

In addition, the values of $[Cs][Ar]L$ were divided by the $[Ar]$ values as determined from the filling pressure of argon to yield values of $[Cs]L$ appropriate to each measured value of A_T . The ratio of A_T for the lines of the second doublet to $[Cs]L$ was then used to calculate the respective oscillator strengths. The accuracy of these oscillator strengths is directly proportional to the accuracy of the $[Cs][Ar]L$ values of Fig. 7 and, therefore, to the assumption of an equilibrium vapor pressure in the experiments using the sealed-off absorption cell. Because of the numerous sources of error present in this comparison, e.g., drift in cesium density and errors in planimeter determination of A_T values, we do not regard this as a measurement of the cesium density, but only as a consistency check on the assumption of an equilibrium vapor pressure.

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³⁶S. D. Tvorogov and V. V. Fomin, Opt. Spektrosk. 30, 228 (1971) [Opt. Spectrosc. 30, 228 (1971)].

³⁷Quoted by G. N. Plass and D. Warner, Phys. Rev. 86, 138 (1952). Their Eq. (2a) should read the equivalent of $k(\Delta\nu) = \frac{1}{15} \kappa N C_6^{1/2} (\Delta\nu^{3/2} \beta) e^{-\beta}$, where κ is the integrated

absorption coefficient for the line (Ref. 30). $\Delta\nu$ is the absolute value of the difference between the frequency of interest and that at line center, N is the perturber density, $\beta = 12\pi \Delta\nu^{5/6} C_6^{1/6} / 5v$, C_6 is the van der Waals constant defined by setting the intermolecular potential equal to $\Delta\nu = C_6/R^6$ and v is the relative velocity of the collision.

Note that in this notation the absorption coefficient for the red wing is $k(\Delta\nu) = \kappa N C_6^{1/2} (3\Delta\nu^{3/2})^{-1}$, i. e., the violet wing is lower by $(7/3\beta)^{-1} e^{*\beta}$. Also, Holstein's result is lower than Lindholm's (Ref. 35) by 0.23 $e^{(6)}$, i. e., by a large factor in the range of validity of the theory. Holstein (private communication) has averaged this result over a thermal distribution of velocities to obtain $\langle k(\Delta\nu) \rangle \approx \kappa (7/15) N C_6^{1/2} (\Delta\nu^{3/2} \beta^{2/3})^{-1} \exp(-\frac{2}{3}\beta^{2/3})$, where here $v = (2kT/\mu)^{1/2}$, k is Boltzmann's constant, T is the gas temperature, and μ is the reduced mass. Note that since the expansion parameter in Holstein's theory, $\frac{5}{3}\beta$, is only about unity at 2 Å from line center, we should not be too surprised as to the discrepancy between theory and experiment. Unfortunately, the shoulder in the absorption curve for the blue wing of the 8944-Å line at about 10 Å caused by the minimum in the ground-state potential^{25,26} prevents a test of Holstein's theory at larger wavelength differences from line center.

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Second-Order Corrections to the Fine Structure of Helium. III. Improved Calculation of Some 3P Contributions

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Spin-dependent perturbations from intermediate 3P states are calculated by expanding the perturbations to the wave function in terms with one negative power of one of the electron or interelectron coordinates, in addition to standard Hylleraas terms. The nonstandard terms reflect singularities of the Breit operators. A method for solving linear equations with "almost-singular" coefficient matrices is devised. Significant improvement in accuracy is achieved for five contributions, but the procedure does not work well in all cases where the coefficient matrix is unsymmetrical.

I. INTRODUCTION

In an earlier paper,¹ referred to as I, the contributions to the fine structure of the 2^3P level of helium from second-order perturbation theory with intermediate 3P states were calculated, and in a subsequent paper,² referred to as II, the contributions from 1P and 3D intermediate states were

also calculated. However, many of the results of I did not have the desired numerical accuracy, which was to match the absolute experimental precision of the two fine-structure separations of the 2^3P level (10^{-6} cm⁻¹ for the large interval and 10^{-7} cm⁻¹ for the small interval). In this paper, we present a method which dramatically increases the accuracy for those contributions that come

from the square of a spin-dependent Breit operator or from the mixture of two operators that are singular in the same region. In practice, this is when $r_{12} \rightarrow 0$, i. e., when the two electrons come close together. The method was extended to two other cases where the two operators mixing in second-order perturbation theory have different singularities; but satisfactory results were obtained for only one such case. This is probably because one has to handle nonsymmetric, "almost-singular" matrices, and this seems to be plagued with numerical roundoff difficulties. The calculations reported here were done on CDC 6600 computers (at the Lawrence Berkeley Laboratory and in Stockholm) in single precision corresponding to about 14 decimals (48 bits) accuracy.

The results of this paper are included in a recent Letter,³ which summarizes the various theoretical contributions to the fine-structure separations and compares the results with the experimental values.

II. METHOD: EXPANSION OF BASIS

In this series of papers, the second-order energies are calculated numerically using the method of Dalgarno and Lewis.⁴ The equation

$$(H_0 - E_0) \Psi_1^{(i)} = -(H_1^{(i)} - E_1^{(i)}) \Psi_0 \quad (1)$$

is solved for $\Psi_1^{(i)}$. The wave function and energy for the unperturbed 2^3P state are Ψ_0 and E_0 , respectively, and H_0 is the nonrelativistic Hamiltonian $H_0 \Psi_0 = E_0 \Psi_0$. $H_1^{(i)}$ is any Breit operator, and $E_1^{(i)}$ is its expectation value in the 2^3P state. The operators that will be used in this paper are the following (in atomic units):

$$H_0 = -\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}},$$

$$H_1^{(1)} = \frac{1}{4} \alpha^2 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \left(\frac{\vec{r}_1 \times \vec{p}_1}{r_1^3} + \frac{\vec{r}_2 \times \vec{p}_2}{r_2^3} \right),$$

$$H_1^{(2)} = -\frac{3}{8} \alpha^2 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot [(\vec{r}_1 - \vec{r}_2) \times (\vec{p}_1 - \vec{p}_2)] \frac{1}{r_{12}^3},$$

$$H_1^{(3)} = \frac{1}{4} \alpha^2 \left(\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \frac{3(\vec{\sigma}_1 \cdot \vec{r}_{12})(\vec{\sigma}_2 \cdot \vec{r}_{12})}{r_{12}^2} \right) \frac{1}{r_{12}^3},$$

