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Double ionization of helium by fully stripped ions in the independent-event model

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Abstract. Double ionization of He by fully stripped ions are studied within the independent-event model. Ionization of each of the two electrons in He are considered to be independent events and probabilities for these events are calculated individually by using the continuum-distorted-wave approximation. Electron-electron correlation has been accounted for through the explicitly correlated two-electron wavefunction of Pluvinage. Good agreement between our results and measurements are attributed to this static correlation as well as to the dynamical correlation of events as against particles.

1. Introduction

In a recent letter (Deb and Crothers 1990, to be referred to as I) and following the work of Dunseath (1990) and Dunseath and Crothers (1991) on transfer ionization we have demonstrated that the independent-event (IEV) model in conjunction with continuum-distorted-wave (CDW) theory can describe successfully a two-electron process such as double ionization in the intermediate and high energy region. The idea of the IEV model is to consider the transition of a single electron as an isolated event and is independent of any subsequent or preceding event of another transition. Probabilities for these transitions are then calculated separately by suitable theoretical models and are multiplied to obtain the total probability for the two-electron process. By doing so one can account for correlation of events as against particles, which is usually ignored in the independent-electron (IEL) model. (This is not to say that some two-electron transitions may not be well described in a two step mechanism based on the IEL method (Shingal 1990).) More specifically, the important difference between the IEV and the IEL models can be seen as follows. For example, let us consider the probability of ionizing one electron from neutral He by He^{2+} as P_1, and in a subsequent process of ionization of the second electron from He^+ ion the probability is P_2. Due to the change of effective charges for the two processes, it is predicted (Basbas *et al* 1973, Ford and Reading 1990) that $P_2 < P_1$ which means $P_1^2 > P_1P_2$. In other words describing double ionization by using P_1^2 (rather than P_1P_2), usually done in the IEL model, could overestimate the cross sections especially in the low and intermediate energy region. In fact calculations in this model give cross sections larger than measurements (cf Shingal and Lin 1991). In the original work of Crothers and McCarroll (1987) where this IEV model was proposed, double capture probabilities were calculated by squaring the single-electron transition probability. This was justified because double capture by alpha particle from helium is a special case resonant transition when the two probabilities are expected to be equal.

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It is now well recognized that double ionization is sensitive to electron–electron correlation (Knudsen *et al* 1984, Heber *et al* 1990). Therefore it is important to account for some sort of correlation in a calculation of double ionization cross sections. There are several ways (McGuire 1987) of accounting for it, for instance (*a*) static correlation which comes through the target wavefunction and (*b*) scattering correlation coming through the transition operator. In the following we shall adopt the static correlation by using the explicitly correlated helium wavefunction due to Pluvinage (1950). This wavefunction has several advantages; it gives more accurate ground state energy than the Hartree–Fock wavefunction and accounts for nearly 50% of the correlation energy. The correlation energy is defined to be the difference between the experimental and the Hartree–Fock energy. From the above points of view the six-parameter Hylleraas (1929) wavefunction might be even better but is computationally far more expensive than the Pluvinage (1950) wavefunction. We shall illustrate this point later in the theory section.

In the next section we present a brief account of the formulation in the notation of I and show how the complicated integrals are evaluated and in section 3 we present details of results of double ionization of He by H^+ and Li^{3+} ions at various energies.

2. Theory

We consider the double ionization of He by a fully stripped ion A^{q+} as a two-step process:

$$A^{q+} + He(1s^2) \rightarrow A^{q+} + He^+(1s) + e^- \tag{1}$$

$$\rightarrow A^{q+} + He^{2+} + 2e^-. \tag{2}$$

Under the independent-event model the two reactions (1) and (2) are considered to be independent and the probabilities for the two reactions P_1 and P_2 respectively are calculated individually using CDW theory. The total double ionization cross sections are then calculated by

$$\sigma_{DI} = 2\pi a_0^2 \int_0^\infty \rho P_1(\rho) P_2(\rho)\, d\rho \tag{3}$$

where

$$P_j(\rho) = \int d\boldsymbol{\kappa}_T |a_j(\rho, \boldsymbol{\kappa}_T)|^2 \qquad j = 1, 2 \tag{4}$$

and

$$a_j(\rho, \boldsymbol{\kappa}_T) = \frac{1}{2\pi v} \int_0^\infty \eta J_0(\eta\rho) T_j(\eta, \boldsymbol{\kappa}_T)\, d\eta \tag{5}$$

where $\boldsymbol{\kappa}_T$ 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.

