# Coulomb perturbation calculations in momentum space and application to quantum-electrodynamic hyperfine-structure corrections*

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Adaptation of the momentum-space Schrödinger-Coulomb Green's function for second-order perturbation calculations of the bound-state energy levels of hydrogenic atoms is demonstrated. The numerical viability of the formulas derived is proven by recalculating the contribution in second order of the spin-spin operator to the hydrogen hyperfine-structure residual $R=(8\nu_{2S}-\nu_{1S})/\nu_{1S}$. Application to positronium hyperfine structure is discussed.

## INTRODUCTION

The general concern of this paper is the technical problem of calculating the energy eigenvalues of the Bethe-Salpeter equations describing the atomic two-body systems hydrogen positronium and muonium. Since these atoms are rather accurately described by the nonrelativistic spinless Schrödinger equation with $1/r$ potential plus well-known fine-structure corrections it is natural that all foregoing work on them[1-7] has proceeded by approximating in some sense the Bethe-Salpeter equation by the Schrödinger equation and developing a perturbation scheme about the Schrödinger solution. Although recent work[8] directed towards calculating with the Bethe-Salpeter equation in a covariant manner appears promising, it is felt that the nonrelativistic approximation procedure is not exhausted, and in any case it is always useful to calculate quantum-electrodynamic (QED) corrections by more than one method if possible. Also it is likely that expressions of the type we shall analyze will arise in alternative perturbation schemes.

Specifically this paper is addressed to one step in the aforementioned procedure, the calculation in second order with Schrödinger wave functions of an arbitrary perturbation operator, i.e.,

$$\Delta E^{(2)}=\sum_{n\neq 0}\frac{\langle\varphi_0|\mathcal{O}|\varphi_n\rangle\langle\varphi_n|\mathcal{O}|\varphi_0\rangle}{E_0-E_n}\,; \qquad (1)$$

the sum over states includes integration over the continuum. As will be discussed in Sec. I it is convenient and perhaps mandatory that the required operators $\mathcal{O}$ be expressed in momentum space:

$$[\mathcal{O}\varphi](\vec{p})=\int O(\vec{p},\vec{p}\,')\varphi(\vec{p}\,')\,d\vec{p}\,'\,. \qquad (2)$$

Although both bound and continuum wave functions are known,[9-11] a direct summation, especially to fairly high precision, appears impractical. Fortunately, it has been found straightforward in cases of interest to replace the resolvent operator occurring in (1) by a single kernel function of two momentum variables, with the result that $\Delta E^{(2)}$ may be expressed as

$$\Delta E^{(2)}=\int\int\int\int d\vec{p}\,d\vec{p}\,'\,d\vec{p}_1\,d\vec{p}_1'\,\varphi_0^\dagger(\vec{p}_1)O(\vec{p}_1,\vec{p})\times G^{(0)}(\vec{p},\vec{p}\,')O(\vec{p}\,',\vec{p}_1')\varphi_0(\vec{p}_1')\,. \qquad (3)$$

The formula for $G^{(0)}$ is obtained by exploiting the formal similarity of the resolvent

$$G^{(0)}(\vec{p},\vec{p}\,')=\sum_{n\neq 0}\frac{\varphi_n(\vec{p})\varphi_n^\dagger(\vec{p}\,')}{E_0-E_n} \qquad (4)$$

and the momentum-space Green's function

$$G_E(\vec{p},\vec{p}\,')=\sum_{\text{all } n}\frac{\varphi_n(\vec{p})\varphi_n^\dagger(\vec{p}\,')}{E-E_n}\,, \qquad (5)$$

for which parametric representations are available.

Unfortunately, because it seems necessary to evaluate $\Delta E^{(2)}$ numerically, one gives up the possibility of developing $\Delta E^{(2)}$ as an expansion in powers of $\alpha$, an important feature of all preceding QED correction calculations. It may be that as specific calculations are carried out techniques will be developed for analytic evaluation; some parts of the demonstration calculations were performed analytically.

Section I contains a more detailed schematic discussion of the motivation for this work. In Sec. II, $G^{(0)}$ is extracted from $G_E$ for the case of $\varphi_0$ equaling the ground and first excited state, and the $s$ and $d$ partial waves of the $G^{(0)}$ are derived. Various numerical checks of the formulas are described. In Sec. III the previously calculated hydrogen hyperfine-structure residual is recalculated. In Sec. IV some preliminary work on application to the second-order positronium hyperfine structure is described.

## I. HYPERFINE STRUCTURE

An important contribution in the high-precision calculation of the quantum-electrodynamic fine structure of hydrogenic atoms is the calculation of certain fine-structure operators in second order. An example of this situation is the case of the hydrogen hyperfine-structure splitting residual

$$R=(8\Delta\nu_{2S}-\Delta\nu_{1S})/\Delta\nu_{1S} \qquad (6)$$

($\Delta\nu_{1S}$, $\Delta\nu_{2S}$ are the hfs splittings of the $1S$ and $2S$ states) calculated by Mittleman,[12] Zwanziger,[13] Schwartz,[14] and Sternheim.[5] The work of Schwartz and part of Sternheim's was the calculation of the second-order contribution to $R$,

$$R^{(2)}=\frac{1}{\Delta\nu_{1S}^{(1)}}\left(8\sum_{n\neq 2S}\frac{|\langle\varphi_{2S}|\Delta H_{nsd}+\Delta H_{\rm hfs}|\varphi_n\rangle|^2}{E_{2S}-E_n}\Bigg|_{F=1-F=0}-\sum_{n\neq 1S}\frac{|\langle\varphi_{1S}|\Delta H_{nsd}+\Delta H_{\rm hfs}|\varphi_n\rangle|^2}{E_{1S}-E_n}\Bigg|_{F=1-F=0}\right), \qquad (7)$$

a contribution of order $\alpha^2 m/M$ emerging from the Bethe-Salpeter two-body formalism. The $\varphi_{1S,\,2S}$ are nonrelativistic Schrödinger-Coulomb functions coupled to two-component spinors for protons and electrons with total angular momentum $\vec{F}=\vec{L}+\vec{S}_e+\vec{S}_p$. $\Delta H_{\rm hfs}$ denotes the dipole-dipole operator

$$\Delta H_{\rm hfs}=\frac{\alpha}{4mM}\left(\frac{8\pi}{3}\vec{\sigma}_1\cdot\vec{\sigma}_2\delta^3(\vec{r})+\frac{\vec{\sigma}_1\cdot\vec{\sigma}_2}{r^3}-3\frac{\vec{\sigma}_1\cdot\vec{r}\vec{\sigma}_2\cdot\vec{r}}{r^5}\right), \qquad (8)$$

and $\Delta H_{nsd}$ denotes the spin-independent part of the lowest-order relativity correction to the Hamiltonian

$$\Delta H_{nsd}=-\frac{p^4}{8m^3}-\frac{p^4}{8M^3}+\pi\alpha\delta^3(\vec{r}),$$
$$\vec{r}=\vec{r}_e-\vec{r}_p,\quad \vec{p}=\vec{\nabla}/i; \qquad (9)$$

the spin-orbit term does not contribute to $S$-state calculations. The terms of type $\Delta H_{nsd}\times\Delta H_{nsd}$ are dropped since they do not contribute to the splittings. The $\Delta H_{\rm hfs}\times\Delta H_{nsd}$ may be thought of as the expectation value of $\Delta H_{\rm hfs}$ with the lowest-order relativity correction to $\varphi$. These calculations were carried out in coordinate space by the method of Dalgarno and Lewis,[15] which does not calculate the sum over states directly, but instead solves the equivalent inhomogeneous equation.

An extremely important property of $R^{(2)}$ is the fact that the $1S$ and $2S$ terms separately diverge, and formation of the residual is required to obtain a finite result. The divergence is provided by the singularity of the operators at $r=0$ coupled with the nonvanishing of the $S$-state wave function at $r=0$; a finite result would be obtained for non-$S$ states. Formation of the residual guarantees that the divergent pieces cancel owing to the fact that $|\varphi_{2S}(0)|^2=\frac{1}{8}|\varphi_{1S}(0)|^2$. Thus we conclude that the Schwartz-Sternheim procedure is inadequate for calculating directly the second-order corrections to $S$-state hyperfine structure. Although not serious for the hydrogen ground-state splitting, where the relative order is $\alpha^2 m/M\sim 2\times 10^{-8}$ and the best possible calculation will have uncertainty ~1 ppm due to the uncertainty in $\alpha$, the problem is important for the hyperfine structure of positronium where the mass ratio is unity, and only the ground-state splitting has been measured. Since this splitting has not yet been calculated to the accuracy of the measurement,[16] resolution of the divergence problem and calculation of the second-order hfs contribution (as well as the numerous other uncalculated contributions[6,17]) remains an outstanding problem in high-precision QED.

The origin of the divergence is well known and becomes clear on examining the rigorous derivation of the hfs. One begins with the sixteen-component Bethe-Salpeter equation. Including in the zero-order equation only the instantaneous Coulomb interaction and integrating over the relative energy variable, one obtains the sixteen-component three-dimensional Salpeter equation[1]

$$[E-H_1-H_2-(\Lambda_{1+}\Lambda_{2+}-\Lambda_{1-}\Lambda_{2-})I_{\rm Coulomb}]\phi=0\,, \qquad (10)$$

similar to the Breit equation ($H_1, H_2$ are Dirac free-particle Hamiltonians and the $\Lambda_\pm$ are positive/negative-energy projection operators). The effects of transverse photon exchange, multiphoton exchange, self-energy and vacuum polarization are taken into account by perturbation theory, with single-photon exchange providing the dominant contribution to hyperfine structure. This derivation is performed and perturbations written down most simply in momentum space, since it is basically a matter of working with Feynman diagrams and propagators, which have their simplest representation in momentum space.

