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Relativistic magnetic quadrupole transitions in Be-like ions

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The multiconfiguration Dirac-Fock method, based on the extended optimal level approximation, is used to calculate magnetic quadrupole transitions ($M2$) from $2s2p(^3P_2)$ to $2s^2(^1S_0)$ states in berylliumlike ions. The calculation of this transition for $Z>6$ uses the Dirac-Fock Hamiltonian which is necessary for highly ionized atoms. The Breit interaction is treated as a first-order perturbation, and its non-negligible contributions to the excitation energies for heavier ions are highlighted. Some of the $M2$ transition probabilities results presented in this paper are calculated for the first time, to our knowledge.

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I. INTRODUCTION

The possibility that magnetic quadrupole radiation might have astrophysical significance for atomic transitions, which satisfy the selection rule $\Delta S=1$, was first pointed out by Mizushima [1]. Transitions from low-lying excited states to the ground state of berylliumlike ions are of interest in astrophysics because of their abundant identifications in the Sun, planetary nebulae (PN), and quasistellar objects [2]. They are useful in the spectral diagnostics of those astronomical objects (for example, the ratio of C/O for most of the PN can be safely approximated by C III/O III [3]). The abundance of carbon and oxygen also determines the type of chemistry in the PN precursor's envelope, whether carbon rich or oxygen rich. Because of the lack of data about the properties of the forbidden lines of highly ionized atoms, insufficient attention was given to their applications to astronomical objects, like hot stars or nebulae, etc. A comprehensive modeling of a star's internal structure needs a precise estimate of its radiative transitions. The evolution of these ions on the stellar surface could have an influence on the evolution of the star. PN and low-density interstellar medium (ISM) exhibit many of the forbidden lines in emission, which infer the abundance of these ions [2]. In dense ISM, these forbidden lines are seen for highly ionized atoms. In a way these lines describe the abundance of these elements in galaxies, which helps in the study of galactic chemical evolution. $M2$ transitions in highly ionized systems occur in ultraviolet and visible emission bands. Therefore, high-resolution spectrographs of satellites can observe these lines, and require that these data be as precise as possible.

Since the strengths of forbidden transitions are rather weak, it is difficult to determine their rates accurately. The accuracies of the computed excitation energies and transition rates depend largely on a balanced treatment of the correlation effects, an adequate size of the orbital basis, and the quality of the valence orbitals. The multiconfiguration Dirac-Fock (MCDF) method is the relativistic counterpart of the multiconfiguration Hartree-Fock (MCHF) theory. Our calculations of the magnetic quadrupole transition probabilities of the berylliumlike ions are calculated with the MCDF method based on the extended optimal level (EOL) approximation described in the Sec. II. In those calculations, the corrections of the energies of the atomic states due to the Breit interation are included using first-order perturbation theory.

Jönsson and Froese Fischer [4] performed calculations for doubly ionized carbon with the MCDF-EOL method followed by the relativistic-configuration-interaction (RCI) calculation. They used a different set of orbitals for the initial and final states. There were a few other calculations for these transitions [5–8]; the majority of these used the intermediate coupling approach. Garstang showed that in the nonrelativistic limit the magnetic quadrupole transition probabilities are approximately proportional to the square of the electric dipole matrix element [5]. However, it was shown by Lin *et al.* [9] that this approximation is not quite accurate. They calculated this line for a few ions of the Be isoelectronic sequence using a semiempirical model potential. The Z-expansion method used by Laughlin [10] appears to be a rough estimate, and its accuracy is uncertain. In the present work we used a fully relativistic one-electron Hamiltonian, and supplemented it with two-electron Coulomb and Breit terms. To ensure the convergence for each of the applied models and to estimate the error, the calculation is performed stepwise. The strong Z dependence (approximately $\propto Z^8$ [11]) of $M2$ transitions is known, and its relativistic nature becomes important near $Z=17$ [5]. We have used the relativistic expression for the magnetic quadrupole moment and the general relativistic atomic structure package [12] for our computations.

