Relativistic configuration-interaction calculation of $K\alpha$ transition energies in berylliumlike iron

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We perform relativistic configuration-interaction calculations of the energy levels of the low-lying and core-excited states of berylliumlike iron, Fe^{22+}. The results include the QED contributions calculated by two different methods, the model QED operator approach and the screening-potential approach. The uncertainties of theoretical energies are estimated systematically. The predicted wavelengths of the $K\alpha$ transitions in berylliumlike iron improve previous theoretical results and compare favorably with the experimental data.

I. INTRODUCTION

Highly charged iron produces some of the brightest x-ray emission lines from hot astrophysical objects, such as compact x-ray binaries, galaxy clusters, and stellar coronae. The $K\alpha$ spectral features of iron have been detected in the spectra of nearly all classes of cosmic x-ray sources, because of their high transition rate, low intergalactic absorption, as well as the high relative abundance of iron in the universe. Moreover, iron has been found an important element for the diagnostics of hot laboratory plasma, notably in magnetic nuclear fusion and tokamaks. Since the Fe $K\alpha$ line typically contains the contributions from different charge states, its analysis provides useful information about the equilibrium and nonequilibrium charge-state distributions of ions as well as about the electron and ion temperatures in the plasma.

In view of this importance of the Fe $K\alpha$ line for astrophysics and laboratory diagnostics, accurate theoretical predictions are needed for the reliable identification and interpretation of experimental spectral data. The simplest ion contributing to the $K\alpha$ line is the heliumlike ion. *Ab initio* QED calculations are available for these ions [1], whose accuracy is significantly higher than the present experimental precision. For more complicated ions, however, no full-scale QED calculations of $K\alpha$ transitions have yet been performed, and one has to rely on some kind of relativistic calculations complemented by an approximate treatment of QED effects.

In our previous investigation [2], we performed a relativistic configuration-interaction calculation of the $K\alpha$ transitions in lithiumlike ions, including iron. In that work, the QED effects were taken into account within the one-electron screening-potential approximation. Theoretical results obtained in there agreed well with the recent experimental data [3], the theoretical precision being slightly better than the experimental one.

In the present study, we apply this approach to a more complicated system, the berylliumlike iron. For this ion, we calculate the energy levels of 5 lowest-lying and 18 core-excited states. When combined with the data available for the helium- and lithiumlike ions, accurate theoretical results cover almost all experimentally observed Fe $K\alpha$ transitions in the region between 1.850 and 1.880 Å [4].

The paper is organized as follows. In the next section, we give a brief outline of our computation method with emphasis

on new features as compared to the previous investigations. Section III then presents the results of our calculations and compares them with the previous theoretical and experimental data. Relativistic units $\hbar = c = 1$ and charge units $e^2/4\pi = \alpha$ are used throughout this paper.

II. METHOD OF CALCULATION

We perform our calculations of the energy levels in two steps. On the first step, we solve the Dirac-Coulomb-Breit eigenvalue problem by means of the configuration-interaction (CI) method. On the second step, we calculate the QED correction, which is then added to to the CI energy. The nuclear recoil effect is small when compared to the total theoretical uncertainty and thus is taken into account by means of the reduced mass prefactor (i.e., nonrelativistically and neglecting the mass polarization).

A. Dirac-Coulomb-Breit energy

In relativistic quantum mechanics, the energy of an atom E is given by the eigenvalue of the Dirac-Coulomb-Breit (DCB) Hamiltonian H_{DCB},

$$H_{DCB}\,\Psi = E\,\Psi, \tag{1}$$

where $\Psi \equiv \Psi(PJM)$ is the N-electron wave function with given parity P, total angular momentum J, and angular momentum projection M. The DCB Hamiltonian is conventionally defined by

$$H_{DCB} = \sum_i h_D(i) + \sum_{i<j}[V_C(i,j) + V_B(i,j)], \tag{2}$$

where the indices $i,j = 1, \ldots, N$ numerate the electrons, h_D is the one-particle Dirac-Coulomb Hamiltonian, and V_C and V_B are the Coulomb and the frequency-independent Breit parts of the electron-electron interaction; see, e.g., [5] for details. It is assumed that H_{DCB} acts in the space of the wave functions constructed from the positive-energy eigenfunctions of some one-particle Dirac Hamiltonian (the so-called no-pair approximation).

