Theoretical study of decay processes in Li-like 
$1s2s^2 \ 2S_{1/2}$ inner-shell excited ions

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Abstract

Based on a Multi-configuration Dirac-Fock method, a systematic study has been carried out for the decay processes of the inner-shell excited state $1s2s^2 \ 2S_{1/2}$ of Li-like ions. It is found that only the Auger decay channel is dominant for the low Z ions, the two-electron one-photon radiative decay caused by a strong electron correlation becomes a competitive channel for the middle and high Z ions, whereas the magnetic quadruple radiative decay is also an important decay channel for the very heavy ions. At the same time, it is noticed that the Breit interaction can give a very important contribution to the Auger decay rate of the heavy ions.

Key words: Decay rate, MCDF, Breit interaction

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1 Introduction

The inner-shell excited states of ions in Li-like isoelectronic sequence are of special interest in both theoretical and experimental study due to their simple level structures and strong relativistic and quantum electrodynamic effects[1]. In the past years there have been many theoretical calculations and experimental measurements for the Li-like $1s2l2l'$ resonance states [1-4]. From these studies, one has obtained various information, such as wavelengths, transition probabilities, autoionization rates and so on. However, those works had not paid special attention on the decay of the $1s2s^2 \ 2S_{1/2}$ state along the whole isoelectronic sequence. Only in very recent studies, such as the experimental observation on the anomalous high intensity of the $1s2s^2 - 1s^22p$ transition of

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Li-like aluminum ion in laser produced plasmas spectra by Rosmej et al. [5] and the observation of dielectronic recombination through two-electron one-photon correlative stabilization in an electron-beam ion trap experiment of Li-like iron ions by Zou et al. [6], the properties of the 1s2s 2S1/2 state are attracted further interest. This is because that the TEOP transition is caused completely by electronic correlation effect, which is very sensitive to multi-electron wave functions used. Therefore, such transitions can provide a very good test for different calculations and experiments.

In the present paper, we present a systematic calculation on the excited energies, the electric-dipole allowed (E1) decay rate, the electric-dipole forbidden (M1, M2) decay rates and the Auger decay rate of the 1s2s 2S1/2 state along the whole Li-like isoelectronic sequence by using the Multi-configuration Dirac-Fock (MCDF) method [7].

2 Theoretical method

The radiative decay rate can be expressed by [8]

\[ A_{jk}^r = \frac{4e^2\varepsilon}{3\hbar c^3 g_j} |\langle \Psi_j | T^{(t)} | \Psi_k \rangle|^2, \quad (1) \]

where \( \Psi_j \) and \( \Psi_k \) are the atomic state wavefunctions (ASFs) of the state \( j \) and the state \( k \), respectively. \( \varepsilon \) is the photon energy, and \( T^{(t)} \) is the multipole radiative tensor operator.

The Auger decay rate from the autoionization state \( j \) to the final state \( i \) can be expressed by [9]

\[ A_{ji}^a = \frac{2\pi}{\hbar} |\langle \Psi_j | \sum_{p<q} V_{pq} | \Psi_i \epsilon_i \rangle|^2, \quad (2) \]

where \( \Psi_j \) is the ASF of the state \( j \), while \( \Psi_{i\epsilon_i} \) is the ASF of the system formed by the autoionized ion and the free electron with energy \( \epsilon_i \). The two-electron operator \( V_{pq} \) in Eq.(2) is the sum of the Coulomb and Breit operators, which in atomic units is expressed by [10]

\[ V_{pq} = \frac{1}{r_{pq}} - \frac{\alpha_p \cdot \alpha_q}{r_{pq}} \cos \left( \frac{\omega r_{pq}}{r_{pq}} \right) + (\alpha_p \cdot \nabla_p)(\alpha_q \cdot \nabla_q) \frac{\cos \left( \frac{\omega r_{pq}}{r_{pq}} \right) - 1}{\omega^2 r_{pq}} \quad (3) \]
where the $\alpha_p$ and $\alpha_q$ are the Dirac matrices, and $\omega$ is the wavenumber of the exchanged virtual photon.