$$H_1^{(4)} = -\frac{1}{2} \alpha^2 \left(\vec{p}_1 \cdot \vec{p}_2 + \frac{(\vec{r}_{12} \cdot \vec{p}_1)(\vec{r}_{12} \cdot \vec{p}_2)}{r_{12}^2} \right) \frac{1}{r_{12}},$$

$$H_1^{(6)} = \pi \alpha^2 [\delta^{(3)}(\vec{r}_1) + \delta^{(3)}(\vec{r}_2)],$$

where α is the fine-structure constant. Once the solutions of (1) have been obtained, the second-order energies are given by two different integrals:

$$\begin{aligned} E_2^{(i,j)} \langle \Psi_0 | \Psi_0 \rangle &= -\langle \Psi_1^{(i)} | H_0 - E_0 | \Psi_1^{(j)} \rangle \\ &= \langle \Psi_0 | H_1^{(i)} - E_1^{(i)} | \Psi_1^{(j)} \rangle, \end{aligned}$$

and by similar expressions for $E_2^{(j,i)} = E_2^{(i,j)}$. In I and II, wave-function perturbations $\Psi_1^{(i)}$ were expanded in standard Hylleraas terms with non-negative powers of r_1 , r_2 , and r_{12} :

$$\Psi_1^{(i)} = \sum_{l,m,n=0}^{l+m+n \leq \omega} X_{lmn}^{(i)} U_{lmn}, \quad (2)$$

where U_{lmn} is given by

$$U_{lmn} = \frac{1 - P_{12}}{4\pi\sqrt{2}} T_1^{(1)}(\vec{r}_1) u_{lmn}(1, 2) \quad (3)$$

and

$$u_{lmn}(1, 2) = e^{-\kappa\sigma r_1/2} e^{-\kappa r_2/2} r_{12}^l r_1^m r_2^n,$$

$$T_1^{(1)}(\vec{r}_1) = -(x_1 + iy_1)/\sqrt{2}.$$

When ω increased from 1 to 8 so that the number of terms

$$N(\omega) = \frac{1}{6} (\omega + 1) (\omega + 2) (\omega + 3)$$

in the expansions (2) increased from 4 to 165, some of the results of I were rather poorly converged. We believe that the cause of this is primarily the singularities of the operators $H_1^{(i)}$, i. e., that $-(H_1^{(i)} - E_1^{(i)}) \Psi_0$ is not well approximated by $(H_0 - E_0) \Psi_1^{(i)}$ when only standard terms [Eq. (3)] with $l \geq 0$, $m \geq 0$, and $n \geq 0$ are used in the expansions for $\Psi_1^{(i)}$.

Let us first look at a simplified problem. Take Ψ_0 to be just a $(2p, 1s)$ product wave function, and let $H_1^{(1)}$ act on it and pick out the P part:

$$P \text{ part of } H_1^{(1)} \Psi_0 = \text{const} \times r_1^{-3} \Psi_0,$$

where

$$\Psi_0 = \alpha(1) \alpha(2) T_1^{(1)}(\vec{r}_1) e^{-\tau r_1} e^{-2\tau r_2}.$$

There is thus the pole term proportional to $T_1^{(1)}(\vec{r}_1) r_1^{-3}$ which will be reproduced by $H_0 \Psi_1^{(1)}$ if

$$\Psi_1^{(1)} = (1/r_1) \Psi_0. \quad (4)$$

But with this expression for $\Psi_1^{(1)}$, $H_0 \Psi_1^{(1)}$ will include other, less singular terms such as $T_1^{(1)}(\vec{r}_1) \times e^{-\tau/r_1}$ with $n = 1, 2$ [and also a term $T_1^{(1)}(\vec{r}_1) \delta^{(3)}(\vec{r}_1) = 0$] which do not have any counterpart in $H_1^{(1)} \Psi_0$. The solution $\Psi_1^{(1)}$ of (1) might thus be a power series starting with a term like (4), but also including terms like $T_1^{(1)}(\vec{r}_1) \ln r e^{-\tau}$, $T_1^{(1)}(\vec{r}_1) r \ln r e^{-\tau}$, and so on; so that an exact solution for $\Psi_1^{(1)}$ (which could exist if the $1/r_{12}$ terms is dropped from H_0) would be very complicated, even in this simplified case.

Turning now to the actual problem, the P part of $H_1^{(1)} \Psi_0$ is

$$\frac{1 - P_{12}}{4\pi\sqrt{2}} \sum_{l,m,n=0}^{l+m+n \leq \omega} C_{lmn} V_{lmn}(1, 2),$$

where $V_{lmn}(1, 2)$ is given by the expression in Eq. (B4) of I [hereafter denoted I(B4)]. When $m = 0$, the first term of I(B4) gives $T_1^{(1)}(\vec{r}_1) u_{10n}(1, 2)/r_1^3$. Looking at I(B2), one sees that this pole term

would result from [fourth term in I(B2)] $H_0 T_1^{(1)}(\vec{r}_1) u_{l-1n}(1, 2)$, along with many other singular terms. This nonstandard term in the expansion for $\Psi_1^{(1)}$, proportional to $(1 - P_{12}) T_1^{(1)}(\vec{r}_1)/r_1$, would also reproduce the terms

$$-\frac{l}{2} \frac{T_1^{(1)}(\vec{r}_1) \vec{r}_1 \cdot \vec{r}_2}{r_1^3 r_{12}^2} u_{l0n}(1, 2) \quad \text{and} \quad \frac{l}{2} \frac{T_1^{(1)}(\vec{r}_1)}{r_1} u_{l0n}(1, 2)$$

in I(B4). [Use $\vec{r}_1 \cdot \vec{r}_2 = \frac{1}{2} (r_1^2 + r_2^2 - r_{12}^2)$.] The two remaining terms in I(B4) cause trouble when $n=0$, in which case they are

$$\frac{l}{2} \frac{1}{r_2^3 r_{12}^2} [T_1^{(1)}(\vec{r}_1) \vec{r}_1 \cdot \vec{r}_2 - T_1^{(1)}(\vec{r}_2) r_2^2] u_{l00}(1, 2). \quad (5)$$

