have computed a value of -1.76098 a.u. for the relativistic energy, and Clementi[16] reports a value of -526.81705 a.u. for the HF energy. The total experimental energy of neutral argon is not known. Moore[14] gives only the first eight ionization potentials, the sum of those potentials being -21.204071 a.u. Sherr, Silverman, and Matsen[17] have calculated a value of -508.06909 a.u. for the total energy, nonrelativistic plus relativistic, of Ar^{8+}. Adding the theoretical results of Scherr *et al.*, to the experimental results from Moore, we obtain a value of -529.30980 a.u. as the total energy of neutral argon. Subtracting the relativistic energy[15] and the HF energy[16] from the total energy yields a value of -0.73 a.u. for the correlation energy of argon. Clementi[18] uses the correlation energy of neon as a basis to estimate the correlation energy of argon and reports a value of -0.692 a.u. We note, however, that in a later work, Clementi[19] reports an estimate of the correlation energy of argon as -0.79 a.u.

Several other properties of argon can be investigated using the basis set of single-particle states used in this calculation. Simons[8] has calculated the dipole polarizability of argon and the London dispersion forces between argon atoms. Further investigations are being carried out.

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Effect of Atomic Correlations on *KLL* Auger Transitions*

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Effect of correlation between the two participating electrons is investigated for *KLL* Auger transitions in the region $12 \leq Z \leq 21$ using a simple ansatz for the correlated two-electron wave function. For simplicity, the screened-hydrogenic model is used for these wave functions in the limit of no correlation. Our results for relative intensities are compared with the uncorrelated hydrogenic intensities and with the results of earlier hydrogenic calculations. An enhancement of these intensities is observed in the right direction.

I. INTRODUCTION

The object of this paper is to investigate the importance of correlation effects between the two participating electrons in a *KLL* Auger transition, particularly for low atomic numbers. It is well known that Auger line intensities are extremely sensitive to the detailed nature of the wave functions used. Ideally, the recent nonrelativistic calculations[1,2] with Hartree–Fock–Slater (HFS) wave functions should provide one with a logical basis for introducing the features associated with correlation into the problem. However, because of the relative simplicity of the screened-hydrogenic model, in this paper we shall try to consider the effects of correlation within the framework of this model by using a simple ansatz for this correlation. Our object in doing this is to try to see how far electronic correlation effects could contribute to the relative line intensities in the *KLL* series(i.e., ratio of the intensities of the individual lines to that of the KL_1L_1 line) for the region $12 \leq Z \leq 21$. The reason for choosing the low-Z region will be made clear in Sec. II. It is hoped that even a simple study of this kind may later on motivate further work on correlation effects based on a more realistic model.

While the scope of our discussion is necessarily restricted by the use of the hydrogenic model, we would like to point out here that even the more sophisticated and successful models often implicitly neglect details of the electronic repulsions.[3] For example, in a self-consistent-field (SCF) calculation, the wave function for each individual electron is determined by (i) the potential of the nucleus and (ii) the potential due to the probability density of the other electrons. On the whole, this allows electrons to come close together more often than is actually the case. Since the Auger process arises basically from the interaction between the two participating electrons, in addition to the fields (i) and (ii) above, the repulsive influence of each of these electrons on the other should play a crucial role in this process. In other words, one should try to construct a wave function here in which the interacting electrons avoid each other more strongly than in the usual SCF formulation. This is the approach we shall try to use in this paper on the much simpler hydrogenic model.

II. THEORY

A. Correlation Energy and Correlated Wave Function

As outlined above, details of the electronic repulsions should have an important bearing on this problem. The energy of this interaction should therefore enter into the over-all energetics of the system. Effectively, this gives rise to a correction in the total Hamiltonian of the system which is commonly called the correlation energy.[3] This correlation energy is quite appreciable for two electrons in the same spatial orbital, particularly so, if they have opposite spins. Incidentally, this is the case with the KL_1L_1 transition. Since the intensity of this line is used as the basis for computing relative intensities, we should like to note here the particular relevance of correlation effects in our discussion of the *KLL* transitions.

That the correlation term should be relatively more important in the lighter atoms is readily understood. The over-all averaging effect of the other "spectator" electrons may not be quite so smooth in these atoms as to give rise to a central field. Viewed against the background of this somewhat weak noncentral field, the two-electron interaction assumes the role of a substantial perturbation with a dependence on the interelectron distance $r_{12} = |\vec{r}_1 - \vec{r}_2|$.

