Two-electron capture by He^{2+}, Li^{3+}, and B^{5+} in the independent-event model

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We apply a single-channel distorted-wave approximation in conjunction with the independent-event model to calculate the double-capture cross sections by He^{2+}, Li^{3+}, and B^{5+} from neutral He. The capture probabilities of the two electrons in two successive independent events are calculated by a single-channel distorted-wave approximation with realistic screening charge parameters. Our T matrix has been evaluated analytically and therefore the present method is much simpler than other available rigorous calculations. Our results are compared with the measurements and other calculations. It is found that the present method gives fairly good agreement with the measurements. [S1050-2947(96)09109-3]

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I. INTRODUCTION

Multielectron transitions from atomic targets have received much attention lately. Understanding the role of electron-electron correlation on these processes is of great topical interest. Double capture by fully stripped ions from atomic helium is the simplest problem of this kind where only two electrons are involved. When the projectile is He^{2+}, the process is a resonant process and the double capture into the ground state would be dominant where the effect of electron-electron correlation is expected to be maximum. As the projectile charge increases, the probability of one of the electrons being captured into the excited state would increase. The effect of electron-electron correlation in the final captured channel is therefore expected to decrease because of relatively large interelectronic separation. In the present calculation our aim is to use our recently developed single-channel distorted-wave approximation [1] in conjunction with independent-event model to calculate the double-capture cross sections by He^{2+}, Li^{3+}, and B^{5+} ions from atomic helium.

In the literature there exist quite a few measurements [2–8] and a number of calculations on double capture by He^{2+} and other fully stripped ions from the helium atom. McGuire and Weaver [9] have presented an independent-particle model (IPM) in which the double-electron capture probability is given by the square of one-electron capture probability. This method therefore does not account for any effect of correlation. The IPM has been used by various groups within a variety of approximations. The continuum distorted-wave (CDW) approximations [10–12] under this model have mixed success. However, all these calculations are restricted to capture into the ground state $(1s^2)$ of the projectile ions. A few calculations taking account of correlation to a certain degree are also reported. Using configuration interaction Deco and Grün [13] calculated cross sections for double capture by He^{2+} from He atoms for the energy range 1.5–6 MeV. In a multistate close-coupling calculation, Shingal and Lin [14] have accounted for some form of correlation through charge screening. They obtained fairly good results for the single electron-transition process only. It was Crothers and McCarroll [15] who have used an explicitly correlated wave function due to Pluvinage [16] to represent the helium target and presented results for double-capture cross sections by He^{2+}. In this work they prescribed a different model called independent-event model (IEM) in which the double capture occurs as a result of two successive one-electron capture events. However, since they have considered the resonant process of He^{2+} on He, they have used the IPM to calculate the double-capture cross sections. This IEM was used later by Dunseath and Crothers [17] under the CDW prescription to calculate double-capture cross sections by He^{2+} and obtained reasonable results. Gravielle and Miraglia [18] have calculated the single-electron capture probability employing a second-order CDW theory and used this probability to calculate double-capture cross sections in IPM. Recently Belkić and co-workers [19–21] have presented a four-body (4B) model within the CDW and boundary corrected first Born prescription. They have presented double-capture cross sections for He^{2+} and Li^{3+} projectiles. However, their results are restricted to both the electrons being captured into the ground state $(1s^2)$. Calculation of this 4B amplitude requires the evaluation of complicated multidimensional integrals even for the ground state. It is, therefore, very difficult to use this formulation to calculate double-capture cross sections into the excited states. Gayet *et al.* [22] have calculated double-capture cross sections into the excited states up to $n=4$ levels within the CDW-IPM model. They have also presented CDW-4B results, but for the $1s^2$ final state only.

In what follows, we present a method to calculate the double-capture cross sections by He^{2+}, Li^{3+}, and B^{5+} within the IEM. The single-electron capture probabilities for two successive events are calculated by using our recently developed single-channel distorted-wave approximation [1] with realistic screened charges.