The next step in the procedure is to perform an algebraic reduction of the sixteen-component system to a more familiar four-component Pauli-type system. There exist several procedures for accomplishing this.[1,2,4,7,18] This would not be necessary if one knew how to solve the sixteen-component equations in some direct fashion. What next transpires is that the reduced system is then approximated nonrelativistically by approximating the widely occurring factor

$$E_p = (p^2 + m^2)^{1/2} = m + \frac{p^2}{2m} - \frac{p^4}{8m^3} + \cdots .$$

This yields the momentum-space form of the Schrödinger equation and fine-structure operators which are immediately Fourier transformable to the forms presented in (8) and (9). We note, however, that the second and succeeding terms of $E_p$ are more divergent as $p \to \infty$ than the exact form, and this makes the coordinate-space form of the operators more singular as $r \to 0$ than the exact operator, giving rise to the divergence in the hfs calculation. [An example of this is the fact that the exact hfs operator contains a denominator $E_p(e)E_p(\text{proton})$ which is customarily approximated by $mM$.] In practice one also finds that the wave functions for the relativistic equation differ from the Schrödinger functions in their asymptotic behavior as $p \to \infty$, and this must be taken into account when one calculates one order or more beyond the lowest fine-structure order $\alpha^4 m$. However, it has been possible to express the revised wave functions simply in terms of the Schrödinger functions.

The situation described above leaves two alternatives if a convergent perturbation scheme is desired. One could Fourier transform the exact operators, a procedure that has not heretofore been employed and seems unmanageable, or one could calculate with exact momentum-space operators. Thus the requirements of high-precision relativistic atomic physics provide an important motivation for studying momentum-space perturbation calculations.

## II. RESOLVENT CALCULATION

The problems we address ourselves to is the momentum-space calculation of the quantity

$$\Delta E^{(2)} = \sum_{n \neq 0} \frac{\langle \varphi_0 | \mathcal{O} | \varphi_n \rangle \langle \varphi_n | \mathcal{O} | \varphi_0 \rangle}{E_0 - E_n} . \tag{11}$$

The $\varphi_n$ satisfy

$$\frac{p^2}{2m} \varphi_{nlm}(\vec{p}) - \frac{\alpha}{2\pi^2} \int \frac{d\vec{p}\,'}{|\vec{p} - \vec{p}\,'|^2} \varphi_{nlm}(\vec{p}\,') = E_n \varphi_{nlm}(\vec{p}) ,$$

$$n = 1, 2, 3 \ldots , \quad l = 0, 1, \ldots , n-1, \quad m = -l, \ldots , +l, \tag{12}$$

$$E_n = (1/n^2) \times \tfrac{1}{2} \alpha^2 m = (1/n^2) \times 1 R_\infty ,$$

where $R_\infty$ is the rydberg, and $\mathcal{O}$ is an arbitrary momentum-space operator of which there are two types: integral,

$$[\mathcal{O}\varphi](\vec{p}) = \int O(\vec{p}, \vec{p}\,') \varphi(\vec{p}\,') \, d\vec{p}\,' , \tag{13}$$

and $c$ number,

$$[O\varphi](\vec{p}) = O(\vec{p}) \varphi(\vec{p}) , \tag{14}$$

i.e.,

$$O(\vec{p}, \vec{p}\,') = f(\vec{p}) \delta(\vec{p} - \vec{p}\,') .$$

As mentioned in the Introduction, our procedure is to find an explicit form for the resolvent operator occurring in (11) and evaluate $E^{(2)}$ as a multiple integral. This is accomplished by extracting the term

$$|\varphi_0\rangle\langle\varphi_0| / (E - E_0)$$

from the full Green's function $G_E(\vec{p}, \vec{p}\,')$ and evaluating the remaining expression at $E = E_0$.

A particularly convenient form for $G_E$ is the one developed by Schwinger,[19] making use of the $O(4)$ symmetry of the Coulomb equation. In the following some familiarity with the notation of Ref. 19 will be assumed. The main result of Schwinger is to show that $G_E$ may be written

$$G_E(\vec{p}, \vec{p}\,') = \frac{-16 m p_{0\nu}^3}{(p_{0\nu}^2 + p^2)^2 (p_{0\nu}^2 + p'^2)^2} \Gamma_\nu(\Omega, \Omega'),$$

$$E = -p_{0\nu}^2 / 2m , \tag{15}$$

where $\Gamma_\nu(\Omega, \Omega')$ obeys a simple four-dimensional Euclidean surface-integral equation whose solution is

$$\Gamma_\nu(\Omega, \Omega') = \sum_{nlm} \frac{Y_{nlm}(\Omega) Y^*_{nlm}(\Omega')}{1 - \nu/n} , \quad \nu = \alpha / p_{0\nu},$$

$$n = 1, 2, 3 \ldots , \quad l < n, \quad -l \leq m \leq l , \tag{16}$$

where the $Y_{nlm}$ are four-dimensional spherical harmonics, and the development of a simple parametric representation for $\Gamma_\nu$ in terms of the more useful variables $\vec{p}, \vec{p}\,', E$. These are related to $\Omega$, $\Omega'$ by the transformation

$$\vec{\xi} = \frac{-2 p_{0\nu} \vec{p}}{p_{0\nu}^2 + p^2}, \quad \xi_0 = \frac{p_{0\nu}^2 - p^2}{p_{0\nu}^2 + p^2} , \tag{17}$$

where $\xi = (\vec{\xi}, \xi_0)$ lies on the four-dimensional unit sphere and is equivalent to the angular variable $\Omega$. Formal contact between (16) and expression (5) for $G_E$ is acquired by evaluating the residue of $\Gamma_\nu$ at the bound-state poles $\nu = n$, with the result

$$Y_{nlm}(\Omega) = \frac{(p_{0n}^2 + p^2)^2}{4 p_{0n}^{5/2}} \varphi_{nlm}(\vec{p}),$$

$$p_{0n}^2 / 2m = (1/n^2)(\tfrac{1}{2} \alpha^2 m) . \tag{18}$$

It is to be noted that, although the sum (16) is over the positive integers $n$ only, the hydrogenic continuum is included in (15). In order to express $\Gamma_\nu$ in closed form one uses the relation

$$\frac{1}{1-\nu/n}=1+\frac{\nu}{n}+\nu^2\frac{1}{n(n-\nu)}$$
$$=1+\frac{\nu}{n}+\frac{\nu^2}{n}\frac{i}{2\sin\pi\nu}\int_c d\rho\,\rho^{-\nu}\rho^{n-1}$$
$$=1+\frac{\nu}{n}+\frac{\nu^2}{n}\int_0^1 d\rho\,\rho^{-\nu}\rho^{n-1}, \qquad (19)$$

for $\nu<1$ (the contour $c$ is described in Ref. 19, but we shall not need it), and the relations

$$\sum_{nlm} Y_{nlm}(\Omega)Y^*_{nlm}(\Omega')=\delta(\Omega-\Omega'), \qquad (20a)$$

$$\sum_{nlm}\frac{1}{2n} Y_{nlm}(\Omega)Y^*_{nlm}(\Omega')=\frac{1}{4\pi^2}\frac{1}{(\xi-\xi')^2}, \qquad (20b)$$

$$\sum_{nlm}\frac{\rho^{n-1}}{n} Y_{nlm}(\Omega)Y^*_{nlm}(\Omega')=\frac{1}{2\pi^2}\frac{1}{(1-\rho)^2+\rho(\xi-\xi')^2}, \qquad (20c)$$

to find

$$\Gamma_\nu(\Omega,\Omega')=\delta(\Omega-\Omega')+\frac{\nu}{2\pi^2}\frac{1}{(\xi-\xi')^2}+\frac{\nu^2}{2\pi^2}\left(\frac{i}{2\sin\pi\nu}\right)\int_c d\rho\frac{\rho^{-\nu}}{(1-\rho)^2+\rho(\xi-\xi')^2}. \qquad (21)$$

Use of

$$(\xi-\xi')^2=\frac{4p_{0\nu}^2(\vec{p}-\vec{p}')^2}{(p_{0\nu}^2+p^2)(p_{0\nu}^2+p'^2)}, \qquad (22a)$$

$$\delta(\Omega-\Omega')=\left(\frac{p_{0\nu}^2+p^2}{2p_{0\nu}}\right)^3\delta(\vec{p}-\vec{p}') \qquad (22b)$$

leads to formulas [Eq. (1), Ref. 19] for $G_E(\vec{p},\vec{p}')$ in terms of $E,\vec{p},\vec{p}'$.