In the CI method, the eigenfunctions $\Psi(PJM)$ of Eq. (1) are represented by a (finite) sum of the configuration-state

functions (CSFs) with the same P, J, and M,

$$\Psi(PJM) = \sum_r c_r \Phi(\gamma_r PJM), \qquad (3)$$

where γ_r denotes the set of additional quantum numbers that determine the CSF. The CSFs are constructed as linear combinations of antisymmetrized products of one-electron orbitals ψ_n. In the present work, the one-electron orbitals ψ_n are solutions of the frozen-core Dirac-Fock equation.

The energy of the system is given by one of the roots of the secular equation

$$\det\{\langle \gamma_r PJM | H_{\mathrm{DCB}} | \gamma_s PJM\rangle - E_r \, \delta_{rs}\} = 0, \qquad (4)$$

where "det" denotes the determinant of the matrix. The elements of the Hamiltonian matrix are represented as linear combinations of one- and two-particle radial integrals (see, e.g., [5]),

$$\langle \gamma_r PJM | H_{\mathrm{DCB}} | \gamma_s PJM\rangle = \sum_{ab} d_{rs}(ab)\, I(ab)$$

$$+ \alpha \sum_k \sum_{abcd} v_{rs}^{(k)}(abcd)\, R_k(abcd). \qquad (5)$$

Here, a, b, c, and d numerate the one-electron orbitals, d_{rs} and $v_{rs}^{(k)}$ are the angular coefficients [6–9], $I(ab)$ are the one-electron radial integrals, and $R_k(abcd)$ are the relativistic generalization of Slater radial integrals [10].

Our implementation of the CI method has been described in the previous papers [2,11,12]. We shall therefore discuss here only those issues that are new to the present calculation. The first difficulty arises in the calculation of the core-excited states, whose energies are well above the autoionization threshold, i.e., above the continuum of the valence-excited states. For a large basis set we are using here, the atomic states of interest turn out to be very far away from the lowest eigenvalue of the Hamiltonian matrix. The numerical approach we were using previously for determining the eigenvalues of a large matrix (the implementation of the Davidson algorithm by Stathopoulos and Froese Fischer [13]) was suitable for the computation of just the lowest (highest) matrix eigenvalues. In the present work, we use the Jacobi-Davidson algorithm as implemented within the JDQZ package [14,15]. The JDQZ package, although significantly slower than the one by Stathopoulos and Froese Fischer, was able to provide us with eigenvalues and the corresponding eigenvectors around an arbitrary energy target far from the lowest eigenvalue.

Another new feature of the present calculations is the identification of computed levels in terms of the nonrelativistic LS coupling scheme. In our relativistic CI calculations we use the jj coupling scheme, which is natural in the relativistic case. In order to compare the computed levels with experiments and previous nonrelativistic calculations, we had to identify our calculated levels within the LS coupling scheme. In the case of the core-exited states of berylliumlike ions such identification is not straightforward (as it was in the case of lithiumlike ions), because of the large number and high density of levels. In order to identify the levels, we calculated the expectation values of the squares of the orbital momentum operator L^2 and the spin operator S^2 with the eigenfunctions of the DCB Hamiltonian. The matrix elements of the L^2 and S^2 operators are obtained

as

$$\langle \gamma_r PJM | L^2 | \gamma_s PJM\rangle = \sum_{ab} d_{rs}(ab)\, I^{(L)}(ab)$$

$$+ \sum_{abcd} v_{rs}^{(1)}(abcd)\, R^{(L)}(abcd) \qquad (6)$$

and

$$\langle \gamma_r PJM | S^2 | \gamma_s PJM\rangle = \frac{3}{4} \sum_a d_{rs}(aa)$$

$$+ \sum_{abcd} v_{rs}^{(1)}(abcd)\, R^{(S)}(abcd), \qquad (7)$$

where the angular coefficients $d_{rs}(ab)$ and $v_{rs}^{(k)}(abcd)$ are the same as in Eq. (5) and the radial integrals $I^{(L)}(ab)$ and $R^{(L,S)}(abcd)$ are presented in the Appendix.