2.1. Calculation of T_1 and T_2

The full CDW approximation has been used to calculate the transition amplitude T_1. The matrix element for ionizing the first electron is given by

$$T_1(\eta, \boldsymbol{\kappa}_T) = \langle \chi_f^{(-)} | W_f^+ | \chi_i^{(+)} \rangle \tag{6}$$

where

$$\chi_i^{(+)} = \tfrac{1}{2}[1+\mathscr{P}_{12}]\Psi_{\text{pluv}}(r_{T1}, r_{T2}, r_{T12}) \exp(\mathrm{i}\boldsymbol{K}_i \cdot \boldsymbol{R}_i) D_P^{(+)}(-\boldsymbol{v}, \boldsymbol{r}_{P1}) \tag{7}$$

$$W_f \chi_f^{(-)} = -\frac{1}{\sqrt{2}}[1+\mathscr{P}_{12}](2\pi)^{-3/2}\phi(r_{T2}) \exp(\mathrm{i}\boldsymbol{\kappa}_T \cdot \boldsymbol{r}_{T1} + \mathrm{i}\boldsymbol{K}_{Tf} \cdot \boldsymbol{R}_i)$$
$$\times \nabla_{r_{T1}} D_T^{(-)}(\boldsymbol{\kappa}_T, \boldsymbol{r}_{T1}) \cdot \nabla_{r_{P1}} D_P^{(-)}(\boldsymbol{\kappa}_P, \boldsymbol{r}_{P1}) \tag{8}$$

$$\Psi_{\text{pluv}}(r_1, r_2, r_{12}) = c(k)(Z_T^3/\pi) \exp(-Z_T r_1 - Z_T r_2 - \mathrm{i}kr_{12})\, {}_1F_1(1+1/2\mathrm{i}k; 2; 2\mathrm{i}kr_{12}) \tag{9}$$

$$D_i^{(\pm)}(\boldsymbol{\kappa}_i, \boldsymbol{r}_i) = N^{(\pm)}(Z_i/\kappa_i)\, {}_1F_1(\pm \mathrm{i}Z_i/\kappa_i; 1; \pm \mathrm{i}\kappa_i r_i - \mathrm{i}\boldsymbol{\kappa}_i \cdot \boldsymbol{r}_i) \tag{10}$$

$$N^{(\pm)}(\nu) = \exp(\pi\nu/2)\Gamma(1 \mp \mathrm{i}\nu). \tag{11}$$

In (9) k is the variational parameter determined to be 0.41 by energy minimization technique and the normalization constant $c(k)$ is then worked out to be $c(0.41) = (0.364\,05)^{1/2}$. The subscript i in (10) stands either for target (T) or projectile (P). The permutation operator $\mathscr{P}_{12}$ in (7) and (8) stands for interchanging coordinates of two indistinguishable electrons 1 and 2. Substituting (7)–(11) in (6) the integrals may be separated as follows:

$$T_1(\eta, \boldsymbol{\kappa}_T) \equiv \frac{1}{\sqrt{2}}(2\pi)^{-3/2} I_P \cdot I_T \tag{12}$$

where

$$I_P = \int \mathrm{d}\boldsymbol{r}_P \exp(-\mathrm{i}\boldsymbol{K}_T \cdot \boldsymbol{r}_P) D_P^{(+)}(-\boldsymbol{v}, \boldsymbol{r}_P) \nabla_{r_P} D_P^{(-)*}(\boldsymbol{\kappa}_P, \boldsymbol{r}_P) \tag{13}$$