In looking for a wave function ψ_C for such an interacting pair of electrons, we can start out by writing

$$\psi_C = \psi_A(\vec{r}_1, \vec{r}_2)\,\chi(r_{12}) , \tag{1}$$

where ψ_A is the antisymmetrized two-electron hydrogenic wave function and $\chi(r_{12})$ is the correlation function. In writing Eq. (1), we note that the atom subjected to an Auger transition has a nearly-closed-shell configuration which can be described in terms of a completely-closed-shell configuration together with the correlated two-electron configuration. Since the completely-closed-shell configuration may be treated for all practical purposes as a vacuum, ψ_C may be regarded as the wave function for the entire atom including the correlated-electron pair. We have in Eq. (1) what is usually called a correlated open shell, the detailed nature of ψ_A depending on the type of coupling used.

As for the correlation function $\chi(r_{12})$, we recall here the arguments made by Hartree and Ingman.[4] The idea is that $\chi(r_{12})$ should approach a constant value for $r_{12} \to \infty$, expressing the separability of the wave function when the electrons are far apart, and should decrease to a smaller value for $r_{12} \to 0$, keeping the electrons apart.

B. Ansatz

On the basis of these considerations, we have tried the following ansatz for the bound-state wave function:

$$\psi_C = \psi_A(nln'l';\; SLJM)\,(1 - \lambda e^{-\mu r_{12}}) , \tag{2}$$

where λ and μ are variational parameters, and $\psi_A(nln'l'; SLJM)$ is the specialized form of $\psi_A(\vec{r}_1, \vec{r}_2)$ corresponding to the *SLJM* representation (we have used in this paper an extreme *LS* coupling without configuration interaction). ψ_A in Eq. (2) may be generally characterized by two different principal quantum numbers n and n', however, since the two electrons participating in the *KLL* Auger process belong to the same major shell, we have here $n = n'$.

Since the purpose of this paper is to explore the validity and limitations of the above ansatz in describing the atomic configuration undergoing *KLL* transitions as a heliumlike systems, we start out by using the ground state of helium as a test for this model. In other words, we make a variational calculation of the ground-state energy of helium using the wave function ψ_C with the appropriate quantum numbers and obtain the best value of λ by minimizing the energy. It is seen that λ may be taken as unity.

For the second parameter μ, we choose $\mu = Z/na_0$, where a_0 is the first Bohr radius of hydrogen. [This choice is valid for *KLL* transitions where $n = n'$. In general we can write $\mu = (Z/2a_0)(1/n + 1/n')$.] This implies accepting a_0 as the unit of length. Obviously, ψ_C is very nearly equal to ψ_A for large Z so that correlation effects become inappreciable. For small Z, ψ_C is rather different from ψ_A. This is quite plausible, since for heavier atoms the Coulomb fields of the nucleus and the other electrons become quite strong, so that the perturbation caused by the mutual repulsion of the two participating electrons may be neglected. For lower Z values, this perturbation is more appreciable when compared to the combined effect of these Coulomb fields. It can also be seen that for larger values of n, where the participating electrons can only "see" a rather weak screened-Coulomb field, correlation effects between these electrons should be more appreciable than for small values of n.

For the final state of the system we do not assume any correlation between the two electrons, because they are now far apart and belong to states which are dynamically different in character, one being bound to the K shell and the other raised to the continuum. For the continuum electron we use a screened-Coulomb wave function normalized to a current of one electron per unit time per unit energy range.

C. Screening

It is well known that the result of such a calculation depends critically on the choice of an appropriate effective nuclear charge $Z_{\text{eff}} = Z - \sigma$, where σ is the screening constant. For the bound-state wave functions, we follow the Hartree prescription and put $\sigma = Z - (\langle r_H\rangle / \langle r\rangle)$. Here $\langle r_H\rangle$ is the mean hydrogenic radius and $\langle r\rangle$ is the mean Hartree-Fock radius. We use $\langle r\rangle$ as computed by Froese[5] for neutral atoms.

The choice of screening for a continuum state is more difficult. However, since the greatest contribution to the matrix element comes for values of r near the orbit from which the Auger electron is ejected, the choice $Z_{\text{eff}} = Z_b$ seems to be realistic,[6] where Z_b denotes the effective nuclear charge for the $2s$ or $2p$ subshells, as the case may be.