An essential part of the present calculation is the systematic estimation of the uncertainties of the obtained theoretical predictions. For each atomic state of interest, we perform our CI calculations with many (typically, about 20) different sets of configuration-state functions. From these computations, we then deduce an estimate of how well our CI results were converged, by analyzing the successive increments of the results obtained with the basis set being increased in various directions.

B. QED effects

The QED effects are calculated in the present work by means of two different approaches. By comparing the results from these approaches, we estimate the uncertainty of our treatment. The first method is based on summing up the self-energy and vacuum-polarization QED corrections calculated for each one-electron orbital in an effective screening potential. The total QED correction for a given many-electron state is obtained by adding the QED contributions from all one-electron orbitals, weighted by their fractional occupation numbers as obtained from the eigenvectors of the CI calculation,

$$\delta E_{\mathrm{QED}} = \sum_a q_a [\langle a | \Sigma_{\mathrm{SE}}(\varepsilon_a) | a\rangle + \langle a | V_{\mathrm{VP}} | a\rangle]. \qquad (8)$$

Here, the index a runs over all one-electron orbitals contributing to the given many-electron state, q_a is the occupation number of the one-electron orbital, Σ_{SE} is the self-energy operator, ε_a is the Dirac energy of the one-electron state a, and V_{VP} is the vacuum polarization potential. This approximate treatment of QED corrections was used in our previous work on lithiumlike ions [2] and similarly also by other authors, in particular, for berylliumlike ions by Chen and Cheng [16].

Our second method of evaluating the QED effects is based on the model QED operator h^{QED} formulated recently by Shabaev *et al.* [17] and implemented in the QEDMOD Fortran package [18]. The QEDMOD package is a tool that efficiently calculates matrix elements of h^{QED} with the (bound-state) one-electron wave functions. In the present work, we add the model QED operator to the DCB Hamiltonian, essentially modifying the one-electron integrals $I(a,b)$ of Eq. (5) in our CI code by

$$I(ab) \rightarrow I(ab) + \delta_{\kappa_a,\kappa_b} \langle a | h^{\mathrm{QED}} | b\rangle, \qquad (9)$$

TABLE I. Contributions to the Dirac-Coulomb-Breit energy for the $1s2s2p^2\ {}^3P_0$ state of berylliumlike iron, Fe^{22+}, for infinite nuclear mass, in atomic units. SD denotes the contribution of single and double excitations, and T denotes the contribution of the triple excitations. L is the maximal value of the orbital angular momentum quantum number of the configuration-state functions.

L	δ E
Coulomb, SD	
1	$-567.743\,35$
2	$-0.024\,67$
3	$-0.003\,51$
4	$-0.000\,82$
$5\ldots\infty$	$-0.000\,58$[a]
Breit, SD	
1	$0.044\,60$
2	$-0.000\,99$
3	$-0.000\,17$
4	$-0.000\,05$
$5\ldots\infty$	$-0.000\,07$[a]
Coulomb, T	
1	$-0.000\,05$
Total	$-567.729\,66\ (90)$

[a]extrapolation.

where κ_a denotes the relativistic angular quantum number of the state a. If either a or b is a continuum state [i.e., $\max(\varepsilon_a, \varepsilon_b) > m$], the matrix element of h^{QED} is assumed to be zero. The QED correction to the energy level is then identified by taking the difference of the CI eigenvalues with and without the h^{QED} operator. A comparison of the results of these two approaches for evaluation of QED correction is presented in the next section.