In order to present $G_E(\vec{p},\vec{p}')$ in a form with the contribution of a given bound state (here $n=1,2$) separated, we expand (20c) in powers of $\rho$ and compare coefficients, finding

$$Y_{100}(\Omega)Y^*_{100}(\Omega')=1/2\pi^2, \qquad (23a)$$

$$\sum_{lm}Y_{2lm}(\Omega)Y^*_{2lm}(\Omega')=-\frac{1}{2\pi^2}[(\xi-\xi')^2-2], \qquad (23b)$$

or, with the definition (22a) and use of the addition theorem for three-dimensional spherical harmonics,

$$\sum_{lm}Y_{2lm}(\Omega)Y^*_{2lm}(\Omega')=\frac{1}{2\pi^2}\left(\frac{4(p_{0\nu}^2-p^2)(p_{0\nu}^2-p'^2)}{(p_{0\nu}^2+p^2)(p_{0\nu}^2+p'^2)}+\frac{64\pi}{3}\frac{pp'p_{0\nu}^2}{(p_{0\nu}^2+p^2)(p_{0\nu}^2+p'^2)}\sum_{m=-2}^{2}Y_{2m}(\theta,\varphi)Y^*_{2m}(\theta',\varphi')\right). \qquad (23c)$$

Evaluating (23a) and (23c) at the poles $\nu=1,2$ one finds the correct correspondence with the standard forms of the Coulomb wave functions (Appendix A), as indicated in (17). Using Eqs. (20), (23a), and (23b), one may slightly alter the derivation of $\Gamma_\nu$ by applying (19) only to the terms $n\neq1,2$ to find $\Gamma_\nu$ in a form with the $n=1$ or $n=2$ pole separated:

$$\Gamma_\nu=\frac{Y_{100}(\Omega)Y^*_{100}(\Omega')}{1-\nu}+\left(\delta(\Omega-\Omega')-\frac{1}{2\pi^2}\right)+\frac{\nu}{2\pi^2}\left(\frac{1}{(\xi-\xi')^2}-1\right)+\frac{\nu^2}{2\pi^2}\left(\frac{i}{2\sin\pi\nu}\right)\int_c d\rho\,\rho^{-\nu}\frac{[2-(\xi-\xi')^2]\rho-\rho^2}{1+\rho[(\xi-\xi')^2-2]+\rho^2}, \qquad (24a)$$

$$\Gamma_\nu=\sum_{l=0}^{1}\sum_m\frac{Y_{2lm}(\Omega)Y^*_{2lm}(\Omega')}{1-\nu/2}+\delta(\Omega-\Omega')-\frac{1}{\pi^2}(2+\nu)+\frac{\nu}{2\pi^2}\frac{1}{(\xi-\xi')^2}+\frac{1}{\pi^2}\left(1+\frac{\nu}{2}\right)(\xi-\xi')^2$$
$$+\frac{\nu^2}{2\pi^2}\left(\frac{i}{2\sin\pi\nu}\right)\int_c d\rho\,\rho^{-\nu}\left(\frac{1}{1+\rho[(\xi-\xi')^2-2]+\rho^2}+\rho[(\xi-\xi')^2-2]\right). \qquad (24b)$$

The terms without the $Y$'s have no pole at $\nu=1,2$, respectively. What remains is to substitute in the momentum variables through Eqs. (22), (23a), and (23c), express $G_E$ in terms of $\Gamma_\nu$ by means of (15), show that the pole terms are of the form

$$P_1=\frac{\varphi_{100}(\vec{p})\varphi^\dagger_{100}(\vec{p}')}{E-E_1}+\delta_1,$$
$$P_2=\frac{\varphi_{200}(\vec{p})\varphi^\dagger_{200}(\vec{p}')}{E-E_2}+\frac{\sum_m\varphi_{21m}(\vec{p})\varphi^\dagger_{21m}(\vec{p}')}{E-E_2}+\delta_2, \qquad (25)$$

where $\delta_{1,2}$ are regular as $E\to E_{1,2}$, and calculate $\delta_{1,2}$. To obtain the required resolvents one discards the pole terms and evaluates the rest at $E=E_{1,2}$. Thus only the terms of $\delta_{1,2}$ zero order in $E-E_{1,2}$ are required.

This procedure is most simply illustrated for the ground state because (23a) implies that one need not consider a variation of $Y_{100}(\Omega)Y^*_{100}(\Omega')$ in the region of the pole and may use (18) without modification. It is convenient to introduce as a variable the binding energy by way of

$$p_{0\nu}^2=2mB,\quad p_{01}^2=2mB_1=\alpha^2m^2,$$
$$B,B_1=-E,-E_1. \qquad (26)$$

With the substitution

$$\nu=\alpha m/p_{0\nu}=(B_1/B)^{1/2}, \qquad (27)$$

the pole term is

$$P_1 = -\frac{1}{2}\left(\frac{B}{B_1}\right)^{5/2} \frac{(2mB_1+p^2)^2(2mB_1+p'^2)^2}{(2mB+p^2)^2(2mB+p'^2)^2}\,\frac{\varphi_{100}(\vec{p})\varphi_{100}(\vec{p}')}{B-(BB_1)^{1/2}}\,. \tag{28}$$

Expanding about $B=B_1$, we find

$$P_1 = \frac{\varphi_{100}(\vec{p})\varphi^\dagger_{100}(\vec{p}')}{B_1-B} + \varphi_{100}(\vec{p})\varphi^\dagger_{100}(\vec{p}')\left(-\frac{9}{4B_1}+4m\,\frac{4mB_1+p^2+p'^2}{(2mB_1+p^2)(2mB_1+p'^2)}\right)+O(B-B_1)+\cdots\,. \tag{29}$$

The calculation for $n=2$ is complicated by the fact that one must in addition expand (23c) about the point $B=B_2$. An intermediate formula that contains all terms through order $(B-B_2)^0$ is

$$\begin{aligned} P_2 = -\left(\frac{8m}{\pi^2}\right)\frac{1}{\sqrt{B_2}}\left(\frac{2B_2}{B-B_2}+\frac{1}{2}+\cdots\right)&\frac{1}{(2mB_2+p^2)^3(2mB_2+p'^2)^3} \\ \times\Big(8\sqrt{2}\,m^{3/2}[B_2^2+2B_2(B-B_2)]\,&[(2mB_2-p^2)(2mB_2-p'^2)-2m(B-B_2)(4mB_2-p^2-p'^2)] \\ +\frac{256\sqrt{2}\pi}{3}m^{5/2}pp'\sum_m Y_{1m}(\theta,\varphi)Y^*_{1m}(\theta',\varphi')&[B_2^3+3B_2^2(B-B_2)]\Big)\left(1-\frac{6m(B-B_2)(4mB_2+p^2+p'^2)}{(2mB_2+p^2)(2mB_2+p'^2)}\right). \end{aligned} \tag{30}$$

Again neglecting terms of $O(B-B_2)$, one finds a formula of the form (29) with the correct pole term plus remainder.

At this point it is convenient to introduce atomic units:

$$\vec{x},\vec{x}'=\vec{p},\vec{p}'/\alpha m\,,\quad p_{01}^2(\text{a.u.})=1,\quad p_{02}^2(\text{a.u.})=\tfrac{1}{4}\,,$$
$$B_1=\tfrac{1}{2},\,B_2=\tfrac{1}{8}\,. \tag{31}$$

Green's functions have dimension

$$G(\vec{p},\vec{p}')=[m/(\alpha m)^5]G(\vec{x},\vec{x}') \tag{32a}$$

and wave functions

$$\varphi(\vec{p})=[1/(\alpha m)^{3/2}]\varphi(\vec{x})\,. \tag{32b}$$

From now on we shall work with resolvents, leaving off the pole terms. The resulting expressions for resolvents corresponding to the ground and first excited states are

$$\begin{aligned} G^{(1)}(\vec{x},\vec{x}') = {} & \frac{4}{\pi^2}\frac{1}{D_1^3D_1'^3}(-5x^2x'^2+3x^2+3x'^2+11)-\frac{2}{D_1}\delta(\vec{x}-\vec{x}')-\frac{2}{\pi^2}\frac{1}{D_1D_1'}\frac{1}{|\vec{x}-\vec{x}'|^2} \\ & -\frac{8}{\pi^2}\frac{1}{D_1^2D_1'^2}\int_0^1 d\rho\,\frac{(2-4|\vec{x}-\vec{x}'|^2/D_1D_1')-\rho}{1+\rho(4|\vec{x}-\vec{x}'|^2/D_1D_1'-2)+\rho^2}\,,\quad D_1,D_1'\equiv 1+x^2,\ 1+x'^2\,; \end{aligned} \tag{33a}$$

$$\begin{aligned} G^{(2)}(\vec{x},\vec{x}') = {} & \frac{512}{\pi^2}\frac{1}{D_2^4D_2'^4}[6D_2^2D_2'^2-9(1-4x^2)(1-4x'^2)D_2D_2'-16(\tfrac{1}{2}-x^2-x'^2)D_2D_2'+48(\tfrac{1}{2}+x^2+x'^2)(1-4x^2)(1-4x'^2)] \\ & +\sum_m Y_{1m}(\theta,\varphi)Y^*_{1m}(\theta',\varphi')\frac{xx'}{D_2^3D_2'^3}\left(-\frac{32678}{3\pi}+\frac{2048\times256}{\pi}\frac{(\frac{1}{2}+x^2+x'^2)}{D_2D_2'}-\frac{256\times512}{\pi}\right) \\ & -\frac{8}{D_2}\delta(\vec{x}-\vec{x}')-\frac{32}{\pi^2}\frac{1}{D_2D_2'}\frac{1}{|\vec{x}-\vec{x}'|^2}-\frac{16384}{\pi^2}\frac{|\vec{x}-\vec{x}'|^2}{D_2^3D_2'^3} \\ & -\frac{1024}{\pi^2}\frac{1}{D_2^2D_2'^2}\int_0^1 d\rho\,\frac{-1+(16|\vec{x}-\vec{x}'|^2/D_2D_2'-2)^2+\rho(16|\vec{x}-\vec{x}'|^2/D_2D_2'-2)}{1+\rho(16|\vec{x}-\vec{x}'|^2/D_2D_2'-2)+\rho^2}\,,\quad D_2,D_2'\equiv 1+4x^2,\ 1+4x'^2\,. \end{aligned} \tag{33b}$$

It should be noted that the first set of square brackets of (33b) includes the term $3072/(\pi^2D_2^2D_2'^2)$, which comes from the $\rho$ integral $(i/2\sin\pi\nu)\int_c d\rho/\rho^2$ by way of (19) and which is obtained by decomposition of the integrand of (24b). The $\rho$ integrands of (33) now have no singularity at $\rho=0$ and are thus evaluated as ordinary real integrals, as indicated.