The first of these can be obtained with $n=-1$ in I(B2). However, this gives terms proportional to $(1 - P_{12}) T_1^{(1)}(\vec{r}_1)/r_2$ in the expansion for $\Psi_1^{(1)}$ which would lead to an infinite value of $E_2^{(1,1)}$ if we use the algorithm of the earlier sections, since $\langle \Psi_1^{(1)} | H_0 | \Psi_1^{(1)} \rangle$ includes integrals with r_2^{-3} in the integrand, coming from the $-2/r_2$ term in H_0 . Finally, to obtain the second term of (5), one would need terms such as $(1 - P_{12}) T_1^{(1)}(\vec{r}_2) u_{l0n-1}(1, 2)$ in the expansion for $\Psi_1^{(1)}$. Thus it would be a rather hopeless task to reproduce all the terms of $H_1^{(1)} \Psi_0$ by adding more and more special terms to the expansion for $\Psi_1^{(1)}$. Even if one managed to do this, there would be very many terms in $H_0 \Psi_1^{(1)}$ without counterpart in $H_1^{(1)} \Psi_0$. Now all but the first term in I(B4) are proportional to $\vec{r}_1 \times (\vec{r}_1 \times \vec{r}_2)$ and only contribute an exchange part to the matrix elements of $H_1^{(1)}$, and this is generally smaller than the direct part because the latter involves folding radial functions (such as $r_1 e^{-\kappa_1/2}$ and $r_1 \times e^{-\kappa_1/2}$) with coinciding peaks, whereas the former involves folding of functions (such as $r_1 e^{-\kappa r_1/2}$ and $e^{-\kappa \sigma r_1/2}$) with maxima occurring for different values of the argument. Therefore we shall only include terms in $\Psi_1^{(1)}$ which will give the leading singularities in $H_1^{(1)} \Psi_0$, which are the terms proportional to $T_1^{(1)}(\vec{r}_1)/r_1^3$. Then the conclusion is that the most important singular part of $\Psi_1^{(1)}$ will be included if the following extended expansion is used [see Eq. (3)]:

$$\Psi_1^{(1)} = \sum_{n=0}^{\omega} x_n^{(1)} U_{0-1n} + \sum_{l, m, n=0}^{l+m+n \leq \omega} X_{lmn}^{(1)} U_{lmn}. \quad (6)$$

Powers of r_{12} in the new terms have been dropped, their inclusion would increase the number of new terms from $\omega+1$ to $\frac{1}{2}(\omega+2)$ while adding little more flexibility. The new terms approximate the behavior of $\Psi_1^{(1)}$ as $r_1 \rightarrow 0$ ($r_2 \rightarrow 0$), in which case $r_{12} \rightarrow r_2(r_{12} \rightarrow r_1)$. The expansion (6) does not lead to many new integrals, beyond the integrals whose evaluation were described in Appendix A of I.

It follows from the work of Schwartz⁵ that the convergence of the second-order energies should

improve when additional trial terms, reflecting the singularities of $H_1^{(1)}$, are introduced in the expansions for $\Psi_1^{(1)}$. If one tries to fit a function $F \sim r^{-d}$ as $r \rightarrow 0$ with functions that are regular at the origin, corresponding to fitting $\Psi_1^{(1)}$ with standard terms, the convergence rate for the one-dimensional model problem, where the volume element is $dv = r^d dr$, is⁵ (see Sec. V of I)

$$c_n^2 \sim 1/n^{d-2d+2}.$$

The additional terms in (6) should change d from 1 to 0, so that a significant improvement of the convergence of $E_2^{(1,1)}$ should occur. However, there may still be singularities, possibly logarithmic ones, to slow down the convergence.

Denoting the nonstandard terms in (6) by V_n and the standard ones by U_k , the system of equations for $\Psi_1^{(1)}$ is now

$$\sum_{n=1}^{\omega+1} \tilde{A}_{ln} x_n^{(1)} + \sum_{k=1}^{N(\omega)} \tilde{A}_{lk} X_k^{(1)} = B_l^{(1)}, \quad l=1, 2, \dots, N(\omega) + \omega + 1, \quad (7)$$

where the three indices in (6) have been mapped into one. We have

$$B_l^{(1)} = -\langle V_l | H_1^{(1)} - E_1^{(1)} | \Psi_0 \rangle, \quad l=1, 2, \dots, \omega+1 \quad (8)$$

and

$$B_l^{(1)} = -\langle U_{l-\omega-1} | H_1^{(1)} - E_1^{(1)} | \Psi_0 \rangle,$$

$$l = \omega+2, \omega+3, \dots, N(\omega) + \omega + 1. \quad (9)$$

Explicitly, the matrix \tilde{A} in (7) is

$$\tilde{A} = \begin{pmatrix} \langle V_n | H_0 - E_0 | V_n \rangle & \langle V_n | H_0 - E_0 | U_k \rangle \\ \langle U_k | H_0 - E_0 | V_n \rangle & \langle U_k | H_0 - E_0 | U_k \rangle \end{pmatrix}, \quad n', n=1, 2, \dots, \omega+1, \quad k', k=1, 2, \dots, N(\omega). \quad (10)$$

We first tried to solve the system (7) as it stands, without deleting any of the equations. In principle, the matrix \tilde{A} is nonsingular; E_0 has a value which makes the lower right-hand block in (10) singular, but this should not stop \tilde{A} from having rank equal to its dimension $N(\omega) + \omega + 1$. However, this leads to quite unreasonable results; the second-order energies came out as huge numbers. The reason for this is probably that \tilde{A} is quite close to being singular.

After some experimentation, it was decided to adjust E_0 in (10) to the lowest value which makes \tilde{A} singular. This number—call it \tilde{E}_0 —is of course the smallest eigenvalue of H_0 in the enlarged basis $(V_1, \dots, V_{\omega+1}, U_1, \dots, U_{N(\omega)})$. An adjustment of $E_1^{(1)}$ in (8) and (9) must also be made, otherwise Eqs. (7) will be overdetermined after E_0 has been changed to \tilde{E}_0 . The elements of the eigenvector $\tilde{\Psi}_0$ of \tilde{A} corresponding to \tilde{E}_0 demonstrate the linear dependence among the rows of \tilde{A} (see Sec. IV of I); thus $E_1^{(1)}$ must be adjusted to $\tilde{E}_1^{(1)}$ determined

by

$$0 = \langle \tilde{\Psi}_0 | H_1^{(i)} - \tilde{E}_1^{(i)} | \Psi_0 \rangle, \quad (11)$$