III. RESULTS AND DISCUSSION

In Table I we present an example of our CI calculation of the Dirac-Coulomb-Breit energy for the $1s2s2p^2\ {}^3P_0$ state of berylliumlike iron. The various contributions in this table are obtained by analyzing the results of calculations with 17 different sets of basis functions. These basis sets are obtained by varying the number of partial waves included (i.e., the largest value of the orbital momentum l of one-electron orbitals), the size of the basis for each partial wave, and by including or omitting the Breit interaction. By extending the basis set and taking the differences of the results, we identify the contributions of individual partial waves and check the

stability of the results for each partial wave with regard to the number of basis functions. The analysis is supplemented by estimating the tail of the expansion by polynomial least-squares fitting of the increments in $1/l$.

The contribution of the triple excitations was found to be very small in all cases relevant for the present work. We thus perform the main part of our calculations with single and double excitations only, and estimate the contribution of the triple excitations separately within a smaller basis. The partial-wave expansion was truncated at $l = 4$, with the contribution of the higher-l multipoles being estimated by extrapolation. The typical size of the basis set was of about $N = 30\,000$ functions. The results presented in Table I are well converged with respect to the number of partial waves as well as to the number of the basis functions. For higher excited states, however, the convergence of the partial-wave expansion becomes slower and, more importantly, the stability of the results with regard to the number of basis functions drops down. The latter problem is associated with the interaction of the reference core-excited state with the continuum of valence-exited states, which is difficult to describe accurately. For each atomic state of interest, we perform a separate analysis of the convergence with different sets of basis functions and estimate the uncertainty of the theoretical result based on this analysis.

In Table II we present results for the QED correction for selected states of berylliumlike iron. As described above, the calculation is performed by two different methods, namely, the model QED potential approach (QEDMOD) and the direct calculation of QED corrections in a screening potential. In the latter case, we use two different screening potentials, the core-Hartree (CH) potential and the localized Dirac-Fock (LDF) potential. The definition of these potentials is the same as in our previous works [2,12]. Indeed, we observe fair agreement between the QED corrections obtained by the different methods. In the case of core-excited states, the difference between the results remains well within the 1% range. For the ground and valence-excited states, the deviation is noticeably larger, on the level of 2%. This is explained by a relatively large effect of screening of one $1s$ electron by another $1s$ electron, which is not well described by approximate methods.

As a final result for the QED correction we take the value obtained by the model QED operator approach. The uncertainty of this value was estimated by taking the maximal difference between the three results. For the ground and the $^{3,1}P_1$ valence-excited states, our calculation can be compared with the previous investigation by Chen and Cheng [16], in which the screening-potential approach with the Kohn-Sham

TABLE II. QED corrections for berylliumlike iron, Fe^{22+}, in atomic units. "QEDMOD" denotes the results obtained with the model QED potential, "LDF" labels the results obtained with the localized Dirac-Fock potential, "CH" denotes results obtained with the core-Hartree potential, and "Final QED" denotes the final result for the QED correction with uncertainty.

Method	$1s^2 2s^2\ {}^1S_0$	$1s^2 2s2p\ {}^3P_1^o$	$1s^2 2s2p\ {}^1P_1^o$	$1s2s^2 2p\ {}^3P_1^o$	$1s2s2p^2\ {}^3P_0$	$1s2s2p^2\ {}^5P_3$
QEDMOD	0.312 25	0.296 24	0.296 60	0.176 80	0.160 77	0.161 02
LDF	0.315 30	0.294 26	0.295 02	0.176 90	0.160 28	0.161 67
CH	0.309 17	0.293 90	0.294 68	0.176 44	0.160 03	0.161 45
Final QED	0.312 2 (30)	0.296 2 (23)	0.296 6 (19)	0.176 8 (4)	0.160 8 (8)	0.161 0 (7)
Ref. [16]	0.308 9	0.292 9	0.293 7			

TABLE III. Energy levels of berylliumlike iron Fe^{22+}, in rydbergs, 1 Ry = 109 737.315 685 39 (55) cm^{-1}. Separately listed are the Dirac-Coulomb energy, the Breit correction, and the QED correction. The total energies are presented for the ground state, whereas for all other states, the energies relative to the ground state are given. The theoretical contributions are presented multiplied by the reduced mass prefactor μ/m, $1 - \mu/m = 0.00000981$.