At this point one can make the first and simplest numerical check of the formulas. Since $G^{(1,2)}$ are resolvents they are orthogonal to $\varphi_{100}(\vec{x})$, $\varphi_{200}(\vec{x})$, and in particular, for $\vec{x}'=0$; that is,

$$\int d\vec{x}\,\varphi_{100}(\vec{x})G^{(1)}(\vec{x},0)=\int d\vec{x}\,\varphi_{200}(\vec{x})G^{(2)}(\vec{x},0)=0\,. \tag{34}$$

The $\rho$ integrals are elementary, and the rest were performed numerically or analytically if simple. The relations (34) are satisfied to a high degree of accuracy (~$1/10^4$). Appendix C contains some particulars of the numerical work.

For the calculations envisioned $O(\vec{p}, \vec{p}')$ has very simple rotational properties {e.g., hfs = (spin scalar) × (orbital scalar) + [(spin tensor) × (orbital tensor)]$_{\text{rank }2}$} and thus partial wave expansion is appropriate by way of

$$G(x, x', \vec{x}\cdot\vec{x}') = \sum_{\substack{\lambda=0,1,2,3\ldots \\ =s,p,d,f}}^{\infty} G_\lambda(x,x') \sum_{\mu=-\lambda}^{+\lambda} Y_{\lambda\mu}(\Omega) Y^*_{\lambda\mu}(\Omega'), \tag{35}$$

$$G_\lambda(x,x') = 2\pi \int_{-1}^{1} G(x,x',y) P_\lambda(y)\, dy, \quad y = \cos\theta_{\vec{x},\vec{x}'}$$

($\Omega, \Omega'$ are now ordinary angles). It has been found simplest to perform the $y$ integrals first and then the $\rho$ integrals. The results are expressible in terms of elementary functions. Appendix B contains some details of these calculations. It was found convenient for the $\rho$, $y$ integrals to introduce the variables

$$\beta_1 = 4(x^2+x'^2)/D_1D_1', \quad \gamma_1 = 8xx'/D_1D_1',$$
$$\beta_2 = 16(x^2+x'^2)/D_2D_2', \quad \gamma_2 = 32xx'/D_2D_2'. \tag{36}$$

These lie within the triangle indicated in Fig. 1, as can be demonstrated by the method of Lagrange

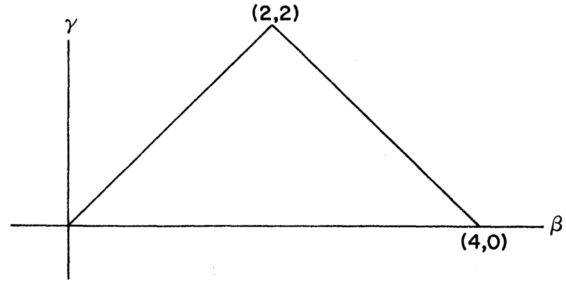


FIG. 1. Domain of $\beta, \gamma$.

multipliers. The expressions are simplified if one introduces the auxiliary definitions

$$b_{1,2\pm} = \beta_{1,2} \pm \gamma_{1,2} - 2, \tag{37a}$$

$$\delta_{1,2\pm} = \tan^{-1}\left(\frac{\beta_{1,2}\pm\gamma_{1,2}}{(4-b^2_{1,2\pm})^{1/2}}\right),$$
$$\omega_{1,2\pm} = \tan^{-1}\left(\frac{b_{1,2\pm}}{(4-b^2_{1,2\pm})^{1/2}}\right),$$
$$-\tfrac{1}{2}\pi < \delta_{1,2\pm}, \omega_{1,2\pm} < \tfrac{1}{2}\pi, \tag{37b}$$

$$Q^{(\pm)}_{1,2} = \delta_{1,2\pm} - \omega_{1,2\pm};$$
$$\theta_{1,2\pm} = \tan^{-1}\left(\frac{(4-b^2_{1,2\pm})^{1/2}}{b_{1,2\pm}}\right), \quad 0 < \theta_{1,2\pm} < \pi. \tag{37c}$$

The $s$ waves are

$$G_s^{(1)}(x,x') = \frac{16}{\pi}\frac{1}{D_1^3 D_1'^3}[-5x^2x'^2+3x^2+3x'^2+11] - \frac{2}{D_1}\frac{\delta(x-x')}{x^2} + \frac{4}{\pi}\frac{1}{D_1D_1'}\frac{1}{xx'}\log\left|\frac{x-x'}{x+x'}\right|$$
$$-\frac{16}{\pi}\frac{1}{D_1^2D_1'^2}\{2+(1/\gamma_1)[\tfrac{1}{2}(\beta_1-\gamma_1)\log(\beta_1-\gamma_1) - \tfrac{1}{2}(\beta_1+\gamma_1)\log(\beta_1+\gamma_1) - (4-b^2_{1-})^{1/2}Q_1^{(-)} + (4-b^2_{1+})^{1/2}Q_1^{(+)}]\}$$
$$\equiv G^{(1)}_{s,1} + G^{(1)}_{s,2} + G^{(1)}_{s,3} + G^{(1)}_{s,5}, \tag{38a}$$

$$G_s^{(2)}(x,x') = \frac{2048}{\pi}\frac{1}{D_2^4D_2'^4}[6D_2^2D_2'^2 - 9D_2D_2'(1-4x^2)(1-4x'^2) - 16(\tfrac{1}{2}-x^2-x'^2)D_2D_2' + 48(\tfrac{1}{2}+x^2+x'^2)(1-4x^2)(1-4x'^2)]$$
$$-\frac{8}{D_2}\frac{\delta(x-x')}{x^2} + \frac{64}{\pi}\frac{1}{D_2D_2'}\frac{1}{xx'}\log\left|\frac{x-x'}{x+x'}\right| - \frac{65536}{\pi}\frac{(x^2+x'^2)}{D_2^3D_2'^3}$$
$$-\frac{2048}{\pi}\frac{1}{D_2^2D_2'^2}\left\{(3-\beta_2) - \frac{1}{\gamma_2}\left[-\log\left(\frac{\beta_2-\gamma_2}{\beta_2+\gamma_2}\right) + \tfrac{1}{4}b^2_{2-}\log(\beta_2-\gamma_2)\right.\right.$$
$$\left.\left. -\tfrac{1}{4}b_2^{+2}\log(\beta_2+\gamma_2) - \tfrac{1}{2}b_{2-}(4-b^2_{2-})^{1/2}Q_2^{(-)} + \tfrac{1}{2}b_{2+}(4-b^2_{2+})^{1/2}Q_2^{(+)}\right]\right\}$$
$$\equiv G^{(2)}_{s,1} + G^{(2)}_{s,2} + G^{(2)}_{s,3} + G^{(2)}_{s,4} + G^{(2)}_{s,5}. \tag{38b}$$

The $d$ waves are

$$G_d^{(1)}(x,x') = -\frac{2}{D_1}\frac{\delta(x-x')}{x^2} - \frac{4}{\pi}\frac{1}{D_1D_1'}\left[-\frac{3}{4}\left(\frac{1}{x^2}+\frac{1}{x'^2}\right) + \left(\frac{1}{2xx'} - \frac{3(x^2+x'^2)^2}{8x^3x'^3}\right)\log\left|\frac{x-x'}{x+x'}\right|\right] - \frac{16}{\pi}\frac{1}{D_1^2D_1'^2}J^{(1)}(\beta_1,\gamma_1)$$
$$\equiv G^{(1)}_{d,1} + G^{(1)}_{d,2} + G^{(1)}_{d,3}, \tag{39a}$$

$$G_d^{(2)}(x,x') = -\frac{8}{D_2}\frac{\delta(x-x')}{x^2} - \frac{64}{\pi}\frac{1}{D_2D_2'}\left[-\frac{3}{4}\left(\frac{1}{x^2}+\frac{1}{x'^2}\right) + \left(\frac{1}{2xx'} - \frac{3(x^2+x'^2)}{8x^3x'^3}\right)\log\left|\frac{x-x'}{x+x'}\right|\right] - \frac{2048}{\pi}\frac{1}{D_2^2D_2'^2}J^{(2)}(\beta_2,\gamma_2)$$
$$\equiv G^{(2)}_{d,1} + G^{(2)}_{d,2} + G^{(2)}_{d,3}. \tag{39b}$$

