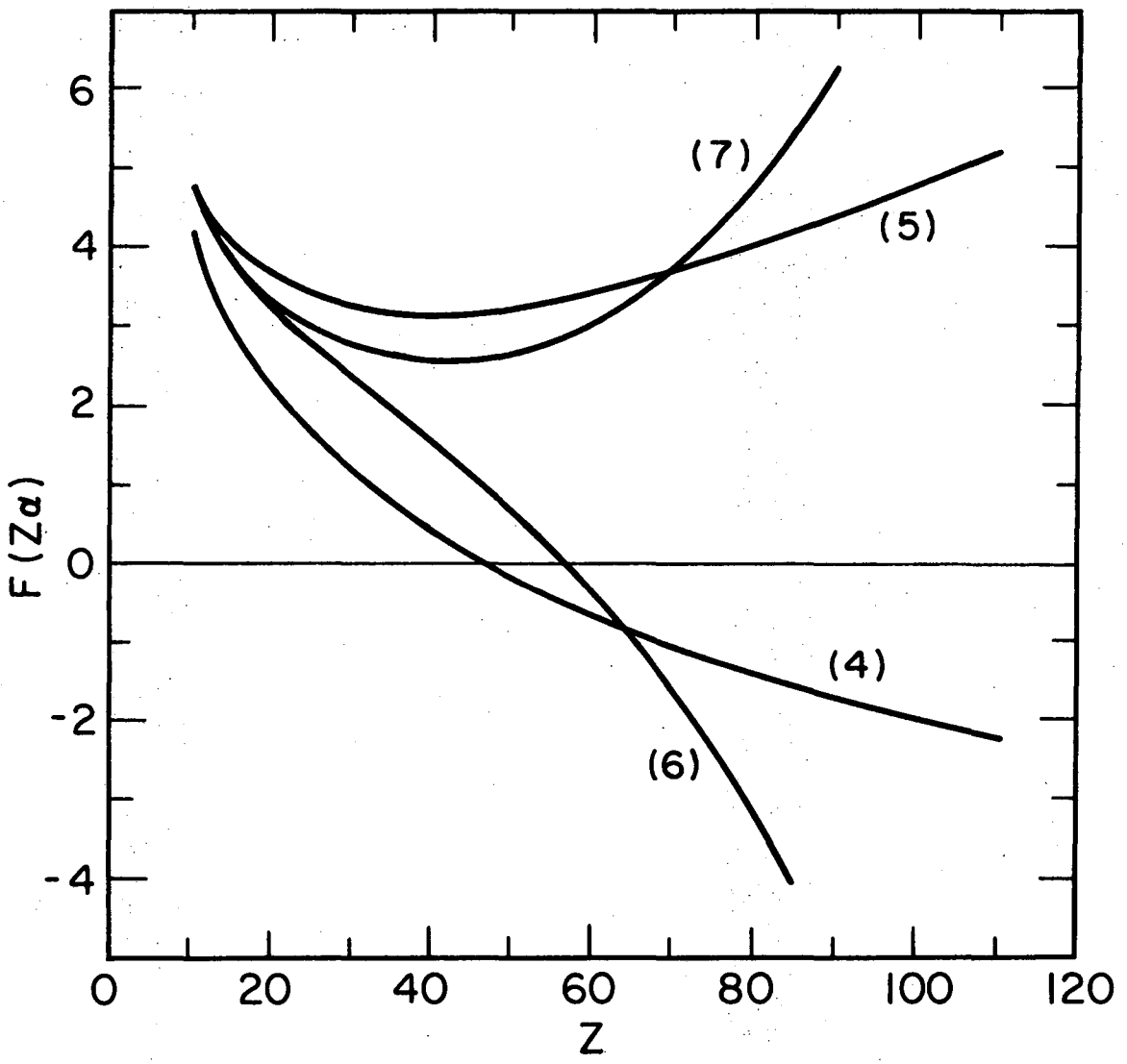

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Fig. 1.2

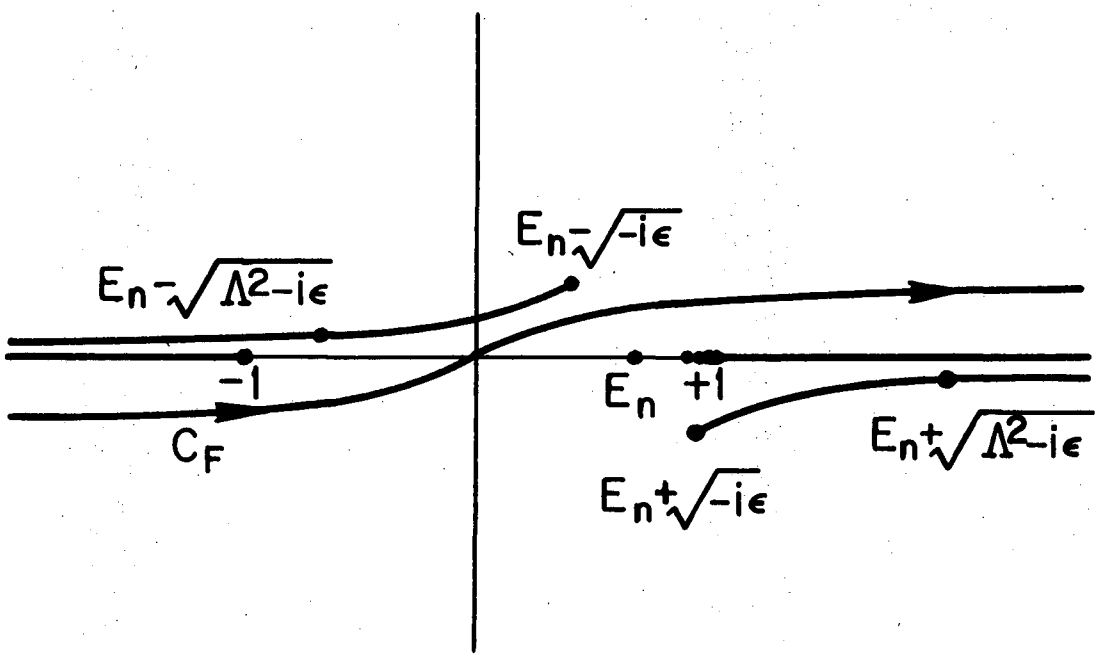

