Negative-energy contributions to transition amplitudes in heliumlike ions

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We derive the leading term in an αZ expansion for the negative-energy (virtual electron-positron pair) contributions to the transition amplitudes of heliumlike ions. The resulting expressions allow us to perform a general analysis of the negative-energy contributions to electric- and magnetic-multipole transition amplitudes. We observe a strong dependence on the choice of the zeroth-order Hamiltonian, which defines the negative-energy spectrum. We show that for transitions between states with different values of total spin, the negative-energy contributions calculated in a Coulomb basis vanish in the leading order while they remain finite in a Hartree basis. The ratio of negative-energy contributions to the total transition amplitudes for some of nonrelativistically forbidden transitions is shown to be of order $1/Z$. In the particular case of the magnetic-dipole transition $3\,^3S_1 \rightarrow 2\,^3S_1$, we demonstrate that the neglect of negative-energy contributions, in an otherwise exact no-pair calculation, would lead one to underestimate the decay rate in helium by a factor of 1.5 in calculations using a Hartree basis and by a factor of 2.9 using a Coulomb basis. Finally, we tabulate revised values of the line strength S for the magnetic-quadrupole (M_2) transition $2\,^3P_2 \rightarrow 1\,^1S_0$. These values include negative-energy contributions from higher partial waves, which were neglected in our previous calculations. [S1050-2947(98)03512-4]

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I. INTRODUCTION

The *ab initio* relativistic consideration of an atomic system requires a careful treatment of negative-energy states (virtual electron-positron pairs), which, if included improperly, lead to the *continuum dissolution* problem discussed by Sucher [1]. An accepted remedy for this problem is to use the *no-pair* Hamiltonian, which excludes negative-energy states [1,2]. The no-pair approach is well justified for determining energies of many-body systems. The leading corrections beyond the no-pair approximation have been studied for the ground state of heliumlike ions in Ref. [3]. However, the effect of negative-energy states on the transition amplitudes still remains an open question. If such corrections were a negligibly small fraction of the total amplitude, the study would be mainly of ''academic'' interest. However, as we demonstrate in this work, the relative contribution for some nonrelativistically forbidden transitions is of order $1/Z$ and thus the practical importance of understanding when to include negative-energy contributions cannot be overstated. To allow general consideration we will derive the leading term in the αZ expansion of the negative-energy contribution to the transition amplitudes in heliumlike ions.

The separation of negative- and positive-energy states depends on the choice of the zeroth-order Hamiltonian. In practical calculations one often employs the Dirac-Coulomb Hamiltonian modified by a model potential, chosen to approximate the interaction between electrons. The question of negative-energy contributions to the magnetic-dipole transition $2\,^3S_1 \rightarrow 1\,^1S_0$ was considered numerically by Lindroth and Salomonson [4] for heliumlike argon and by Indelicato [5] in systematic multiconfigurational Hartree-Fock (MCHF) calculations. Employing a Dirac-Coulomb basis set, the former work demonstrated numerically that the negative-energy contribution vanishes. By contrast, Indelicato's MCHF calculations revealed contributions from negative-energy states that were comparable to the ''regular'' positive-energy values, especially for light ions. We will address this difference by deriving negative-energy corrections both for the Dirac-Coulomb basis and for a basis modified by a spherically symmetric model potential.

The transition amplitudes, although calculated by employing exact eigenfunctions of the no-pair Hamiltonian, depend on the gauge of the electromagnetic field, as noted in Ref. [6]. This gauge dependence is reflected in slight differences between the length-form and velocity-form transition amplitudes. In Ref. [7] it was demonstrated that the gauge dependence is a direct consequence of the omission of contributions from negative-energy states in the no-pair Hamiltonian. In that work the configuration-interaction (CI) method was used to determine the contribution to transition amplitudes from positive-energy states and perturbation theory was used to obtain the contribution from the negative-energy states. Based on numerical analysis, the authors of Ref. [7] noted that the negative-energy contributions were negligible for length-form transition amplitudes compared to those calculated in the velocity form. They recommended using the length-form no-pair amplitudes in calculations of the electric-dipole transition amplitudes. We extend this recommendation to all electric-multipole transitions.

For magnetic-multipole transition amplitudes, we find that when calculated in a Dirac-Coulomb basis, the leading term vanishes for transitions between states with different values of total spin due to the cancellation between Coulomb and Breit contributions. Since all magnetic-multipole transitions to the ground state of heliumlike ions ($1\,^1S_0$) involve the

upper state with total spin $S=1$, we make a general assertion that, for such M_J transitions, the leading contribution due to negative-energy states vanishes. This fact allows us to correct the numerical results of Ref. [7] for the magnetic-quadrupole (M_2) transition $2\,^3P_2 \to 1\,^1S_0$. We tabulate revised values of the line strength S for this transition. The negative-energy corrections are of particular importance in the case of nonrelativistically forbidden magnetic-dipole transitions. We consider the transition $3\,^3S_1 \to 2\,^3S_1$ using both Dirac-Coulomb and Hartree basis sets. We find the ratio of negative- to positive-energy contributions to be of order $1/Z$ in both calculations. Furthermore, we find that for this transition the neglect of contributions from the negative-energy states would underestimate the decay rate by a factor of 1.54 for helium in the Hartree case and by a factor of 2.91 in the Coulomb case.

We also demonstrate that modification of the zeroth-order Hamiltonian by a model potential introduces an additional correction that gives rise to the leading order for magnetic-multipole transitions between states with different total spin. Thus, even for the well-studied magnetic-dipole transition $2\,^3S_1 \to 1\,^1S_0$, the ratio of negative- to positive-energy state contributions is shown to scale as $1/Z$.

We derive the analytical expressions in Sec. II. The discussion of negative-energy contributions to electric-multipole transitions is given in Sec. III and to magnetic-multipole transitions in Sec. IV. Predictions based on analytical results are illustrated by direct summation over negative-energy states in second-order many-body perturbation theory. The numerical methods employed are discussed in Sec. V. Conclusions are given in Sec. VI.