III. CALCULATION

For the lighter atoms, the electrostatic interaction dominates and we can realistically use the *LS* coupling to describe the initial and final two-hole states of the atom. (The second hole in the initial state belongs to the continuum.) In the *SLJM* representation, the antisymmetrized wave function ψ_A introduced in Eq. (2) is given by

$$\psi_A\,(nlnl';\ SLJM) = \frac{1}{\sqrt{2}} \sum_{M_L M_S} C^{SLJ}_{M_S M_L M}\left[\varphi\,(nlnl'LM_L) + (-1)^{l+l'-L+S}\varphi(nl'nlLM_L)\right]\chi\,(\tfrac{1}{2}\tfrac{1}{2}SM_S)\,, \tag{3}$$

where

$$\varphi(nlnl'LM_L) = \sum_{m_l m_{l'}} C^{ll'L}_{m_l m_{l'} M_L} Y^{m_l}_l(\theta_1, \varphi_1)\, Y^{m_{l'}}_{l'}(\theta_2, \varphi_2) \times R_{nl}(r_1) R_{nl'}(r_2) \tag{4}$$

and

$$\chi(\tfrac{1}{2}\tfrac{1}{2}SM_S) = \sum_{m_S m_{S'}} C^{(1/2)(1/2)S}_{m_S m_{S'} M_S}\, \chi_1(m_S)\, \chi_2(m_{S'})\,. \tag{5}$$

Here R and Y are the single-particle radial and angular functions, and χ_1 and χ_2 are the single-particle spin functions.

The total transition probability into all possible states of L and S for a given final configuration of the atom then is

$$W = \sum_{LS} \frac{(2S+1)(2L+1)}{2(2l''+1)} \sum_\nu \frac{1}{N_C^2} \left| \frac{1}{\hbar} \langle \psi_f | \frac{e^2}{r_{12}} | \psi_C \rangle \right|^2 . \tag{6}$$

Here ψ_f is the final-state wave function which may be written

$$\psi_f = \psi_A(n''l''\infty\nu;\ SLJM)\,. \tag{7}$$

N_C is the normalization factor given by

$$N_C^2 = \int \psi_C^\dagger \psi_C\, d\vec{r}_1 d\vec{r}_2\,. \tag{8}$$

In the above $n''l''$ are the quantum numbers characterizing the bound electron in the final state (for *KLL* transitions, $n'' = 1$, $l'' = 0$ and ν denotes the angular momentum of the ejected electron).

Specializing now to the *KLL* transitions, the total transition probability into states of all possible L and S for a final configuration of the atom is

$$W = \sum_{LS} \frac{(2S+1)(2L+1)}{2} \sum_\nu \times \left| \frac{1}{\hbar} \sum_p \left[d_p (D_p - D_p^c) \pm (-1)^{l+l'} e_p (E_p - E_p^c) \right] \right|^2 . \tag{9}$$

Here p is a discrete index denoting the multipolarity of the virtual photon, and its range is determined by the conservation of angular momentum. D_p is the direct radial integral corresponding to uncorrelated electronic orbitals and D_p^c the same for correlated electronic orbitals. Similarly, E_p and E_p^c represent the uncorrelated and correlated exchange integrals. (The plus sign goes with even $L+S$ and the minus sign with odd $L+S$.) The uncorrelated integrals D_p and E_p are exactly the ones used by Kostroun *et al.*[7] The correlated integrals are given in the Appendix. The angular factors d_p and e_p are as follows:

$$d_p=(-)^{l+l'+L}\langle l''\|C^p\|l\rangle\langle\nu\|C^p\|L'\rangle\begin{Bmatrix} l'' & \nu & L \\ l' & l & p \end{Bmatrix},$$

$$e_p=(-)^{\nu+l'+L}\langle l''\|C^p\|l'\rangle\langle\nu\|C^p\|l\rangle\begin{Bmatrix} l'' & \nu & L \\ l & l' & p \end{Bmatrix}. \tag{10}$$

Here $\langle l\|C^p\|l'\rangle$ is the reduced matrix element of the spherical harmonic, multiplied by $4\pi/(2p+1)^{1/2}$ and

$$\begin{Bmatrix} l_1 & l_2 & L \\ l_3 & l_4 & S \end{Bmatrix}$$

is the 6-j symbol.