so that, explicitly,

$$\begin{aligned} \tilde{E}_1^{(i)} \langle \tilde{\Psi}_0 | \Psi_0 \rangle = & \sum_{m=1}^{N(\omega)} C_m \left(\sum_{n=1}^{\omega+1} \tilde{c}_n \langle V_n | H_1^{(i)} | U_m \rangle \right. \\ & \left. + \sum_{k=1}^{N(\omega)} \tilde{C}_k \langle U_k | H_1^{(i)} | U_m \rangle \right) \end{aligned}$$

and a similar expression for $\langle \tilde{\Psi}_0 | \Psi_0 \rangle$. Here $(\tilde{c}_1, \dots, \tilde{c}_{\omega+1}, \tilde{C}_1, \dots, \tilde{C}_{N(\omega)})$ is the eigenvector $\tilde{\Psi}_0$, and $(C_1, \dots, C_{N(\omega)})$ are the coefficients in the expansions of Ψ_0 into standard terms [Eq. (3)]. One can now delete any one of the $N(\omega) + \omega + 1$ equations [Eqs. (7)], but we choose to put $X_1^{(i)} = 0$ and drop the $(\omega + 2)$ th equation in (7), so that the $(\omega + 2)$ th row and column of \tilde{A} in (10) are deleted. This choice is made for the reasons stated in Sec. IV of I; the first standard term in the expansion for $\tilde{\Psi}_0$ is the most important one, corresponding to a $(1s, 2p)$ wave function. Finally, $E_2^{(i,j)}$ is now given by

$$\begin{aligned} E_2^{(j,i)} \langle \Psi_0 | \Psi_0 \rangle = E_2^{(i,j)} \langle \Psi_0 | \Psi_0 \rangle = \langle \Psi_0 | H_1^{(i)} - \tilde{E}_1^{(i)} | \Psi_1^{(j)} \rangle \\ = - \langle \Psi_1^{(i)} | H_0 - \tilde{E}_0 | \Psi_1^{(j)} \rangle, \quad (12) \end{aligned}$$

where $\tilde{E}_1^{(i)}$ must be used rather than $E_1^{(i)}$ because, if $E_1^{(i)}$ is used, $E_2^{(i,j)}$ will change if an arbitrary multiple of $\tilde{\Psi}_0$ (the solution of the homogeneous equation corresponding to the inhomogeneous equation for $\Psi_1^{(i)}$) is added to $\Psi_1^{(i)}$. Using $\tilde{E}_1^{(i)}$, the resulting $E_2^{(i,j)}$ are unique in this sense.

This provides an algorithm resembling the one used in Secs. IV and VI of I; but, in addition to Ψ_0 (E_0 is not required), one also needs \tilde{E}_0 and $\tilde{\Psi}_0$ as input. This eigenvalue problem was solved by the iterative method⁶ used to determine Ψ_0 and E_0 in I. However, the search for eigenvalues and eigenvectors consumes much computer time; so the need to know \tilde{E}_0 and $\tilde{\Psi}_0$ is a serious drawback of the present method.

III. CALCULATIONS AND RESULTS FOR SYMMETRIC CASES

In this section, we give the results obtained by this method for the cases where the same expansions (i. e., the same additional terms) could be used for both $\Psi_1^{(i)}$ and $\Psi_1^{(j)}$ when calculating $E_2^{(i,j)}$. The results for $E_2^{(1,1)}$, using the expansion (6) for $\Psi_1^{(i)}$, are given in Table I. The numbers calculated according to the different expression in (12) did agree to the digits quoted, a convention used in all the tables of this paper. The eigenvalues \tilde{E}_0 were rather close to E_0 (for the same ω); they agreed to four digits for $\omega = 1$ and 2, to six digits for $\omega = 3, 4$, and 5, to seven digits for $\omega = 6$ and 7, and to eight digits for $\omega = 8$. The differences between $\tilde{E}_1^{(1)}$ and $E_1^{(1)}$ were greater, ranging from two digits of agreement for $\omega = 1-6$ to four digits

TABLE I. Second-order energy $E_2^{(1,1)}$ calculated with expansion (6) for $\Psi_1^{(1)}$.

ω	No. of terms in $\Psi_1^{(1)}$	$E_2^{(1,1)} (\frac{1}{2}\alpha^2 R)\frac{1}{2}\alpha^2$
1	6	-0.511 973 988 24
2	13	-0.568 854 763 28
3	24	-0.616 881 834 82
4	40	-0.640 110 546 2
5	62	-0.652 223 2
6	91	-0.658 084
7	128	-0.660 772
8	174	-0.662 040
∞		-0.663 2(2) fast

for $\omega = 7$ and 8.

Table I represents an impressive improvement over the corresponding results in Table IV of I. With 24 terms in the expansion (6), the value of $E_2^{(1,1)}$ was closer to the final extrapolated value (of this paper) than the results obtained with 165 standard terms [Eq. (3)] in Table IV of I. The ratio of successive differences of computed values for $E_2^{(1,1)}$ was fairly constant (ranging from 0.45 to 0.52 for $2 \leq \omega \leq 8$); so the results have been extrapolated according to the "fast" scheme, where the differences between computed energies for successive variational calculations, labeled by ω , are assumed to be proportional to α^ω , where $|\alpha| < 1$ (see Sec. V of I). Note that the results for $E_2^{(1,1)}$ from Table IV of I came closest to the present results when the "slow" scheme of extrapolation was used, i. e., when the differences are assumed to be proportional to ω^{-p} with $p > 1$. This is a qualitative confirmation of Schwartz's theory of convergence of variational calculations.⁵

Next, we try two different expansions for $\Psi_1^{(2)}$ and $\Psi_1^{(3)}$. The operators $H_1^{(2)}$ and $H_1^{(3)}$ are singular when $r_{12} \rightarrow 0$, and from I(B5) and I(B6) it is seen that $H_1^{(i)} \Psi_0$ contains terms proportional to $1/r_{12}^3$ when $l=0$ ($i=2, 3$). Similar terms are obtained from $H_0 \Psi_1^{(i)}$ if functions proportional to $1/r_{12}$ are included in $\Psi_1^{(i)}$. This should take care of the dominant singularities that slow down the convergence of $E_2^{(2,2)}$, $E_2^{(3,3)}$, and $E_2^{(2,3)}$, although terms with $\ln r_{12}$ should probably also be included. We try two simple expansions:

$$\Psi_1^{(i)} = \sum_{n=0}^{\omega} x_n^{(i)} U_{-10n} + \sum_{l,m,n=0}^{l+m+n \leq \omega} X_{lmn}^{(i)} U_{lmn}, \quad (13)$$

$$\Psi_1^{(i)} = \sum_{m=0}^{\omega} x_m^{(i)} U_{-1m0} + \sum_{l,m,n=0}^{l+m+n \leq \omega} X_{lmn}^{(i)} U_{lmn}. \quad (14)$$

