The Effect of Correlation on the Double Ionization of Helium by Fast Electrons*

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The double ionization of helium by fast electrons is studied by using a correlated double continuum wave function describing the two ejected electrons.

Key words: Double-ionisation processes; Scattering cross-section; Electron scattering, inelastic; Electron correlation.

Introduction

The double ionization constitutes a problem of considerable importance in many branches of physics such as astrophysics, plasma and fusion studies. The recent progress in multiple detection in coincidence [1] permits us to perform measurements revealing the nature of the mechanism of this process. Preliminary theoretical studies [2, 3] have shown the importance of electronic correlation in the description of the initial state of a colliding system consisting of a fast incident electron and a stable atom. Recent results [4] have also shown the importance of correlation in the description of the final state, that is the double continuum of the two ejected electrons.

The purpose of our present work is to perform, for the first time, calculations in which the correlation in both states is taken into account. This is possible by the use of Hylleraas-type solutions for the initial state and a correlated double continuum function proposed by Brauner, Briggs, and Klar [6], which consists of a product of three Coulomb wave functions containing r_{12} and r_{12} and r_{12} .

Method

The first Born approximation permits us to write the differential cross-section in the form

$$\frac{\mathrm{d}^5 \sigma}{\mathrm{d}\Omega_{\mathrm{s}} \, \mathrm{d}\Omega_{\mathrm{1}} \, \mathrm{d}\Omega_{\mathrm{2}} \, \mathrm{d}(k_1^2/2) \, \mathrm{d}(k_2^2/2)} = \frac{(2 \, \pi)^4 \, k_{\mathrm{s}} \, k_{\mathrm{1}} \, k_{\mathrm{2}}}{k_{\mathrm{i}}} \, | \, T_{\mathrm{fi}} |^2 \,,$$

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where Ω and k represent the solid angles and the moduli of the different wave vectors, respectively (Figure 1). The conservation of energy imposes

$$\frac{k_{\rm i}^2}{2} = I^{2+} + \frac{k_{\rm s}^2}{2} + \frac{k_{\rm 1}^2}{2} + \frac{k_{\rm 2}^2}{2} \,, \tag{2}$$

 I^{2+} being the ionization energy, and

$$T_{\rm fi} = \langle \Psi_{\rm f}^- | V | \Psi_{\rm i} \rangle , \qquad (3)$$

with

$$V = -\frac{Z}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}}. (4)$$

We describe the initial state by

$$|\Psi_{i}\rangle = \left|\frac{e^{i\mathbf{k}_{i}\cdot\mathbf{r}_{0}}}{(2\pi)^{3/2}}\,\varphi_{i}(\mathbf{r}_{1},\mathbf{r}_{2})\right\rangle \tag{5}$$

and the final state by

$$\langle \Psi_{\mathbf{f}}^{-}| = \left\langle \frac{e^{i \mathbf{k_s} \cdot \mathbf{r_0}}}{(2\pi)^{3/2}} \, \varphi_{\mathbf{f}}(\mathbf{r_1}, \mathbf{r_2}) \right|, \tag{6}$$

where (7)

$$\varphi_{\rm i}({\pmb r}_1\,,{\pmb r}_2) = N[e^{-a{\pmb r}_1}\,e^{-b{\pmb r}_2} + e^{-b{\pmb r}_1}\,e^{-a{\pmb r}_2}]\,[1 + c\,{\pmb r}_{12}]\,.$$

The values of the variational parameters a, b, and c are given by Bonham et al. [5].

$$\varphi_{\mathbf{f}}(\mathbf{r}_1 \cdot \mathbf{r}_2) = M e^{i\mathbf{k}_1 \cdot \mathbf{r}_1} e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} \chi(\mathbf{r}_1, \mathbf{r}_2)$$
(8)

with

$$\chi(\mathbf{r}_{1}, \mathbf{r}_{2}) = \prod_{j=1}^{3} {}_{1}F_{1}(-i\alpha_{j}, 1; i(k_{j} r_{j} + \mathbf{k}_{j} \cdot \mathbf{r}_{j})), \quad (9)$$

where j=3 corresponds to r_{12} and k_{12} .

For the T matrix element we finally obtain the expression (10)

$$T_{\text{fi}} = A \left[-Z G(k_1, k_2) + G(k - k_1, k_2) + G(k_1, k - k_2) \right],$$

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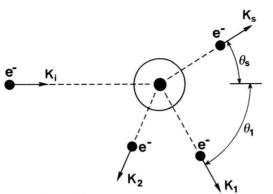


Fig. 1. The incident, scattered and ejected electron's wave vectors.

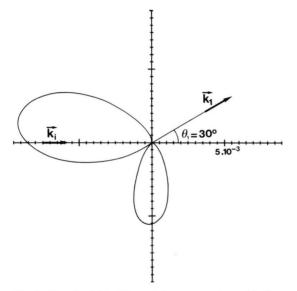


Fig. 2. The fivefold differential cross-section of helium in polar coordinates $(\sigma^{(5)}, \Theta_2)$, for an incident-electron energy of 5109 eV, the energies of the two ejected electrons being 10 eV and 20 eV, respectively. The first electron ejection angle is fixed to 30 degrees. The axes are calibrated in $5 \cdot 10^{-4}$ atomic units of the fivefold differential cross-section per division.

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where
$$G(\mathbf{k}_{1}, \mathbf{k}_{2}) = \omega(\mathbf{k}_{1}, \mathbf{k}_{2}, a, b, 0) + \omega(\mathbf{k}_{1}, \mathbf{k}_{2}, b, a, 0)$$
 (11)

$$+ c(\omega(\mathbf{k}_1, \mathbf{k}_2, a, b, 1) + \omega(\mathbf{k}_1, \mathbf{k}_2, b, a, 1))$$

with

$$\omega(\mathbf{k}_1, \mathbf{k}_2, a, b, n) \tag{12}$$

$$= \int e^{-i\mathbf{k}_1 \cdot \mathbf{r}_1 - a\mathbf{r}_1} e^{-i\mathbf{k}_2 \cdot \mathbf{r}_2 - b\mathbf{r}_2} r_{12}^n \chi(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2.$$

We have been able to perform this integration following the methods elaborated in [6-11].

Results

After having performed some preliminary verifications by applying our procedure to situations for which theoretical results were available [4] we proceeded in the determination of the five-fold differential cross-section (5 DCS) for the double ionization of helium

Using typical experimental conditions [1] of high incident-electron energy (5109 eV) and scattering angle $\Theta_s = 1^\circ$, and fixing the ejection angle of the first electron to $\Theta_1 = 30^\circ$ and the energy values of the two ejected electrons to 10 eV and 20 eV, respectively (Fig. 2), we determined the 5 DCS for different values of the solid ejection angle of the second electron, Θ_2 , varying between 0° and 360° .

Figure 2 represents the variation of the 5DCS in polar coordinates. Here Θ_2 is taken as polar angle and the 5DCS as polar distance.

Comparing our results to those obtained by procedures using other types of final-state wave functions constructed by products of two Coulomb wave functions with variable nuclear charges [4], we observe large differences in the angular distributions, revealing the importance of the correlation in the final state.

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