In obtaining Eq. (9) from Eq. (6), we have used in ψ_C the approximate expansion

$$r_{12}=r_> - r_< \cos\theta_{12} , \tag{11}$$

where θ_{12} is the angle between $r_>$ and $r_<$, the latter denoting the greater and smaller of the two quantities r_1 and r_2, respectively. The neglect of higher terms in this expansion may be justified by remembering that the initial wave function is very small for small values of r_{12}. Most of the contribution to the matrix element from this wave function is therefore made in the region of large r_{12}.

IV. RESULTS AND DISCUSSION

Transition rates for the lines ${}^1S_0(KL_1L_1)$, ${}^1S_0(KL_2L_2)$, ${}^1D_2(KL_2L_3)$, ${}^1P_1(KL_1L_{2,3})$, and the triplet ${}^3P_{0,1,2}(KL_1L_{2,3})$ obtained by using the correlated two electron wave functions are given in Table I. The corresponding rates in the limit of no correlation ($\lambda=0$) are also displayed in the table. The only experimental results for transition rates available in this region are those of Cleff and Mehlhorn[8] for Cl ($Z=17$).

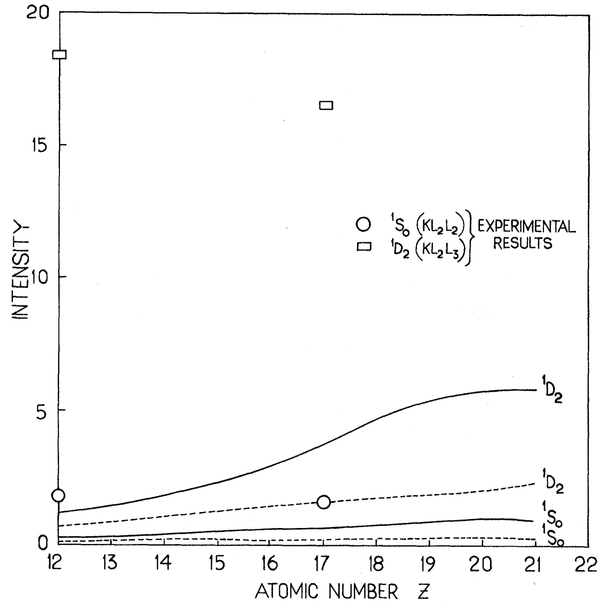

FIG. 1. Intensities of ${}^1D_2(KL_2L_3)$ lines relative to the line ${}^1S_0(KL_1L_1)$ for $12\leq Z\leq 21$ are shown as a function of atomic number Z. We have included the only available experimental values for ${}_{12}$Mg of Fahlman *et al.* (Ref. 9) and those for ${}_{17}$Cl of Mehlhorn *et al.* (Ref. 8). The solid lines represents the correlated result and the broken lines the uncorrelated ones. The same notation applies to Fig. 2.

Figure 1 shows calculated intensities of the lines ${}^1S_0(KL_2L_2)$ and ${}^1D_2(KL_2L_3)$ relative to the line ${}^1S_0(KL_1L_1)$; Fig. 2 shows the same for the lines ${}^1P_1(KL_1L_{2,3})$ and ${}^3P_J(KL_1L_{2,3})$. In these figures we have also included the experimental values of relative intensities given by Fahlman *et al.*[9] for $Z=12$ in addition to those for Cl ($Z=17$). Our uncorrelated results (which is a pure hydro-

TABLE I. K-auger transition probabilities (in multiples of 10^{-3} a.u.) for $2s^0\,2p^6$, $2s\,2p^5$, and $2s^2\,2p^4$ final configuration of the atom.