Term		J	Coulomb	Breit	QED	Total	NIST[a]	Other theory[b]	Experiment
$1s^2 2s^2$	^1S	0	-1625.6818	0.5181	0.6245	$-1624.539\,(6)$		-1624.547	
$1s^2 2s2p$	$^3P^o$	0	3.1650	0.0424	-0.0325	3.175 (9)	3.173		
		1	3.4632	0.0247	-0.0320	3.456 (9)	3.455	3.455	3.4550 (2)[c]
		2	4.3382	-0.0077	-0.0298	4.301 (9)	4.299		
$1s^2 2s2p$	$^1P^o$	1	6.8856	0.0039	-0.0313	6.858 (9)	6.856	6.858	6.8561 (5)[c]
$1s2s^2 2p$	$^3P^o$	1	485.6460	-0.4349	-0.2709	484.940 (19)	484.786		484.934 (5)[d]
$1s2s^2 2p$	$^1P^o$	1	487.9367	-0.4578	-0.2688	487.210 (23)	487.200		487.208 (5)[d]
$1s2s2p^2$	^5P	1	486.7934	-0.3794	-0.3051	486.109 (7)			
		2	487.3533	-0.3851	-0.3035	486.665 (7)			
		3	487.9174	-0.4802	-0.3025	487.135 (7)	487.200		
$1s2s2p^2$	^3P	0	490.1470	-0.4315	-0.3030	489.413 (7)	489.414		
		1	490.4131	-0.4291	-0.3029	489.681 (6)			
		2	491.4503	-0.4509	-0.3004	490.699 (7)			
$1s2s2p^2$	^3D	1	490.8672	-0.3908	-0.3026	490.174 (7)	490.260		
		2	490.5592	-0.4403	-0.3034	489.816 (8)	489.815		
		3	490.9252	-0.5124	-0.3025	490.110 (8)	490.134		
$1s2s2p^2$	^3S	1	492.0479	-0.3831	-0.3038	491.361 (9)	491.401		
$1s2s2p^2$	^1D	2	492.7697	-0.3958	-0.3019	492.072 (7)	492.053		
$1s2s2p^2$	^3P	0	492.1343	-0.3658	-0.3052	491.463 (8)			
		1	493.1155	-0.4072	-0.3022	492.406 (9)			
		2	493.6276	-0.4056	-0.3006	492.921 (8)			
$1s2s2p^2$	^1P	1	494.4470	-0.4880	-0.3025	493.656 (10)	493.743		
$1s2s2p^2$	^1S	0	494.8880	-0.3519	-0.2994	494.237 (11)	494.381		

[a]NIST Atomic Spectra Database [21] and Shirai *et al.* [22].
[b]Chen and Cheng [16].
[c]Denne *et al.* [23].
[d]Rudolph *et al.* [3].

screening potential was used. We observe that their results are smaller and slightly outside of our error bars.

From our analysis, we conclude that the uncertainty of the theoretical predictions for the ground and the valence-excited states of berylliumlike iron mainly arises from the uncertainty of the QED treatment. A more rigorous QED calculation, similar to that for lithiumlike ions [19,20], would improve the theoretical accuracy for these states. In contrast, for most of the core-excited states, the theoretical uncertainty comes both from the QED effect and from the Dirac-Coulomb-Breit energy.

Table III presents the calculated energy levels of berylliumlike iron. For the ground $1s^2 2s^2 \, ^1S$ state, the total energy is listed, whereas the *relative* energies (with respect to the ground state) are given for the excited states. Our results are compared with the NIST compilation based on experimental and theoretical data [21,22], with the relativistic CI calculation by Chen and Cheng [16], as well as with the experimental results [3,23]. The estimated fractional accuracy of our theoretical energies of the core-excited states is of about 2×10^{-5}. The overall agreement with the NIST compilation data is quite good, although we observe significant deviations up to ten times our estimated uncertainty for a number of core-excited states. Notably, this is the case for the $1s2s^2 2p \, ^3P_1^o$ state, where excellent agreement is found with the recent measurement [3], well within the given error bars.