II. THEORY

Under the IEM the double-capture cross sections by fully stripped ions from atomic He is given by

TABLE I. Double-electron capture cross sections (in cm^2) for He^{2+}-He collisions. E is the projectile impact energy (in keV). Experimentals are taken from (a) McDaniel *et al.* [2], (b) Faria, Freire, and de Pinho [4], and (c) Schuch *et al.* [5]. CM, the calculations of Crothers and McCarroll [15] with Pluvinage electronic wave functions within CDW approximation; GM, the second-order calculations of Gravielle and Miraglia [18] with impulse approximation using HF wave function; BCIS-4B, the results of boundary corrected continuum intermediate state (BCIS) method of Belkić [21]; CDW-IPM, results with the CDW as reported by Gayet, Rivarola, and Salin [10] using (i) hydrogenic wave function and (ii) Hartee-Fock-type wave function. $a[-b]$ stands for $a\times 10^{-b}$.

E (keV)	Experiment	Present result	CM	GM	BCIS-4B	CDW-IPM
500	5.1[−18][a]	8.69[−18]	5.8[−18]	5.0[−18]		(i) 1.6[−17] (ii) 1.3[−17]
750	9.5[−19][a]	1.16[−18]	7.4[−19]	7.6[−19]		(i) 1.8[−18] (ii) 1.1[−18]
1000	2.6[−19][a]	2.34[−19]	1.5[−19]	1.6[−19]	1.1[−19]	(i) 3.1[−19] (ii) 1.7[−19]
1400	3.6[−20][a]	4.15[−20]	2.1[−20]	1.9[−20]		(i) 3.4[−20] (ii) 1.7[−20]
2000	0.82[−21][b]	2.24[−21]			1.57[−21]	
2500	2.5[−22][b]	3.85[−22]			3.17[−22]	
3000	6.5[−23][b]	8.74[−23]			7.96[−23]	
4000	1.3[−24][c]	6.52[−24]			8.11[−24]	
6000	0.54[−25][c]	1.66[−25]			2.95[−25]	

$$\sigma_2 = 2\pi a_0^2 \int_0^\infty P_1(\rho) P_2(\rho)\rho\, d\rho, \tag{1}$$

where the transition probability that depends on the impact parameter (ρ) is given by

$$P_i(\rho) = |a_i(\rho)|^2, \quad i=1,2 \tag{2}$$

with

$$a_i(\rho) = \int_0^\infty \eta\, d\eta\, J_m(\eta\rho) T_i(\eta)/(2\pi v). \tag{3}$$

Here η is the transverse component of the change in the linear momentum and m is the change in azimuthal quantum numbers between the initial and final states and $J_m(\eta\rho)$ is the Bessel function of order m, v is the impact velocity, and $T_i(\eta)$ is the transition amplitude obtained by the wave treatment. Atomic units are used throughout the calculation.