and

$$I_T = \int \mathrm{d}\boldsymbol{r}_{T1}\, \mathrm{d}\boldsymbol{r}_{T2}\, \phi^*(\boldsymbol{r}_{T2}) \Psi_{\text{pluv}}(\boldsymbol{r}_{T1}, \boldsymbol{r}_{T2}) \exp(\mathrm{i}\boldsymbol{K}_T \cdot \boldsymbol{r}_{T1} - \mathrm{i}\boldsymbol{\kappa}_T \cdot \boldsymbol{r}_{T1})$$
$$\times \nabla_{r_{T1}} D_T^{(-)*}(\boldsymbol{\kappa}_T, \boldsymbol{r}_{T1}). \tag{14}$$

Apart from the vector derivative, (13) is a limiting case of the Nordsieck (1954) type of integrals and can be evaluated analytically and then performing the derivative we arrive at

$$I_P = 2\pi\mathrm{i}Z_P N^{(+)}(\nu_P) N^{(+)}(\omega_P) \alpha^{-1} (\alpha+\gamma)^{-1} \left(\frac{\alpha}{\alpha+\beta}\right)^{\mathrm{i}\nu_P} \left(\frac{\alpha}{\alpha+\gamma}\right)^{\mathrm{i}\omega_P}$$
$$\times \{A\boldsymbol{K}_T - Bv(\hat{\boldsymbol{v}} - \hat{\boldsymbol{\kappa}}_P)\} \tag{15}$$

where

$$A = {}_2F_1(\mathrm{i}\nu_P; \mathrm{i}\omega_P; 1; Z) - \left(\frac{\beta+\delta}{\alpha+\gamma}\right) B$$

$$B = \mathrm{i}\nu_P \left(\frac{\alpha}{\alpha+\beta}\right) {}_2F_1(1+\mathrm{i}\nu_P; 1+\mathrm{i}\omega_P; 2; Z)$$

$$\alpha = K_T^2/2 \qquad \beta = -\boldsymbol{v} \cdot \boldsymbol{K}_T \qquad \gamma = -\boldsymbol{\kappa}_P \cdot \boldsymbol{K}_T \qquad \delta = \boldsymbol{v} \cdot \boldsymbol{\kappa}_P - v\kappa_P$$

$$\boldsymbol{\kappa}_P = \boldsymbol{\kappa}_T - \boldsymbol{v} \qquad \boldsymbol{K}_T = \boldsymbol{K}_i - \boldsymbol{K}_{Tf} \qquad \omega_P = Z_P/\kappa_P \qquad \nu_P = Z_P/v$$

$$Z = \frac{\beta\gamma - \alpha\delta}{(\alpha+\beta)(\alpha+\gamma)}.$$

Here $\boldsymbol{K}_i$ is the initial relative momentum and $\boldsymbol{K}_{Tf}$ is the final relative momentum of the aggregate heavy particles.

Following the appendix of Crothers and McCarroll (1987) the six-dimensional integral I_T in (14) is then reduced to a two-dimensional one:

$$I_T = 8\pi i C \kappa_T \nabla_{\kappa_T} \frac{\partial}{\partial \mu} \int_{\Gamma-i\infty}^{\Gamma+i\infty} dq\, \tilde{f}(q) \left\{ -\frac{1}{2\mu}\left[\ln\left(\frac{\mu+q}{\mu-q}\right) + i\pi \right] \right.$$
$$\left. \times \frac{(\mu+ik)^{-1+1/2ik}}{(\mu-ik)^{1+1/2ik}} + \int_{\Gamma-i\infty}^{q} dp(\mu^2-p^2)^{-1} \frac{(-p+ik)^{-1+1/2ik}}{(-p-ik)^{1+1/2ik}} \right\} \tag{16}$$

where

$$\tilde{f}(q) = \{Q^2 + (Z_T+q)^2\}^{-1+i\omega_P} \{Q^2 + (Z_T+q)^2 + 2\boldsymbol{\kappa}_T \cdot \boldsymbol{Q} - 2i\kappa_T(Z_T+q)\}^{-i\omega_T}$$

$$C = c(k)\left(\frac{Z_T}{\pi}\right)^{3/2} N^{(+)}(\omega_T) \qquad \omega_T = Z_T/\kappa_T \qquad \boldsymbol{Q} = \boldsymbol{K}_T - \boldsymbol{\kappa}_T$$

and $-Z_T < \Gamma < 0$.