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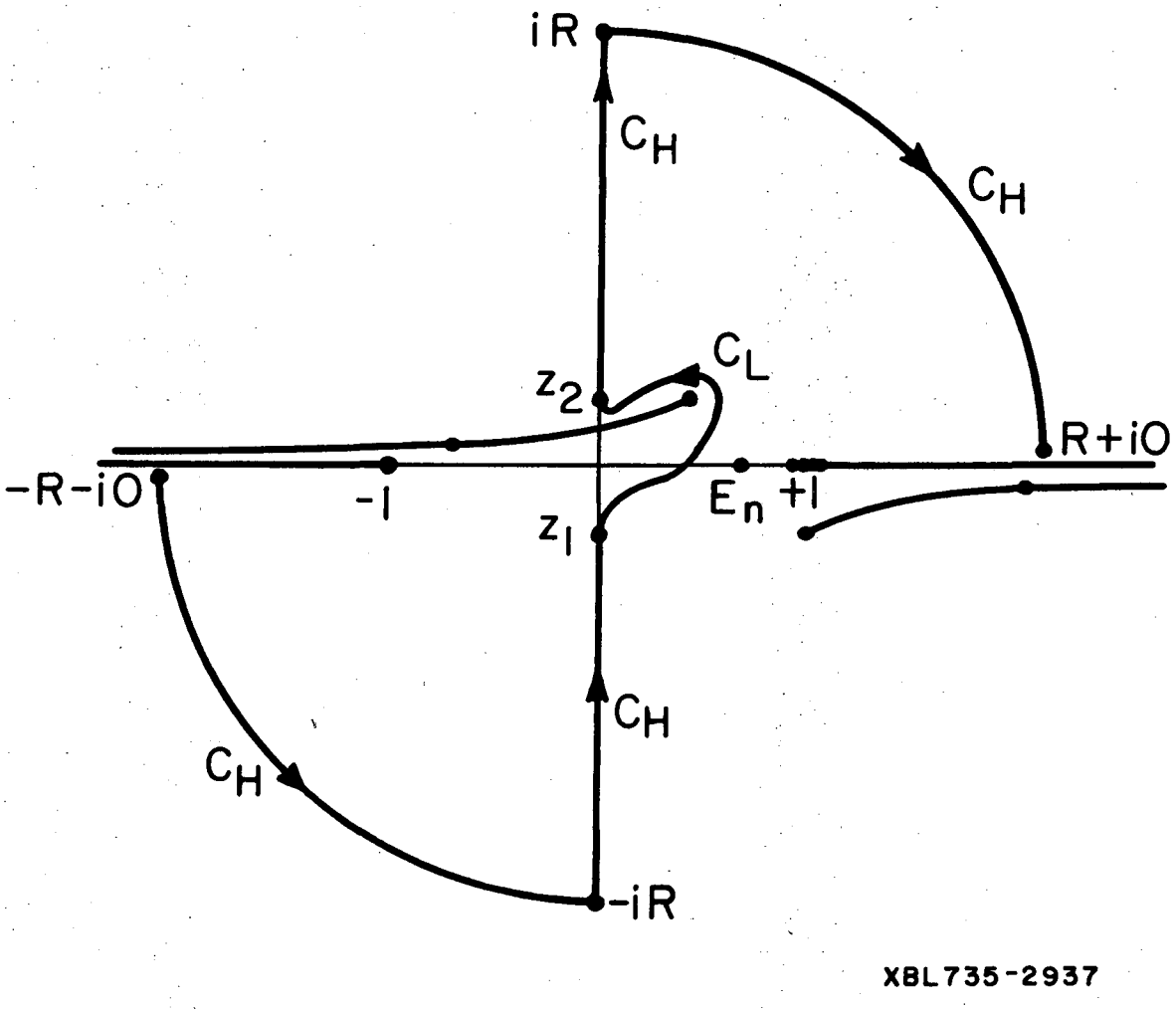
Fig. 2.1