II. THEORY

The MCDF method uses the relativistic, no-pair Hamiltonian. The Hamiltonian for an N-electron atom is written in atomic units as

$$H=\sum_{i=1}^{N} H_i+\sum_{i,j;i<j}^{N}\frac{1}{r_{ij}}, \tag{2.1}$$

where $r_{ij}=|r_i-r_j|$, r_i's are the positions of the ith particle. H_i is the Dirac Hamiltonian of the ith particle, defined as

$$H_i=c\alpha\cdot\mathbf{p_i}+(\beta-1)c^2+V_{nuc}(r_i), \tag{2.2}$$

where V_{nuc} is the potential due to the nucleus. Expression (2.2) is also called the *Dirac-Coulomb Hamiltonian*. The atomic wave function for the N electron is obtained by solving the equation

$$H\Psi(\Pi,J,M)=E\Psi(\Pi,J,M), \tag{2.3}$$

where Π is the parity, J is the total angular momentum eigenvalue, and M is the eigenvalue of its projection on the z axis.

In the MCDF method, the trial wave function is taken to be a linear combination of configuration state functions (CSF's):

$$|\Psi(\Pi,J,M)\rangle=\sum_{r=1}^{n} c_r\Phi_r(\Pi,J,M)\rangle. \tag{2.4}$$

The CSF's are eigenfunctions of the parity, total angular momentum J^2, and J_z. The CSF's are expressed as a linear combination of Slater determinants of Dirac spinors,

$$\Phi_r(\Pi,J,M)\rangle=\sum_{i=1}^{N_\gamma} d_i|D_i\rangle, \tag{2.5}$$

where $|D_i\rangle$ is a determinantal wave function built from single-particle states, and its coefficients d_i are obtained by requiring that the CSF's are eigenstates of J^2 and its projection J_z. The variational principle is used to determine the radial wave functions and the mixing coefficients c_r self-consistently. The energy functional that is minimized is given by

$$E_\alpha=\int \Psi_\alpha^\dagger H\Psi_\alpha d\tau=\sum_{r,s} c_r^*(\alpha)H_{rs}c_s(\alpha)=c_\alpha^\dagger Hc_\alpha \tag{2.6}$$

in matrix notation, where the Hamiltonian matrix element is defined by

$$H_{rs}=\langle\Phi_r|H|\Phi_s\rangle. \tag{2.7}$$

Keeping the orbitals fixed, the variation of the energy functional E_α with respect to the mixing coefficients with the normalization condition $\langle\Psi_\alpha|\Psi_\alpha\rangle=1$ yields

$$(H-E_\alpha I)c_\alpha=0, \tag{2.8}$$

i.e., c_α is an eigenvector of the Hamiltonian with eigenvalue E_α.

Self-consistent field (SCF) equations are obtained by requiring that the energy functional should be stationary when subject to variations in the radial functions (P_a,Q_a), such that the orbitals form an orthonormal set. Consider the energy functional

$$\mathbf{E}=E_{opt}+\sum_a \overline{q_a}\epsilon_a N(aa)+\sum_{a,b;a\neq b}\epsilon_{ab}N(ab), \tag{2.9}$$

with

$$E_{opt}=\sum_r d_r^2H_{rr}+\sum_{r,s;r\neq s} d_{rs}H_{rs}, \tag{2.10}$$

where $\overline{q_a}=\Sigma_r d_r^2 q_a(r)$ is the generalized occupation number for orbital a, and d_r $(r=1,\ldots,n)$, the real coefficients, depend on the configuration mixing coefficients and are chosen so that $\Sigma_r d_r^2=1$. The Lagrange multipliers ϵ_a and ϵ_{ab} ensure the normalization and orthogonality conditions, respectively.

The EOL approximation of the MCDF approach is an extension of the well known optimal level version [13]. For the latter case, $E_{opt}=E_\alpha$ yields $d_r=c_r(\alpha)$ and $d_{rs}=c_r(\alpha)c_s(\alpha)$, so that the wave function and mixing coefficients are optimum for the state α. In the EOL approach, optimization is done on a sum of energies $\Sigma_iE(\alpha_i)$, $i=1,\ldots,n_L$, where $n_L<n$, and for that case

$$E_{opt}=\frac{1}{n_L}\sum_{i=1}^{n_L} E_{\alpha i}, \tag{2.11}$$

so that

$$d_r=\left[\frac{1}{n_L}\sum_{i=1}^{n_L} c_r^2(\alpha_i)\right]^{1/2} \tag{2.12}$$