II. THEORY

We perform a perturbation theoretic analysis of transition amplitudes similar to that given in Ref. [7]. The summation over negative-energy states appears for the first time in the second-order expression. Here we briefly recapitulate the derivation of the second-order perturbation expression for transition amplitudes. The many-electron Hamiltonian H is represented as a sum of a zeroth-order Hamiltonian $\mathcal{H}_0$ and a perturbation $\mathcal{V}$,

$$\mathcal{H}_0 = \sum_i h_0(i) = \sum_i [h^D(i) + U(i)], \tag{2.1}$$

$$\mathcal{V} = \sum_{i<j} V(i,j) - \sum_i U(i), \tag{2.2}$$

where h^D is the Dirac Hamiltonian of an electron in the Coulomb potential of a nucleus, U is a model potential, and the two-electron interaction $V(i,j)$ is a sum of Coulomb and Breit interactions. The eigenfunctions of h_0 serve as a basis for perturbation theory. They include both negative- and positive-energy states. The inclusion of the model potential U in the zeroth-order Hamiltonian can improve the convergence of perturbation theory if the model potential approximates the Coulomb interaction between atomic electrons. For heliumlike systems, we will consider both the Coulomb case, where the model potential U is set to zero, and the Hartree case, with the self-consistent Hartree potential of the ground state $v_0(1s,r)$. In the no-pair approach the perturbation $\mathcal{V}$ is surrounded by positive-energy projection operators, thus eliminating contributions from negative-energy states completely to all orders of perturbation theory. However, even the process of separation of positive- and negative-energy states depends on the choice of model potential U and would be acceptable if the final result were modified only slightly. In contrast, we will demonstrate that the contribution of negative-energy states to transition amplitudes depends sensitively on the choice of the model potential, especially for nonrelativistically forbidden transitions.

In the zeroth-order approximation, the uncoupled states are antisymmetrized combinations of products of eigenfunctions of the Hamiltonian h_0. In the second-quantized form, the initial state is represented as $\Psi^{(0)}_{va} = a^\dagger_v a^\dagger_a |0\rangle$ and the final state as $\Psi^{(0)}_{wb} = a^\dagger_w a^\dagger_b |0\rangle$. Orbital labels a and b refer to the $1s$ state and w and v to excited states. The possibility of v being a $1s$ electron is also allowed in the following. We treat the interaction $\mathcal{V}$ as a perturbation and obtain the first-order correction to wave functions. For example, the correction to the initial state is

$$\Psi^{(1)}_{va} = -\sum_{ij\neq va} \frac{v_{ijva}}{\varepsilon_i+\varepsilon_j-\varepsilon_v-\varepsilon_a} a^\dagger_i a^\dagger_j |0\rangle + \sum_{i\neq v} \frac{U_{iv}}{\varepsilon_i-\varepsilon_v} a^\dagger_i a^\dagger_a |0\rangle + \sum_{i\neq a} \frac{U_{ia}}{\varepsilon_i-\varepsilon_a} a^\dagger_v a^\dagger_i |0\rangle. \tag{2.3}$$

Here the summation is performed over eigenstates of h_0 with energies ε_i and v_{ijkl} are matrix elements of the two-particle interaction $V(i,j)$ in that basis.

We consider a matrix element of a one-body operator $H^I = \Sigma_i h^I(i)$ between two states of a heliumlike ion. With the aid of the first-order correction to wave functions, we form the expression for the second-order matrix element

$$T^{(2)} = \langle \Psi^{(1)}_{wb} | H^I | \Psi^{(0)}_{va} \rangle + \langle \Psi^{(0)}_{wb} | H^I | \Psi^{(1)}_{va} \rangle \tag{2.4}$$

and obtain

$$\begin{aligned} T^{(2)} = & \sum_{ia\neq wb} \frac{v_{wbia}(h^I)_{iv} - v_{wbai}(h^I)_{iv}}{\varepsilon_w-\varepsilon_i} \\ & - \sum_{iv\neq wb} \frac{v_{wbvi}(h^I)_{ia} - v_{wbiv}(h^I)_{ia}}{\varepsilon_i+\varepsilon_v-\varepsilon_w-\varepsilon_b} \\ & + \sum_{ib\neq va} \frac{(h^I)_{wi}v_{ibva} - (h^I)_{wi}v_{biva}}{\varepsilon_v-\varepsilon_i} \\ & - \sum_i \frac{(h^I)_{bi}v_{wiva} - (h^I)_{bi}v_{iwva}}{\varepsilon_i+\varepsilon_w-\varepsilon_v-\varepsilon_a} \\ & + \sum_{i\neq w} \frac{U_{wi}(h_I)_{iv}\delta_{ab} - U_{wi}(h_I)_{ia}\delta_{bv}}{\varepsilon_i-\varepsilon_w} \\ & + \sum_{i\neq v} \frac{(h_I)_{wi}U_{iv}\delta_{ab}}{\varepsilon_i-\varepsilon_v} - \sum_{i\neq a} \frac{(h_I)_{wi}U_{ia}\delta_{bv}}{\varepsilon_i-\varepsilon_a}. \end{aligned} \tag{2.5}$$

The summation over intermediate states i includes both negative- and positive-energy states. It is our aim to estimate the leading term in the αZ expansion due to summation over the negative-energy states. In the second-order expressions

above we have omitted the derivative term given in Ref. [7] since it does not affect the negative-energy state contribution. When considering transition between states represented in the lowest order by a combination of product wave functions, e.g., the $2\,^3P_1$ state, the above expressions should be generalized. Such gauge-independent multiconfigurational generalization for Be-like systems can be found in Ref. [8].

A. Summation over negative-energy states

We approximate the differences between positive and negative energies in the denominators of Eq. (2.5) by $2mc^2$. In this paper we will use atomic units ($m_e=\hbar=e/\sqrt{4\pi\epsilon_0}=1, c=1/\alpha$). The Pauli approximation for a positron wave function becomes

$$\phi^-=\begin{pmatrix} -\frac{1}{2}\frac{\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}}{c} \\ 1 \end{pmatrix}\varphi^-. \tag{2.6}$$

Nonrelativistic positron wave functions φ^- form a complete basis set and thus satisfy the closure relation

$$\sum_i \varphi_i^-(r,s)[\varphi_i^-(r',s')]^\dagger=\delta(r-r')\,\delta_{s,s'}, \tag{2.7}$$

where s is a spin variable. This relation allows us to express a summation over negative-energy states of electrons in the Pauli approximation as

$$\sum_{\epsilon_i<0}\phi_i(r,s)[\phi_i(r',s')]^\dagger=\Lambda(r,s)\,\delta(r-r')\,\delta_{s,s'}. \tag{2.8}$$

Here the matrix operator Λ is defined as

$$\Lambda(r,s)=\begin{pmatrix} \frac{1}{4}\frac{\hat{p}^2}{c^2} & -\frac{1}{2}\frac{\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}}{c} \\ -\frac{1}{2}\frac{\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}}}{c} & 1 \end{pmatrix}. \tag{2.9}$$

The operator Λ, when acted upon a wave function, decreases the size of the large component by an order of $(\alpha Z)^2$, making the large and small components of the result comparable. Employing the modified closure relation (2.8), we find that the entire contribution from negative-energy states to the second-order matrix element (2.5) is

$$T_-^{(2)}=\frac{1}{2c^2}(W_{wbva}+W_{bwav}-W_{wbav}-W_{bwva}), \tag{2.10}$$

where the operator W is

$$W=V(1,2)\Lambda(1)h^I(1)+h^I(1)\Lambda(1)V(1,2) -U(1)\Lambda(1)h^I(1)-h^I(1)\Lambda(1)U(1). \tag{2.11}$$

Here and below the arguments 1 and 2 stand for coordinate and spin variables of electrons 1 and 2, respectively. The operator W can be represented in a form symmetric with respect to interchange of electrons 1 and 2; however, we find the representations (2.10) and (2.11) more convenient. At this point, we have performed a summation over negative-energy states for an arbitrary one-body operator H^I. Now we turn to the calculation of the correction from negative-energy states to transition amplitudes.

