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Note on electron impact excitation for transition $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ of Be-like isoelectronic sequence

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Abstract. Relativistic distorted-wave method was used to calculate the electron impact excitation collision strengths for transitions $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ of Be-like isoelectronic ions. The target states were described, respectively, by 10-level, 46-level and 133-level MCDF configuration-expansion. The relativistic continuum orbitals were calculated in the potential field of frozen target-ion charge distribution with semi-classical exchange potential. The influence of the target states on this collision process along the isoelectronic sequence was investigated in the above three MCDF configuration-expansion modes. It was found that the configurations in the $n = 3$ and the $n = 4$ complexes have great influence on both the high and the low Z ions but the influence is relatively small for intermediate Z ions. The latter phenomenon was attributed to competition between opposing correlation and relativistic effects on the collision strengths.

PACS. 34.50.Fa Electronic excitation and ionization of atoms (including beam-foil excitation and ionization) – 34.80.Kw Electron-ion scattering; excitation and ionization

In this note we present some recent results computed by relativistic distorted-wave (RDW) procedures for electron impact excitation (EIE) for transitions $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ of atomic ions with Be-like isoelectronic sequence. The collision strength calculations of Be-like ions are of importance in interpreting and diagnosing the line ratios in the solar spectrum and various kinds of plasmas [1]. The behaviour of collision strengths for these transitions is discussed in three target describing modes, namely, 10-level, 46-level and 133-level multi-configuration Dirac-Fock (MCDF) configuration-expansion (CE). Also, the collision strength behaviour as a function of the scattered electron energy E_f is analyzed. These calculation modes are compared with one another to investigate the influence of target states on the excitational collision strengths.

The collision strengths for transitions $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ of some Be-like ions have previously been calculated by several methods, such as for Be-like C, O, Si, Fe ions by the R-matrix method [2,3], and O, Ne, Fe, Xe ions by the relativistic distorted-wave (RDW) method [4–6]. However, most of these calculations were based on the target described by coupling the lowest 10 states, or the lowest 20 states, the latter also including 10 states in configurations $2s3l(l = s, p, d)$. Up to now, no results obtained by using higher-level MCDF CE performed by either R-matrix or RDW methods have been reported in the literature. It is therefore desirable to check the influence on the collision strengths when the target states are described, respectively, by 46- or 133-level MCDF CE. Furthermore, no systematic study on this EIE transition along Be-like isoelectronic sequence have appeared in the literature. Such a systematic study can provide us a clear picture on how the correlation effect and relativistic effect affect the final collision strengths, and thus enhance our understanding of the collision processes involved.

The present RDW calculational procedures were given in detail in references [6–8]. In RDW theory, the target states are frozen in the collision dynamics. In order to make our RDW calculation more realistic, theoretically generalized occupation numbers instead of fictitious occupation numbers [6] were used in determining the distorted potentials, where a semi-classical method was used in determining the exchange potentials which is free electron energy-dependent. Continuum orbitals were calculated in these distorted potentials. In the present relativistic bound state calculations we used the GRASP[2] code [9,10] based on MCDF theory. Multiconfiguration self-consistent-field (SCF) calculations are based on the Dirac-Coulomb Hamiltonian. The nuclear potential is modeled as a spherically symmetric distribution of nuclear charge. The one-body operator is based upon the Dirac kinetic-energy operator. The transverse photon interaction (generalized Breit Hamiltonian between bound electrons) is added to the two-body operators. The calculations are performed in two separate sections. The atomic structures are calculated perturbatively in the first section, and the electron collisions are calculated in the second section. With the addition of the transverse photon interaction, the mixing coefficients may be somewhat

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Table 1. Checking the influence of the target states by three calculational modes on the collision strengths for four scattered electron energies E_f (in eV) for transition $2s^2\ {}^1S_0$-$2s2p\ {}^3P_1$ of Be-like isoelectronic sequence. For each ion, the first, second and third entries were obtained by the modes (C), (B), and (A), respectively. The configurations used in modes (A)-(C) are explained in the text. Transition energies ΔE (in eV) in the second column were obtained from mode (C). $a-b$ means $a\times 10^b$.

