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TWO-ELECTRON PROCESSES IN He\textsuperscript{2+} + He COLLISIONS AT INTERMEDIATE IMPACT ENERGIES\textsuperscript{(1)}

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Abstract - Two electron processes in He\textsuperscript{2+} + He collisions are investigated theoretically within the independent electron approximation. The transition probabilities for double capture, transfer ionization and double ionization processes are expressed in terms of products of single electron transition probabilities which are calculated using the atomic orbital expansion method (AO). The effect of relaxation due to the change of screening in the second electron is examined by using a different effective charge in the calculation of single electron transition probabilities for the second electron. The role of electron correlation is partially explored for the double electron capture process by performing a two-electron version of the AO+ code.

1. INTRODUCTION

In ion-atom collisions involving many-electron systems, multi-electron transitions occur frequently. For the simplest two-electron transitions, processes such as double electron capture, double ionization and simultaneous ionization and capture can be observed experimentally when bare projectiles collide with two-electron atoms. The collision of He\textsuperscript{2+} + He at intermediate impact energies is one of the simplest systems where such two-electron transitions can be studied.

Theoretical studies of two-electron transitions are hampered by three difficulties. First, the transition probabilities for two-electron processes are in general much smaller than those for one-electron transitions, particularly at intermediate energies, making accurate calculations of these probabilities harder. Second, the role of electron correlation has to be properly treated. This requires elaborate wave functions for describing two-electron states. Third, the importance of "two-step" mechanism where two-electron transitions can be viewed as two successive one-electron transitions in a single collision has to be evaluated. This requires collision models beyond the first-order perturbation theory.

A complete theoretical model describing two-electron transitions would require the solution of the time-dependent Schrödinger equation for the two-electron system. The atomic and molecular orbital expansion methods used in the one-electron and quasi-one-electron systems have been generalized to two-electron systems for collisions at intermediate and low energies, respectively\textsuperscript{1,2}. In actual applications, the two-electron close coupling codes have been applied mostly to one-electron transitions only\textsuperscript{3}. To study processes such as double capture in He\textsuperscript{2+} + He collisions to doubly excited states\textsuperscript{4}, or transfer excitation to He**(2\textsuperscript{2}P\textsuperscript{2}) in He\textsuperscript{+} + H collisions\textsuperscript{5}, the two-electron AO+ code has been applied. In these selective applications, a large number of basis functions including both the single- and two-electron transitions have been included. Such more accurate calculation, though plausible, is not suitable for studying many variety of collision systems. Furthermore, the two-electron close coupling code so far has not been applied to processes involving ionizations. We thus have to examine the feasibility of adopting the simpler independent particle approximation\textsuperscript{6} to study these two-electron transitions.

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II. THEORY

There are a number of possible variants of the independent particle model for applications to multiple processes. Consider first the double electron capture process. Assume that there is no correlation and that there is no change of screening after the first electron is captured, we can obtain the double capture cross section \( \sigma_{cc} \) from the single electron capture probability \( P_c(b) \),

\[
\sigma_{cc} = 2\pi \int P_c^2(b) b db. \tag{1}
\]

If we assume that the second electron has relaxed and thus there is a change in the screening before it is captured, then there is a change of binding energy for the second electron from -0.904 au to -2.0 au, and hence a different capture probability \( P'_c(b) \), from the remaining target He\(^+\) ion. In this model, the double capture probability is calculated by employing the relation,

\[
\sigma_{cc} = 2\pi \int P_c(b)P'_c(b) b db. \tag{2}
\]

Similarly, we can obtain the cross sections for double ionization and transfer ionization as

\[
\sigma_{ii} = 2\pi \int P_i^2(b) b db. \tag{3}
\]

and

\[
\sigma_{ei} = 4\pi \int P_c(b)P_i(b) b db. \tag{4}
\]

if one assumes that the second electron is not relaxed (i.e., no change in screening). If one assumes that the second electron has relaxed, then the expressions for double ionization and transfer ionization are given by

\[
\sigma_{ii} = 2\pi \int P_i(b)P'_i(b) b db. \tag{5}
\]

and

\[
\sigma_{ei} = 2\pi \int (P_c(b)P'_i(b) + P_i(b)P'_c(b)) b db. \tag{6}
\]

respectively. In the equations above, \( P_c \) and \( P_i \) refer to single electron capture and single ionization probabilities, respectively.

For double capture to specific doubly excited states, a special consideration is needed. Assume that \( 2\Sigma^+ \) doubly excited states are formed in a collision. In the independent electron model the electronic wave function for the first electron in the \( n-2 \) subspace after the electron capture is given by

\[
\psi_1(\vec{r}_1; b) = \sum_{l,m} a_{2lm}(b)\phi_{2lm}(\vec{r}_1). \tag{7}
\]

where \( \phi_{nlm}(\vec{r}) \) are hydrogenic orbitals and the sum is over all allowed \( l \) and \( m \) values for \( n=2 \). A similar expression can be written for the second electron. The two-electron wave
functions are the symmetrized products (for singlet states) of single electron wave functions $\psi_1(\vec{r}_1; b)$ and $\psi_2(\vec{r}_2; b)$

$$\psi(1, 2) = \frac{1}{\sqrt{2}}[\psi_1(\vec{r}_1; b)\psi_2(\vec{r}_2; b) + \psi_1(\vec{r}_2; b)\psi_2(\vec{r}_1; b)].$$