The $J$ are given by

$$\begin{aligned} J^{(1)}(\beta_1,\gamma_1) &= (1/\gamma_1^2)[6-\tfrac{2}{3}\gamma_1^2+2(\beta_1-2)+(\beta_1-2)^2] \\ &+(1/\gamma_1^3)\log(\beta_1-\gamma_1)[2-\tfrac{1}{2}\gamma_1^2+(\beta_1-2)(3-\tfrac{3}{4}b_{1-}^2+\tfrac{1}{2}\gamma_1 b_{1-})+(\beta_1-2)^2(\tfrac{3}{2}+b_{1-})] \\ &+(1/\gamma_1^3)\log(\beta_1+\gamma_1)[-2+\tfrac{1}{2}\gamma_1^2-(\beta_1-2)(3-\tfrac{3}{4}b_{1+}^2+\tfrac{1}{2}\gamma_1 b_{1-})-(\beta_1-2)^2(\tfrac{3}{2}-b_{1+})] \\ &+(1/\gamma_1^3)Q_1^{(-)}\{-8+b_{1-}^2+\tfrac{1}{4}b_{1-}^4+[\gamma_1^2-3\gamma_1(\beta_1-2)](1-\tfrac{1}{4}b_{1-}^2)\} \\ &-(1/\gamma_1^3)Q_1^{(+)}\{-8+b_{1+}^2+\tfrac{1}{4}b_{1+}^4+[\gamma_1^2-3\gamma_1(\beta_1-2)](1-\tfrac{1}{4}b_{1+}^2)\}-(3/\gamma_1^3)(\beta_1-2)[\tfrac{1}{2}(\theta_{1+}^2-\theta_{1-}^2)]\,, \end{aligned} \tag{40a}$$

$$\begin{aligned} J^{(2)}(\beta_2,\gamma_2) &= (1/\gamma_2^2)[-\tfrac{1}{4}\gamma_2^2+3+(\beta_2-2)(\tfrac{5}{12}\gamma_2^2+\tfrac{15}{4})+\tfrac{1}{4}(\beta_2-2)^2-\tfrac{1}{4}(\beta_2-2)^3] \\ &+(1/\gamma_2^3)\log(\beta_2-\gamma_2)[3-\tfrac{1}{2}\gamma_2^2-\tfrac{3}{16}b_{2-}^4+\tfrac{1}{8}\gamma_2^2 b_{2-}^2+(\beta_2-2)(4+\tfrac{1}{2}b_{2-}^3)+(\beta_2-2)^2(\tfrac{3}{2}-\tfrac{3}{8}b_{2-}^2)] \\ &-(1/\gamma_2^3)\log(\beta_2+\gamma_2)[3-\tfrac{1}{2}\gamma_2^2-\tfrac{3}{16}b_{2+}^4+\tfrac{1}{8}\gamma_2^2 b_{2+}^2+(\beta_2-2)(4+\tfrac{1}{2}b_{2+}^3)+(\beta_2-2)^2(\tfrac{3}{2}-\tfrac{3}{8}b_{2+}^2)] \\ &-\tfrac{3}{2}(1/\gamma_2^3)[\tfrac{1}{2}(\theta_{2+}^2-\theta_{2-}^2)]\,. \end{aligned} \tag{40b}$$

It should be observed that despite appearances all the above expressions remain finite as $\gamma_{1,2}\to 0$.

Some simple numerical computations have been performed to check the formulas and assess the accuracy obtainable. In the case of the $s$ waves one may calculate

$$W^{(1,2)}=\int d\vec{x}\,\varphi_{100,200}(\vec{x})G^{(1,2)}(\vec{x},\vec{x}')=W^{(1,2)}_{1+2+3+4+5}=0\,. \tag{41}$$

Values for $|\vec{x}'|=0.5, 1.0$ are given in Table I. By appropriate modification of the Balmer formula (12) [using $\mathcal{O}(\vec{p})=\lambda p^2$ as a perturbation and comparing with the $\lambda^2$ term in the expansion of the modified Balmer formula] one may conclude that

$$\begin{Bmatrix} V^{(1)} \\ V^{(2)} \end{Bmatrix}=\int d\vec{x}\,d\vec{x}'\begin{Bmatrix}\varphi_{100}(\vec{x}) \\ \varphi_{200}(\vec{x})\end{Bmatrix}x^2\begin{Bmatrix}G^{(1)}(\vec{x},\vec{x}') \\ G^{(2)}(\vec{x},\vec{x}')\end{Bmatrix}x'^2\begin{Bmatrix}\varphi_{100}(\vec{x}') \\ \varphi_{200}(\vec{x}')\end{Bmatrix}=\begin{Bmatrix}-2 \\ -\tfrac{1}{2}\end{Bmatrix}. \tag{42}$$

The calculated values are $V_2^{(1)}=-1.25$, $V^{(1)}_{1+3+5}=-0.741$, $V^{(1)}=-1.991$; $V_2^{(2)}=-0.375$, $V^{(2)}_{1+3+4+5}=-0.121$, $V^{(2)}=-0.496$. Similar checks may be performed on non-$s$ waves by inserting them between states of the same angular momentum but different $n$. For example, to check the $d$ waves we calculated

$$\begin{aligned} D^{(1,2)} &= \int \varphi_{32}^{\dagger}(\vec{x})G_d^{(1,2)}(\vec{x},\vec{x}')\varphi_{32}(\vec{x}')\,d\vec{x}\,d\vec{x}' \\ &= \sum_{n=d\text{ states}}\frac{|\langle\varphi_{32}|\varphi_n\rangle|^2}{E_{1,2}-E_n} \\ &= \frac{1}{E_{1,2}-E_3}=-2.25,\,-14.40\,, \end{aligned} \tag{43}$$

with the results $D^{(1)}_{1+2+3}=-1.811-0.342-0.087=-2.24$, $D^{(2)}_{1+2+3}=-5.813-3.318-5.240=-14.371$. Note that calculation of $V^{(1,2)}$, unlike the rest of the checks, must include the sum over the continuum; the accuracy of the result indicates that it is properly included automatically.

### III. CALCULATION OF RESIDUAL

In calculating $R^{(2)}$ one develops techniques that will be required for the general hyperfine-structure calculation. However, for this calculation it is found that double vector integrals are all that is required and the general situation implied by (3) has not yet been treated. In momentum space the hfs operator may be expressed as[9] (for convenience we let the proton have $g=2$)

$$[\Delta H_{\rm hfs}\varphi](\vec{p})=\frac{\alpha}{2\pi^2}\left(\frac{1}{4mM}\right)\int\frac{d\vec{p}}{|\vec{p}-\vec{p}'|^2}\times[\vec{\sigma}_1\cdot\vec{\sigma}_2-\vec{\sigma}_1\cdot(\vec{p}-\vec{p}')\vec{\sigma}_2\cdot(\vec{p}-\vec{p}')]\varphi(\vec{p}')\,, \tag{44}$$

TABLE I. Resolvent orthogonality check.

| $x'$ | | $W_1(i)$ | $W_2(i)$ | $W_3(i)$ | $W_4(i)$ | $W_5(i)$ | Total |
|---|---|---|---|---|---|---|---|
| 0.5 | $i=1$ | 1.8430 | −0.9219 | −0.7483 | 0.0 | −0.1726 | −0.0001 |
| | $i=2$ | 10.186 03 | 0.0000 | −1.698 04 | −10.186 20 | 1.697 93 | 0.0003 |
| 1.0 | $i=1$ | 0.4499 | −0.2251 | −0.2248 | 0.0 | 0.0000 | 0.0000 |
| | $i=2$ | 2.5091 | 0.1956 | 0.0216 | −2.6077 | −0.1197 | −0.001 |

the Fourier transform of (8). The second term contains both a scalar and a tensor part, which we may separate by way of the general tensor decomposition

$$\vec{\sigma}_1 \cdot \vec{A}\vec{\sigma}_2 \cdot \vec{A} = \left(\frac{8\pi}{15}\right)^{1/2} A^2 \sum_{\mu=-2}^{2} T_\mu^{(2)}(\vec{\sigma}_1, \vec{\sigma}_2) Y_{2,-\mu}(\theta_{\vec{A}}, \varphi_{\vec{A}}) + \tfrac{1}{3}\vec{\sigma}_1 \cdot \vec{\sigma}_2 A^2 \tag{45}$$

(see Ref. 20 for the conventions employed), arriving at the more workable expression

$$[\Delta H_{\rm hfs}\varphi](\vec{p}) = \frac{1}{2\pi^2}\left(\frac{e}{2m}\right)\left(\frac{e}{2M}\right)\int d\vec{p}'\left[\tfrac{2}{3}\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \left(\frac{8\pi}{15}\right)^{1/2} \sum (-1)^\mu T_\mu^{(2)} Y_{2,-\mu}(\Omega_{\vec{p}-\vec{p}'})\right]\varphi(\vec{p}') \,. \tag{46a}$$

The coordinate-space tensor form is

$$\Delta H_{\rm hfs} = \frac{\alpha}{4mM}\left[\frac{8\pi}{3}\vec{\sigma}_1 \cdot \vec{\sigma}_2 \delta^3(\vec{r}) + \frac{3\alpha}{4mM}\left(\frac{8\pi}{15}\right)^{1/2}\frac{1}{r^3} \times \sum (-1)^\mu T_\mu^{(2)} Y_{2,-\mu}(\Omega)\right]. \tag{46b}$$

The $T \times Y$ part does not contribute to $\Delta E$ in first order, and in second order there are no scalar-tensor cross terms. In second order the scalar part contains only intermediate $s$ states and the tensor part only $d$ states.