$$d_{rs}=\frac{1}{n_L}\sum_{i=1}^{n_L} c_r(\alpha_i)c_s(\alpha_i). \tag{2.13}$$

The relativistic two-electron operator cannot be written down in closed form. In QED, the interaction between two electrons can be expressed as a series expansion. The first term is the Coulomb interaction, and the leading correction to it is known as the Breit interaction [14–16]. It is linear in the fine-structure constant. In the present work, we consider the Breit interaction as a first-order perturbation. We have used the expressions given by Grant and McKenzie to evaluate the Breit contributions [17]. The Hamiltonian matrix is constructed and diagonalized to obtain estimates of the mixing coefficients for the required atomic states [Eq. (2.8)]. Starting with these values of the mixing coefficients, the SCF equations are solved to obtain new estimates for the orbitals. This process is repeated until self-consistency is achieved. The eigenvalues and orbitals obtained in this way are used to calculate different atomic properties. The magnetic quadrupole emission coefficient is given by the expression [18]

$$A_{fi}=\frac{1}{[J_f]}\sum_{M_i,M_f} 2\pi|\langle\Psi_f|M2|\Psi_i\rangle|^2 \tag{2.14}$$

where $[j]=2j+1$. The matrix element of the magnetic quadrupole operator, $M2$, with respect to initial ($|\Psi_i\rangle$) and final ($|\Psi_f\rangle$) wave functions, can be written in terms of the CSF as

$$\langle\Psi_f|M2|\Psi_i\rangle=\sum_{rs} c_{rf}c_{si}\langle\Phi_r|M2|\Phi_s\rangle, \tag{2.15}$$

where

$$\langle \Phi_r || M2 || \Phi_s \rangle = \sum_{ab} d^k_{rs}(ab) \langle \phi_b || M2 || \phi_a \rangle. \quad (2.16)$$

The expressions for this single matrix element are

$$\langle \phi_b | M2 | \phi_a \rangle = \left(\frac{\omega}{\pi c} \right)^{1/2} [j_b]^{1/2} (-1)^{(2j_a + J_b - 1/2)} |\overline{M}_{ab}| \times \begin{pmatrix} j_b & L & j_a \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \quad (2.17)$$

and

$$\overline{M}_{\alpha\beta} = \frac{5}{\sqrt{6}} (\kappa_\alpha + \kappa_\beta) I_L(\omega) \quad (2.18)$$

and

$$I_L(\omega) = \int_0^\infty (P_a Q_b + Q_a P_b) J_L\left(\frac{\omega r}{c} \right) dr. \quad (2.19)$$

P and Q are the large and small components of the wave function, respectively, and J_L is the spherical Bessel function of order L.

III. RESULTS AND DISCUSSION

We have employed the MCDF approach in the EOL approximation to calculate excitation energies and the magnetic quadrupole transition rates for selected ions of the berrylium sequence. The advantage of this approach is that it is capable of taking into account a large class of electron correlation effects with a relatively small number of virtual orbitals. The intermediate coupling method was used to calculate magnetic quadrupole transition probabilities for a few Be-like ions [6–8]. In this method, different basis sets are used for the diagonalization of the different parts of the Hamiltonian. The Coulomb part is diagonalized with respect to the *LS*-coupled basis, and the spin-orbital part with respect to the *JJ*-coupled basis. For $Z \leqslant 12$ Tachiev and Froese Fischer [19] used this approach in the framework of the multiconfiguration Hartree-Fock method supplemented by the the Breit-Pauli corrections (the MCHF+BP approach). There is a small difference between those results and ours, mainly because of the choice of the orbital basis and the incomplete treatment of the relativistic effects in their approaches. Our calculated excitation energies are in better agreement with the experimental values (wherever available) than the other calculations. The superiority of the MCDF-EOL method (with the Breit interaction) over the MCHF+BP method is obvious from Table I (MCHF+BP excitation energies data are taken from Froese Fischer's web page : http://www.vuse.vanderbilt.edu/ cff/cff.html). This table shows the percentage of the differences of the calculated excitation energies from the experimental values. The accuracy is much better in the case of the MCDF-EOL method, and it steadily improves for higher Z values.

TABLE I. Comparison of the percentages of differences of calculated excitation energies from experimental values between the MCHF+BP and MCDF+Breit (first-order correction) methods.

Z	MCHF+BP	MCDF+Breit
6	0.287	0.119
7	0.231	0.075
8	0.187	0.057
9	0.219	0.057
10	0.284	0.029

TABLE II. Contributions of the Breit interaction to the excitation energies (in cm^{-1}).