B. Negative-energy corrections to transition amplitudes

For a single electron, the interaction Hamiltonian with an electromagnetic field described by the vector potential $\boldsymbol{A}$ and scalar potential Φ is given by

$$h^I=-\Phi+c\,\boldsymbol{\alpha}\cdot\boldsymbol{A}. \tag{2.12}$$

The two-electron interaction V is a sum of Coulomb C and Breit B interactions

$$C_{12}=\frac{1}{r_{12}}, \tag{2.13}$$

$$B_{12}=-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2\frac{1}{r_{12}}-\frac{1}{2}(\boldsymbol{\alpha}_1\cdot\nabla_1)(\boldsymbol{\alpha}_2\cdot\nabla_2)r_{12}. \tag{2.14}$$

We employ the Pauli approximation in calculations of matrix elements of the operator W, where this approximation for the electron wave function is given by

$$\phi=\begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}}{2c} \end{pmatrix}\varphi, \tag{2.15}$$

φ being the nonrelativistic wave function of the electron. Below we give a breakdown of contributions to the operator W arising from various combinations of interactions

$$W=W^{C\Phi}+W^{B\Phi}+W^{U\Phi}+W^{CA}+W^{BA}+W^{UA}. \tag{2.16}$$

The derivation of these contributions is based on commutator identities for Pauli matrices $\boldsymbol{\sigma}$. $W^{C\Phi}$ is a contribution arising from Coulomb interaction and scalar potential

$$W^{C\Phi}=-\frac{\alpha^2}{2}\nabla_1\Phi(1)\cdot\nabla_1\frac{1}{r_{12}}. \tag{2.17}$$

There is a similar contribution from the model potential $W^{U\Phi}$,

$$W^{U\Phi}=\frac{\alpha^2}{2}\nabla_1\Phi(1)\cdot\nabla_1U(1). \tag{2.18}$$

These terms contribute to $T_-^{(2)}$ corrections of order $\alpha(\alpha Z)^3\langle\Phi\rangle$, where $\langle\Phi\rangle$ designates scaling of the scalar potential Φ. The contribution from the Breit interaction and scalar potential $W^{B\Phi}$ is $(\alpha Z)^2$ smaller than $W^{C\Phi}$ and does not contribute to the leading order. The situation is different for the vector potential part of the interaction Hamiltonian: The contribution from the vector potential and Coulomb interaction W^{CA} is of the same order as the contribution from the vector potential and Breit interaction W^{BA}. We have

$$W^{CA}=-\boldsymbol{\sigma}_1\cdot\left[\boldsymbol{A}(1)\times\nabla_1\frac{1}{r_{12}}\right], \tag{2.19}$$

$$W^{BA}=-\boldsymbol{\sigma}_2\cdot\left[\boldsymbol{A}(1)\times\nabla_1\frac{1}{r_{12}}\right]-\frac{1}{r_{12}}\boldsymbol{A}(1)\cdot\hat{\boldsymbol{p}}_2 - \frac{1}{r_{12}}\boldsymbol{n}_{12}\cdot\boldsymbol{A}(1)\boldsymbol{n}_{12}\cdot\hat{\boldsymbol{p}}_2, \tag{2.20}$$

where $\boldsymbol{n}_{12}$ is the unit vector along $\boldsymbol{r}_{12}=\boldsymbol{r}_1-\boldsymbol{r}_2$. Finally, the model potential combined with the vector potential term results in an effective operator

$$W^{UA}=\boldsymbol{\sigma}_1\cdot[\boldsymbol{A}(1)\times\nabla_1 U(1)]. \tag{2.21}$$

The contribution to $T_-^{(2)}$ due to the vector potential scales as $\alpha(\alpha Z)\langle c\boldsymbol{\alpha}\cdot\boldsymbol{A}\rangle$, where we explicitly separated scaling of $c\boldsymbol{\alpha}\cdot\boldsymbol{A}$.

For further discussion, it is important to note that in the absence of a model potential the entire negative-energy contribution vanishes for transitions between states with different values of total spin S. Indeed, combining Coulomb and Breit contributions for the vector potential and expressing the sum in terms of the total spin $\boldsymbol{S}$, we obtain $W^{(C+B)A}=W^{CA}+W^{BA}$,

$$W^{(C+B)A}=-2\boldsymbol{S}\cdot\left[\boldsymbol{A}(1)\times\nabla_1\frac{1}{r_{12}}\right]-\frac{1}{r_{12}}\boldsymbol{A}(1)\cdot\hat{\boldsymbol{p}}_2 - \frac{1}{r_{12}}\boldsymbol{n}_{12}\cdot\boldsymbol{A}(1)\boldsymbol{n}_{12}\cdot\hat{\boldsymbol{p}}_2. \tag{2.22}$$

The last two terms in the above expression do not depend on spin and vanish for transitions between states with $\Delta S\neq 0$. The first term is proportional to the total spin $\boldsymbol{S}$ and also vanishes for such transitions since the reduced matrix element $\langle S_1||\boldsymbol{S}||S_2\rangle\propto\delta_{S_1S_2}$. Thus the leading negative-energy contribution vanishes for transitions between states with different values of the total spin when calculations are performed in a Coulomb basis. The model potential term W^{UA}, however, does not possess this property and results in significantly different contributions to amplitudes for transitions with $\Delta S\neq 0$, as discussed in the following sections. The analysis of the above expressions allows us to make general qualitative predictions about the role of negative-energy states in calculations of transition amplitudes. We performed angular reductions of the negative-energy contributions and the resulting expressions can be found in the Appendix. Alternatively, the direct numerical summation in second-order expressions (2.5) over the negative-energy part of basis set of h_0 can be done to obtain the results for model potential case and to evaluate the higher-order corrections.

