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Ab-initio Calculations for Forbidden M1 Transitions in Ar^{13+} and Ar^{14+} Ions

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Abstract

A multi-configuration Dirac–Fock (MCDF) method has been used to study the $2s^22p$ ($^2P_{3/2}$–$^2P_{1/2}$) M1 transitions of Ar^{13+} and all the M1 transitions among the 2s2p levels of Ar^{14+} by including correlation effects to a rather large extent. Some detailed comparisons of the present theoretical results with the newest experiments and a few existing calculations are presented.

1. Introduction

Electric-dipole *forbidden* intercombination and magnetic dipole (M1) transitions of highly charged ions have been found to be very useful in the diagnostics of astrophysical and laboratory plasmas [1,2]. These transitions often represent optically *thin* lines, i.e. isolated lines with low transition probabilities, due to low self-absorption effects in the plasma. M1 lines, moreover, frequently occur at longer wavelengths, if compared with the electric-dipole allowed transitions, since they may connect the levels within the same electron configuration. Thus, by having lines in the visible or near–uv range, high resolution techniques can be employed in order to obtain detailed information including even the shape of the lines.

The M1 transitions among the 2s2p levels in the beryllium isoelectronic sequence are of particular interest. Their intensity ratios, for example, relative to the allowed E1 transitions, have been used to determine the electron density of plasma [3]. To investigate these forbidden M1 transitions, several measurements and calculations have been carried out during the last years [4–10]. However, a rather large scattering of the available theoretical and experimental data still exists up to now. For example in the 2s2p ($^3P_2 - {}^3P_1$) transition of Ar^{14+}, the deviations between two semi-relativistic [7,8] and relativistic [6] theoretical transition probabilities amount to almost 60%, while the experiment [4] differs from the theoretical data by 16% and 42%, respectively.

In this paper, we report about a multi-configuration Dirac–Fock (MCDF) study of M1 transitions in beryllium- and boron-like argon. Detailed computations have been performed for the $2s^22p$ ($^2P_{3/2} - {}^2P_{1/2}$) transition of Ar^{13+} and the 2s2p ($^3P_2 - {}^3P_1$), 2s2p ($^3P_1 - {}^3P_0$) and 2s2p ($^1P_1 - {}^3P_{0,1,2}$) transitions of Ar^{14+}, respectively by including correlation effects to a rather large extent.

2. Theoretical method and computational procedures

In this study, the atomic state wavefunctions (ASF) have been generated by the widely–used atomic structure package GRASP92 [11] which is based on the multi-configuration Dirac–Fock (MCDF) method. Here an atomic state wavefunction is approximated by a linear combination of configuration state functions (CSF) with the same symmetry

$$\psi_\alpha(PJM) = \sum_{r=1}^{n_c} c_r(\alpha)\,|\gamma_r PJM>, \qquad (1)$$

where n_c is the number of CSF and $\{c_r(\alpha)\}$ denotes the representation of the atomic state in this basis. In a standard calculation, the CSFs are antisymmetrized products of a common set of orthonormal orbitals which are optimized on the basis of the Dirac–Coulomb Hamiltonian. Further relativistic contributions to the representation $\{c_r(\alpha)\}$ of the atomic states due to (transverse) Breit interactions are added by diagonalizing the Dirac–Coulomb–Breit Hamiltonian matrix. The dominant quantum electrodynamic (QED) contributions, i.e. self-energy and vacuum polarization effect, have also been included in the computations of the total energy as a perturbation.

In the practical expansion of wavefunctions of the interesting atomic states in this study, namely the $2s^22p\ ^2P_{1/2,\,3/2}$ of Ar^{13+} and the 2s2p $^3P_{0,1,2}$ and 2s2p $^1P_1$ of Ar^{14+}, all the single and double excitations from the occupied $2l$ shells up to the unoccupied $5l$ shells have been included. Then, these occupied (spectroscopic) and unoccupied (correlation) orbitals are decided by a series of J-dependent optimizations corresponding to the levels with different parity and total angular momenta. As a result, the relaxation effects caused by radiation from an initial state into a final state can be considered in the calculations of the wavefunctions at first. Finally, to incorporate these effects also in the calculations of the transition probability, a newly developed determinant wavefunctions expansion program CESD [12] and transition probability program REOS [13] are used.