III. RESULTS AND DISCUSSIONS

In a recent calculation [1] we have applied a single-channel distorted-wave model to calculate the charge transfer cross sections by fully stripped ions with high-Z value from atomic hydrogen. In the present calculation we put this model to a further test by applying it in conjunction with the IEM to calculate double-capture cross sections by He^{2+}, Li^{3+}, and B^{5+} from atomic helium. We therefore calculate both T_1 and T_2 following the method described by Das *et al.* [1]. One might argue that the two transition matrix elements in two successive events should not be treated on the same footing. However, very recently Afrosimov *et al.* [23] used the target continuum distorted-wave approximation [24,25] for calculating similar matrix elements with realistic charge parameters and obtained reasonably good results. In our calculation we use the target charge $Z_T=1.687$ for both events. This is justified because after one electron is captured by the first event, only very few target atoms will be singly ionized and the probability of capturing the second electron from a neutral helium atom would be dominant in the second event. For the projectile charge we take $Z_P=q$ in the first event that allows one electron to be captured either in the ground state or in the excited state where q is the nuclear charge of the fully stripped projectile. When the first electron is captured in the ground state (with $Z_P=q$), the second event allows another electron (from neutral helium) to be captured either in the ground state with new projectile charge, $Z_P'=(q-\frac{5}{16})$ or in the excited state with $Z_P'=(q-1)$. On the other hand, when the first electron is captured in the excited state (by the first event with $Z_P=q$) we consider the second electron is captured only in the ground state by the second event. For this second event we take $Z_P'=q$ assuming that the second electron that is captured in the ground state will not feel any screening by the electron already captured in the excited state. This assumption is consistent with the Franc-Condon principle. In our calculation we have taken into account the contributions from the product projectile states up to $n=4$ levels. This means that one of the two electrons is captured into the $1s$ level and the other electron is captured into any state up to $n=4$. However, contributions from both electrons being captured into excited states are not accounted for because this contribution is likely to be very small. Here it is to be mentioned that in the present two-step model it is very difficult to account for the antisymmetrization of the wave function. However, we expect that the effect of antisymmetrization will not be significant in the high-energy range considered here.

In Table I we present our results for double-capture cross sections by He^{2+} from He together with the measured values and other available theoretical results. From this table we see that our capture cross sections are somewhat larger than the available measurements of McDaniel *et al.* [2], Faria, Freire,

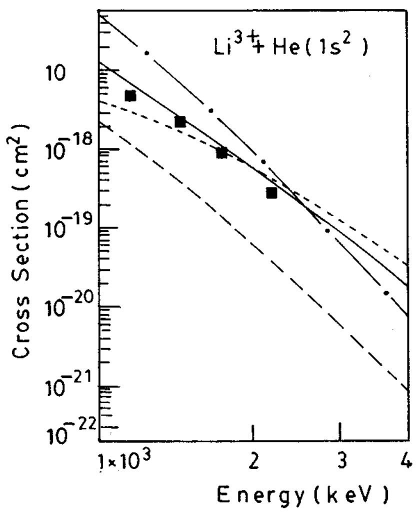

FIG. 1. Double-capture cross sections for Li^{3+}-He collisions vs incident energy. Theories: —, present calculations; –·–, CDW-IPM ($n,n'=1$–4) [22]; ----, CB1-4B [20]; ‒‒‒, CDW-4B [22]. Experiment: ■ Shah and Gilbody [6].

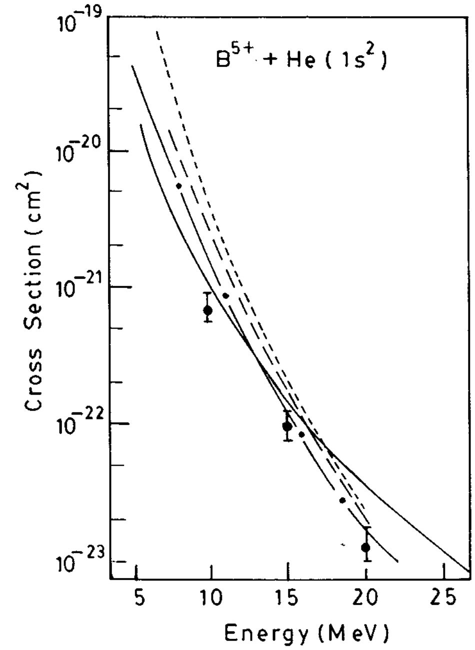

FIG. 2. Double-capture cross sections for B^{5+} -He collisions vs incident energy. Theories: —, present calculations; –·–··, OBK calculations for capture of one or both electrons into 1s [7]; ----, OBK calculations for capture into all n states [7]; ‒‒‒, CDW-IPM ($n,n'=1$–4) [22]. Experiments: ⧳ Hippler *et al.* [7].