At this point we note that the q-integrand involves a derivative with respect to $\mu(=2Z_T)$ which originates from one of the single-parameter hydrogenic 1s orbitals in (9) and (14). A six-parameter Hylleraas (1929) wavefunction would lead to several more terms with multiple derivatives at this stage. We also recall that after the q-integration is performed we still need to perform four more numerical integrations (three over $\boldsymbol{\kappa}_T$ and one over ρ, the impact parameter). The typical CPU time in the CRAY X-MP for the calculation of a double ionization cross section at one energy with the Pluvinage wavefunction is 90 min. This means the addition of several more terms at this stage (as a result of using the Hylleraas wavefunction) would significantly increase the CPU time.

We then perform the derivatives with respect to $\boldsymbol{\kappa}_T$ and μ in (16) and after doing the scalar product with (15) we finally get

$$T_1 = -\frac{8i}{\pi} Z_P Z_T^{11/2} c(k) N^{(+)}(\nu_P) N^{(+)}(\omega_P) N^{(+)}(\omega_T) \alpha^{-1} (\alpha+\gamma)^{-1} \left(\frac{\alpha}{\alpha+\beta}\right)^{i\nu_P} \left(\frac{\alpha}{\alpha+\gamma}\right)^{i\omega_P}$$
$$\times \int_{\Gamma-i\infty}^{\Gamma+i\infty} dq [a(q)]^{-1-i\omega_T} [b(q)]^{-1+i\omega_T} L_1(q)$$
$$\times \{A(K_T^2 - [\kappa_T + i(Z_T+q)]\hat{\boldsymbol{\kappa}}_T \cdot \boldsymbol{K}_T)$$
$$- B(v \cdot \boldsymbol{K}_T - v\hat{\boldsymbol{\kappa}}_P \cdot \boldsymbol{K}_T - [\kappa_T + i(Z_T+q)][v \cdot \hat{\boldsymbol{\kappa}}_T - v\hat{\boldsymbol{\kappa}}_P \cdot \hat{\boldsymbol{\kappa}}_T])\} \tag{17}$$

where

$$L_1(q) = \frac{1}{8Z_T^2} \frac{(2Z_T+ik)^{-1+1/2ik}}{(2Z_T-ik)^{1+1/2ik}}$$
$$\times \left\{ \left[\ln\left(\frac{2Z_T+q}{2Z_T-q}\right) + i\pi \right] \left[1 + \frac{2Z_T(4Z_T+1)}{4Z_T^2+k^2} \right] + \frac{4Z_T q}{4Z_T^2-q^2} \right\}$$
$$- 4Z_T \int_{\Gamma-i\infty}^{q} dp(4Z_T^2-p^2)^{-2} \frac{(-p+ik)^{-1+1/2ik}}{(-p-ik)^{1+1/2ik}}$$

$$a(q) = K_T^2 - \{\kappa_T + i(Z_T+q)\}^2 \qquad b(q) = K_T^2 + \kappa_T^2 - 2\boldsymbol{\kappa}_T \cdot \boldsymbol{K}_T + (Z_T+q)^2.$$

The transition amplitude T_2 for ionizing the second electron from the He^+ ion (reaction (2)) is calculated again by using CDW approximation but with an eikonal initial state (CDW-EIS). Details of this calculation were presented by Crothers and McCann (1983). This approximation is found to be quite satisfactory in recent calculations (Fainstein *et al* 1987, 1988a, b) as well as in measurement (Andersen *et al* 1990).