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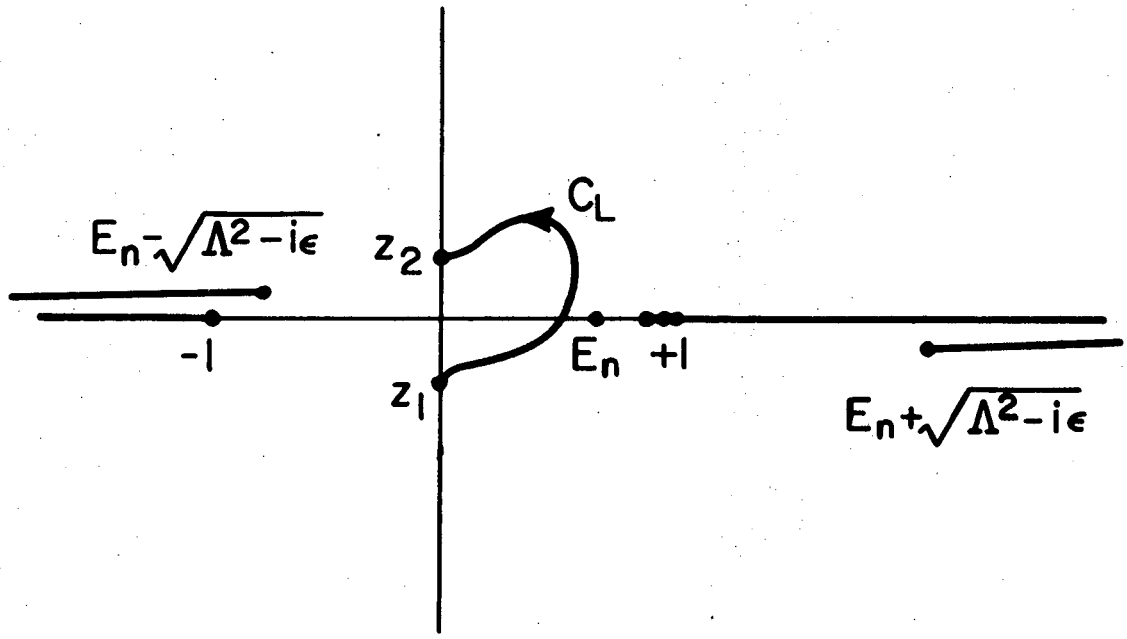