and de Pinho [4] and Schuch *et al.* [5]. It is to be pointed out that Schuch *et al.* [5] mentioned that their measurements are likely to give somewhat lower values of the cross sections due to some technical problem. On the theoretical side, our results are fairly close to the CDW-IPM results of Gayet, Rivarola, and Salin [10] in low-energy regions whereas in the high-energy region boundary corrected continuum intermediate state (BCIS)-4B results of Belkić [21] agrees best with those of ours. Up to 1400 keV the other available results are due to Crothers and McCarroll [15] and Gravielle and Miraglia [18]. These two sets of results agree within a few percent, but are significantly lower than our results, as well as the measurements of McDaniel *et al.* [2]. This discrepancy may be attributed to the fact that these calculations [15,18] consider only ground-state capture. However, double capture by He^{2+} into the ground state from neutral He being a resonance process, is expected to be dominant. Interestingly the BCIS-4B [21] results of double capture into ground state agree well with our results that include contributions up to $n=4$ levels. It is clear from Eq. (1) that the present IEM differs from the IPM in calculating the total probability of double capture. While IEM calculates the total probability as P_1P_2, the IPM takes P_1^2. While calculating the P_1 and P_2 in the IEM we use different realistic screening charges for two different events that expect to take account of the correlation effect to a certain extent. In addition, by taking the product P_1P_2 (instead of P_1^2) correlation of events are, to a certain degree, also accounted for. However for a special case of resonant collision such as $He^{2+}+He(1s^2)\rightarrow He(1s^2)+He^{2+}$ if $P_1 \sim P_2$ then IEM is equivalent to IPM. But as the projectile charge increases the IPM usually overestimates the measurements.

In Fig. 1 we present our total double-capture cross sections (solid line) by Li^{3+} on He. In this figure we also present CDW-4B ($1s^2$) results (short dashed line) of Gayet *et al.* [22], CDW-IPM ($n,n'=1,\ldots,4$) results of (dashed-doted line) Gayet *et al.* [22], and CB1-4B ($1s^2$) results (dotted line) of Belkić [20]. The CDW-IPM results of Gayet *et al.* [22] accounted for the contributions up to $n=4$ levels. They have systematically presented the contributions for $n=1$, 2, 3, and 4 levels and found reasonable convergence up to $n=4$ level. We also find that the total double-capture cross section should include the contributions up to at least the $n=4$ level. However, our results show better agreement than those of Gayet *et al.* [22] with the measurement of Shah and Gillbody [6] (full squares). The four-body calculation (CB1-4B) of Belkić [20] shown in this figure exhibits different energy dependence. The CDW-4B results ($1s^2$) of Gayet *et al.* [22] are lower by a factor of about 3 throughout the energy range considered here. It is expected that these results would improve if contributions from excited states are taken into account. However, such a calculation in the CDW-4B approximation would be a difficult problem.

In Fig. 2 double-capture cross sections by B^{5+} are presented together with the experimental results (closed circles) and Oppenheimer-Brinkman-Kramers (OBK) calculations (short dash) of Hippler *et al.* [7]. We also present the results of Gayet *et al.* [22] (long dash). It is found that our results agree well with the measurements in the lower-energy side. In this case we calculate the double-capture cross sections also up to $n=4$ levels. Both the OBK calculations and the CDW-IPM results of Gayet *et al.* [22] overestimate the measured values. It is to be noted that the CDW-4B results are only for double capture into $1s^2$ levels.

IV. CONCLUSION

We have presented a method to calculate double-capture cross sections by fully stripped ions from the helium atom. The independent-event model is used with a recently developed single channel distorted-wave method. The present calculations account for electron-electron correlation through some realistic charge screening. The correlation of events is also accounted for by taking double-capture probability as a product of two single-electron capture probabilities in two successive events. Under the independent-event model our method being analytic is by far the simplest. As the projectile charge increases, our method shows better agreement with measurements as expected.

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