3. Results and discussions

We apply the above technique to calculate the double ionization cross sections for H^+ and Li^{3+} impact on He. In figure 1 we present our results for proton impact and compare with the measurements of Shah and Gilbody (1985) and in table 1 we compare our results of Li^{3+} impact with available calculation and measurements. The general agreement in the former case is satisfactory over 200 keV/amu whereas in the latter case the results tend to agree in the MeV/amu region. This behaviour is consistent

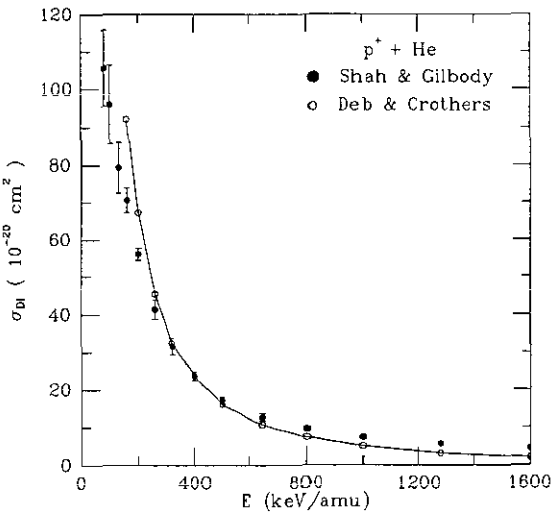

Figure 1. Total cross sections for double ionization of He by H^+ impact as a function of incident energy E (keV/amu). Full circles: measurement of Shah and Gilbody (1985); open circles: present calculation. A full curve is drawn through the present results to guide the eye.

Table 1. Total double ionization cross sections in units of 10^{-19} cm^2 for Li^{3+} impact on helium atoms. DC, present calculation; SL, Shingal and Lin (1991); SG, Shah and Gilbody (1985); KD, Knudsen *et al* (1984).

E (keV amu^{-1})	DC	SL	SG	KD
200.0	236.2	303.0	192.0 ± 8.0	—
313.0	131.8	374.0	153.0 ± 8.0	—
390.0	99.73	260.0	126.0 ± 4.0	—
640.0	46.9	—	—	74.0 ± 8.1
1440.0	12.5	—	—	18.0 ± 2.0
2310.0	5.53	—	—	8.5 ± 0.9

with the analysis of Knudsen *et al* (1984). Based on the results of Bohr (1948) they analysed that the perturbative approaches should be valid for the region where a parameter $\kappa(=2qv_0/v)$ is well below unity. Here q is the projectile ion charge, v_0 and v are the Bohr velocity and the ion velocity respectively. Clearly, as q increases, v has to be increased significantly to maintain κ being well below unity. Considering our results presented here and our results of He^{2+} impact (presented in I) we note that the best regions of agreement are over 400 keV/amu for proton impact, 700 keV/amu for alpha particle impact and 1 MeV/amu for Li^{3+} impact. On the other hand the region, where $\kappa \geqslant 1$, corresponds to $v \leqslant 2, 4, 6$ for H^+, He^{2+} and Li^{3+} impact respectively. In these cases our results start to deviate from the measurements. However, down to 200 keV/amu our results are closer to the measurements than those of Shingal and Lin (1991). We have not yet considered the question of the ratio R of double to single ionization for both proton and antiproton projectiles, which has been well discussed by Reading and Ford (1987) in the forced impulse method and by Olson (1987) in the classical trajectory Monte Carlo method. However, we note that single ionization is to be discussed within the current model (Dunseath and Crothers 1991) and that CDW-EIS has been considered successful in accounting for the difference between proton and antiproton impact (Fainstein *et al* 1988b).

4. Conclusion

The independent event model has been applied for the first time to calculate double ionization cross sections of helium by fully stripped ions. Results are found to be in very good agreement with the measurements in the intermediate and high energy region. We attribute the good agreement between our results and measurements to the new approaches in our calculation: first, accounting the electron-electron correlation through the initial target wavefunction; and second, adopting the independent event model which accounts correlation of events as against particles.

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