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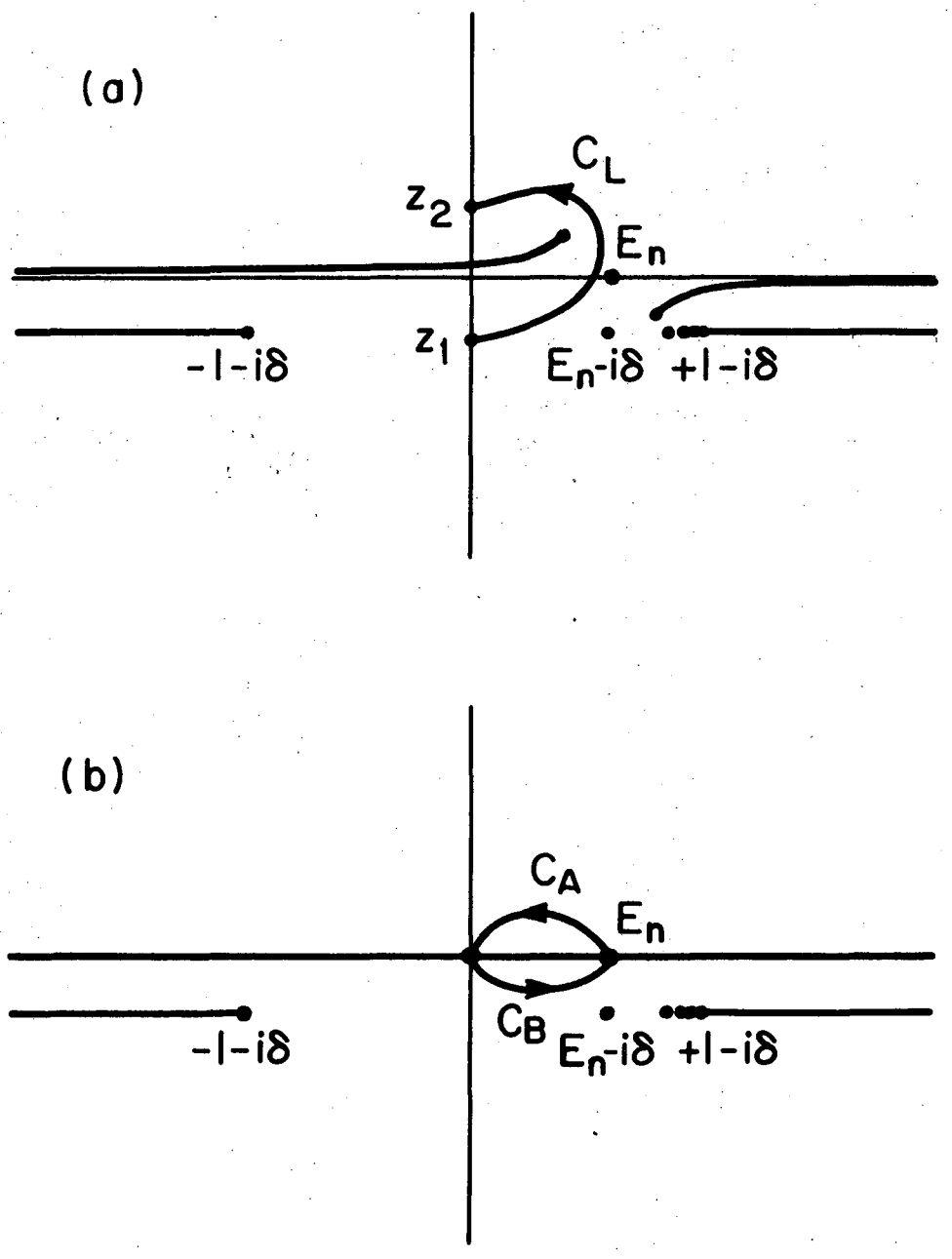