The first-order hfs splittings implied by (46) are

$$\Delta\nu_{1S,2S}^{(1)} = \Delta E_{1S,2S}^{(1)}\big|_{\rm triplet} - \Delta E_{1S,2S}^{(1)}\big|_{\rm singlet} = \tfrac{8}{3}\alpha^2(m/M)\{1, \tfrac{1}{8}\} \text{ a.u.} \,. \tag{47}$$

The scalar part of the second-order hfs is the simplest to calculate:

$$\Delta\nu_{1S,2S}^{(2,s)} = \left(\frac{1}{2\pi^2}\right)^2\left(\frac{e}{2m}\right)^2\left(\frac{e}{2M}\right)^2\left(\frac{2}{3}\right)^2(-8)\sum_{n\neq 1S,2S}\frac{[\int\int d\vec{p}\,d\vec{p}'\,\varphi_{1S,2S}^\dagger(\vec{p})\varphi_n(\vec{p}')][\int\int d\vec{p}_1\,d\vec{p}_1'\,\varphi_n^\dagger(\vec{p}_1)\varphi_{1S,2S}(\vec{p}_1')]}{E_{1S,2S}-E_n} \tag{48}$$

the factor −8 coming from spin algebra. The $\vec{p}$, $\vec{p}_1'$ integrals may be performed immediately with the result

$$\int d\vec{x}\,\varphi_{1S,2S}(\vec{x}) = (8\pi^2, \pi^2) \,. \tag{49}$$

Forming the residual (6), (7) we find

$$R^{(2,s)} = -\tfrac{1}{12}\alpha^2\frac{m}{M}\frac{8\pi^2}{(2\pi^2)^2}\int\int d\vec{x}\,d\vec{x}'\left(\sum_{n\neq 2S}\frac{\varphi_n(\vec{x})\varphi_n^\dagger(\vec{x}')}{E_{2S}-E_n} - \sum_{n\neq 1S}\frac{\varphi_n(\vec{x})\varphi_n^\dagger(\vec{x}')}{E_{1S}-E_n}\right)$$
$$= -[(2 = g_I)/3]\,\alpha^2(m/M)(3 - 2\log 2) \tag{50}$$

according to Ref. 14. Inserting the $s$-wave part of the resolvents and simplifying,

$$R^{(2,s)} = \frac{-1}{6\pi^2}\int\int d\vec{x}\,d\vec{x}'\;Y_{00}(\Omega)Y_{00}^*(\Omega')[G_s^{(1)}(x,x') - G_s^{(2)}(x,x')]$$
$$\equiv R_1^{(2,s)} + R_2^{(2,s)} + R_3^{(2,s)} + R_4^{(2,s)} + R_5^{(2,s)} = -\tfrac{2}{3}(3 - 2\ln 2) = -1.0758 \,, \tag{51}$$

the subscripts on $R^{(2,s)}$ correspond to the individual terms of the $G_s$ [Eq. (38)]. All the terms have been calculated analytically except $R_5^{(2,s)}$. The results presented in Table II appear to verify the correctness of our approach.

Note that the $n=1$, $n=2$ contributions to $R_2^{(2,s)}$, $R_3^{(2,s)}$, which are precisely the zeroth- and first-order Born terms in a scattering expansion of $G_{E=E_1,E_2}(\vec{p},\vec{p}')$, separately diverge, but adding the integrands yields convergent results. The remaining terms converge separately. This suggests the conjecture that an adequate resolvent for the "relativistic Schrödinger-Pauli equation" mentioned in Sec. I [see, e.g., Eqs. (4.11) and (4.12), Ref. 7, minus the spin terms] may be obtained by using the zeroth and first Born scattering terms from that equation, which may be written down immediately, and what we have calculated here as an adequate nonrelativistic approximation for the rest. For the Born terms one would then require the correct operators and wave functions.

TABLE II. Scalar contribution to second-order residual.

| | $R_1^{(2,s)}$ | $R_2^{(2,s)}$ | $R_3^{(2,s)}$ | $R_4^{(2,s)}$ | $R_5^{(2,s)}$ | Total |
|---|---|---|---|---|---|---|
| $G_s^{(1)}$ | $-\frac{2}{3}$ | $+\frac{1}{3}$ | $+0.9242$ | 0.0 | −1.3033 | −1.0767 |
| $G_s^{(2)}$ | $+4$ | | $=+\frac{4}{3}\ln 2$ | $-\frac{19}{3}$ | 1.9687 | |

The calculation of the tensor contribution is rather more complicated owing to the coupling between the required angular integrations. The major problem encountered is to perform the integral

$$V_{10,\,20}(\vec{x}) = \int x'^2\,dx'\,d\Omega'\,Y_{2m}(\Omega_{\vec{x}-\vec{x}'}) \times\{\varphi_{10,\,20}(\vec{x}') = Y_{00}(\Omega')R_{10,\,20}(x')\}\,. \quad (52)$$

Our approach is to develop a spherical harmonic expansion for $Y_{2m}(\Omega_{\vec{x}-\vec{x}'})$; in our special case only the terms containing $Y^*_{00}(\Omega')$ will contribute since the resulting expression is multiplied by $Y_{00}(\Omega')$ and integrated. Recalling the rectangular form of the spherical harmonics, expressing the resulting functions of $\theta, \varphi, \theta', \varphi'$ in terms of $Y_{lm}(\Omega)$ and $Y_{lm}(\Omega')$, one finds

$$Y_{22}(\Omega_{\vec{x}-\vec{x}'}) = \frac{1}{|\vec{x}-\vec{x}'|^2}\left[x^2Y_{22}(\Omega) + x'^2Y_{22}(\Omega') - xx'(\tfrac{40}{3}\pi)^{1/2}Y_{11}(\Omega)Y_{11}(\Omega')\right],$$

$$Y_{21}(\Omega_{\vec{x}-\vec{x}'}) = \frac{1}{|\vec{x}-\vec{x}'|^2}(\tfrac{20}{3}\pi)^{1/2}[xY_{10}(\Omega) - x'Y_{10}(\Omega')][xY_{11}(\Omega) - x'Y_{11}(\Omega')]\,, \quad (53)$$

$$Y_{20}(\Omega_{\vec{x}-\vec{x}'}) = \frac{1}{|\vec{x}-\vec{x}'|^2}\left[x^2Y_{20}(\Omega) + x'^2Y_{20}(\Omega') - xx'(20\pi)^{1/2}Y_{10}(\Omega)Y_{10}(\Omega') + (5\pi)^{1/2}(x^2+x'^2)Y_{00}(\Omega)Y_{00}(\Omega')\right] - (5/16\pi)^{1/2}\,,$$

$$Y_{2,-m} = (-1)^{\mu}Y^*_{2,m}\,.$$

The next step is to expand $1/|\vec{x}-\vec{x}'|^2$ in spherical harmonics (up to $l=2$ is all that is required). The terms thus generated involving a product of two spherical harmonics of the same argument must be reexpanded. On employing the selection rules for integrals over products of three $Y$'s and dropping all terms that do not have $Y^*_{00}(\Omega')$ dependence, very few terms remain; the general result is

$$Y_{2m}(\Omega_{\vec{x}-\vec{x}'}) = [1/(4\pi)^{1/2}]g(x,x')Y_{2m}(\Omega)Y^*_{00}(\Omega')\,,$$

$$g(x,x') = 2\pi\left[\left(\frac{5}{4} - \frac{3}{4}\frac{x'^2}{x^2}\right) + \left(\frac{3}{4}\frac{x'}{x} - \frac{3}{8}\frac{x}{x'} - \frac{3}{8}\frac{x'^3}{x^3}\right)\log\left|\frac{x-x'}{x+x'}\right|\right]$$
$$= x^2Q_0(x,x') - 2xx'Q_1(x,x') + x'^2Q_2(x,x')\,, \quad (54)$$

the $Q_i$ being the expansion coefficients of $1/|\vec{x}-\vec{x}'|^2$. The calculation of the radial integrals indicated in (52) is straightforward but long; the results are

$$K_{10}(x) = \int x'^2\,dx'\,g(x,x')R_{10}(x')$$
$$= -\left(\frac{\pi^3}{2}\right)^{1/2}\left[5 + \frac{9}{x^2} + \frac{3}{x^2}\frac{1}{1+x^2} + \frac{6}{1+x^2} + \frac{3x^2}{1+x^2} - 12\left(\frac{1}{x} + \frac{1}{x^3}\right)\tan^{-1}x\right], \quad (55a)$$

$$K_{20}(x) = \int x'^2\,dx'\,g(x,x')R_{20}(x')$$
$$= (\pi^3)^{1/2}\left[-\frac{5}{4} - \frac{27}{16x^2} - \frac{12}{(1+4x^2)^2}\left(x^4 + \frac{9}{4}x^2 + \frac{15}{16} + \frac{7}{64x^2}\right) + 3\left(\frac{1}{x} + \frac{1}{2x^3}\right)\tan^{-1}2x\right]. \quad (55b)$$

A simple check of this procedure can now be made by calculating the matrix element of the hfs tensor part between $\varphi_{10}$, $\varphi_{20}$, and $\varphi_{32}$ in both momentum and coordinate space and checking that they are equal. Using Eqs. (46) and (55) and canceling various constants and spin factors, it is required that

$$3\int r^2\,dr\,\tilde{R}_{32}(r)\begin{Bmatrix}\tilde{R}_{10}(r)\\ \tilde{R}_{20}(r)\end{Bmatrix}\frac{1}{r^3}$$
$$= -\frac{1}{2\pi^2}\int\int dx\,dx'\,x^2x'^2R_{32}(x)\begin{Bmatrix}R_{10}(x')\\ R_{20}(x')\end{Bmatrix}g(x,x')$$
$$= -\frac{1}{2\pi^2}\int dx\,x^2R_{32}(x)\begin{Bmatrix}K_{10}(x)\\ K_{20}(x)\end{Bmatrix} = \begin{Bmatrix}0.030429\\ -0.005508\end{Bmatrix}. \quad (56)$$

The equality is satisifed rather precisely.

