J. Phys. B: At. Mol. Opt. Phys. 23 (1990) L799–L803. Printed in the UK

LETTER TO THE EDITOR

Double ionization of helium by alpha-particle impact

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Received 2 October 1990

Abstract. We present cross sections for double ionization of helium by alpha-particle impact within the independent-event model. Within this model the probability of ionizing the first electron (P_1) from neutral helium is calculated in the continuum distorted-wave (CDW) approximation using an explicitly correlated wavefunction of Pluvinage, whereas the probability of ionizing the second electron (P_2) from the He^+ ion is calculated in the CDW approximation with an eikonal initial state (CDW-EIS). The total probability for double ionization is then $P_1 P_2$ rather than the P_1^2 which is usually assumed in the independent-electron model. The calculated cross sections in the present model show excellent agreement with the measurement of Shah and Gilbody, at all energies above 200 keV/amu.

Two-electron transfer from a helium atom by fully stripped ions has recently received much attention, one of the motivations being to understand the role of electron–electron correlation in a variety of collision processes. Double ionization is one of these processes where electron–electron correlation may be expected to contribute to the total cross section in the lower and intermediate energy regions. Indeed, Fritsch and Lin (1990) found very recently that electron–electron correlation also plays an important role in other processes, such as double excitation, for projectiles of smaller charges. Because of the complexity of a correlated two-electron wavefunction, most of the theoretical investigations so far available are based on the independent-electron model. In this model the target wavefunction is described either by a one-electron hydrogenic wavefunction or by an uncorrelated Hartree–Fock type of wavefunction. Having calculated the single ionization probability by using these wavefunctions, one then squares this probablity, weights it by the impact parameter (ρ), and finally one integrates it over the impact parameter to get the double-ionization cross sections. In other words, and in particular if an uncorrelated Hartree–Fock type of two-electron wavefunction is considered for the target atom, the independent-electron model does not account for correlation, as it squares the single-ionization probability to get the corresponding double ionization probability. Very recently Shingal and Lin (1991) have reported a coupled-channel calculation with a large number of basis sets on each centre for one- and two-electron transfer processes within the independent-electron model. Using two different models with different screening charges and ionization energies they claimed that better agreement can be achieved for the two-electron transfer processes, such as double ionization, with their model B. However, they also pointed out that this change of screening charge and averaging the double ionization energy does not account for the effect of correlation. For very fast projectiles the effect

0953-4075/90/230799+05$03.50

of electron–electron correlation may not be significant. In this case the independent-electron model might be a reasonable description for double ionization (cf Salin 1987).

After the first ionization event occurs, the Hamiltonian, energy and target charge all change. The interacting system is now He^{++} on He^{+} with the other electron removed to the continuum. This is a purely Coulombic system and may be handled by an appropriate simple theoretical model. Besides, the probability of ionizing the second electron (P_2) from He^{+} by an alpha particle is expected to be smaller (cf Basbas *et al* 1973) than the probability of ionizing the first electron (P_1) from neutral helium. It is therefore advisable to calculate the two probabilities separately using suitable theoretical models and multiply them to get the double-ionization probability, especially when one does not account for the continuum electron–electron correlation explicitly through the wavefunction. In the present letter, however, we address these points in the independent-event model originally proposed by Crothers and McCarroll (1987). In our interpretation and extension of this model the two probabilities are calculated by applying two variants of the continuum distorted wave (CDW) approximation. To calculate P_1 we use the conventional CDW theory where we represent the target helium atom by the explicitly correlated two-electron Pluvinage (1950) wavefunction which is given by

$$\Psi_{\mathrm{Pluv}}(r_1, r_2, r_{12}) = c(k)(Z_{\mathrm{T}}^3/\pi)\exp(-Z_{\mathrm{T}}r_1 - Z_{\mathrm{T}}r_2 - \mathrm{i}kr_{12})\,{}_1F_1\left(1 + \frac{1}{2\mathrm{i}k}; 2; 2\mathrm{i}kr_{12}\right) \tag{1}$$

where $r_{12} = |\,\boldsymbol{r}_1 - \boldsymbol{r}_2\,|$, $c(k)$ is the normalization constant and the variational parameter k is determined by the usual energy minimization process. In (1) electron j has position coordinate $\boldsymbol{r}_j$ relative to the nucleus of the target with charge Z_{T}.