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Fig. 3.2

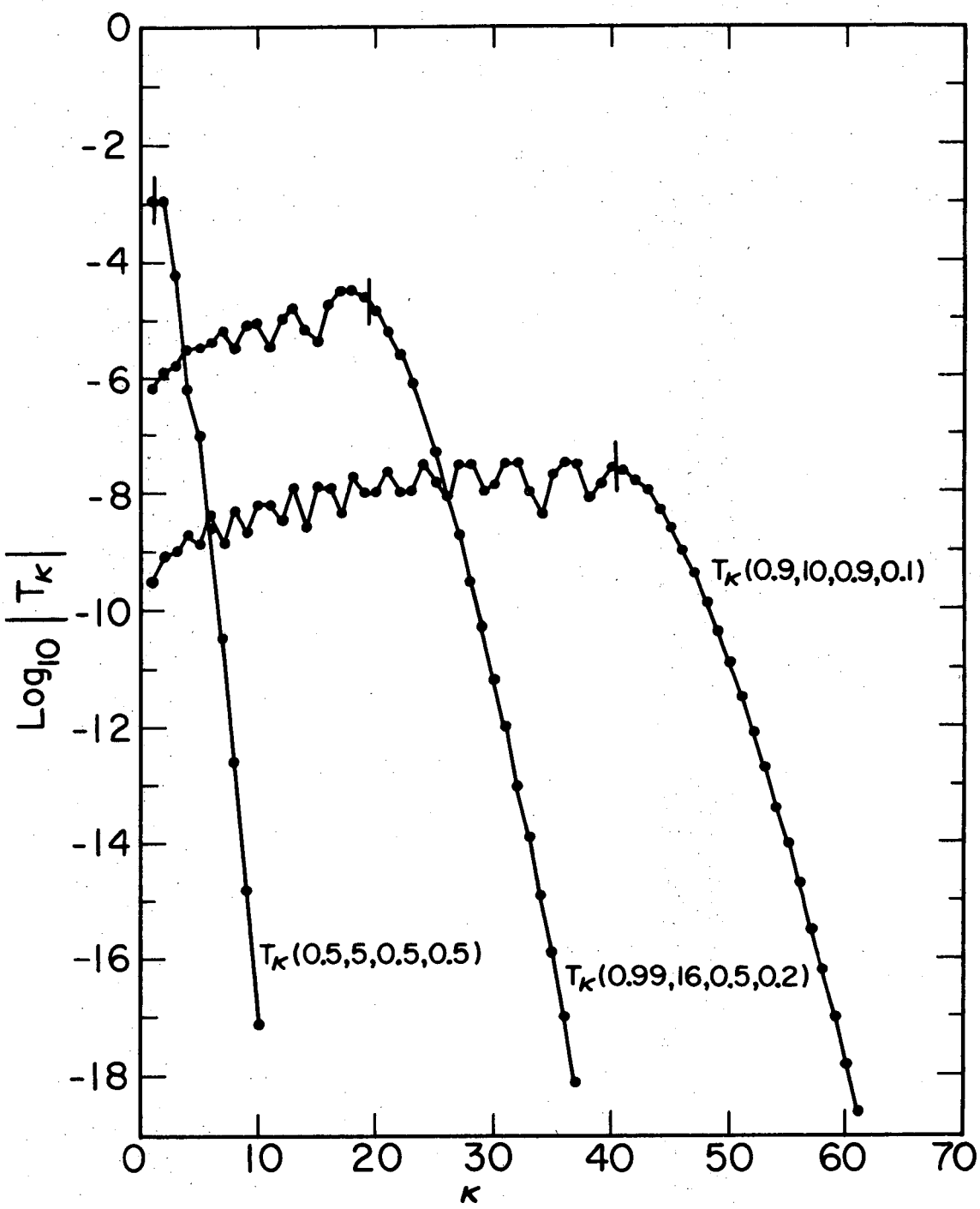

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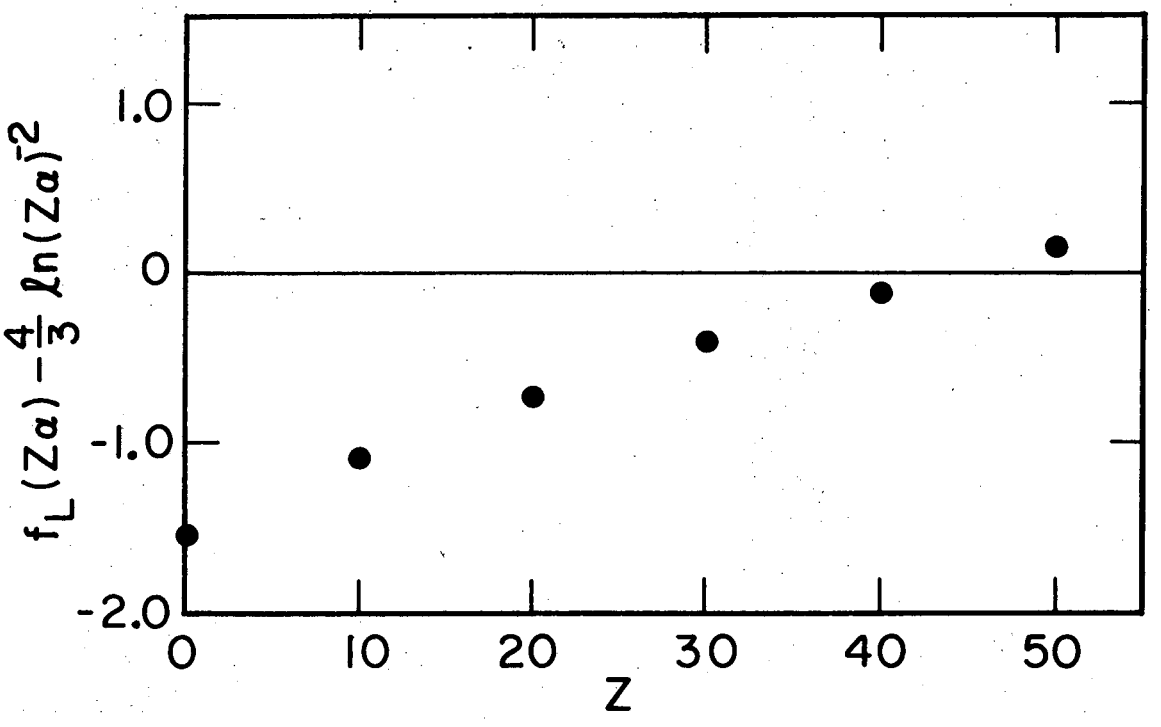
Fig. 5.1