To complete setting up the tensor part, one needs to perform the required spin algebra and remaining angular integrations. The second-order energy shift may be written

$$\Delta E^{(2,t)}_{\substack{\text{triplet}\\ \text{singlet}}}\,(1S,2S) = \left(\frac{1}{2\pi^2}\right)^2\left(\frac{e}{2m}\right)^2\left(\frac{e}{2M}\right)^2\left(\frac{8\pi}{15}\right)\sum_{n\neq 1S,\,2S}\frac{|\int d\vec{x}[K_{10,\,20}(x)\chi_{t,\,s}][(1/4\pi)^{1/2}\sum T^{(2)}_{\mu}Y_{2,-\mu}(\Omega)][\Phi_{JM,\,n}(\Omega)R_n(x)]|^2}{E_{10,\,20} - E_n}\,. \quad (57)$$

$\Phi_{JM,n}$ is the total angular momentum wave function of the state $n$. Since $T^{(2)}$ is rank 2 and the spin parts of $\Phi_{JM,n}$ are either $S=0$ or $S=1$, it follows that $\chi_{\rm singlet}$ has no matrix element with $\Phi_{JM,n}$, and the spin of $\Phi$ is 1. The orbital part of $\Phi$ must have $l=2$, and since $T\times Y$ is a rotational scalar the contributing states have (taking $M=1$)

$$\Phi_{J=1,M=1,n}(l=2,S=1)=\sqrt{\tfrac{1}{10}}\,\chi_{11}Y_{20}(\Omega)-\sqrt{\tfrac{3}{10}}\,\chi_{10}Y_{21}(\Omega)+\sqrt{\tfrac{6}{10}}\,\chi_{1-1}Y_{22}(\Omega)\,. \qquad (58)$$

Performing the spin sum and $\Omega$ integration and replacing the sum over states by the resolvent kernel, one finds

$$\Delta E^{(2,t)}_{\rm triplet}(1S,2S)=\left(\frac{1}{2\pi^2}\right)^2\left(\frac{e}{2m}\right)^2\left(\frac{e}{2M}\right)^2\frac{8\pi}{15}\frac{1}{4\pi}\frac{20}{3}\times\int dx\,dx'\,x^2x'^2K_{10,20}(x)\times G_d^{(1,2)}(x,x')K_{10,20}(x')\,. \qquad (59)$$

We note that if one retains the sum over states and performs the corresponding coordinate-space calculation, the result agrees with the expression preceding Eq. (16) of Ref. 14 if one takes $g_I=2$ and inserts a factor $(e/2M)^2=\mu_N^2$. This form was arrived at by starting with a different form of the tensor interaction. Using (59) to construct the residual, we find

$$\begin{aligned}R^{(2,t)}&=R_1^{(2,t)}+R_2^{(2,t)}+R_3^{(2,t)}\\&=\left(\frac{1}{2\pi^2}\right)^2\frac{1}{48}\int dx\,dx'\,x^2x'^2\\&\quad\times[8K_{20}(x)G_d^{(2)}(x,x')K_{20}(x')\\&\quad-K_{10}(x)G_d^{(1)}(x,x')K_{10}(x')]\\&=-\tfrac{1}{8}(g_I=2)(\tfrac{17}{16}-\tfrac{5}{3}\log 2)=0.02319\,,\end{aligned} \qquad (60)$$

where the last line is the analytic result of Ref. 14. Again the subscripts on the $R^{(2,t)}$ correspond to the individual terms of the $G_d$ [Eq. (39)]. Again one finds the integrals of the zeroth and first Born terms separately divergent, but the indicated combinations convergent. Table III contains the results; in this case all integrations were numerical. Again the agreement is reasonable. There is, however, room for improvement (see Appendix C), and it is felt that refinement of our preliminary numerical procedure should yield better accuracy.

## IV. POSITRONIUM

The formulas that give the splittings for the positronium ground state are (48) and (59),

$$\Delta\nu^{(2)}_{\rm scalar}=-\tfrac{2}{9}(\tfrac{1}{4}\alpha^6m)\frac{1}{\pi}\int dx\,dx'\,G_s^{(1)}(x,x')\,, \qquad (61a)$$

$$\Delta\nu^{(2)}_{\rm tensor}=\left(\frac{1}{2\pi^2}\right)^2\frac{1}{144}(\tfrac{1}{4}\alpha^6m)\times\int\int dx\,dx'\,K_{10}(x)G_d^{(1)}(x,x')K_{10}(x')\,,$$

$$\tfrac{1}{4}\alpha^6m=4.6645\text{ MHz}\,. \qquad (61b)$$

We have attempted to obtain some idea of the order of magnitude of the scalar term (the tensor term is smaller owing to the small overlap between $s$ and $d$ radial functions). The convergent pieces are easily calculated:

$$\Delta\nu^{(2)}_{\rm scalar,1}=1.03\text{ MHz}\,,\quad \Delta\nu^{(2)}_{\rm scalar,5}=2.02\text{ MHz}\,.$$

The zeroth Born term is linearly divergent, and thus one cannot reasonably expect that any cutoff calculation would yield a good approximation to the relativistically correct expression, and thus we omit it. The first Born term is logarithmically divergent, and one might expect to obtain a fair answer by cutting off the integrals at $p\sim m$ or $x=1/\alpha\equiv\Lambda$. The Born-term integral thus cut off is

$$\Delta\nu^{(2)}_{\rm scalar,3}=(-2/9\pi)(\tfrac{1}{4}\alpha^6m)(4/\pi)2I(\Lambda),$$

$$\begin{aligned}I(\Lambda)&=\int_0^\Lambda dx\int_0^x dx'\,\frac{xx'}{(1+x^2)(1+x'^2)}\log\left|\frac{x-x'}{x+x'}\right|\\&=-\int_0^\Lambda\frac{x\,dx}{1+x^2}(\tan^{-1}x)^2\\&=-\tfrac{1}{2}\log(1+x^2)(\tan^{-1}x)^2\Big|_0^\Lambda\\&\quad+\int_0^\infty dx\log(1+x^2)\frac{\tan^{-1}x}{1+x^2}+O\left(\frac{1}{\Lambda}\right).\end{aligned}$$

Evaluation of $I(\Lambda)$ gives

$$I(\Lambda)=-\tfrac{1}{4}\pi^2\log(1/\alpha)+2.76\,,$$

with the consequent splitting

$$\Delta\nu^{(2)}_{\rm scalar,3}=7.87\text{ MHz}\,.$$

This added to the convergent terms gives a total of 10.92 MHz, which is about two standard deviations of the experimental result. The form of the Born term may indicate the presence of a logarithmic contribution in the corresponding term of a relativistic calculation. This requires further investigation since, although Fulton *et al.*[6] found a logarithmic term in the diagram representing successive transverse exchange with free-particle propagation in between, presumably corresponding in

TABLE III. Tensor contribution to second-order residual.

| | $R_1^{(2,t)}$ | $R_2^{(2,t)}$ | $R_3^{(2,t)}$ | Total |
|---|---|---|---|---|
| $G_d^{(1)}$ | 0.02131 | 0.00175 | 0.00897 | 0.0229 |
| $G_d^{(2)}$ | | | −0.00914 | |

part to the zeroth Born term we have omitted, they found none corresponding to exchange of a single Coulomb photon between the transverse exchanges.

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### APPENDIX A: COULOMB WAVE FUNCTIONS

We tabulate here the wave functions[9,10] required for the calculations described. With $\varphi_{nlm}(\vec{x}) = R_{nl}(x)Y_{lm}(\hat{x})$, $\tilde{\varphi}_{nlm}(\vec{r}) = \tilde{R}_{nl}(r)Y_{lm}(\hat{r})$ defined as the momentum- and coordinate-space forms, we have (in atomic units)

$$R_{10}(x) = -4\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{(1+x^2)^2}, \quad \tilde{R}_{10}(r) = 2e^{-r},$$

$$R_{20}(x) = \frac{32}{\sqrt{\pi}}\frac{1-4x^2}{(1+4x^2)^3}, \quad \tilde{R}_{20}(r) = \frac{1}{\sqrt{2}}e^{-r/2}(1-\tfrac{1}{2}r),$$

$$R_{21}(x) = \frac{128i}{\sqrt{3\pi}}\frac{x}{(1+4x^2)^3}, \quad \tilde{R}_{21}(r) = \frac{1}{2\sqrt{6}}e^{-r/2}r,$$

$$R_{32}(x) = \left(\frac{2}{\pi 5!}\right)^{1/2} 81\times 2^7\frac{x^2}{(1+9x^2)^4},$$

$$\tilde{R}_{32}(r) = \frac{4}{81\sqrt{30}}e^{-r/3}r^2.$$

The phase indicated makes these exact Fourier transforms of one another [Ref. 10, Eq. (28)].