It is important to note that the Pluvinage wavefunction is in various ways a better approximation to the exactly correlated helium wavefunction than the Hartree–Fock or any other independent-electron model wavefunction. Firstly, it accounts for the static angular correlation (McGuire 1987). Secondly, it gives a more accurate estimation of the ground state energy than the Hartree–Fock wavefunction. Thirdly, it accounts for nearly 50% of the total correlation energy. The second ionization probability P_2 has been calculated by using the hybrid form of CDW and eikonal approximations (CDW-EIS) introduced by Crothers and McCann (1983). Total double-ionization cross sections are then calculated by

$$\sigma_{\mathrm{DI}} = 2\pi a_0^2 \int_0^\infty \rho P_1(\rho) P_2(\rho)\,\mathrm{d}\rho \tag{2}$$

where

$$P_j(\rho) = \int \mathrm{d}\boldsymbol{\kappa}_{\mathrm{T}}\,|\,a_j(\rho, \boldsymbol{\kappa}_{\mathrm{T}})\,|^2 \qquad j = 1, 2 \tag{3}$$

and

$$a_j(\rho, \boldsymbol{\kappa}_{\mathrm{T}}) = \frac{1}{2\pi v}\int_0^\infty \eta J_0(\eta\rho) T_j(\eta, \boldsymbol{\kappa}_{\mathrm{T}})\,\mathrm{d}\eta \tag{4}$$

where $\boldsymbol{\kappa}_{\mathrm{T}}$ is the momentum of the ionized electron and η is the transverse component of the change in momentum of the relative motion of the heavy particles.

The transition amplitude for the first ionization event is given by

$$T_1(\eta, \boldsymbol{\kappa}_\mathrm{T}) = \langle \chi_f^{(-)} \mid W_f^\dagger \mid \chi_i^{(+)} \rangle \tag{5}$$

where

$$\chi_i^{(+)} = \tfrac{1}{2}(1+\mathcal{P}_{12})\Psi_{\mathrm{Pluv}}(r_{\mathrm{T}1}, r_{\mathrm{T}2}, r_{\mathrm{T}12}) \exp(\mathrm{i}\boldsymbol{K}_i \cdot \boldsymbol{R}_i)\, D_P^{(+)}(\boldsymbol{\kappa}_\mathrm{P}, \boldsymbol{r}_{\mathrm{P}1}) \tag{6}$$

$$\begin{aligned} W_f\chi_f^{(-)} = &-\frac{1}{\sqrt{2}}(1+\mathcal{P}_{12})\,(2\pi)^{-3/2}\,\phi(r_{\mathrm{T}2}) \exp(\mathrm{i}\boldsymbol{\kappa}_\mathrm{T}\cdot\boldsymbol{r}_{\mathrm{T}1} + \mathrm{i}\boldsymbol{K}_{\mathrm{T}f}\cdot\boldsymbol{R}_i) \\ &\times \boldsymbol{\nabla}_{r_{\mathrm{T}1}} D_\mathrm{T}^{(-)}(\boldsymbol{\kappa}_\mathrm{T}, \boldsymbol{r}_{\mathrm{T}1}) \cdot \boldsymbol{\nabla}_{r_{\mathrm{P}1}} D_P^{(-)}(\boldsymbol{\kappa}_\mathrm{P}, \boldsymbol{r}_{\mathrm{P}1}) \end{aligned} \tag{7}$$

$$D_i^{(\pm)}(\boldsymbol{\kappa}_i, \boldsymbol{r}_i) = N^{(\pm)}(Z_i/\kappa_i)\, {}_1F_1(\pm\mathrm{i}Z_i/\kappa_i; 1; \pm\mathrm{i}\kappa_i r_i - \mathrm{i}\boldsymbol{\kappa}_i\cdot\boldsymbol{r}_i) \tag{8}$$

$$N^{(\pm)}(\nu) = \exp(\pi\nu/2)\,\Gamma(1 \mp \mathrm{i}\nu). \tag{9}$$

Here the subscript i refers to the corresponding quantities associated with either the target (T) or the projectile (P) nucleus. Accordingly, $\boldsymbol{r}_{\mathrm{T}1}, \boldsymbol{r}_{\mathrm{P}1} \ldots$ are the position vectors of the electron 1 with respect to target and projectile nucleus respectively and $r_{\mathrm{T}12} = \mid \boldsymbol{r}_{\mathrm{T}1} - \boldsymbol{r}_{\mathrm{T}2} \mid$. $\boldsymbol{K}_i$ is the initial relative momentum and $\boldsymbol{K}_{\mathrm{T}f}$ is the final relative momentum of the aggregate heavy particles and $\boldsymbol{\kappa}_P = \boldsymbol{\kappa}_\mathrm{T} - \boldsymbol{v}$ where v is the impact velocity. The permutation operator $\mathcal{P}_{12}$ in (6) and (7) stands for interchanging coordinates of two indistinguishable electrons 1 and 2 .