XBL 735 - 2933

Fig. 5.2

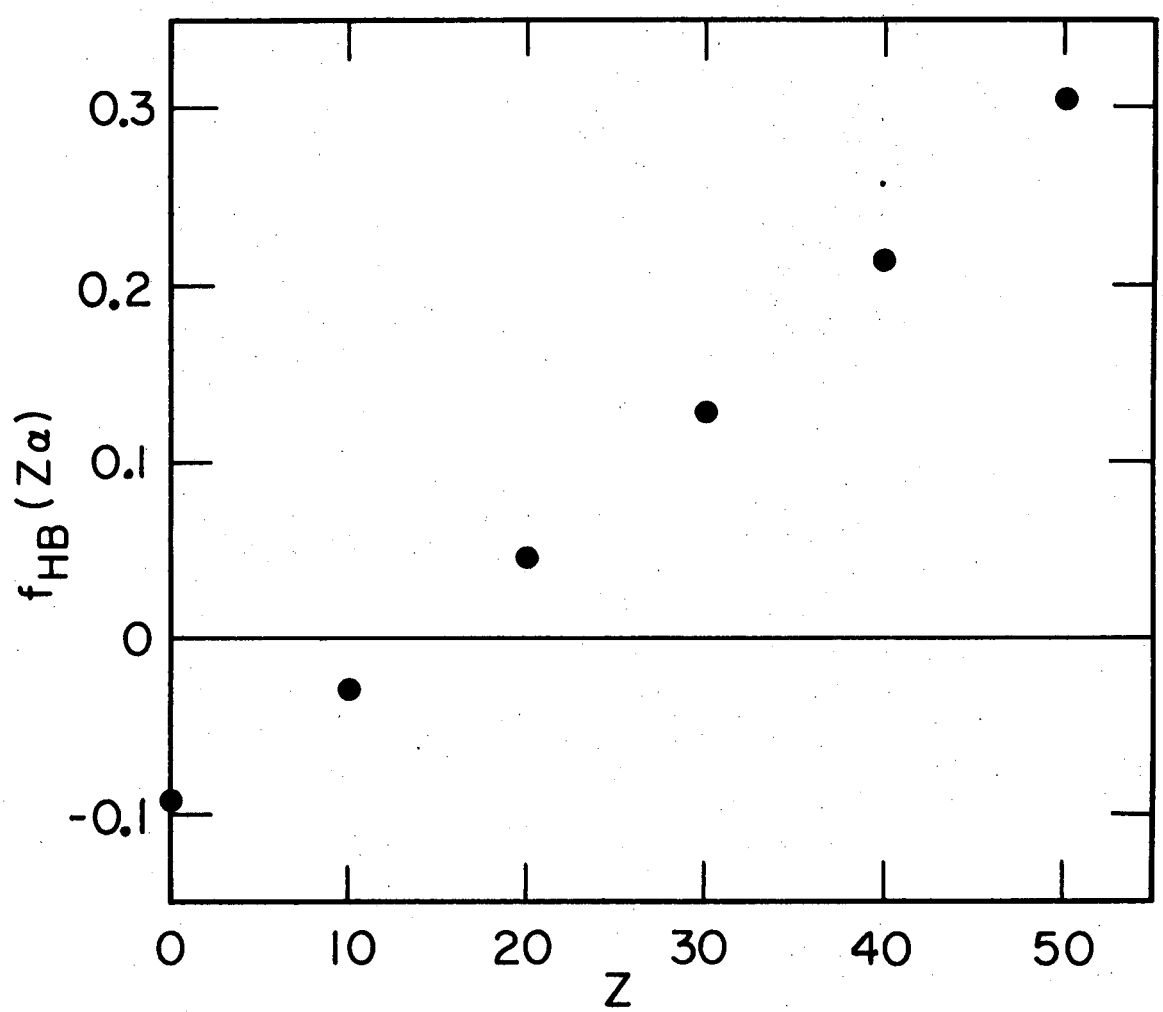


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Fig. 9.1

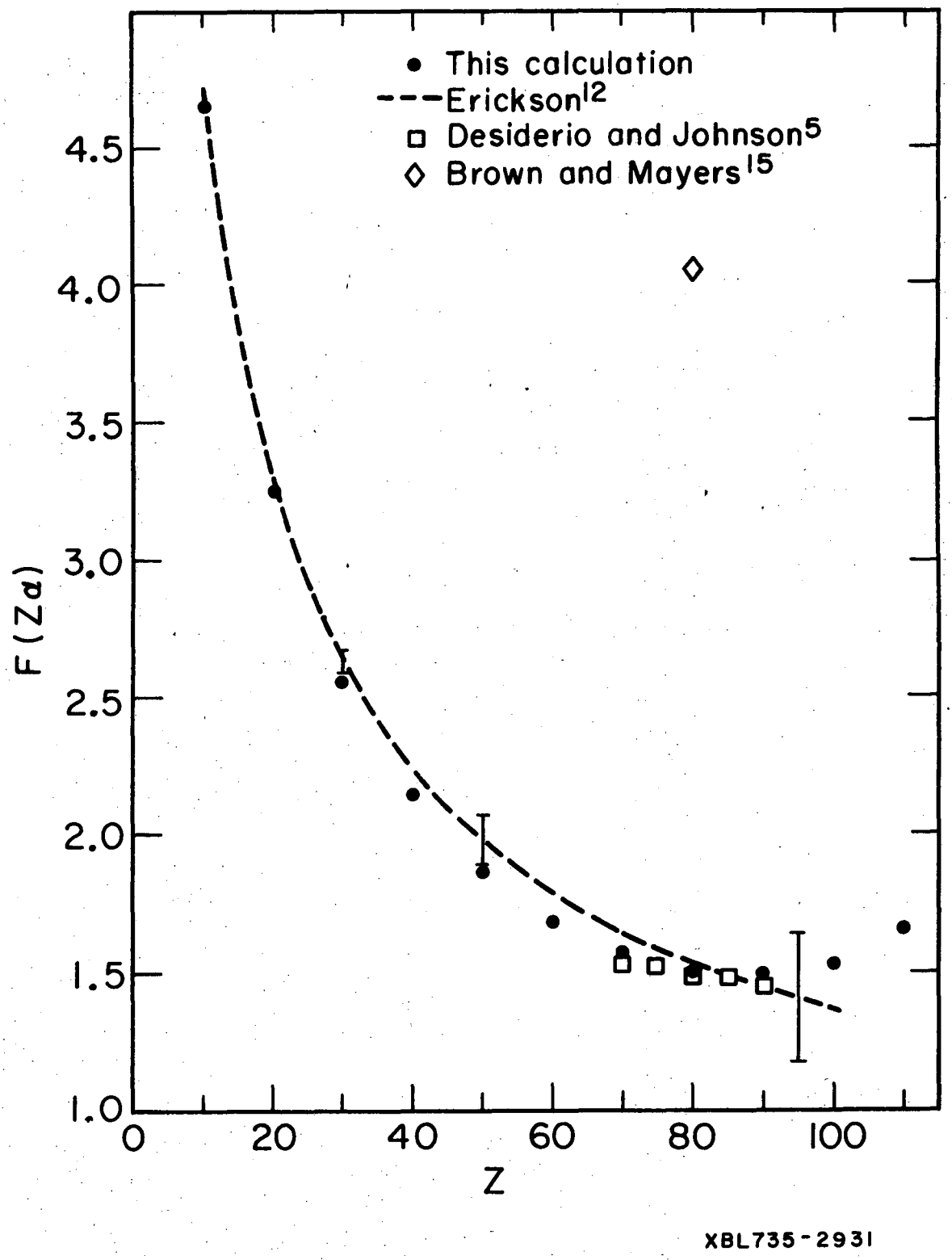