### APPENDIX B: INTEGRATIONS FOR PARTIAL WAVES

Intermediate results for $J^{(1,2)}(\beta,\gamma)$ of the $d$ waves are given here. The $s$-wave integrals are similar but much simpler. We have

$$J^{(2)}(\beta,\gamma) = \int_0^1 d\rho\int_{-1}^1 dy\,[P_2(y) = \tfrac{3}{2}y^2 - \tfrac{1}{2}]\frac{-1+(\beta-2-\gamma y)^2+\rho(\beta-2-\gamma y)}{1+(\beta-2)\rho+\rho^2-\gamma\rho y}$$
$$= \int_0^1 d\rho\left[\left(-\frac{3}{\gamma^2\rho^4}-\frac{3(\beta-2)}{\gamma^2\rho^3}-\frac{3}{\gamma^2\rho^2}\right)+\left(-\frac{3}{2}\frac{1}{\gamma^3\rho^5}-\frac{3(\beta-2)}{\gamma^3\rho^4}+\frac{1}{2}\frac{1}{\gamma\rho^3}-\frac{3}{\gamma^3\rho^3}-\frac{3}{2}\frac{(\beta-2)^2}{\gamma^3\rho^3}-\frac{3(\beta-2)}{\gamma^3\rho^2}-\frac{3}{2}\frac{1}{\gamma^3\rho}\right)\right.$$
$$\left.\times\log\left|\frac{1+(\beta-\gamma-2)\rho+\rho^2}{1+(\beta+\gamma-2)\rho+\rho^2}\right|\right], \tag{B1}$$

$$J^{(1)}(\beta,\gamma) = \int_0^1 d\rho\int_{-1}^1 dy\,P_2(y)\frac{-(\beta-2+\rho)+\gamma y}{1+(\beta-2)\rho+\rho^2-\gamma\rho y}$$
$$= \int_0^1 d\rho\left[\left(-\frac{3}{\gamma^2\rho^3}-\frac{3(\beta-2)}{\gamma^2\rho^2}-\frac{3}{\gamma^2\rho}\right)+\left(-\frac{3}{2}\frac{1}{\gamma^3\rho^4}-\frac{3(\beta-2)}{\gamma^3\rho^3}-\frac{3}{\gamma^3\rho^2}-\frac{3}{2}\frac{(\beta-2)^2}{\gamma^3\rho^2}+\frac{1}{2\gamma\rho^2}-\frac{3(\beta-2)}{\gamma^3\rho}-\frac{3}{2}\frac{1}{\gamma^3}\right)\right.$$
$$\left.\times\log\left|\frac{1+(\beta-\gamma-2)\rho+\rho^2}{1+(\beta+\gamma-2)\rho+\rho^2}\right|\right]. \tag{B2}$$

Both integrands are convergent in the limit $\rho\to 0$. To proceed we need the integrals

$$M_{a,b,c,d,e,f} = \lim_{\lambda\to 0}\int_\lambda^1 d\rho\left\{\frac{1}{\rho^5},\frac{1}{\rho^4},\frac{1}{\rho^3},\frac{1}{\rho^2},\frac{1}{\rho},1\right\}\times\log\frac{1+b_-\rho+\rho^2}{1+b_+\rho+\rho^2}. \tag{B3}$$

All but $M_e$ may be calculated straightforwardly by partial integration to eliminate the logarithm. The integrals then required are

$$Q_{1,2,3,4,5,6,7} = \lim_{\lambda\to 0}\int_\lambda^1 d\rho\left\{\frac{1}{\rho^4},\frac{1}{\rho^3},\frac{1}{\rho^2},\frac{1}{\rho},1,\rho,\rho^2\right\}\times\frac{1}{1+b\rho+\rho^2},$$

which in terms of

$$Q_5 = \frac{2}{(4-b^2)^{1/2}}\left(\tan^{-1}\frac{2+b}{(4-b^2)^{1/2}}-\tan^{-1}\frac{b}{(4-b^2)^{1/2}}\right)$$

are

$$Q_7 = 1-\tfrac{1}{2}b\log(2+b)+\tfrac{1}{2}(b^2-2)Q_5,$$
$$Q_6 = \tfrac{1}{2}\log(2+b)-\tfrac{1}{2}bQ_5,$$
$$Q_4 = -\tfrac{1}{2}\log(2+b)-\log\lambda-\tfrac{1}{2}bQ_5,$$
$$Q_3 = -1+1/\lambda-Q_5-bQ_4$$
$$Q_2 = -\tfrac{1}{2}+1/2\lambda^2-Q_4-bQ_3$$
$$Q_1 = -\tfrac{1}{3}+1/3\lambda^3-Q_3-bQ_2.$$

Upon combination with the surface terms of the $M_i$ and insertion into (A1) and (A2) all $\lambda$ dependence drops out and the results of (40) are found, with the $Q^{(\pm)}_{1,2}$ coming from $Q_5$.

A rather complex procedure was employed to evaluate $M_e$, even though the simple form of the result indicates that something far simpler might have been done, although forms presented in standard tables are based on Taylor expansion of the integrand. Our procedure is to develop a generalized power series expansion for $\log(1+b\rho+\rho^2)$, which reduces to the small-$\rho$ Taylor expansion for any value of $b$, which, due to the properties of $\beta, \gamma$ (Fig. 1), lies between $-2$ and $+2$. We may write

$$\log(1+b\rho+\rho^2)=\log(1+\rho/d_-)(1+\rho/d_+)$$
$$=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\frac{\rho}{d_-}\right)^n+\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\frac{\rho}{d_+}\right)^n,$$

where the expansion is valid since $\rho<1$ and

$$d_\pm=\tfrac{1}{2}b\pm\tfrac{1}{2}i(4-b^2)^{1/2}$$

lie on the unit circle. To proceed, note that

$$\frac{1}{d_+^n}+\frac{1}{d_-^n}=\left(\frac{1}{d_+}\right)^n+\left(\frac{1}{d_+}\right)^{n*}=2\,\mathrm{Re}\left(\frac{1}{d_+}\right)^n=2\,\mathrm{Re}(d_-)^n$$

since

$$(d_+^*/d_+d_+^*)^n=(d_+^*)^n=(d_-)^n.$$

Writing

$$d_-=re^{i\theta'}$$

we have

$$r=1,\quad \theta'=\tan^{-1}[-(4-b^2)^{1/2}/b],\quad -\pi<\theta'<0,$$

and

$$2\,\mathrm{Re}(d_-)^n=2\cos n\theta'.$$

Since the cosine is an even function,

$$2\,\mathrm{Re}(d_-)^n=2\cos n\theta,$$
$$\theta=\tan^{-1}[(4-b^2)^{1/2}/b],\quad 0<\theta<\pi,$$

and thus

$$\log(1+b\rho+\rho^2)=2\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\rho^n\cos n\theta.$$

Integrating term by term

$$M_e=2\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2}(\cos n\theta_- - \cos n\theta_+),$$

$$\theta_\pm=\tan^{-1}[(4-b_\pm^2)^{1/2}/b_\pm],\quad 0<\theta_\pm<\pi.$$

The simplicity of the coefficients of $\cos n\theta$ suggests that this series is the Fourier series of a simple function defined on a suitable interval, and this turns out to be true. One can show that

$$2\sum_{n=1,\,\mathrm{odd}}^{\infty}\frac{\cos n\theta}{n^2}\equiv f_{\mathrm{odd}}(\theta)=\tfrac{1}{4}\pi^2-\tfrac{1}{2}\pi\theta,\quad 0<\theta<\pi$$

$$2\sum_{n=2,\,\mathrm{even}}^{\infty}\frac{\cos n\theta}{n^2}\equiv f_{\mathrm{even}}(\theta)=\tfrac{1}{2}(\theta-\tfrac{1}{2}\pi)^2-\tfrac{1}{24}\pi^2,\quad 0<\theta<\pi.$$

The appropriate interval of definition is $0<\theta<2\pi$, and the appropriate extension of $f_e$ and $f_0$ is defined by requiring them to be even about $\theta=\pi$. Note that $f_{e-0}$ is even-odd about $\theta=\frac{1}{2}\pi,\frac{3}{2}\pi$. Combining these

$$M_e=\tfrac{1}{2}(\theta_+^2-\theta_-^2),$$
$$\theta_\pm=\tan^{-1}[(4-b_\pm^2)^{1/2}/b_\pm],\quad 0<\theta_\pm<\pi.$$

## APPENDIX C: NUMERICAL INTEGRATIONS

The numerical integrations were performed in double-precision Fortran on a Digital Scientific Meta IV computer. A standard trapezoidal routine RIEMANN,[21] was used. This routine employs one iteration of self-correction and was especially valuable for this work in that it handled the logarithmic singularities automatically with no special programming required. For double integrals it was advantageous to compile two of these and let the first call the second for its integrand.

As yet no systematic effort has been made to optimize computer time and accuracy. A major source of error is the fact that the individual terms of the $G_{s,d;5}^{(1,2)}$ diverge badly as $\gamma_{1,2}\to 0$, although the sum does not. This could be remedied by using a Taylor series expansion about $\gamma_{1,2}=0$ for $\gamma_{1,2}$ less than some preassigned value.


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