From (7) it is to be noted that in the final channel we considered a ground-state hydrogenic orbital $\phi(r_{\mathrm{T}2})$ for the second electron remaining bound to the target nucleus and we describe the ionized electron 1 by a hydrogenic target continuum orbital simultaneously distorted by the projectile in the usual CDW manner (Crothers and McCann 1983). However, we do not account for the so called scattering correlation (McGuire 1987) i.e. the explicit correlation of these two electrons through the Coulomb repulsion $(1/r_{12})$ in the scattering operator. The integrals in (5) are then separable into one-centre integrals: a three-dimensional integral with respect to the projectile nucleus and a six-dimensional integral with respect to the target nucleus. The first one is evaluated analytically while, following closely the appendix of Crothers and McCarroll (1987), the second integral has been reduced to a two-dimensional integral (Dunseath and Crothers 1991, Dunseath 1990). Ionization of the second electron from the residual He^+ ion by an alpha particle is considered to be an isolated second event with the first electron removed to the continuum and the transition amplitude for this system is calculated using the CDW-EIS model of Crothers and McCann (1983). This, after all, follows the prescription of the first event, in the absence of electron 1, but with a normalized eikonal initial state (EIS). This approximation has had considerable success in describing single ionization in a one-active-electron situation (Crothers and McCann 1983, Fainstein *et al* 1987, 1988a,b). Recent measurements of Andersen *et al* (1990) have also provided strong evidence of the suitability of the CDW-EIS approximation for single ionization.

In figure 1 we present our total cross sections for double ionization of He by alpha particle impact together with the measurements of Shah and Gilbody (1985) and the multi-state coupled-channel calculation of Shingal and Lin (1991). The impact energy is denoted by E (keV/amu). Above 200 keV/amu our results give excellent agreement with the measurement at all the energies at which the measurements are reported. However, below 200 keV/amu our results start to overestimate the data and also

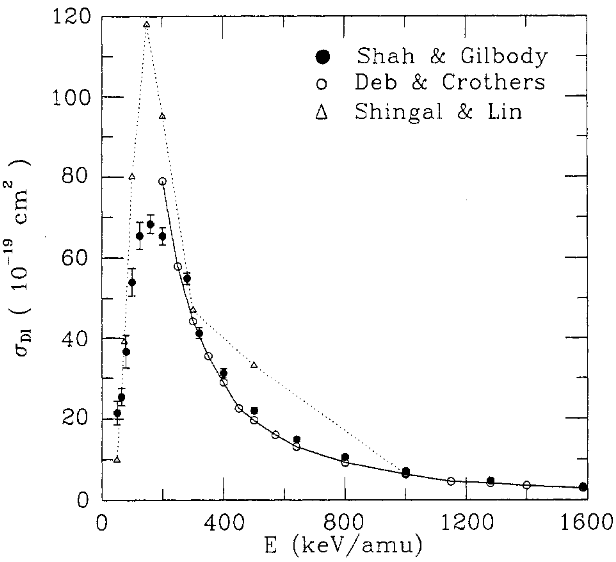

Figure 1. Total cross sections for double ionization of He by He^{++} impact as a function of incident energy E (keV/amu). Full circles: measurement of Shah and Gilbody (1985); open circles: present calculation; open triangles: Shingal and Lin (1991). Full and dotted curves are drawn through the theoretical results to guide the eye.

Table 1. Total double ionization cross sections in units of $10^{-19}cm^2$ for alpha particle impact on helium atoms. DC: present calculation; SG: measurement of Shah and Gilbody (1985).

E (keV/amu)	DC ($10^{-19}cm^2$)	SG ($10^{-19}cm^2$)
400.0	28.83	31.1 ± 1.1
500.0	19.52	21.9 ± 0.7
640.0	13.03	14.8 ± 0.5
800.0	9.15	10.53 ± 0.47
1000.0	6.29	7.07 ± 0.5

fail to peak at lower energies. This is due in part to the usual CDW normalization problem at the lower energies. It is interesting to note that the coupled-channel calculation of Shingal and Lin (1991) involves as many as 79 atomic states (pure and pseudo) based on each of the alpha particle nuclei. Their results, however, do not appear to be as accurate, compared to the measurement, as the results we are reporting here. Further modifications have been made (Shingal 1990) to this coupled-channel calculation, by employing a two-step mechanism, to account to some extent for correlation; the preliminary results show some improvement over the results of Shingal and Lin (1991). The excellent agreement of our results with the measurements indicates the importance of the role of correlation in two-electron processes like double ionization. The essence of the present calculation is not only that we account for correlation through the initial target wavefunction, but also that we include dynamic correlation by our very formulation of the independent-event model in which first one electron is ionized and then the second one; that is, we invoke the concept of correlation of events, as against particles. For completeness we also present our numerical cross sections for double ionization in table 1 together with measurements of Shah and Gilbody at several energies.

We thank Dr R Shingal for communicating the results of Shingal and Lin (1991) prior to publication and Dr K M Dunseath for his assistance with the calculation of P_1. Most of the computing was done on the CRAY X-MP/48 and 416 at RAL. This work is supported by the Science and Engineering Research Council, UK, through grant GR/E 94388.

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