A better expansion would include terms U_{-1mn} with $m \geq 0$, $n \geq 0$, and $m+n \leq \omega$, but it is desirable, from a practical point of view, to keep the number of extra terms small. The operator $H_1^{(4)}$ is also singular when $r_{12} = 0$, but from I(B7) it is seen that all terms in $H_1^{(4)} \Psi_0$ with $1/r_{12}^3$ are proportional to

$(r_1^2 - r_2^2)/r_{12}^3$ when $l=0$. The angular average of $(r_1^2 - r_2^2)/r_{12}^3$ is equal to that of $1/r_{12}$, so that an expansion such as (13) or (14) is not required for $\Psi_1^{(4)}$. Nevertheless, we calculate $E_2^{(2,4)}$, $E_2^{(3,4)}$, and $E_2^{(4,4)}$ along with $E_2^{(2,2)}$, $E_2^{(3,3)}$, and $E_2^{(2,3)}$ with both the expansions (13) and (14) for $\Psi_1^{(i)}$, $i=2, 3, 4$. No more work (calculation of integrals) is involved for the three energies $E_2^{(i,4)}$ ($i=2, 3, 4$) once $E_2^{(2,2)}$, $E_2^{(3,3)}$, and $E_2^{(2,3)}$ are done. These six second-order energies are computed by the same algorithm that was used to compute $E_2^{(1,1)}$. One could also use a mixed representation—say, (13) for $\Psi_1^{(i)}$ and (14) for $\Psi_1^{(j)}$ ($i, j=2, 3, 4$)—and compute $E_2^{(i,j)}$ by the method described in Sec. IV. Some additional integrals are required for the matrix element of H_0 and $H_1^{(i)}$ between standard terms and the functions with $1/r_{12}$ and of H_0 with new terms on both sides. Great care is required in the evaluation of these integrals, since they are divergent unless certain combinations are taken. This is described in the Appendix. It is interesting to note that the matrix of H_0 is no longer automatically symmetric; denoting the additional terms in (13) or (14) by V_n , we have

$$\int d^3r_1 (V_n^* \nabla_1^2 V_m - V_m^* \nabla_1^2 V_n) \\ = \int d\vec{\sigma}_1 \cdot (V_n^* \nabla_1 V_m - V_m^* \nabla_1 V_n).$$

The surface(s) integral over the faraway surface vanishes as usual, but there is also an integral over a small spherical surface of radius ϵ , say, surrounding the singularity at $r_{12}=0$. It turns out that this contribution vanishes because of the angular integration, but the integrand does not go to zero as $\epsilon \rightarrow 0$. For the same reason, there is never any contribution to the matrix elements of H_0 from a δ function $\delta^{(3)}(\vec{r}_{12})$ resulting from the action of H_0 on V_n .

In Table II, we give some of the results of these calculations. For the unmixed energies $E_2^{(i,i)}$, what we compute is always an upper bound (see Appendix C of I for a formal proof of this statement); therefore we have only quoted the results for $E_2^{(i,i)}$ ($i=2, 3$) when the expansion (13) was used for $\Psi_1^{(i)}$, since these were slightly smaller (larger

in magnitude) than the values obtained with (14). The extrapolated results from both sets of calculations [using (13) and (14)] were the same for $E_2^{(2,2)}$, $E_2^{(3,3)}$, and $E_2^{(2,3)}$. In the latter case, the calculated numbers obtained with (13) were slightly closer to the extrapolated results than the ones from (14) for the higher values of ω ; so again only the results from (13) are quoted. For $\omega=8$, the values obtained using (14) were $E_2^{(2,2)} = -1.12280$, $E_2^{(3,3)} = -0.006057$, and $E_2^{(2,3)} = 0.08100$. For these three sequences of numbers, it was found that the successive differences were better fitted by a slow convergence scheme. Again, the results of Table IV of I came closest to the results of Table II of this paper when the slow extrapolation was used.

The results obtained for $E_2^{(2,4)}$, $E_2^{(3,4)}$, and $E_2^{(4,4)}$ (which does not contribute to the fine structure), using both expansions (13) and (14) for $\Psi_1^{(i)}$ ($i=2, 3, 4$), were rather close to the results of Table IV and VI of I. Some of these results are given in Table III; since they do not represent a significant improvement over the results of I, they have not been extrapolated. The differences between E_0 and \tilde{E}_0 , as well as between $E_1^{(i)}$ and $\tilde{E}_1^{(i)}$ ($i=2, 3, 4$), were of the same orders of magnitude (for $\omega=1-8$) as the corresponding quantities used in the calculation of $E_2^{(1,1)}$. It is not surprising that the expansions (13) and (14) should give essentially the same results, since the nonstandard terms approximate the behavior of $\Psi_1^{(i)}$ at $r_{12} \approx 0$, where $r_1 \approx r_2$.

One could probably not expect any significant improvement over the accurate values for $E_2^{(2,4)}$ and $E_2^{(3,4)}$ obtained in Table IV of I. This is because in

$$E_2^{(i,4)} = -\langle \Psi_1^{(i)} | H_0 - \tilde{E}_0 | \Psi_1^{(4)} \rangle / \langle \Psi_0 | \Psi_0 \rangle \quad (i=2 \text{ or } 3),$$

$\Psi_1^{(2)}$ or $\Psi_1^{(3)}$ is improved when the expansions (13) or (14) are used rather than just standard terms; but this is not true for $\Psi_1^{(4)}$. Since one of the two perturbed wave functions is improved, one might anticipate a slight improvement, and this seems to be the case; i. e., the differences between the results for $\omega=7$ and 8 in Table III are smaller than the corresponding quantities in I.

The results of this section are in excellent agreement with the corresponding results from I, and we have achieved a significant improvement in accuracy with only a few extra trial functions. In fact, $E_2^{(1,1)}$ and $E_2^{(3,3)}$ were improved by two orders of magnitude, and $E_2^{(2,2)}$ and $E_2^{(2,3)}$ were improved by one order.