Z	Contributions to ΔE
6	19.84
7	35.93
8	59.11
9	91.28
10	131.67
11	185.67
12	253.70
13	340.02
14	443.40
15	570.07
17	895.77
18	1090.02
19	1322.64
20	1593.19
22	2247.92
26	4117.06
28	5363.68
30	6903.70
35	12047.52
40	19560.90
45	30095.86
50	44362.98
55	63024.75

Our computations consist of several steps. We start with the Dirac-Fock calculation, and then optimize the two $2s^2(^1S_0)$ and $2s2p(^3P_2)$ states (levels) with respect to stationary criteria [see Eq. (2.9)]. In each of the following steps, one new orbital (to avoid the problem of computational convergence) is added to the old set and optimization is done on the required sum of the state energies using that basis. In our EOL calculations we have optimized the lowest five energy states [i.e., $n_L = 5$ in Eq. (2.11)].

Since we are interested in optimizing the $2s^2(^1S_0)$ and $2s2p(^3P_2)$ states, we have chosen CSF's which contribute to these two states. As the states are of opposite parities, only those CSF's will contribute which have the same parity and total angular momentum as either one of the above two states. Our orbital basis is constructed from $1s$, $2s$, $3s$, $4s$, $2p$, $3p$, $4p$,$3d$, $4d$, and $4f$ orbitals. The CSF's are constructed by taking all the possible excitations from the $1s$

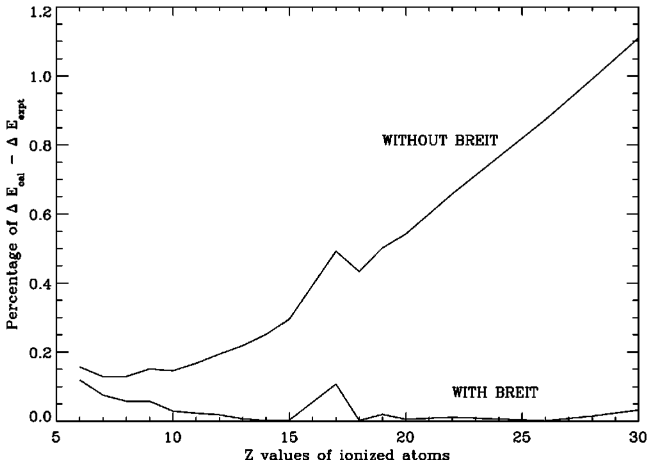

FIG. 1. The effect of Breit interaction on the excitation energies.

and $2s$ orbitals to the other virtual orbitals apart from quadrupole excitations to the $4d$ and $4f$ orbitals.

The convergence of the MCDF orbitals is significantly improved as the value of Z increases. In Table II, we give the contributions of the Breit interaction to the excitation energies. As expected, they increase with Z. This leads to a significant change in the $M2$ transition rates as they are proportional to the fifth power of the excitation energies. The effect of Breit interaction on the excitation energies is plotted for various ionized atoms in Fig. 1. This figure shows that the calculation gives very good agreement with the NIST tabulated values for the excitation energies when the Breit interaction is taken into consideration.

In Table III, we present the excitation energies of the $2s2p\ ^3P_2$ state from the ground states for different Z values. The standard values are taken from NIST online database and, in a few cases, where there are some differences between our calculated excitation energies and the standard values, we compare our results with the unpublished data of Kelly (indicated as ‡). For Z values of 35, 40, 45, 50, and 55 there are no data available in the literature. Table III shows excellent agreement between our calculations and the NIST data. For low-Z ions, the difference between the standard values and our calculated values is on average $<50\ \mathrm{cm}^{-1}$, which is well within the limit of the former. We can improve these calculations if we consider some more orbitals in the active space, but that is computationally expensive and can create convergence problems. In our calculation there is a change in the ordering of $1s^2 2p^2_{1/2}(^1S_0)$ and $1s^2 2s_{1/2} 2p_{3/2}(^3P_2)$ states for highly ionized Be-like atoms ($Z=45$, 50, and 55). This is because of the rather large contraction of the $2p_{1/2}$ orbital for ions with large Z.

TABLE III. Excitation energies (in cm^{-1}) from the ground state.

	$2s2p(^3P_2)$	
Z	NIST	EOL
6	52447.11	52509.6
7	67416.3	67467.1
8	82385.3	82432.7
9	97437	97493.2
10	112704	112736.7
11	128218	128247.4
12	144091	144117.4
13	160429	160439.9
14	177318	177320.6
15	194856	194861.8
17	232660[a]	232410.5
18	252683	252688.1
19	274090[a]	274143.4
20	296950	296933.5
22	347240	347200.8
26	471780	471784.7
28	549500	549579.8
30	640470	640263.8
35		938933.4
40		1373896.5
45		1995158.4
50		2864042.8
55		4054174.1

[a] From Kelly's unpublished work (http://physics.nist.gov/cgi-bin/AtData/main-asd).