III. ELECTRIC-MULTIPOLE TRANSITIONS

For practical purposes we consider the multipole expansion of the electromagnetic field, discussed, for example, in Ref. [9], and find the matrix elements of the operator

$$Q_{JM}^{(\lambda)}=\sum_{i,j}(q_{JM}^{(\lambda)})_{ij}a_i^\dagger a_j,$$

with

TABLE I. Scaling of the ratio of negative- to positive-energy states contributions for electric-multipole E_J transition amplitudes in heliumlike ions.

Gauge	Basis	$\Delta S=0$	$\Delta S\neq 0$
length	Coulomb	α^4Z^3	α^4Z^3
velocity	Coulomb	α^2Z	α^2Z
length	model potential	α^4Z^3	α^4Z^3
velocity	model potential	α^2Z	$1/Z$

$$(q_{JM}^{(\lambda)})_{ij}=i\sqrt{\frac{4\pi J}{(2J+1)(J+1)}}\frac{(2J+1)!!}{k^J}\frac{1}{c} \times\{\Phi_{JM}^{(\lambda)}(\boldsymbol{r},\omega)-c\boldsymbol{\alpha}\cdot\boldsymbol{A}_{JM}^{(\lambda)}(\boldsymbol{r},\omega)\}_{ij}. \tag{3.1}$$

Here J is the multipolarity, with $\lambda=1$ for electric and $\lambda=0$ for magnetic transitions. The particular form of electromagnetic multipole potentials depends on the choice of gauge and we refer the reader to Ref. [7] for explicit expressions. We will consider two forms of electromagnetic potentials: length and velocity (transverse) forms. In the velocity form the electric scalar potential is identically zero. In the length form the above expressions reproduce the electric J-pole moment operator ($\lambda=1$) in the long-wavelength approximation ($kr\ll 1$). The transition amplitude must remain invariant under gauge transformation. However, the calculations performed in the no-pair approach lack this important property because of omission of negative-energy states, as has been demonstrated in Ref. [7]. In this section we determine the effect of negative-energy states on calculations of the reduced matrix elements of $Q_J^{(1)}$ for electric-multipole E_J transitions.

The scaling of the ratio of negative- to positive-energy contributions for electric-multipole transitions in both length and velocity gauges is summarized in Table I. In this table the scaling of the positive-energy states contribution for the nonrelativistically forbidden intercombination ($\Delta S\neq 0$) transitions is assumed to be $(\alpha Z)^2$ times smaller than that of spin-allowed transitions. Also, the order of the next term in the negative-energy contributions is assumed to be a factor of $(\alpha Z)^2$ smaller than the order of the leading term.

It has been shown numerically in Ref. [7] that for electric-dipole transitions $2\,^3P_0\rightarrow 2\,^3S_1$ and $2\,^3P_2\rightarrow 2\,^3S_1$, negative-energy corrections to transition amplitudes calculated in the length gauge are much smaller than those obtained in the velocity gauge. With the help of our analytical result, this observation can be extended for all electric-multipole E_J transitions. Indeed, the ratio of negative-energy contributions in the length form to those obtained in the velocity form is $(\alpha Z)^2$ or less. Qualitatively, such a substantial difference between negative-energy state contribution in length and velocity forms can be understood from the fact that the electric-dipole operator in velocity form mixes large and small components of wave functions, while the length-form operator does not. On the other hand, the ''large'' and ''small'' components of positron wave function have the opposite meaning. This leads to the fact that the matrix element of dipole operator between negative- and positive-energy states in the

TABLE II. Contributions from negative-energy states to the reduced matrix element of the electric-dipole moment for the $2\,^3P_1 \rightarrow 1\,^1S_0$ transition in heliumlike ions calculated with the Hartree basis set. $(Q_1)_+^{\rm np}$ is the no-pair contribution from the second-order perturbation theory calculations. $(Q_1)_-^C$, $(Q_1)_-^B$, and $(Q_1)_-^U$ are the negative-energy contributions due to Coulomb and Breit interactions and the model potential, respectively. The breakdown for both length and velocity forms is presented. The notation $a[-b]$ designates $a \times 10^{-b}$.

Gauge	Z	$(Q_1)_+^{\rm np}$	$(Q_1)_-^C$	$(Q_1)_-^B$	$(Q_1)_-^U$	$(Q_1)^{\rm tot}$
Length	2	1.362[−4]	−4.602[−11]	−9.325[−10]	5.371[−11]	1.362[−4]
Velocity	2	1.432[−4]	1.413[−5]	−1.413[−5]	−7.064[−6]	1.362[−4]
Length	10	4.107[−3]	−2.824[−9]	−5.773[−8]	3.602[−9]	4.107[−3]
Velocity	10	4.118[−3]	2.088[−5]	−2.167[−5]	−1.049[−5]	4.107[−3]
Length	50	1.872[−2]	−1.013[−7]	−1.198[−6]	1.943[−7]	1.872[−2]
Velocity	50	1.875[−2]	−1.737[−5]	−3.508[−5]	−9.529[−6]	1.872[−2]
Length	100	8.633[−3]	−6.477[−7]	−3.264[−6]	9.107[−7]	8.630[−3]
Velocity	100	8.656[−3]	1.539[−5]	−3.145[−5]	−1.005[−5]	8.630[−3]

second-order expressions is $(\alpha Z)^2$ times smaller in the length form than in the velocity form.

There is a very surprising effect for intercombination transition amplitudes calculated in the velocity form in a model potential basis: The relative contribution of negative-energy states scales as $1/Z$. This fact implies a significant correction for light ions. The reason is that even though the contributions from Breit and Coulomb interactions cancel each other owing to $\Delta S \neq 0$, the correction from the model-potential term still remains and contributes in leading order. A similar behavior is found for nonrelativistically forbidden magnetic-dipole transitions discussed in Sec. IV.

As an example, we consider the $2\,^3P_1 \rightarrow 1\,^1S_0$ electric-dipole intercombination transition. The calculation requires a generalization of the second-order expressions to a multiconfigurational case since the $2\,^3P_1$ state is represented in the lowest order as a combination of $(2p_{1/2}1s_{1/2})_1$ and $(2p_{3/2}1s_{1/2})_1$ j-j coupled states. We employed the approach of Ref. [8] with an obvious reduction to the case of helium. The results of the direct numerical summation over a basis set in the second-order expressions are presented in Table II. First we note that the negative-energy contributions bring the results of calculations in length and velocity form into agreement. In contrast to relatively tiny corrections found in Ref. [7] for allowed transitions, these contributions are at the level of 5% in velocity form for $Z=2$, due to a specific choice of transition. We also note that for low Z, the negative-energy contributions in velocity form from the Coulomb interaction cancels that from the Breit interaction, so that the total negative-energy correction arises from the model potential term, as discussed earlier. The negative-energy contribution would vanish if a Dirac-Coulomb basis set were used. The relative contribution of negative-energy states is amplified in the velocity form and is substantially smaller in the length form, as discussed earlier.