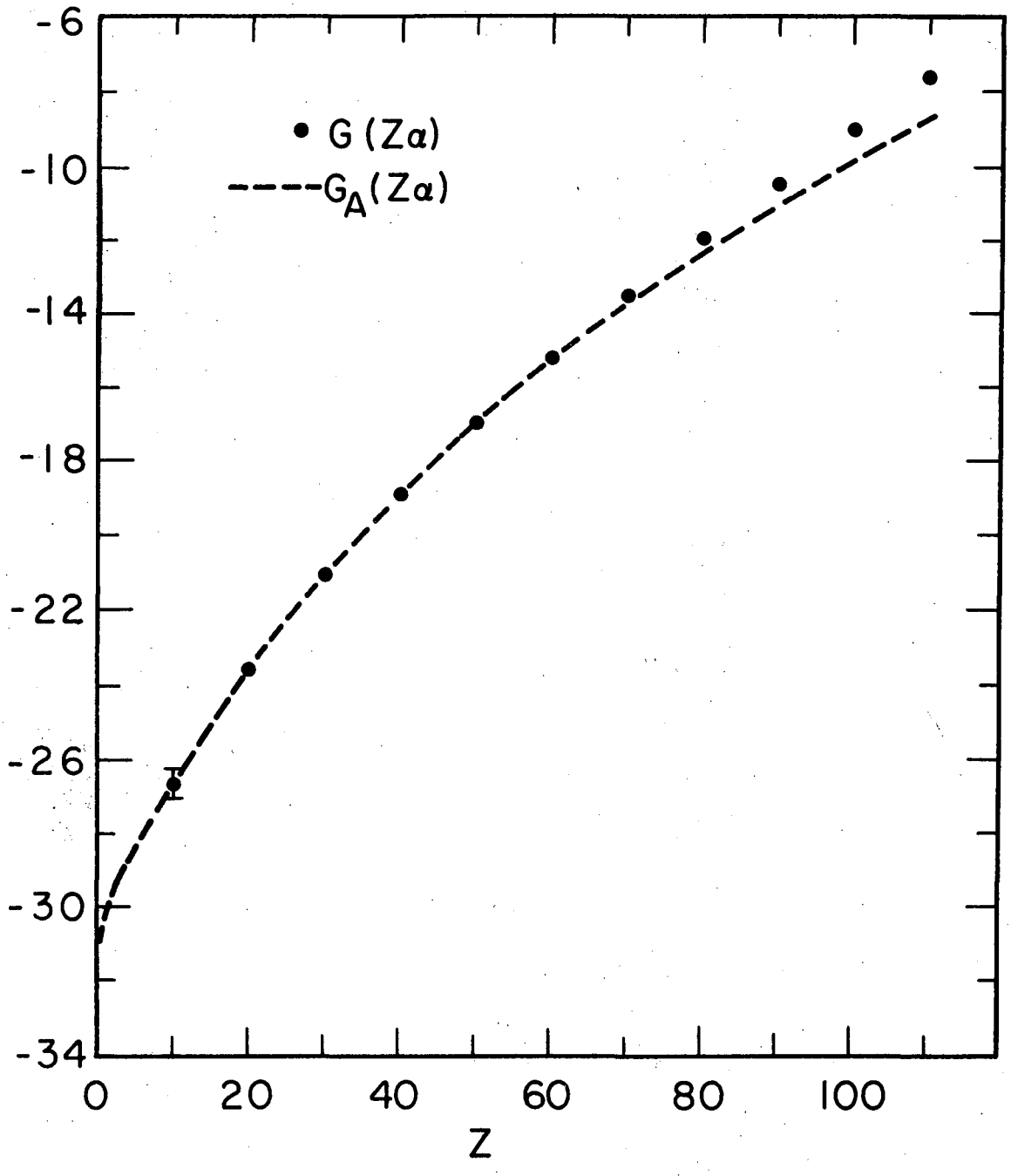

This calculation
Erickson[12]
Desiderio and Johnson[5]
Brown and Mayers[15]
F (Zα)
Z
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0
20
40
60
80
100
XBL735-2931

Fig. 10.1



XBL735-2941

Fig. 10.2

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