In a practice calculation, the energies and the wavefunctions have been generated by the widely used atomic structure package GRASP92 \cite{7}, which is an implementation of the MCDF method. In the method, the ASF has been constructed by a linear combination of configuration state functions (CSFs), while the CSFs are antisymmetrized products of a common set of orthonormal orbitals which are optimized on the basis of the Dirac-Coulomb Hamiltonian. Further the (transverse) Breit interactions were added by diagonalizing the Dirac-Coulomb-Breit Hamiltonian Matrix. The dominant quantum electrodynamic (QED) contributions, i.e. self-energy and vacuum polarization effects, have also been included in the computations of the total energy as a perturbation. The radiative decay rates and the Auger decay rates are calculated by using the recently developed REOS99 \cite{8} and AUGER \cite{9} programs, which are based on the obtained MCDF wavefunctions.

3 Results and discussion

In Figure 1, as an example, the level structure and the important decay channels of Li-like iron ion are shown. It can be seen that the $1s2s^2 2S_{1/2}$ state can not only decay to the $1s^2 1S_0$ state by an no-radiative Auger transition, but also decay to the lower $1s^22s 2S_{1/2}$ and $1s^22p^2 2P_{3/2}$ states by the electric dipole forbidden M1 and M2 radiative transitions, respectively. It is especially need to be noticed that this inner-shell excited state can also decay to the $1s^22p^2 2P_{1/2}$ and $1s^22p^2 2P_{3/2}$ states by the so-called two-electron one-photon (TEOP) transitions, which are caused completely by electron correlation effect. According to a further analysis for the wavefunction components of the $1s2s^2 2S_{1/2}$ state, it is found that although its main component $1s2s^2 2S_{1/2}$ is dominant absolutely, it also includes a little mixture with the $1s2p^2 2S_{1/2}$ and $1s2p^2 4P_{1/2}$ states. Whereas the transitions from the $1s2p^2 2S_{1/2}$ and $1s2p^2 4P_{1/2}$ to the $1s^22p^2 2P_{1/2}$ and $1s^22p^2 2P_{3/2}$ states are very strong, therefore these TEOP transitions become possible. Of course, for different ions of the same sequence, although they have similar level structure and decay processes, due to the fast increasing relativistic effects along the sequence, their decay properties may become quite different as we will discuss below, especial for the heavy ions.

In Table 1, the calculated total radiative decay rate, Auger decay rate, Auger energy and the excited energy of the $1s2s^2 2S_{1/2}$ state are shown for five selected ions. Also some available theoretical and experimental results are tabulated for comparison. It is found that the agreement with both the different calculations and experiments is good in general for both the rates and energies. Especial for the Auger energies, the difference between the present calculation
Fig. 1. Level structure and decay channels of $1s^2 2s^2 2S_{1/2}$ state in Li-like iron ion. and the existing experiment is even less than $0.5\,\text{eV}$ whether for the lighter $Ar^{15+}$ and $Fe^{23+}$ ions or the heavier $Hg^{80+}$ ions. This indicates that the correlation effects and QED effects have been considered very accurately in the present calculations. Therefore, the present predictions for the remaining ions should be reliable.

Fig. 2. Decay rates of the $1s^2 2s^2 2S_{1/2}$ state as functions of atomic number $Z$.