Therefore, in order to reduce the effect of negative-energy states on high-precision no-pair calculations, the length form of multipole-electric transition operator should be employed. Also, in relativistic multiconfigurational Hartree-Fock calculations similar to Ref. [5] one should take additional care for negative-energy contributions to intercombination transition amplitudes calculated in the velocity form.

IV. MAGNETIC-MULTIPOLE TRANSITIONS

In this section we consider the negative-energy correction to the magnetic-multipole operator $M_J = 2cQ_J^{(0)}$. For magnetic-multipole transitions, the velocity and length forms of the multipole potentials are identical, the scalar potential being zero. The scaling of ratios of negative-energy to positive-energy contributions for magnetic-multipole transitions is summarized in Table III. In this table we explicitly separate the magnetic-dipole (M_1) transition since it is nonrelativistically forbidden. There are several surprising effects, which we will further explore in this section.

It is worth noting that all magnetic-multipole transitions to the ground state of He-like ions have $\Delta S \neq 0$. Therefore, the leading order of the negative-energy correction calculated in the Coulomb basis vanishes. In other words, for transitions with $\Delta S \neq 0$ the contribution arising from the Coulomb interaction given by Eq. (2.19) exactly cancels the contribution from the Breit interaction (2.20). As mentioned before, such detailed cancellation for the magnetic-dipole transition $2\,^3S_1 \rightarrow 1\,^1S_0$ has been observed in the numerical calculations of Ref. [4] for heliumlike Ar ($Z=18$). To illustrate this point further, we perform a direct numerical summation over a set of negative-energy states in Eq. (2.5). We present the absolute values of the ratios of negative-energy contributions to the total value of the reduced matrix element in Fig. 1. The total value of the reduced matrix element has been taken from Ref. [7]. From Fig. 1 it is clear that the cancellation between the Coulomb and Breit negative-energy contributions is nearly complete for low values of Z, with the total negative-energy contribution being less than one-

TABLE III. Scaling of the ratio of negative- to positive-energy state contributions for magnetic-multipole M_J transition amplitudes in heliumlike ions obtained in the transverse gauge.

Basis	$\Delta S=0$	$\Delta S\neq 0$
M_1, Coulomb	$1/Z$	$\alpha^2 Z$
M_1, model potental	$1/Z$	$1/Z$
$J\neq 1$, Coulomb	$\alpha^2 Z$	$\alpha^4 Z^3$
$J\neq 1$, model potential	$\alpha^2 Z$	$\alpha^2 Z$

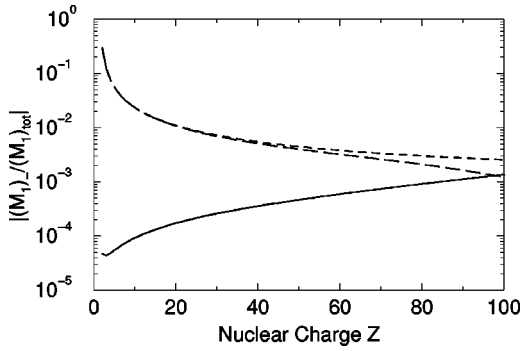

FIG. 1. Comparison of the relative contributions of the negative-energy states due to the Coulomb and Breit interactions to the total value of the reduced matrix element M_1 for the magnetic-dipole transition $2\,^3S_1 \rightarrow 1\,^1S_0$ along the helium isoelectronic sequence. All contributions are scaled to the total value of M_1 from Ref. [7]. The dotted line represents the Coulomb contribution, the dashed line, the Breit contribution, and the solid line, the total relative contribution from the negative-energy states.

thousandth the individual Coulomb and Breit contributions for $Z \leqslant 5$. For larger values of Z, there is only a partial cancellation because terms of the higher powers of αZ contribute to the negative-energy correction. It is worth noting that if there were no such cancellation, the relative contribution of negative-energy states would scale as $1/Z$.

However, when the calculations of magnetic-multipole transition amplitudes for $\Delta S \neq 0$ are performed with the model potential basis set, the term W^{UA} gives a leading negative-energy contribution and must be taken into account. Indeed, for nonrelativistically forbidden magnetic-dipole transitions, e.g., $2\,^3S_1 \rightarrow 1\,^1S_0$, one expects the ratio of negative- to positive-energy contributions to be of order of $1/Z$. In Table IV we give a numerical breakdown for the $2\,^3S_1 \rightarrow 1\,^1S_0$ transition for selected values of Z. Again, we find a strong cancellation between the Coulomb and Breit contributions at low Z, with less cancellation as we increase the value of Z. Unlike the case of starting from a Coulomb basis, however, starting from the Hartree basis provides us with an additional component that is not negligible. In the particular case of helium, the negative-energy states in a Hartree basis contribute 1% to the total transition amplitude and 2% to the total transition rate. By contrast, the negative-energy contributions are entirely negligible (at least in the second order) in a Coulomb basis. It is worth emphasizing that the no-pair CI values are calculated with a high degree of accuracy. For high Z the final total in the Table IV is independent of the choice of basis. The 0.3% difference of total values for $Z=2$ represents a limitation of the present second-order treatment of the negative-energy contributions.

Recently, the effect of negative-energy contributions for the $2\,^3S_1 \rightarrow 1\,^1S_0$ M_1 transition in the case of multiconfigurational Hartree-Fock calculations has been considered by Indelicato [5]. His results also exhibit a $1/Z$-like ratio of negative- to positive-energy contributions that can be attributed to a breakdown of detailed cancellation between Coulomb and Breit terms by the MCHF effective model potential.

The leading term of the negative-energy contribution in a Coulomb basis should also vanish for the magnetic-quadrupole transition (M_2) transition $2\,^3P_2 \rightarrow 1\,^1S_0$. Such a cancellation is demonstrated numerically in Table V. In Table V we also make a comparison with the data given in Ref. [7]. The contributions are different by several orders of magnitude for low-Z ions. The error was traced to an insufficient number of partial waves employed in calculating the negative-energy contributions in Ref. [7]. We revise the numerical calculations and find agreement with the analytical predictions. Incorrect values of negative-energy contributions were used in [7] to determine the transition rate (A coefficient) and the line strength S. Being small, the negative-energy state contribution did not change the values of A at the level of significant figures quoted; however, the line strength S was quoted to a higher degree of accuracy and we find some difference due to negative-energy corrections. Revised values of line strength are presented in Table VI. The difference between the current results and those of Ref. [7] is in the last one or two significant figures and amounts to 0.02% for $Z=100$ and less for other ions.