Finally, our theoretical results for the wavelengths of the $K\alpha$ transition lines of berylliumlike iron are presented in Table IV, together with the experimental results [3,4,24], the previous calculation by the $1/Z$ perturbation theory [25], as well as the NIST spectral line compilation. The labeling of the transition lines was taken from Ref. [4]. As seen from this table, different transition lines are often very close to each other, so that small shifts in the theoretical predictions might cause changes in the line ordering. In particular, our calculations lead to reassignment (interchange) of the E3 and E4 lines as well as the E8 and E9 lines, respectively. The overall agreement of our calculations with the experimental results is very good, our results being more accurate than the older astronomical measurements [4,24] but several times less precise when compared with the latest laboratory data [3].

IV. CONCLUSION

In summary, we performed relativistic CI calculations of the energy levels of the ground, 4 valence-excited and 18 core-excited states in berylliumlike iron, Fe^{22+}. Dirac-Coulomb-Breit energies from extended CI calculations were combined with separately computed QED corrections. The QED corrections were obtained by two approximate methods, the model QED operator approach and the screening-potential approach. From the comparison of these two approaches we

TABLE IV. Transition line wavelengths of berylliumlike iron Fe^{22+}, in Å. Line labeling is from Ref. [4].

Line	Transition	Present work	Experiment	Other theory[d]	NIST[e]
	$1s^2 2s2p\ ^3P_1 - 1s2s2p^2\ ^3S_1$	1.86771 (3)		1.86835	
E2	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^1D_2$	1.86823 (2)		1.86795	
E4	$1s^2 2s2p\ ^1P_1 - 1s2s2p^2\ ^1S_0$	1.86973 (3)		1.86975	1.8692
E3	$1s^2 2s^2\ ^1S_0 - 1s2s^2 2p\ ^1P_1^o$	1.87038 (9)	1.87035 (8)[a]		1.8705
			1.87035 (11)[b]		
			1.87039 (2)[c]		
E5	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^3S_1$	1.87095 (3)		1.87155	1.8708
	$1s^2 2s2p\ ^1P_1 - 1s2s2p^2\ ^1P_1$	1.87196 (3)			1.8714
E6	$1s^2 2s2p\ ^3P_1 - 1s2s2p^2\ ^3D_1$	1.87227 (2)	1.87246 (35)[a]	1.87255	1.8724
			1.87226 (23)[b]		
E7	$1s^2 2s2p\ ^3P_0 - 1s2s2p^2\ ^3P_1$	1.87308 (2)	1.87246 (35)[a]	1.87285	
E9	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^3P_2$	1.87350 (2)	1.87347 (35)[a]	1.87385	
E8	$1s^2 2s2p\ ^3P_1 - 1s2s2p^2\ ^3D_2$	1.87365 (2)	1.87347 (35)[a]	1.87355	1.8736
			1.87347 (15)[b]		
E10	$1s^2 2s2p\ ^1P_1 - 1s2s2p^2\ ^3P_2$	1.87479 (2)		1.87470	
E11	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^3D_1$	1.87552 (2)		1.87575	1.8752
E12	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^3D_3$	1.87577 (3)	1.87574 (20)[a]	1.87585	1.8757
			1.87552 (12)[b]		
E13	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^3D_2$	1.87691 (2)		1.87675	
E14	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^3P_1$	1.87743 (2)		1.87715	
E15	$1s^2 2s2p\ ^1P_1 - 1s2s2p^2\ ^1D_2$	1.87807 (2)	1.87812 (20)[a]	1.87814	1.8781
			1.87798 (14)[b]		
E16	$1s^2 2s^2\ ^1S_0 - 1s2s^2 2p\ ^3P_1^o$	1.87913 (7)	1.87933 (30)[a]		1.8797
			1.87957 (25)[b]		
			1.87916 (2)[c]		
E17	$1s^2 2s2p\ ^3P_2 - 1s2s2p^2\ ^5P_3$	1.88733 (2)	1.88690 (35)[b]	1.88745	

[a]Beiersdorfer *et al.* [4].