IV. EXTENSIONS TO NONSYMMETRIC CASES

When different nonstandard terms—say, V_n and W_n —must be used to reflect different singularities in $\Psi_1^{(i)}$ and $\Psi_1^{(j)}$, the method described in Sec. III must be modified. The matrix \tilde{A} of $H_0 - \tilde{E}_0$ used

TABLE II. Second-order energies calculated with expansion (13) for $\Psi_1^{(i)}$, $i=2, 3$.

ω	$E_2^{(2,2)} (\frac{1}{2}\alpha^2 R) \frac{1}{4}\alpha^2$	$E_2^{(3,3)} (\frac{1}{2}\alpha^2 R) \frac{1}{4}\alpha^2$	$E_2^{(2,3)} (\frac{1}{2}\alpha^2 R) \frac{1}{4}\alpha^2$
1	-0.885 763 807 0	-0.005 239 656 190	0.067 865 863 045
2	-0.992 239 130 6	-0.005 741 438 702	0.074 763 980 404
3	-1.054 458 292 2	-0.005 931 330 644	0.078 126 662 368
4	-1.087 089 128 7	-0.006 006 971 263	0.079 681 310 8
5	-1.104 900 2	-0.006 033 454	0.080 365 93
6	-1.116 37	-0.006 049 15	0.080 787
7	-1.121 70	-0.006 056 81	0.080 985
8	-1.126 23	-0.006 063 16	0.081 148
∞	-1.143(5) slow	-0.006 085(5) slow	0.081 7(2) slow

TABLE III. Some second-order energies calculated with expansion (14) for $\Psi_1^{(i)}$, $i=2,3,4$.

ω	$E_2^{(2,4)}(\frac{1}{2}\alpha^2 R)\alpha^2$	$E_2^{(3,4)}(\frac{1}{2}\alpha^2 R)\alpha^2$	$E_2^{(4,4)}(2\alpha^2 R)$
1	0.120 544 656 05	-0.009 245 201 190	-0.022 694 206 586
2	0.162 973 502 22	-0.012 177 821 040	-0.032 068 331 173
3	0.171 402 524 33	-0.012 633 621 644	-0.034 825 336 001
4	0.178 467 714	-0.012 955 451 55	-0.036 706 560 7
5	0.182 135 04	-0.013 079 891	-0.037 762 334
6	0.184 026	-0.013 143 19	-0.038 252 80
7	0.184 86	-0.013 170 5	-0.038 432
8	0.185 34	-0.013 184	-0.038 523 9

when solving $(H_0 - \tilde{E}_0)\Psi_1^{(i)} = -(H_1^{(i)} - E_1^{(i)})\Psi_0$ is no longer symmetric. The two lower blocks in (10) are unchanged, but the upper-left block is $\langle W_n | H_0 - \tilde{E}_0 | V_n \rangle$ and the one at the upper right is $\langle W_n | H_0 - \tilde{E}_0 | U_k \rangle$. One must now distinguish between the left and right eigenvectors $\tilde{\Psi}_0^r$ and $\tilde{\Psi}_0^l$, corresponding to \tilde{E}_0 , in this extended mixed representation. In (11) the value of $\tilde{E}_1^{(i)}$ was determined by multiplication from the left, so that

$$\tilde{E}_1^{(i)} = \langle \tilde{\Psi}_0^l | H_1^{(i)} | \Psi_0 \rangle / \langle \tilde{\Psi}_0^l | \Psi_0 \rangle.$$

Note that the matrix elements of $H_1^{(i)}$ ($H_1^{(j)}$) between the new and the standard terms are $\langle W_n | H_1^{(i)} | U_k \rangle$ ($\langle U_k | H_1^{(j)} | V_n \rangle$), where W_n (V_n) reflects the singularity of $H_1^{(j)}$ ($H_1^{(i)}$). The algorithms for calculating $E_2^{(i,j)}$ and $E_2^{(j,i)}$ are now slightly different. When one solves for $\Psi_1^{(j)}$, the matrix \tilde{A} is the transpose of the one used in solving for $\Psi_1^{(i)}$, and furthermore,

$$\tilde{E}_1^{(j)} = \langle \Psi_0 | H_1^{(j)} | \tilde{\Psi}_0^r \rangle / \langle \Psi_0 | \tilde{\Psi}_0^r \rangle.$$

When the eigenvalue \tilde{E}_0 and eigenvectors $\tilde{\Psi}_0^r$ and $\tilde{\Psi}_0^l$ are determined iteratively, one must solve for both $\tilde{\Psi}_0^r$ and $\tilde{\Psi}_0^l$ at each stage of the iteration, and this further increases the computer time required.

The second-order energy $E_2^{(1,6)}$ was calculated by this method, with some success. Since

$$\begin{aligned} H_1^{(6)}\Psi_0 &= \sum_{l,m,n=0}^{l+m+n \leq \omega} C_{lmn} H_1^{(6)} U_{lmn} \\ &= \alpha^2 \frac{1-P_{12}}{4\sqrt{2}} \delta^3(\vec{r}_2) \\ &\quad \times \sum_{l,m=0}^{l+m \leq \omega} C_{lm0} T_1^{(1)}(\vec{r}_1) r_1^{m+l} e^{-\kappa \sigma r_1/2}, \end{aligned}$$

we see that additional terms in $\Psi_1^{(6)}$ proportional to $T_1^{(1)}(\vec{r}_1)/r_2$ will produce $\delta^{(3)}(\vec{r}_2)$ when acted upon by H_0 . There will also be other, less singular terms produced which are undesirable but unavoidable. So the extended expansion used for $\Psi_1^{(6)}$ is

$$\Psi_1^{(6)} = \sum_{m=0}^{\omega} x_m^{(6)} U_{0m-1} + \sum_{l,m,n=0}^{l+m+n \leq \omega} X_{lmn}^{(6)} U_{lmn}. \quad (15)$$

The results for $E_2^{(1,6)}$ are given in Table IV. There is no result for $\omega=1$ because the iterative solution for \tilde{E}_0 , $\tilde{\Psi}_0^r$, and $\tilde{\Psi}_0^l$ did not converge for the six-dimensional matrix in this case. The difference

between calculated results were not regular enough to permit extrapolation; so we just guessed at the final value. For $\omega=8$, the calculated values for $E_2^{(1,6)}$ and $E_2^{(6,1)}$ were 0.272 78 and 0.272 90. For $\omega=2$ and 3, E_0 and \tilde{E}_0 agreed to three digits, for $\omega=4, 5$, and 6 to five digits, and for $\omega=7$ and 8 to six and seven digits, respectively.