There is an interesting case in which calculations starting from either a Coulomb basis or a model potential basis would lead to negative-energy contributions that are comparable to those of the positive-energy states. This is the case of the magnetic-dipole transitions between states of the *same* value of total spin.

TABLE IV. Contributions from negative-energy states to the reduced matrix element of the magnetic-dipole moment for the $2\,^3S_1 \rightarrow 1\,^1S_0$ transition in heliumlike ions calculated with Hartree and Dirac-Coulomb basis sets. $(M_1)_-^{CA}$ and $(M_1)_-^{BA}$ are the negative-energy contributions due to the Coulomb and Breit interactions, respectively. $(M_1)_-^{UA}$ is a contribution from the Hartree model potential. $(M_1)_-^{\rm tot}$ is the sum of negative-energy contributions. $(M_1)_+^{\rm np}$ is the no-pair contribution from CI calculations. The notation $a\,[-b]$ designates $a \times 10^{-b}$.

	$Z=2$		$Z=50$		$Z=100$	
Contributions	Hartree	Coulomb	Hartree	Coulomb	Hartree	Coulomb
$(M_1)_-^{CA}$	−4.264[−6]	−1.730[−5]	−1.981[−4]	−2.061[−4]	−5.136[−4]	−5.243[−4]
$(M_1)_-^{BA}$	4.263[−6]	1.730[−5]	1.777[−4]	1.846[−4]	2.447[−4]	2.476[−4]
$(M_1)_-^{UA}$	−5.736[−7]	0	3.870[−5]	0	2.745[−4]	0
$(M_1)_-^{\rm tot}$	−5.741[−7]	−2.732[−9]	1.824[−5]	−2.159[−5]	5.646[−6]	−2.767[−4]
$(M_1)_+^{\rm np}$	5.928[−5]	5.890[−5]	4.655[−2]	4.658[−2]	2.055[−1]	2.058[−1]
$(M_1)^{\rm tot}$	5.871[−5]	5.889[−5]	4.656[−2]	4.656[−2]	2.056[−1]	2.055[−1]

TABLE V. Contributions from negative-energy states to the reduced matrix element of the magnetic-quadrupole moment for the $2\,^3P_2 \rightarrow 1\,^1S_0$ transition in heliumlike ions calculated with the Coulomb basis set. $(M_2)_-^{CA}$ and $(M_2)_-^{BA}$ are the negative-energy contributions due to Coulomb and Breit interactions, respectively, and $(M_2)_-^{\rm tot}$ is their sum. The last column gives the (erroneous) negative-energy contribution of Ref. [7]. The notation $a[-b]$ designates $a\times 10^{-b}$.

Z	$(M_2)_-^{CA}$	$(M_2)_-^{BA}$	$(M_2)_-^{\rm tot}$	$(M_2)_-^{\rm tot}$ [a]
2	−6.645[−5]	6.645[−5]	−1.702[−10]	
3	−3.492[−5]	3.492[−5]	−2.120[−10]	
4	−2.699[−5]	2.699[−5]	−3.100[−10]	
5	−2.346[−5]	2.346[−5]	−4.490[−10]	−9.372[−6]
10	−1.822[−5]	1.821[−5]	−2.163[−9]	−7.246[−6]
20	−1.625[−5]	1.623[−5]	−1.851[−8]	−6.368[−6]
30	−1.567[−5]	1.560[−5]	−7.753[−8]	−6.032[−6]
40	−1.540[−5]	1.518[−5]	−2.212[−7]	−5.846[−6]
50	−1.522[−5]	1.472[−5]	−4.998[−7]	−5.791[−6]
60	−1.508[−5]	1.411[−5]	−9.681[−7]	−5.900[−6]
70	−1.495[−5]	1.327[−5]	−1.681[−6]	−6.223[−6]
80	−1.482[−5]	1.213[−5]	−2.696[−6]	−6.812[−6]
90	−1.468[−5]	1.062[−5]	−4.061[−6]	−7.718[−6]
100	−1.454[−5]	8.715[−6]	−5.825[−6]	−8.989[−6]

[a]Reference [7].

For nonrelativistically forbidden magnetic-dipole transitions between states of the same value of total spin, the leading term in the αZ expansion of the *positive-energy* contribution to the transition amplitude vanishes, reducing the transition amplitude by a factor of $(\alpha Z)^2$. Thus one could expect the ratio of negative-energy contribution to the total transition amplitude be of order of $1/Z$ in either the Coulomb or model potential basis. We consider the particular magnetic-dipole transition $3\,^3S_1 \rightarrow 2\,^3S_1$. It is straightforward to check that, due to angular selection rules, the spin-independent terms in Eq. (2.20) vanish. Thus the negative-energy contributions from the Breit and Coulomb interactions are equal in leading order. The calculations based on Eq. (2.19) show that both contribute the value of $1.71\times 10^{-6}Z$ a.u. to the transition amplitude. The analytical value for the reduced matrix element for helium, obtained with the Eq. (A4), is 2.126×10^{-5} a.u. This value closely agrees with the numerical value obtained by a direct summation over the negative spectrum 2.125×10^{-5} a.u. using a Coulomb basis set.

TABLE VI. Revised values of line strength S in a.u. for the magnetic-quadrupole (M_2) transition $2\,^3P_2 \rightarrow 1\,^1S_0$ in heliumlike ions. The notation $a[-b]$ designates $a\times 10^{-b}$.

10	3.4577[−1]	60	7.2035[−3]
15	1.5046[−1]	65	5.8356[−3]
20	8.3070[−2]	70	4.7566[−3]
25	5.2138[−2]	75	3.8924[−3]
30	3.5427[−2]	80	3.1914[−3]
35	2.5392[−2]	85	2.6166[−3]
40	1.8901[−2]	90	2.1414[−3]
45	1.4465[−2]	95	1.7457[−3]
50	1.1302[−2]	100	1.4146[−3]
55	8.9700[−3]		

TABLE VII. Breakdown of contributions to the reduced matrix element of the magnetic-dipole moment and the corresponding transition rate for the $3\,^3S_1 \rightarrow 2\,^3S_1$ transition in heliumlike ions calculated with Hartree basis sets. $(M_1)_+^{\rm np}$ is the no-pair contribution from CI calculations, $(M_1)_-^{\rm tot}$ is the contribution of negative-energy states, and $(M_1)^{\rm tot}$ is their sum. The notation $a[-b]$ designates $a\times 10^{-b}$.