3. Results and discussions

3.1. $2s^22p$ ($^2P_{3/2}$ – $^2P_{1/2}$) *M1 transition of* Ar^{13+}

The ground configuration $2s^22p$ of Ar^{13+} consists of two levels, $^2P_{1/2}$ and $^2P_{3/2}$. These two states have the same parity, the upper $^2P_{3/2}$ level can not decay radiatively through an electric dipole (E1) transition so it decays to the $^2P_{1/2}$ level either via a magnetic dipole (M1) or an electric quadrupole (E2) transition. Since the M1 decay is about five orders of magnitude faster than the E2 decay, only the former transition is important for the lifetime of the $^2P_{3/2}$ state

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Table I. *Comparison of the present calculated transition energy E* (cm^{-1}) *and probability A* (s^{-1}) *with available experiments and calculations in the* $2s^22p$ ($^2P_{3/2} - {}^2P_{1/2}$) *M1 transition of* Ar^{13+}.

Method and author		*E*	*A*
Theory	This work	22636	104.10
	Bhatia *et al.* (1986) [7]		106.8
	Kaufman *et al.* (1986) [8]		104
	Verhey *et al.* (1987) [9]		104
	Froese Fischer (1983) [10]		105.15
Experiment	Moehs *et al.* (1998) [4]		110
	Serpa *et al.* (1998) [5]	22663[a]	114.9

[a]: Experimental transition energy in Ref. [15].

which has been measured in two recent experiments [4,5], and has been calculated in the present study.

In Table I, we list the theoretical transition energy and probability of the $2s^22p$ ($^2P_{3/2} - {}^2P_{1/2}$) M1 transition of Ar^{13+}. For comparison, several available experiments [4,5] and calculations [7–10] are also included.

As seen from the table, the present calculated transition probability is in good agreement with the previous calculations within 3%. The theoretical transition energy is also very close to the experiment. But the theoretical transition probability is small, about 5–10% compared with the available experiments. Clearly, this systematic deviation does not come from the theoretical calculation itself, it is at least not caused by the relativistic, relaxation and correlation effects which were not considered very well in previous calculations.

3.2. *M1 transitions among the* 2s2p *levels of* Ar^{14+}

The 2s2p configuration of Ar^{14+} has 4 fine-structure levels, i.e. $^1P_1$ and $^3P_{0,1,2}$. These levels are separated in two groups by the different multiplicities. The possible M1 transitions among these 2s2p levels include the 2s2p ($^3P_2 - {}^3P_1$), 2s2p ($^3P_1 - {}^3P_0$) and 2s2p ($^1P_1 - {}^3P_{0,1,2}$) lines.

For the 2s2p ($^3P_2 - {}^3P_1$) transition, due to the 2s2p $^3P_2$ level can only decay into lower levels by some weak forbidden transitions, i.e. an M1 transition to 2s2p $^3P_1$, an E2 transition to the 2s2p $^3P_{0,1}$ and a M2 transition to the ground state, and although these latter rates are very small, one can measure its transition probability in experiment and can compare these measurements with different calculations very well. But for the 2s2p $^3P_1$ and 2s2p $^1P_1$ levels, not only can they decay by 2s2p ($^3P_1 - {}^3P_0$) and 2s2p ($^1P_1 - {}^3P_{0,1,2}$) M1 transitions, but also can emit very strong E1 transitions into the ground state. As a result, the probabilities of these M1 transitions are unimportant for the lifetimes of the upper transition levels, and are very difficult to determine in experiments. For the sake of comparison with existing calculations, however, we still calculate these transitions.

In Table II, we present our theoretical transition energies and probabilities of these different M1 transitions of Ar^{14+}. The available experiment [4] and calculations [6–8] are also included for comparison in the Table.

As seen from Table II, the calculated transition energies among the lower triplet states $^3P_{0,1,2}$ are in very good agreement with the experimental values. But the calculated transition energies from the single state to the triplet states are slight big; A good agreement of the present probabilities with the calculations of Bhatia *et al.* [7] for all these transitions and of Kaufman *et al.* [8] for the $^3P_2 - {}^3P_1$ transition are also found. However, all these calculations are rather different from the earlier relativistic extended average energy (EAL) calculation of Idrees *et al.* [6] in both the $^3P_2 - {}^3P_1$ and $^3P_1 - {}^3P_0$ transitions. To explain this latter discrepancy, we also performed a similar calculation. It is found that our new calculation is still different from that of Idrees *et al.* [6], and is nearly the same with our original result. In this case, we believe that the calculations of Idrees *et al.* [6] are unreliable; In addition, a difference of about 13% is found for 2s2p ($^3P_2 - {}^3P_1$) transition when comparing the theoretical result and the new experiment of Moehs et al. [4]. As we will see in the following analysis, this difference can not be compensated by the inclusion of the relativistic, relaxation and correlation effects.