	Uncorrelated transition rates					Values of the transition rates taking correlation into account				
Z	${}^1S_0$ (KL_1L_1)	${}^1S_0$ (KL_2L_2)	${}^1P_1$ $(KL_1L_{2,3})$	${}^3P_J$ $(KL_1L_{2,3})$	${}^1D_2$ (KL_2L_3)	${}^1S_0$ (KL_1L_1)	${}^1S_0$ (KL_2L_2)	${}^1P_1$ $(KL_1L_{2,3})$	${}^3P_J$ $(KL_1L_{2,3})$	${}^1D_2$ (KL_2L_3)
12	2.442	0.125	2.774	0.888	1.668	1.187	0.139	2.149	1.070	1.320
13	2.492	0.169	3.166	0.971	2.213	1.180	0.192	2.297	1.196	1.760
14	2.525	0.210	3.493	1.023	2.758	1.133	0.247	2.477	1.286	1.916
15	2.560	0.250	3.786	1.082	3.272	1.120	0.370	2.582	1.415	2.644
16	2.583	0.290	4.031	1.117	3.720	1.105	0.457	3.104	1.578	2.967
17	2.600	0.328	4.264	1.163	4.249	1.075	0.552	3.669	1.763	3.183
17[a]						0.64 ± 01	1.1 ± 0.3	3.0 ± 0.3	1.4 ± 0.2	10.6 ± 1.2
18	2.609	0.368	4.471	1.197	4.734	1.050	0.602	4.084	1.937	4.973
19	2.614	0.402	4.633	1.213	5.165	1.009	0.818	4.890	2.199	5.724
20	2.619	0.434	4.785	1.239	5.552	0.983	0.931	5.366	2.382	5.790
21	2.620	0.460	4.912	1.248	5.887	0.956	0.944	5.683	2.634	5.948

[a] The experimental results of Mehlhorn *et al.* (Ref. 8).

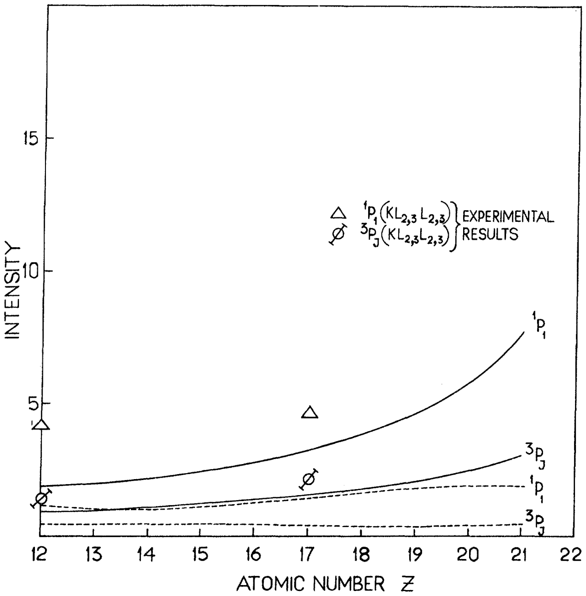

FIG. 2. Intensities of $^1P_1(KL_1L_{2,3})$ and $^3P_J(KL_1L_{2,3})$ relative to $^1S_0(KL_1L_2)$ are shown as a function of atomic number Z. We have included the only available experimental values for $_{12}$Mg of Fahlman *et al.* (Ref. 9) and those for $_{17}$Cl of Mehlhorn *et al.* (Ref. 8).

genic case) agree closely with those of Asaad[10] or of Callan.[11] In fact the two sets of numbers are not discernible on a graphical plot. So in our figures we have not included the transition rates of Callan or of Asaad. It may be noted here that Asaad's intermediate-coupling calculations are actually based on LS-coupling transition amplitudes computed by Callan using a screened-hydrogenic model. In the low-Z region under consideration Asaad's results come quite close to the LS-coupling values.

Our hydrogenic values do not agree with those obtained recently by Kostroun, Chen and Crasemann,[7] because they have used a different type of screening for the continuum electron. Interestingly, looking at the correlated transition rates for the $^1S_0(KL_1L_1)$ line we can see that its intensity decreases as we go to the heavier atoms. This is also the trend exhibited by the corresponding rates of Kostroun *et al.*, although the numbers are different. Actually, our relative intensities are better than the ones which can be obtained from their values of transition rates.

From existing experimental data in the low-Z region it can be seen that the line $^1S_0(KL_1L_1)$ is about the weakest. Although in our correlated calculation this is not the weakest line, Table I shows that it is consistently weaker than in the uncorrelated hydrogenic case. The effect, of course. is to enhance the relative intensities of the other lines, which is a change in the right direction so far as experimental trends are concerned.

While the relative intensities obtained in our correlated calculation exhibit an enhancement in the right direction, their general behavior with increasing Z is quite similar to that of the uncorrelated intensities. In Fig. 1, relative intensities of the $^1S_0(KL_2L_2)$ and $^1D_2(KL_2L_3)$ lines increase with Z, but the rate of increase appears to level off near $Z=21$. This is understandable, because this is the region where the lines $^3P_0(KL_3L_3)$ and $^3P_2(KL_3L_3)$ belonging to the same configuration $(2s)^2(2p)^4$ begin to build up at the expense of $^1S_0(KL_2L_2)$ and $^1D_2(KL_2L_3)$.