Z	$(M_1)_+^{\rm np}$	$(M_1)_-^{\rm tot}$	$(M_1)^{\rm tot}$	A (s^{-1})
2	8.119[−6]	1.947[−6]	1.007[−5]	1.17[−8]
3	2.926[−5]	3.824[−6]	3.308[−5]	4.80[−6]
4	6.299[−5]	5.710[−6]	6.870[−5]	1.90[−4]
5	1.093[−4]	7.600[−6]	1.169[−4]	2.73[−3]
10	5.295[−4]	1.710[−5]	5.466[−4]	6.22
20	2.321[−3]	3.650[−5]	2.358[−3]	9.40[3]
30	5.408[−3]	5.671[−5]	5.464[−3]	6.35[5]
40	9.842[−3]	7.790[−5]	9.920[−3]	1.27[7]
50	1.571[−2]	1.001[−4]	1.581[−2]	1.33[8]
60	2.312[−2]	1.233[−4]	2.324[−2]	9.34[8]
70	3.225[−2]	1.471[−4]	3.240[−2]	5.06[9]
80	4.333[−2]	1.714[−4]	4.350[−2]	2.29[10]
90	5.670[−2]	1.954[−4]	5.689[−2]	9.15[10]
100	7.282[−2]	2.184[−4]	7.304[−2]	3.38[11]

The numerical results for the reduced matrix element of magnetic-dipole moment and the corresponding transition rate for the $3\,^3S_1 \rightarrow 2\,^3S_1$ transition are presented in the Table VII. The calculations were performed in a Hartree model potential. The no-pair contributions and the energies used for tabulation of transition rates were obtained with relativistic configuration-interaction method [10,11]. The Lamb shift was estimated using screened Coulomb field values following tabulations [12]. The inclusion of the Lamb shift modifies the third significant figure of the rate values for $Z>50$. The negative-energy contribution to the matrix element was calculated by a direct numerical summation over negative-energy states in the second-order expressions (2.5). The numerical details of the calculations are described in Sec. V. The relative negative-energy contribution to transition amplitude is 20% for neutral helium and becomes smaller for larger Z, modifying the amplitude by 0.3% for $Z=100$.

We also perform a similar analysis for the Coulomb basis. For helium, the sum of the CI no-pair (0.590×10^{-5} a.u.) and second-order contribution from negative-energy states (2.125×10^{-5} a.u.) amounts to 2.715×10^{-5} a.u. This value is almost by a factor of 3 larger than the corresponding value from calculations in the Hartree basis. For high-Z ions such a comparison becomes much better, e.g., for $Z=100$; the calculations in the Coulomb and Hartree bases agree to four significant figures. We emphasize again that the no-pair CI values presented here are converged to a high accuracy. The differences between the resulting total amplitudes are due to the limitation of the second-order perturbation theory treatment of the negative-energy states. In other words, bringing the total values of the reduced matrix element calculated with different starting potentials into agreement with one another requires consideration of negative-energy contributions

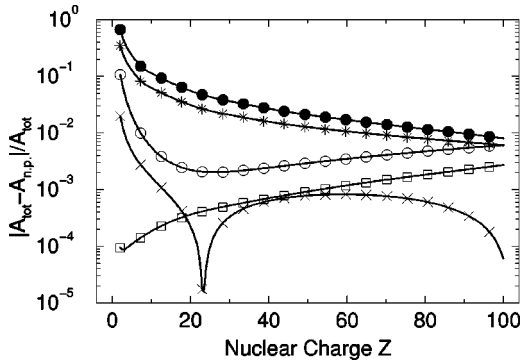

FIG. 2. Comparison of the relative contributions of the negative-energy states to the transition rates (A coefficients) for various transitions along the helium isoelectronic sequence. The ratio of $|A_{\rm tot}-A_{\rm no\ pair}|/A_{\rm tot}$ is plotted. ●, M_1 $3\,^3S_1\rightarrow 2\,^3S_1$, Coulomb basis set; *, M_1 $3\,^3S_1\rightarrow 2\,^3S_1$, Hartree basis set; ○, E_1 $3\,^3P_1\rightarrow 1\,^1S_0$, velocity form, Hartree basis set; ×, M_1 $2\,^3S_1\rightarrow 1\,^1S_0$, Hartree basis set; □, M_1 $2\,^3S_1\rightarrow 1\,^1S_0$, Coulomb basis set.

in higher orders of perturbation theory.

To estimate theoretical uncertainty of the results calculated in the Hartree basis, we compare the second-order no-pair calculations with the all-order no-pair CI result. For helium, the second-order result (7.777×10^{-6} a.u.) recovers 96% of the all-order value (8.119×10^{-6} a.u.), with better agreement for higher Z. Since the negative-energy states contribute at the level of 20% for He, we estimate the theoretical uncertainty of the total value of the reduced matrix element to be at 1% level. Such relative theoretical error in the total value of transition amplitude scales as $1/Z^2$ for higher Z.

The relative modification of the total rate by the inclusion of negative-energy states for $3\,^3S_1\rightarrow 2\,^3S_1$ transition is shown in Fig. 2. Both Coulomb and Hartree cases are considered. The no-pair values for both cases are taken from CI calculations. The total rate is obtained from the reduced matrix element values presented in Table VII. The neglect of contributions from negative-energy states would underestimate the decay rate in the Hartree case by a factor of 1.54 for neutral helium and underestimate the rate by 0.6% for $Z=100$. The rates calculated in the Coulomb basis are affected more strongly and the omission of negative-energy states would underestimate the decay rate in the Hartree case by a factor of 2.91 for neutral helium and underestimate the rate by 0.8% for $Z=100$.

V. NUMERICAL DETAILS

For our numerical calculations, the B-spline basis set has been employed for both the CI and many-body perturbation theory (MBPT) calculations. The B-spline basis functions approximate the eigenfunctions of h_0 in a spherical cavity. The reader is referred to Ref. [13] for details. For the transitions considered previously in Ref. [7], the same basis sets and cavity radii are used. As noted previously, an insufficient number of partial waves were employed in the negative-energy calculations of Ref. [7] for the $2\,^3P_2\rightarrow 1\,^1S_0$ magnetic-quadrupole transition. The addition of these partial waves marks the only change in the present calculations for this transition from those of Ref. [7].