In order to probe the influences of various theoretical approximations on the transition energy and probability, the 2s2p ($^3P_2 - {}^3P_1$) M1 transition is considered in detail as an example. In this analysis, the following approxi-

Table II. *Comparison of the present calculated transition energies E* (cm^{-1}) *and probabilities A* (s^{-1}) *with available experiment and calculations in the* 2s2p ($^3P_2 - {}^3P_1$), 2s2p ($^3P_1 - {}^3P_0$) *and* 2s2p ($^1P_1 - {}^3P_{0,1,2}$) *M1 transitions of* Ar^{14+}.

		Theory				Experiment
Transition		This work	Bhatia *et al.* (1986) [7]	Kaufman *et al.* (1986) [8]	Idrees *et al.* (1989) [6]	Moehs *et al.* (1998) [4]
$^3P_2 - {}^3P_1$	E	16782				16820[a]
	A	63.45	64.3	62	105	74
$^3P_1 - {}^3P_0$	E	7180				7189[a]
	A	6.66	7.77		20.1	
$^1P_1 - {}^3P_0$	E	224983				223538[a]
	A	556.84	584			
$^1P_1 - {}^3P_1$	E	218191				216350[a]
	A	388.97	396			
$^1P_1 - {}^3P_2$	E	201607				199529[a]
	A	504.12	524			

[a]: Experimental transition energy in Ref. [15].

Table III. *Influences of different approximations on the transition energy E* (cm^{-1}) *and probability A* (s^{-1}) *of the* 2s2p ($^3P_2 - {}^3P_1$) *M1 transition in* Ar^{14+}.

Method	*E*	*A*
DF[a]	17649	73.81
DF[a] + Breit	16699	62.54
DF[a] + Breit + QED	16754	63.15
3SD	16772	63.34
4SD	16777	63.40
5SD	16782	63.45

[a]: The correlation between the two $J = 1$ levels, i.e. $^1P_1$ and $^3P_1$, is so strong that we have to include this effect in the approximations for getting a positive transition energy.

mations, namely Dirac–Fock (DF[a]), Dirac–Fock plus Breit interaction (DF[a] + Breit), Dirac–Fock plus Breit interaction and quantum electrodynamics contribution (DF[a] + Breit+ QED) as well as the single and doubly excitations (nSD ($n = 3, 4, 5$)) from the occupied $2l$ shells up into the unoccupied nl shells, have been included, respectively as shown in Table III.

As seen from the table, the transition energy can be corrected seriously by the Breit interaction, QED effect and various correlation effects, but the transition matrix element can not be affected by the different approximations much. This indicates that the transition matrix element is not sensitive for the different approximations at all, a systematic inclusion for relativistic, relaxation and correlation effects still can not reduce the difference between the theoretical calculation and experimental result.

In addition, a complete inclusion of the Breit interaction in optimization of the wavefunctions can modify both one-electron radial functions and the configuration mixing coefficients. Consequently, they should also give some modifications for the transition probability. But as it has been pointed out by Indelicato [14] in the calculation of the $1s2s\ ^3S_1 - 1s^2\ ^1S_0$ M1 transition of Ar^{16+}, such effect gives just an improvement of about 2% for the M1 transition probability. Therefore, we can expect that the influence of such effect should be unimportant also for the present theoretical result.

4. Conclusion

In summary, a multi-configuration Dirac–Fock (MCDF) method has been used to study the $2s^22p$ ($^2P_{3/2} - {}^2P_{1/2}$) M1 transitions of Ar^{13+} and all the M1 transitions among the 2s2p levels of Ar^{14+} by including correlation effects to a rather large extent. By applying an independent optimization procedure and a newly-developed relaxed-orbital transition code, we also incorporated the rearrangement of the electron density due to the transition.

For the $2s^22p$ ($^2P_{3/2} - {}^2P_{1/2}$) transition of Ar^{13+}, our result shown a good agreement with the existed experiments and calculations; For the M1 transitions of Ar^{14+}, the present calculations also are in good agreement with the earlier theoretical results besides that of Idrees *et al*. Comparing the present calculation with the new experiment in the 2s2p ($^3P_2 - {}^3P_1$) transition of Ar^{14+}, a difference of about 13% has been found. A further analysis show that the inclusions of the relativistic, relaxation and correlations effects can not reduce much of the difference. Therefore, a further high precision experiment may be necessary for explaining this discrepancy.

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