Similar calculations were carried out for $E_2^{(1,2)}$, $E_2^{(1,3)}$, and $E_2^{(1,4)}$ using expansions (6) for $\Psi_1^{(1)}$ and (13) for $\Psi_1^{(i)}$ ($i=2,3,4$). The results were quite unsatisfactory. The numbers obtained agreed roughly with the corresponding results in Table IV of I, but roundoff errors increased rapidly with ω ; i. e., the agreement between the four different values for $E_2^{(1,i)}$ calculated according to (12) fell off sharply with increasing ω . Furthermore, the three sequences of (eight) numbers were no longer monotonic, as they were in I. The final extrapolated values of $E_2^{(1,2)}$, $E_2^{(1,3)}$, and $E_2^{(1,4)}$ obtained from these calculations would then have much larger uncertainties than the values given in Table V of I, even though they are consistent with the results of I.

It was assumed that these anomalies were caused by serious numerical roundoff errors, occurring when systems of linear algebraic equations are solved, which is done both when $\tilde{\Psi}_0^r$ and $\tilde{\Psi}_0^l$ are determined iteratively and when the $\Psi_1^{(i)}$'s are obtained. This suspicion was confirmed by an accidental discovery. The eigenvector program was used with two different FORTRAN compilers (FTN and RUN). The results produced after just one iteration, using E_0 from Table I of I as input, were radically different. For $\omega=8$, the first 20 elements of the eigenvectors produced by the RUN code agreed with those produced by the FTN code to no more than one digit, and the remaining 154 elements were totally uncorrelated. This was true for both $\tilde{\Psi}_0^r$ and $\tilde{\Psi}_0^l$. The two compilers generate different machine codes from the same FORTRAN program. Since the matrix \tilde{A} in (7) is "close" to being singular, even with one row and column deleted, different sequences of arithmetic operations might make a big difference. When solving linear equations we used Gaussian

TABLE IV. Second-order energy $E_2^{(1,6)}$ calculated with expansions (6) for $\Psi_1^{(1)}$ and (15) for $\Psi_1^{(6)}$.

ω	$E_2^{(1,6)}(\frac{1}{2}\alpha^2 R)\alpha^2$
2	0.234 99
3	0.258 032
4	0.268 858 5
5	0.270 082 967
6	0.272 51
7	0.272 80
8	0.272 8(1)
∞	0.272 8(2)

elimination with pivotal condensation.

From the results presented here it is evident that these roundoff errors are much less serious for symmetric matrices. We do not fully understand why the method worked fairly well for $E_2^{(1,6)}$ but failed for $E_2^{(1,2)}$, $E_2^{(1,3)}$, and $E_2^{(1,4)}$, except that the matrix used to calculate $E_2^{(1,6)}$ was "less close to being singular" than the one used to obtain $E_2^{(1,i)}$ ($i = 2, 3, 4$).

V. CONCLUSIONS

In the absence of further calculations, somewhat improved accuracy was obtained by extrapolating the sums $E_2^{(3,5)} + E_2^{(3,6)}$ and $E_2^{(1,7)} + E_2^{(2,7)}$, rather than the individual energies—as was done in Table V of I. The results, using the second-order energies of I, together with the improvements of this paper, are listed in Table V. We also tried to use formulas like I(38) for each value of ω and to extrapolate the fine-structure intervals $\Delta\nu_{01}$ and $\Delta\nu_{12}$, but this did not prove profitable. The results of Table V of this paper and of Table V of I were collected to give the total 3P contributions to the fine-structure intervals given in Ref. 3.

Since at present all the uncertainty in the theoretical values comes from the second-order sums, a major effort to increase the accuracy of these contributions is now an urgent project. In view of the difficulties associated with the methods of this paper, it appears that the easiest way to increase the accuracy is to use the straightforward method of I. The number of terms in the expansions for the $\Psi_1^{(i)}$'s will have to increase drastically, and the calculations must be done in double-precision arithmetic. Since the agreement between the theory and experiment³ already is quite impressive, the amount of computer time required for such a project is eminently justified. A new value for the fine-structure constant, good to one part per million, is within reach. This work is in progress.

TABLE V. Contributions of the improved results to the fine-structure intervals. $E_2^{(3,5)}$, $E_2^{(3,6)}$, $E_2^{(1,7)}$, and $E_2^{(2,7)}$ were taken from Table IV of I.

Second-order energy	Final value from Tables I-III	Contribution to $\Delta\nu_{01}$ in 10^{-4} cm $^{-1}$	Contribution to $\Delta\nu_{12}$ in 10^{-4} cm $^{-1}$
$E_2^{(1,1)}$	-0.6632(2)	-0.7738(2)	0
$E_2^{(2,2)}$	-1.143(5)	-1.333(6)	0
$E_2^{(2,3)}$	0.0817(2)	-1.589(4)	0.2542(6)
$E_2^{(3,3)}$	-0.006085(5)	-0.1775(1)	0.05680(5)
$E_2^{(1,6)}$	0.2728(2)	-0.8488(6)	-1.698(1)
$2(E_2^{(3,5)} + E_2^{(3,6)})$	0.0283(3)	0.660(7)	-0.264(3)
$2(E_2^{(1,7)} + E_2^{(2,7)})$	-0.1745(7)	0.694(3)	1.388(6)
Experimental values for separations	9879.121(12)	764.2606(17)	

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APPENDIX: DIVERGENT INTEGRALS

When the expansions (13) or (14) are used for $\Psi_1^{(2)}$, $\Psi_1^{(3)}$, or $\Psi_1^{(4)}$, one runs into integrals with $(r_1^2 - r_2^2)/r_{12}^4$ in the integrand when calculating the matrix elements of H_0 , $H_1^{(2)}$, $H_1^{(3)}$, and $H_1^{(4)}$. So a new type of integral $G(M, N; \alpha, \beta)$ must be introduced, defined by

$$\int \frac{dv_1}{4\pi} \int \frac{dv_2}{4\pi} \frac{r_1^2 - r_2^2}{r_{12}^4} r_1^{M-3} r_2^{N-3} e^{-ar_1} e^{-br_2} = -G(M, N; a, b) + G(N, M; b, a), \quad (\text{A1})$$

where

$$G(M, N; \alpha, \beta) = \int_0^\infty dr e^{-\alpha r} \int_0^\infty ds e^{-\beta s} s^{N-1} (s^2 - r^2)^{-1} = \frac{1}{2} \frac{(M+N-3)!}{\alpha^{M+N-2}} \int_0^1 \frac{du}{u} \frac{(1-u)^{M-1} (1+u)^{N-1}}{[1-u+\beta/\alpha(1+u)]^{M+N-2}}. \quad (\text{A2})$$