Unlike the allowed electric dipole transition between $1s^2 2s^2(^1S_0)$ and $1s^2 2s2p(^1P_1)$ states, the most important contributions to the $M2$ transition between $1s^2 2s^2(^1S_0)$ and $1s^2 2s2p(^3P_2)$ do not come from the Hartree-Fock configurations. In the latter case one of the dominant contributions come from the matrix element $\langle 1s2s3s3p_{1/2}(^3P_2)|M2|1s2s3p_{1/2}3p_{3/2}(^1S_0)\rangle$ for all the ions. Table IV shows how this contribution changes with the value of Z. This contribution decreases as the value of Z increases.

In Table V, transition decay rates are given from $2s2p\,^3P_2$ state to the ground state. It is clear that all the calculations are in fairly good agreement. The small discrepancies are due to the way in relativistic and the many-electron effects are incorporated in the different methods. Most of the other calculations have used relativistic corrections to the nonrelativistic interaction Hamiltonian term to obtain the magnetic quadrupole moment operator. For doubly ionized carbon, Jönsson and Froese Fischer [4] calculated the same transition probability with the MCDF-EOL +RCI method (with the Breit interaction and biorthogonal

TABLE IV. $\langle 1s2s3s3p_{1/2}(^3P_2)|M2|1s2s3p_{1/2}3p_{3/2}(^1S_0)\rangle$ matrix element values for different Z's.

Z	Value
6	1.15736 (−2)[a]
16	4.12406 (−3)
28	2.23929 (−3)
40	1.50165 (−3)
50	1.17056 (−3)

[a] The notation $\alpha(\beta)$ implies $\alpha\times10^{\beta}$.

TABLE V. Transition rate (in sec^{-1}) from $2s2p(^3P_2)$ to the ground state.

Z	λ(Å)	EOL	MCHF+BP	Glass	Others
6	1906.7	5.176(−3)	5.193(−3)	5.261(−3)	5.139[a],5.215(−3)[b]
7	1483.3	1.147(−2)	8.772(−3)	1.161(−2)	1.13(−2)[c]
8	1213.8	2.152(−2)	1.602(−2)	2.171(−2)	2.17(−2)[c]
9	1025.7	3.633(−2)	2.897(−2)	3.700(−2)	
10	887.0	5.720(−2)	5.235(−2)	5.838(−2)	5.76(−2)[c]
11	779.7	8.572(−2)	7.997(−2)		
12	693.9	1.239(−1)	1.177(−1)	1.269(−1)	1.25(−1)[c]
13	623.3	1.745(−1)			
14	563.9	2.410(−1)		2.460(−1)	4.8[d],2.38(−1)[c]
15	513.2	3.281(−1)			
16	466.5	4.461(−1)			4.55(−1)[c]
17	430.3	5.906(−1)			
18	395.7	7.858(−1)			7.993(−1)
19	364.8	1.0423			
20	336.8	1.3804		1.405	1.41[c]
22	288.0	2.4234			
24	244.8	4.433			
26	211.9	7.6459		7.930	7.69[c],10.2[d]
28	181.9	1.3824(1)			13.8[c]
30	156.2	2.5289(1)			
35	106.5	1.1899(2)			
40	72.8	5.8742(2)			
45	50.1	2.8789(3)			
50	34.9	1.3675(4)			
55	24.7	6.2006(4)			

[a] Reference [4].

[b] Reference [8].

[c] Reference [7].

[d] Reference [10].

basis set). There is very good agreement between our result and theirs. Our result agrees with their result (they also have calculated transition probability using the observed transition energy) if we use the standard excitation energy value for the $M2$ transition probability calculation. Thus the small discrepancy is mainly due to the details of the optimization of the orbitals. As expected for low-Z ions, our results are not different from all the other results obtained using relativistic corrections. But for heavier ions the discrepancies are larger. $M2$ transition probabilities are not available in the literature for many of the highly ionized atoms.

IV. CONCLUSION

The MCDF-EOL method was applied to compute the excitation energies and the $M2$ transition probabilities of Be-like ions. The accuracy of the computed excitation energies is in excellent agreement with the NIST database. This work highlights a number of unique and desirable features of the MCDF-EOL method for highly ionized atoms. For instance, the MCDF-EOL calculations yield results with reasonable accuracy using a fewer number of virtual orbitals than some of the other atomic many-body approaches. Also, the importance of the Breit interaction has been highlighted.

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