In Figure 2, the various decay rates of the $1s^2 2s^2 2S_{1/2}$ state as functions of atomic number $Z$ are plotted. It can be seen that the Auger decay is an unique dominant decay channel for the low $Z$ ions ($Z < 30$). With increasing
Table 1
The total radiative decay rate, Auger decay rate, Auger energy and the excited energy of the $1s2s^2 2S_{1/2}$ state in five selected Li-like ions. The total radiative decay rate is defined as the sum of all the possible radiative decay rates. The values in square brackets denote the powers of ten.

| Ions | Method | $\sum A^o$ (s$^{-1}$) | $A^a$ (s$^{-1}$) | Auger Energy (eV) | Excited energy (eV) |
|------|--------|------------------------|-----------------|-------------------|--------------------|
| Ar$^{15+}$ | This work | 4.93[12] | 1.33[14] | 2159.2 | 3076.49 |
| Theo.[6] | 4.42[12] | 2162.5 | 3079.0 |
| Theo.[11] | 5.11[12] | 1.08[14] | |
| Exp.[6] | 4.76[12] | 2159.7 | |
| Fe$^{23+}$ | This work | 1.85[13] | 1.46[14] | 4553.2 | 6597.81 |
| Theo.[2] | 1.78[13] | 1.47[14] | 6600.40 |
| Theo.[12] | 1.89[13] | 1.41[14] | |
| Theo.[13] | | 4554.5 | |
| Theo.[14] | | 4554.6 | |
| Exp.[16] | | 4553.4 | |
| Kr$^{33+}$ | This work | 5.33[13] | 1.56[14] | 8819.4 | 12927.26 |
| Theo.[17] | 5.05[13] | 1.46[14] | |
| Theo.[18] | 5.11[13] | 1.59[14] | |
| Hg$^{77+}$ | This work | 6.07[14] | 4.00[14] | 46357.8 | 69898.5 |
| Exp.[15] | | 46358.0 | |
| U$^{89+}$ | This work | 1.60[15] | 5.68[14] | 63048.8 | 95887.4 |
| Theo.[14] | | 6.21[14] | 63077.0 |
| Theo.[19] | | 6.26[14] | 63062.9 |

of the atomic number $Z$, the E1 TEOP decay to the state $1s^22p^2 2P_{1/2}$ becomes almost the same important as the Auger decay in the range of $30 < Z < 80$. But meanwhile the other E1 TEOP decay to the state $1s^22p^2 2P_{3/2}$ becomes weak gradually. When $Z$ close to 90, the M1 decay to the state $1s^22s^2 2S_{1/2}$ becomes also very important. While the M2 decay to the state $1s^22p^2 2P_{3/2}$ is always very weak along the whole sequence.

It is need to mention that the effect of the Breit interaction on the Auger decay rate of the $1s2s^2 2S_{1/2}$ state is quite striking. In Figure 3, the calculated Auger rates are plotted as functions of atomic number $Z$ in the cases with and without the Breit interaction in the Auger matrix elements. It is shown that the contribution of the Breit interaction to the Auger rate increases very fast with increasing of the atomic number $Z$. For the Li-like uranium ion, for instance, the Auger rate with Breit interaction is almost twice as much as that without Breit interaction. Of course, this effect of Breit interaction has also been studied before for different ionic systems and different atomic processes in both theory and experiment, usually they are state-dependent.


Fig. 3. Contributions of Breit interaction to Auger decay rate of the $1s2s^2 2S_{1/2}$ state.

4 Conclusion

In summary, a systematic MCDF study of the decay properties of the inner-
shell excited state $1s2s^2 2S_{1/2}$ of Li-like ions has been carried out along the
whole isoelectronic sequence. Due to a detailed consideration for the correla-
tion effects and QED effects, the present results show a very good agreement
compared with the several existing experimental Auger energies.

From this study, it is found that only the Auger decay channel is dominant for
the low $Z$ ions, the two-electron one-photon radiative decay caused by a strong
electron correlation becomes a competitive channel for the middle and high
$Z$ ions, whereas the magnetic quadruple radiative decay is also an important
decay channel for the very heavy ions. At the same time, the Breit interaction
can give a very important contribution to the Auger decay rate of the heavy
ions. We hope these properties can be tested in experiment.

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