[b]Seely *et al.* [24], with a 0.16 mÅ shift according to Ref. [4].

[c]Rudolph *et al.* [3].

[d]Shlyaptseva *et al.* [25].

[e]NIST Atomic Spectra Database [21] and Shirai *et al.* [22].

were able to estimate the uncertainty of the overall QED shift. The uncertainty of the Dirac-Coulomb-Breit energies was estimated on the basis of an analysis of the convergence of the CI results with respect to the number of terms of the partial-wave expansion and the number of the one-electron basis functions. The results obtained for the wavelengths of the $K\alpha$ transitions improve the previous theoretical calculations and compare favorably with the experimental data.

APPENDIX: RADIAL INTEGRALS FOR L^2 AND S^2

The radial integrals for the matrix elements of the L^2 operator are

$$I^{(L)}(ab) = \delta_{\kappa_a,\kappa_b}\left[l_a(l_a+1)\int_0^\infty dr\, r^2\, g_a(r)\, g_b(r) \right.$$
$$\left. + \bar{l}_a(\bar{l}_a+1)\int_0^\infty dr\, r^2\, f_a(r)\, f_b(r)\right] \quad \text{(A1)}$$

and

$$R^{(L)}_{abcd} = (-1)^{l_a+l_b+j_c+j_d}\, 2\, \Pi_{j_a j_b j_c j_d}\, \mathcal{R}^{(L)}_{ac}\, \mathcal{R}^{(L)}_{bd}, \quad \text{(A2)}$$

with

$$\mathcal{R}^{(L)}_{ac} = \delta_{l_a,l_c}\left[\Xi(l_a)\begin{Bmatrix} l_a & 1/2 & j_c \\ j_a & 1 & l_a \end{Bmatrix} \int_0^\infty dr\, r^2\, g_a(r)\, g_c(r) \right.$$
$$\left. - \Xi(\bar{l}_a)\begin{Bmatrix} \bar{l}_a & 1/2 & j_c \\ j_a & 1 & \bar{l}_a \end{Bmatrix} \int_0^\infty dr\, r^2\, f_a(r)\, f_c(r)\right]. \quad \text{(A3)}$$

The radial integrals for the S^2 operators are written in a similar form,

$$R^{(S)}_{abcd} = (-1)^{l_a+l_b+j_a+j_b}\, 2\, \Pi_{j_a j_b j_c j_d}\, \mathcal{R}^{(S)}_{ac}\, \mathcal{R}^{(S)}_{bd}, \quad \text{(A4)}$$

with

$$\mathcal{R}^{(S)}_{ac} = \delta_{l_a,l_c}\left[\Xi(1/2)\begin{Bmatrix} 1/2 & l_a & j_c \\ j_a & 1 & 1/2 \end{Bmatrix} \int_0^\infty dr\, r^2\, g_a(r)\, g_c(r) \right.$$
$$\left. - \Xi(1/2)\begin{Bmatrix} 1/2 & \bar{l}_a & j_c \\ j_a & 1 & 1/2 \end{Bmatrix} \int_0^\infty dr\, r^2\, f_a(r)\, f_c(r)\right]. \quad \text{(A5)}$$

The notations are as follows: $\Pi_{ab\ldots} = [(2a+1)(2b+a)\ldots]^{1/2}$, $\Xi(l) = [l(l+1)(2l+1)]^{1/2}$, κ_a is the relativistic momentum quantum number of the state a, $j_a = |\kappa_a| - 1/2$, $l_a = |\kappa_a + 1/2| - 1/2$, $\bar{l}_a = 2j_a - l_a$, and $g_a(r)$ and $f_a(r)$ are the upper and the lower radial components of the one-electron Dirac wave function.

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