		E_f(eV)			
Z	ΔE(eV)	100	500	1000	5000
6	6.587	$3.777-2$	$3.148-3$	$9.134-4$	$6.815-5$
		$4.036-2$	$3.257-3$	$9.500-4$	$9.707-5$
		$4.233-2$	$3.131-3$	$8.895-4$	$6.961-5$
8	10.262	$3.322-2$	$4.945-3$	$1.637-3$	$1.526-4$
		$3.508-2$	$5.070-3$	$1.663-3$	$1.575-4$
		$3.711-2$	$5.053-3$	$1.588-3$	$9.594-5$
14	21.424	$1.402-2$	$6.581-3$	$3.643-3$	$1.310-3$
		$1.440-2$	$6.736-3$	$3.697-3$	$1.293-3$
		$1.489-2$	$6.902-3$	$3.722-3$	$1.204-3$
20	33.502	$9.249-3$	$7.611-3$	$6.719-3$	$5.686-3$
		$9.359-3$	$7.792-3$	$6.940-3$	$5.710-3$
		$9.866-3$	$8.771-3$	$7.946-3$	$5.845-3$
23	40.097	$9.412-3$	$9.307-3$	$9.247-3$	$9.742-3$
		$9.755-3$	$9.614-3$	$9.550-3$	$9.847-3$
		$1.027-2$	$1.156-2$	$1.135-2$	$1.043-2$
30	57.108	$1.325-2$	$1.520-2$	$1.727-2$	$2.252-2$
		$1.349-2$	$1.630-2$	$1.873-2$	$2.351-2$
		$1.625-2$	$2.216-2$	$2.607-2$	$2.727-2$
47	105.308	$1.824-2$	$2.030-2$	$2.317-2$	$3.202-2$
		$1.963-2$	$2.291-2$	$2.738-2$	$3.451-2$
		$2.751-2$	$3.498-2$	$4.475-2$	$4.493-2$
54	127.746	$1.647-2$	$1.826-2$	$2.005-2$	$2.805-2$
		$1.811-2$	$2.125-2$	$2.385-2$	$3.101-2$
		$2.612-2$	$3.356-2$	$3.988-2$	$4.373-2$
64	163.918	$1.324-2$	$1.442-2$	$1.592-2$	$2.260-2$
		$1.466-2$	$1.655-2$	$1.903-2$	$2.611-2$
		$2.300-2$	$2.846-2$	$3.424-2$	$4.409-2$
79	230.717	$8.922-3$	$9.541-3$	$1.033-2$	$1.365-2$
		$1.024-2$	$1.122-2$	$1.269-2$	$1.639-2$
		$1.571-2$	$1.838-2$	$2.201-2$	$2.714-2$
92	299.922	$6.635-3$	$6.654-3$	$7.050-3$	$9.466-3$
		$7.599-3$	$7.791-3$	$8.543-3$	$1.200-2$
		$1.261-2$	$1.347-2$	$1.540-2$	$2.309-2$

changed. In addition to the nonrelativistic Coulomb interaction, the electron undergoes relativistic interactions with the target nucleus and other bound electrons, such as spin-orbit, spin-spin, and spin-other-orbit interactions. The Dirac Hamiltonian $H_{\rm D}$ adequately describes the relativistic interaction. In the electron collision section, we exclude Møller scattering (transverse photon interaction between free and bound electrons) because the incident energy ($< 10^4$ eV) is not high enough to make the Møller interaction between the incident electron and bound electrons very significant.

In MCDF CE theory, the ion atomic state functions (ASFs) Ψ_ν are a linear combination of configuration state functions (CSFs) Φ_μ sharing common values of parity and total angular momentum J,

$$\Psi_\nu = \sum_\mu c_{\mu\nu}\Phi_\mu, \tag{1}$$

where $c_{\mu\nu}$ are the mixing coefficients. To investigate the influence of the target states by different configuration description modes on the electron impact excitation, three CE calculation modes were used, namely,

(A): $2s^2$, $2s2p$, $2p^2$: 6 terms or 10 levels;
(B): (A) + $2s3l + 2p3l$ ($l = s, p, d$): 26 terms or 46 levels;
(C): (B) + $3l3l'$ ($l, l' = s, p, d$) + $2s4l + 2p4l$ ($l = s, p, d, f$): 133 levels.

In the above notation, the K-shell core is omitted for brevity. The resulting collision strengths so obtained are presented in Table 1. The computational procedure took into account all possible contributions from the ground state and excited-state configurations considered in modes (A)-(C), respectively.