On the other hand, Fig. 2 indicates that the lines $^1P_1(KL_1L_{2,3})$ and $^3P_J(KL_1L_{2,3})$ belonging to the configuration $(2s)(2p)^5$ keep growing in intensity even at $Z=21$. This is in contrast to the uncorrelated case, where the rate of growth of these lines is considerably slower, the group ^3P_J showing an almost stationary intensity.

It can be seen that no definitive calculation in accord with experiments has yet been worked out. Quite possibly, choice of continuum wave functions with appropriate screening[7] may be one of the factors having to do with the discrepancies which persist. However, as conjectured by Callan *et al.*,[12] the simple e^2/r_{12} interaction given originally by Wentzel for the Auger effect may not hold very nicely in the low-Z region. In particular for small interelectronic distance r_{12}, the Hartree–Fock radial integral overshoots its final steady value. This seems to indicate that the kind of cutoff built into our model for small r_{12} is a venture in the right direction. That this "correlation" has been tagged onto an otherwise simple hydrogenic system serves to keep the field of vision clear for judging the relative importance of the different elements of the calculation. For example, introduction of intermediate coupling and configuration interaction would be the next logical step enabling us to see how crucial this correlation is when compared to these other features. How one could go about introducing correlations into a full-grown Hartree–Fock system should be an interesting question.

APPENDIX: RADIAL INTEGRALS

The correlated direct radial integral D_p^C introduced in Eq. (9) is given by

$$D_p^c=\alpha_{n''l''}\,\alpha_{n'l'}\,\alpha_{nl}\sum_{S''=0}^{n''-l''-1}\;\sum_{S'=0}^{n'-l'-1}\;\sum_{S=0}^{n-l-1}\beta_{n''l''S''}\beta_{n'l'S'}\beta_{nlS}\left(\frac{(l''+S''+l+S+2+p)!}{[\frac{1}{2}(C_1+C_2)]^{l''+S''+l+S+3+p}}\;Q^c(l',S',\nu)\right.$$

$$-(l''+S''+l+S+2+p)!\sum_{j=1}^{l''+S''+l+S+3+p}\frac{Q_j^c}{[\frac{1}{2}(C_1+C_2)]^j(l''+S''+l+S+3+p-j)!}$$

$$+(l''+S''+l+S+1-p)!\sum_{j=1}^{l''+S''+l+S+2-p}\frac{Q_j^c}{[\frac{1}{2}(C_1+C_2)+\mu/k]^j(l''+S''+l+S+2-p-j)!}\Bigg), \qquad \text{(A1)}$$

$$Q^c(l',S',\nu)=G(\nu,\eta)\frac{(l'+S'+\nu+1-p)!}{[\frac{1}{2}C_3+\mu/k+i]^{l'+S'+\nu+2-p}}\;{}_2F_1\left(\begin{matrix}\nu+1+i\eta\\ l'+S'+\nu+2-p\end{matrix}, 2\nu+2;\frac{2i}{\frac{1}{2}C_3+\mu/k+i}\right), \qquad \text{(A2)}$$

and

$$Q_j^c=G(\nu,\eta)\frac{(l''+S''+l'+S'+l+S+\nu+4-j)!}{[\frac{1}{2}(C_1+C_2+C_3)+\mu/k+i]^{l''+S''+l'+S'+l+S+\nu+5-j}}$$

$$\times{}_2F_1\left(\begin{matrix}\nu+1+i\eta\\ l''+S''+l'+S'+l+S+\nu+5-j\end{matrix}, 2\nu+2;\frac{2i}{\frac{1}{2}(C_1+C_2+C_3+\mu/k+i}\right). \qquad \text{(A3)}$$

where $G(\nu,\eta)$, C_1, C_2, C_3, etc., are exactly as in Ref. 7. Similarly one can write down the expressions for E_p and E_p^c where the role of C_2 and C_3 are interchanged. [For the exchange integrals, $Q^c(l', S', \nu)\rightarrow Q^c(l, S, \nu)$. Q_j and Q_j^c are obviously symmetric under this mapping.] The Sommerfeld parameter η is also correspondingly modified.

All expressions are given in atomic units. The ordinary hypergeometric functions with complex arguments ${}_2F_1$ which occur in the radial integrals can be computed by the matrix method of Callan *et al.*[13]

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