G integrals are only calculated for $M+N \geq 3$; they are logarithmically divergent at the lower limit ($r = s$ or $u = 0$). Writing

$$(1+u)^{N-1} = u(1+u)^{N-2} + (1+u)^{N-2},$$

we obtain after one partial integration

$$G(M, N; \alpha, \beta) = \frac{1}{2} \frac{(M+N-3)!}{\alpha^{M+N-2}} \int_0^1 \frac{dx}{1+x} \frac{x^{M-1}}{(x+\beta/\alpha)^{M+N-2}} + \text{div}(M, N) + \frac{1}{4} [- (M-1)F_L(M-1, N-1; \alpha, \beta) + (N-2)F_L(M, N-2; \alpha, \beta) - (\beta-\alpha)F_L(M, N-1)], \quad (\text{A3})$$

where the logarithmic F_L integrals are defined in Appendix A of I. The first integral is convergent and is evaluated by the numerical method of Schwartz,⁷ the F_L integrals are tabulated, and the divergence is contained in the surface term

$$\begin{aligned} \text{div}(M, N) &= -\frac{1}{2} \frac{(M+N-3)!}{\alpha^{M+N-2}} \\ &\times \lim_{u \rightarrow 0} \ln u \frac{(1-u)^{M-1} (1+u)^{N-2}}{[1-u+\beta/\alpha(1+u)]^{M+N-2}} \\ &= -\frac{1}{2} \frac{(M+N-3)!}{(\alpha+\beta)^{M+N-2}} \lim_{u \rightarrow 0} \ln u. \end{aligned}$$

Thus the logarithmic divergences will cancel between the two G integrals in (A1) if u goes to zero at the same rate in the divergent parts $\text{div}(M, N)$ of the two G integrals, i. e., if the principal value of the integral on the left-hand side in (A1) is taken at $r_1 = r_2$.

Looking at the expression for a typical matrix element,

$$\left\langle \frac{1-P_{12}}{4\pi\sqrt{2}} T_1^{(1)}(\vec{r}_1) u_{l'm'n'}(1, 2) \right| H \left| \frac{1-P_{12}}{4\pi\sqrt{2}} T_1^{(1)}(\vec{r}_1) u_{lmn}(1, 2) \right\rangle,$$

where H is H_0 or $H_1^{(i)}$, it is seen that the principal value should in fact be taken. Writing out this expression without commuting $1 - P_{12}$ through H , one gets two direct and two exchange parts. These occur under the same integral signs and are equal, except that r_1 and r_2 are interchanged. So, if we put $u = \epsilon_1$ in one of the G integrals in (A1) and $u = \epsilon_2$ in the other, we get a term proportional to $\ln(\epsilon_1/\epsilon_2)$ from the lower limit, but then from the other integrals with exchanged variables we get another term proportional to $\ln(\epsilon_2/\epsilon_1)$; so we are justified in taking the principal value.

Formula (A3) cannot be used for $N = 1$, but a similar formula, valid for $N = 1$ (but not for $M = 1$), can be obtained by using

$$(1-u)^{N-1} = -u(1-u)^{N-2} + (1-u)^{N-2}$$

in (A2) and doing the partial integration. The G integrals are only evaluated by these formulas along $M+N = \text{const}$; a backwards recursion formula [similar to I(A7)] is used for $M+N < \text{const}$. There is a formula similar to (A1) for the case where there is a factor $\cos\theta_{12}$ in the integrand on the left-hand side of (A1); this formula contains four G integrals and two A integrals (see Appendix A of I for the definition of A integrals). Again, the divergences cancel among the G integrals. In all cases where G integrals are required, the divergences cancel for the exchange and direct parts separately, except for the matrix element of $1/r_{12}$ in H_0 with functions with $1/r_{12}$ on both sides, when the divergences cancel between the direct and exchange integrals. If the functions $\Psi_1^{(i)}$ had been symmetric (singlet intermediate states), this cancellation would not have taken place.

To evaluate the matrix elements of $H_1^{(3)}$ and $H_1^{(4)}$ between standard terms and functions with $1/r_{12}$, we have to define yet another class of divergent

integrals

$$H(M, N; \alpha, \beta) = \int_0^\infty dr e^{-\alpha r} \int_0^\infty ds e^{-\beta s} s^{N-1} (s^2 - r^2)^{-2},$$

which are calculated along $M+N = \text{const}$, after which a backwards recursion formula is used. These integrals are evaluated by doing the same tricks as for the G integrals, but two partial integrations are required. The surface terms now give a pole-type singularity as well as a finite contribution. After some algebra, we find

$$H(M, N; \alpha, \beta) = -\frac{1}{2} \frac{(M+N-5)!}{\alpha^{M+N-4}} \times \left(\int_0^1 \frac{dx}{(1+x)^2} \frac{x^{M-2}}{(x+\beta/\alpha)^{M+N-4}} + \text{div}(M, N; \alpha, \beta) \right) + \left(\frac{1}{2}N-1\right)G(M-1, N-1; \alpha, \beta) - \frac{1}{2}\beta G(M-1, N; \alpha, \beta),$$

where the first integral is done numerically and the surface term is

$$\begin{aligned} \text{div}(M, N; \alpha, \beta) &= \frac{1}{4} \lim_{u \rightarrow 0} \frac{1}{u} \frac{(1-u)^{M-1} (1+u)^{N-1}}{[1-u+\beta/\alpha(1+u)]^{M+N-4}} \\ &= \frac{1}{4} \frac{1}{(1+\beta/\alpha)^{M+N-4}} \\ &\times \left(\lim_{u \rightarrow 0} \frac{1}{u} + N - M + \frac{\alpha - \beta}{\alpha + \beta} (M+N-4) \right). \quad (\text{A4}) \end{aligned}$$

By looking at the actual combination of integrals involved in the matrix elements, one finds that the logarithmic divergences included in the G integrals cancel separately for the direct and exchange integrals whenever H integrals are used, and that the pole divergences in (A4) cancel between exchange and direct parts. The finite part of (A4) is important and should of course be included. The H integrals are only evaluated for $M \geq 2$, $N \geq 2$, and $M+N \geq 5$.

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