The scattering amplitude $A(b)$ for each doubly excited state within the $2l2l'$ configuration is then obtained from the expansion

$$\psi(1, 2) = \sum_{LM} A_{LMS}(b)\phi_{LMS}(\vec{r}_1, \vec{r}_2),$$

where $\phi_{LMS}(\vec{r}_1, \vec{r}_2)$ is the wave function of each doubly excited state. We assume that configuration interaction (CI) within the intrashell $(n-2)$ is included, i.e.,

$$\phi_{LMS}(\vec{r}_1, \vec{r}_2) = \sum_i c_i \Phi(1, 2).$$

where $\Phi(1, 2)$ is the symmetrized two-electron product wave function. It is then straightforward to derive amplitudes $A_{LMS}(b)$ as

$$A_{LMS}(b) = \sqrt{2} \sum_i c_i \sum_{l_{1m_1}l_{2m_2}} c_{m_1m_2}^{l_1l_2} a_{2l_11m_1}(b)a_{2l_21m_2}(b).$$

where the $C$'s are the Clebsch-Gordan coefficients. The double electron capture cross section for each doubly excited state with usual quantum numbers $L, M$ and spin $S=0$ is then obtained from the amplitude $A_{LMS}$.

III. RESULTS AND DISCUSSION

A. State-Selective Double Electron Capture Cross Section

In a simplified calculation using the AO+ basis set for the He$_{2}^{+}$ + He(1s$^2$) system we use 19 states (12 states on the projectile, ten atomic orbitals for $n=1,2$ and 3 and two 1s UA's; 7 states on the target i.e., two 1s orbitals describing He ground state, three $n=2$ AO orbitals representing excited channels of the target and two UA orbitals, same as on the projectile). The UA orbitals give some representation of the continuum pseudostates. Following the analysis of the previous section we can evaluate the double electron capture cross section to each final doubly excited state. However, in order to compare with experiment, we note that the zero-degree Auger electron spectroscopy can only measure the cross section for the $M=0$ component (quantization axis is in the incident beam direction) and thus only the $M=0$ component from the calculation is compared with the experiment. The cross section obtained using two different independent electron model, without (solid line) and with- (dashed lines) screening, is shown in Fig. 1. We do not show the CDW results as they are far off the scale. Also shown in Fig. 1 are the calculated values of the cross section at two energies, obtained with the two-electron AO code. Despite the general agreement, we note that there is still a large quantitative discrepancy with the experimental data, the calculated cross section being about two to eight times larger than the measured values.
Fig. 1 State-selective double-electron capture cross sections (for 'S, 'P, and 'D states) in the collision process \( ^3\text{He}^{2+} + \text{He}(1s^2) \rightarrow ^3\text{He}(222^+)^* + \text{He}^{2+} \) at 100-500 keV energies. The theoretical curves (solid and dash) are determined without and with screenings in the calculation of the scattering amplitudes of the second electron. The results from the two-electron model are shown by crosses. The experimental data (full symbols) are taken from Zouros et al. (Ref. 7).

The discrepancies in Fig. 1 illustrate the difficulties of obtaining accurate state-selective double-electron capture cross sections from \textit{ab initio} calculations and the limitations of the independent electron model. (We stress that both models work quite well for the single electron capture and double capture to the ground state). This difficulty is mainly due to the smallness of the cross sections involved. We note that double electron capture to doubly excited states for the present collision system is more than two orders of magnitude smaller than the double capture to the ground state. Such small cross sections are sensitive to the convergence of the basis set used in the coupled channel calculations and to the independent electron model.

B. Transfer Ionization and Double Ionization Cross Section.

To calculate cross section involving ionization, a better representation of the continuum using a larger set of pseudostates is required. In view of this and the desire to understand the disagreement between the predicted and the measured state selective double electron capture cross section an elaborate atomic orbital calculation within the independent electron model has been performed (R. Shingal, C. D. Lin and Ashok Jain; to be submitted). A total number of 79 travelling atomic orbitals (60 on the target -10 s-, 10 p- and 10 d- type orbitals, and 19 on the projectile -5 s-, 4 p- and 2 d- type orbitals) have been used. These calculations have been performed using computer codes developed by Shingal (1984, unpublished ). The scattering amplitudes from such a one-electron model were combined to obtain transfer ionization, double ionization and total double capture cross section. The results at two energies and the comparison with experimental data is given in Table I. At the lower energies, we need to include double capture to doubly excited states as transfer ionization since the experiments measured the charge states of the projectile and the target after the collision. Given the fact that all these cross section were obtained from the amplitude computed in a single calculation, the agreement with the experimental data is remarkable.
Table I. Cross sections (in units of $10^{-16}\text{cm}^2$) for single capture $\sigma_c$ (summed over all states), single ionization $\sigma_i$, double capture $\sigma_{cc}$ (summed over double capture to ground and singly excited states), transfer ionization $\sigma_{ti}$ (including double capture to doubly excited states) and double ionization cross sections $\sigma_{ii}$ for $\text{He}^{2+} + \text{He}$ collisions at different energies. The experimental data is taken from Shah and Gilbody.\(^8\)

<table>
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<th>Impact Energy</th>
<th>Single Capture $\sigma_c$</th>
<th>Single Ionization $\sigma_i$</th>
<th>Double Capture $\sigma_{cc}$</th>
<th>Transfer Ionization $\sigma_{ti}$</th>
<th>Double Ionization $\sigma_{ii}$</th>
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References