To our knowledge, the magnetic-dipole $3\,^3S_1\rightarrow 2\,^3S_1$ transition has not been discussed previously in the literature and we present the calculations in details. For this transition, convergence with respect to basis set size, cavity radius, and number of partial waves included was not as straightforward as for the other transitions. Our aim was to obtain an accuracy of a part in 10^5. Because of the inclusion of $n=3$ states into the lowest-order wave function, the cavity radius was increased to $120/Z$ a.u. in size. Unlike the other transitions, however, 40 splines were insufficient in converging our solutions for low Z. Even when a 50 spline basis was used, the second-order MBPT values differed by as much a 1% when varying the cavity radius between 40 and 60 a.u. for the case of neutral He. We therefore used an 11th-order, 70-spline basis set to obtain both our MBPT and CI results for $Z=2-5$. While such a large basis was required however, we only needed to sum over 30 of the 70 splines to obtain the desired level of accuracy. For $Z=10$, only a 50-spline basis was required, summing over the lowest 25 splines. For $Z\geqslant 20$, a 40-spline basis was used, again summing only over the lowest 25 splines.

The relativistic configuration-interaction method, employed for calculations in this paper, has been described in Refs. [10,11]. The expression for matrix elements in the CI framework is given in Ref. [7]. For the CI calculations of the $3\,^3S_1\rightarrow 2\,^3S_1$ transitions, the basis orbitals were limited to those having orbital angular momentum $l\leqslant 4$ for neutral He. For all other $Z\leqslant 50$, including only orbitals with $l\leqslant 3$ was sufficient. For $Z>50$, only orbitals with $l\leqslant 2$ were required.

VI. CONCLUSIONS

We have discussed the role of negative-energy states in calculations of transition amplitudes for heliumlike ions by deriving the leading term of their contribution. The scaling of ratios of negative- to positive-energy state contributions to transition amplitudes is presented in Table I for electric-multipole transitions and in Table III for magnetic-multipole transitions. We determined several situations where the contributions of negative-energy states are comparable to the total value of transition amplitude and must be taken into account. In contrast to the usual understanding of relativistic effects, the negative-energy states contributions for the following cases are most important for low-Z calculations: (i) electric-multipole (E_J) intercombination transition amplitudes calculated in velocity form in a model potential basis, (ii) magnetic-dipole (M_1) transition amplitudes calculated in a model potential basis between states with different values of total spin, and (iii) magnetic-dipole (M_1) transition amplitudes calculated in any basis between states with the same value of total spin.

Figure 2 demonstrates how the inclusion of negative-energy states in the calculations modifies the transition rate for the enumerated cases. It is clear that the negative-energy states play a significant role in the determination of the total rate, contributing for low Z at the level of a few percent for the magnetic-dipole $2\,^3S_1\rightarrow 1\,^1S_0$ transition (Hartree basis), 10% for the velocity form of the electric-dipole intercombination $2\,^3P_1\rightarrow 1\,^1S_0$ transition (Hartree basis), and 100% for the magnetic-dipole $3\,^3S_1\rightarrow 2\,^3S_1$ transition (both Coulomb and Hartree sets). The ''nonsmooth'' behavior of the curve for the magnetic-dipole $2\,^3S_1\rightarrow 1\,^1S_0$ transition (Hartree ba-

sis) is explained by the change of sign of the negative-energy contribution at $Z=23$.

The negative-energy contribution to transition amplitudes calculated in a Coulomb basis is smaller than or comparable to that calculated in a model potential basis. In order to decrease the effect of negative-energy states in electric-multipole transitions, one should employ the length form for electric-multipole potentials, as noted in Ref. [7].

Finally, we have tabulated revised values for line strengths of magnetic-quadrupole $2\,^3P_2 \rightarrow 1\,^1S_0$ transitions in heliumlike ions. These values were obtained from the relativistic no-pair configuration-interaction calculations with negative-energy contributions added from the second-order perturbation theory.

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APPENDIX: ANGULAR REDUCTION OF THE NEGATIVE-ENERGY CONTRIBUTION TO MAGNETIC-DIPOLE MATRIX ELEMENT

In this section we present the results of angular reduction for the leading order in an αZ expansion for matrix element of magnetic dipole. The starting expressions are given by Eqs. (2.17)–(2.19) for the operator W. The results below are expressed in terms of radial integrals

$$\mathcal{R}(ijkl)=\int_0^\infty P_i(r_1)P_k(r_1)r_1\frac{d}{dr_1}\times\left[\int_0^\infty P_j(r_2)\frac{1}{r_>}P_l(r_2)dr_2\right]dr_1. \tag{A1}$$

Here $P(r)$ is the radial part of the nonrelativistic wave function of the zeroth-order Hamiltonian and $r_>=\max(r_1,r_2)$. Also ω_0 is the zeroth-order transition energy and $\delta\omega_1$ is the first-order correction to the transition energy. The analytical expressions for ω_0 and $\delta\omega_1$ can be found, for example, in Ref. [7].

For the $2\,^3S_1 \rightarrow 1\,^1S_0$ magnetic-dipole transition the negative-energy contribution due to the Coulomb $\langle F||M_1||I\rangle_-^{CA}$ and Breit $\langle F||M_1||I\rangle_-^{BA}$ interactions cancel each other, as discussed in Sec. IV. The contribution due to the Coulomb interaction is given by

$$\langle F||M_1||I\rangle_-^{CA}=\frac{2}{\sqrt{6}}\frac{\alpha^2}{1+\dfrac{\delta\omega_1}{\omega_0}}[\mathcal{R}(2s,1s,1s,1s)-\mathcal{R}(1s,2s,1s,1s)]. \tag{A2}$$

If the zeroth-order Hamiltonian includes a spherically symmetric model potential U, there is also a contribution $\langle F||M_1||I\rangle_-^{UA}$. The total negative-energy contribution is represented by this term. In the particular case of the self-consistent Hartree potential

$$U(r)\equiv v_0(1s,r)=\int_0^\infty P_{1s}^2(r')\frac{1}{r_>}dr'$$

we obtain

$$\langle F||M||I\rangle_-^{\rm tot}=\langle F||M||I\rangle_-^{UA}=\frac{2}{\sqrt{6}}\frac{\alpha^2}{1+\dfrac{\delta\omega_1}{\omega_0}}\mathcal{R}(2s,1s,1s,1s). \tag{A3}$$

In the case of the magnetic-dipole transition $3\,^3S_1 \rightarrow 2\,^3S_1$, the contributions from Coulomb and Breit interactions are equal and

$$\langle F||M||I\rangle_-^{CA}=-\sqrt{\frac{2}{3}}\frac{\alpha^2}{1+\dfrac{\delta\omega_1}{\omega_0}}[\mathcal{R}(3s,1s,2s,1s)-\mathcal{R}(1s,3s,2s,1s)-\mathcal{R}(3s,1s,1s,2s)+\mathcal{R}(1s,3s,1s,2s)]. \tag{A4}$$

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