In Table 1, the collision strengths of the resonance excitation from ground state to the $2s2p\ ^3P_1$ state for eleven Be-like ions are presented. For each Z, the atomic number of the ion, the three entries are calculated by modes (A)-(C), respectively. First, let us investigate the results along isoelectronic sequence. When we compare the results by the three modes for each Z, we find that the discrepancies among those modes are more than 10% at low Z. This is mainly due to the incomplete catch of the nonrelativistic correlation effect. As a general fact, more correlation effect was caught in mode (C) by using 133-level MCDF CE. This evidence indicates that the target configurations $2s3l, 2p3l (l = s, p, d)$ as well as configurations $3l3l' (l, l = s, p, d)$ and $2s4l, 2p4l (l = s, p, d, f)$ are important in the electron impact excitation calculation for Be-like ions. The importance of including configurations $2s3l (l = s, p, d)$ for EIE of low Z was also noted by Berrington *et al*. [2,3]. If we next make these comparisons for higher Z, we find that the discrepancies among the three modes increase with increasing Z. The discrepancies are much larger than those in low Z. This curious behaviour is not understandable at first because of the fact that correlation effect is ordinarily important at low Z and generally not important at high Z. The real reason is that, in the present MCDF atomic structure calculation, the nonrelativistic correlation effect does indeed decrease with increasing Z, but at the same time the relativistic effect increases rapidly with increasing Z and it is inextricably coupled with the correlation effect so the two effects cannot be separated clearly. So, the main reason why large discrepancies among the three modes exist at high Z is due to the so-called many-body relativistic effect or relativistic correlation. However, the discrepancies among the three calculation modes are small when Z is about 14-20 because nonrelativistic correlation effects are relatively small at intermediate Z compared with low Z whereas the many-body relativistic effect does not begin to manifest its large influence at these Z's.

Next, let us investigate the collision strengths as a function of the scattered electron energy. At low Z, the discrepancies among the three modes are smaller at high free electron energies than those at low energies. (One exception exists for $Z = 6$ at high energies, but in this case the collision strengths are extremely small.) The reason for this behaviour lies in the fact that the nonrelativistic effect has more influence on the EIE collision strengths when impact electron energy is small than on those when impact electron energy is large. However, in the case of high Z, the situation is quite different. The discrepancies among the three modes are larger at high free electron energies than those at low energies. Again, this is due to the rapidly increasing many-body relativistic effect as the electron impact energy increases.

Another interesting behaviour of the collision strengths as a function of free electron energy is that, at low Z, the collision strengths decrease with increasing scattered electron energy whereas at high Z they increase with increasing scattered electron energy. At intermediate Z (around $Z = 23$ as shown in Tab. 1), the collision strengths first decrease with increasing free electron energy and then increase with increasing free electron energy. These tendencies can be explained from MCDF CE in equation (1). For low-Z ions, the state $2s2p\ ^3P_1$ is close to pure LS-coupling and almost not mixed with the various states $^1P_1$ in the configurations $2s2p, 2s3p, 2s4p, 2p3s, 2p4s, 2p4d$ with the same parity, so the transition $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ is nearly a spin-forbidden transition and thus the collision strengths decrease with increasing free electron energy. On the other hand, for high-Z ions, the state $2s2p\ ^3P_1$ is close to pure jj-coupling and has large mixing coefficients $c_{\mu\nu}$ with the various states $^1P_1$ in the configurations with the same parity. The transitions $2s^2\ ^1S_0$-$2s2p\ ^1P_1$ are dipole-allowed transitions with large collision strengths thus making the collision strengths of transition $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ increase with increasing free electron energy. For intermediate-Z ions, the state $2s2p\ ^3P_1$ begins to deviate from pure LS-coupling but not very seriously, so, the collision strengths firstly decrease with increasing free electron energy in the low free electron energy region. However, in the high electron energy region, the dipole-allowed transitions $2s^2\ ^1S_0$-$2s2p\ ^1P_1$ contribute more compared with those at the low energy region so that the collision strength for transition $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ increases with increasing free electron energy in accordance with the same tendency for high-Z ions.

In summary, the RDW method is used in the present calculations for electron impact excitation of Be-like isoelectronic sequence. The influence of target states on the collision dynamics is investigated. Inclusion of contributions from the configurations in the $n = 3$ and $n = 4$ complexes is found to be very important to catch both the nonrelativistic correlation effect as well as the many-body relativistic effect in the frame of MCDF calculation. The great influence of the many-body relativistic effect is for the first time highlighted on the EIE calculation, especially when the calculations are made for high-Z ions at high impact energies. The different tendencies of the collision strengths for transition $2s^2\ ^1S_0$-$2s2p\ ^3P_1$ as a function of free electron energy among low-Z, intermediate-Z, and high-Z ions can be explained from MCDF configuration-expansion theory. More reasonable comparisons may be made for the Z^2-scaled collision strengths for the transition mentioned above along the Be-like isoelectronic sequence and some further results may be obtained.

The state $2s2p\ ^3P_1$ is nearly pure LS-coupling for low-Z ions and nearly pure jj-coupling for high-Z ions, in which the state $2s2p\ ^3P_1$ is strongly mixed with the $^1P_1$ states with the same parity. since EIE cross sections for

dipole-allowed transitions from the ground state to the $^1P_1$ states are very large [6], the cross section for dipole-forbidden transition from the ground state to $^3P_1$ may be greatly influenced due to the spin-orbit coupling. Also, for high impact energies, the Breit/Møller interaction should play an increasingly important role in both the atomic structure [11] and the EIE calculations. We will continue these investigations on this subject.

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