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On the orthogonality of initial and final states in (e,3e) and (γ,2e) collisions

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Abstract

We present a comparative study of multiple differential cross-sections in (e,3e) and (γ,2e) processes. We make use of initial states with different angular and radial electron–electron correlation factors in a perturbative model, and a C3 wave function to describe the final state. We also compute orthogonality factors between initial and final states. All the calculations show that a simple angular correlation can be used to achieve good qualitative as well as quantitative agreement with experimental results.

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1. Introduction

In recent years there has been an increasing number of experiments that involve quantum states of two electrons in the continuum of an ionic target. Besides the well-known double photoionization of atoms, multiple differential cross-sections of double ionization of electrons by charged projectiles have been obtained [1].

From a theoretical point of view, perturbative models have proven to be both accurate as well as reliable in the description of many different collision environments involving the double ionization of many-electron atoms, either by charged projectiles or photons. Assuming this perturbative regime, the initial and final states of the system can be modeled with a variety of wave functions. The electron–nucleus interaction can be represented in helium-like atoms by a Coulomb wave functions, while the correlation between the electrons can be introduced in different ways [2]. In the initial state, correlation has been included in a wide range of approximations, starting from simple perturbation models to Hylleraas functions of many parameters [3–6]. These functions usually provide a good qualitative agreement with experiments in (e,2e), (e,3e) and (γ,2e) processes. However, many quantitative discrepancies remain, and, although some of them have been pointed out before [7], many more need to be thoroughly analyzed.

In this work we perform a comparative analysis of differential cross-sections of (e,3e) and (γ,2e) processes on He atoms. We make use of initial states with different e–e correlations. In Section 2 we introduce the basic elements of perturbative theories, and in Section 3 we present the results of our calculations. We draw some conclusions in Section 4, and envision possible solutions for the discrepancies obtained. Atomic units are used through the paper, unless otherwise noted.

2. Theory

Perturbative models for the computation of differential cross-sections rely on the accurate description of initial and final wave functions of the system. The transition matrix in these models can be written as

$$T_{\mathrm{if}} = \langle \Psi_{\mathrm{f}}^{-} | V_{\mathrm{i}} | \psi_{\mathrm{i}} \rangle. \tag{1}$$

The wave function Ψ_{f}^{-} is the exact solution for the three-body continuum, while V_{i} is the initial channel perturbation potential

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that is left aside when computing the approximate solution ψ_i of the Schrödinger equation.

The potential V_i for (e,3e) processes can be written as

$$V_\mathrm{i} = -\frac{Z}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}}, \tag{2}$$

where we have assumed the Born approximation. r_0 is the coordinate of the projectile, whose relative distance from the two ejected electrons are r_{01} and r_{02}, respectively. As usual, Z is the charge of the ionic core. Within the Born approximation, the calculation of the five-fold differential cross-sections (FDCS) is performed representing the projectile by plane waves, both in the initial and final channel. Calculation of the transition matrix involves a 9D integration. However, for high projectile energies and small momentum transfers, it is possible to calculate analytically a 6D integral and hence, the numerical work is reduced to a 3D integral evaluation [8].

There are different ways to write V_i for the (γ,2e) process in the dipolar approximation, by using the well-known acceleration, velocity and length gauges [9]. The computation of the triply differential cross-sections (TDCS) in this case is performed by direct numerical integration in the coordinates space with an adaptive Monte Carlo method.

2.1. Final states

The final state of the ionized electrons is modeled by a C3 wave function [10–12]:

$$\Psi_{\mathrm{C3}}(\mathbf{r}_1,\mathbf{r}_2) = N_{\mathrm{C3}}C(-\alpha_1,\mathbf{k}_1,\mathbf{r}_1)C(-\alpha_2,\mathbf{k}_2,\mathbf{r}_2) \times D(\alpha_{12},\mathbf{k}_{12},\mathbf{r}_{12}) \tag{3}$$

where the electron–nucleus interactions are described by the two-body Coulomb functions $C(-\alpha_i,\mathbf{k}_i,\mathbf{r}_i)$ of Sommerfeld parameter $\alpha_i = Z\mu/k_i$, $i=1,2$, and N_{C3} is a normalization factor. The electron–electron correlation is represented by a Coulomb distortion factor D.

We make use of the First Born Approximation in the (e,3e) calculation. Then, the interaction between the projectile and each active charged particle (two electrons and the nucleus) is considered a perturbation, and the projectile is described by a plane wave function. The complete wave function in the (e,3e) case is then $\Psi_\mathrm{f}^{-(\mathrm{e,3e})} = \exp(i\mathbf{k}_0\mathbf{r}_0)\times\Psi_{\mathrm{C3}}(\mathbf{r}_1,\mathbf{r}_2)$. There are different proposals to modify this C3 function, introducing momentum-dependent or distance-dependent effective Sommerfeld parameters[13]. However, in this work we focus our attention on the different approximate solutions to the initial state.

2.2. Initial states

We choose different initial wave functions for the bound electrons with positions $\mathbf{r}_1$ and $\mathbf{r}_2$. There is a variety of approximate wave functions for the $1s^2$ of He. They range from the simple product of hydrogenic 1s states to the very sophisticated, Hylleraas-like functions of Chuluunbaatar et al. [6] (see, for example, ref. [5] and references therein). Usually they can be written as

$$\psi_\mathrm{i}(\mathbf{r}_1,\mathbf{r}_2) = N_i\psi_{\mathrm{unc}}(r_1,r_2)\psi_{\mathrm{corr}}(r_1,r_2,r_{12}), \tag{4}$$

where the uncorrelated wave function $\psi_{\mathrm{unc}}(r_1,r_2)$ for the electrons is represented by the usual product of hydrogenic states $\psi_{\mathrm{unc}} \propto \exp(-Zr_1 - Zr_2)$ [1]. The choice of correlation factors $\psi_{\mathrm{corr}}(r_1,r_2,r_{12})$ can be performed according to different criteria. However, the complete function $\psi_\mathrm{i}(\mathbf{r}_1,\mathbf{r}_2)$ has to be an approximate, physically sound, solution of the ground state Hamiltonian of the He atom:

$$\left(-\left[\frac{D_1}{2}+\frac{Z}{r_1}+E_1\right]-\left[\frac{D_2}{2}+\frac{Z}{r_2}+E_2\right]-\left[D_{12}-\frac{1}{r_{12}}+E_{12}\right] - \frac{\mathbf{r}_{12} < MML{:}MSPACECLASS{=}\text{"NBSP"}/ > \mathbf{r}_1}{2r_{12}r_1}\frac{\partial^2}{\partial r_{12}\partial r_1} - \frac{\mathbf{r}_{12}\mathbf{r}_2}{2r_{12}r_2}\frac{\partial^2}{\partial r_{12}\partial r_2}\right)\varphi_i(\mathbf{r}_1,\mathbf{r}_2)=0 \tag{5}$$

where $D_i = ((\partial^2)/(\partial r_i^2)) + ((2/r_i)(\partial/\partial r_i))$, $i=1, 2$ or 12 and the total energy is $E = E_1 + E_2 + E_{12}$. The first three terms of this equation can be viewed as three independent two-body Coulomb problems. The mixed derivatives, as we can see from the equation, introduce the correlation. We define *angular correlation* as the factors of the wave function ψ_{corr} that only depend on the r_{12} coordinate, and *radial correlation* as those ones that depend only on r_1 or r_2.

One of the first proposals for a correlated ground state of the He atom is due to Pluvinage [14,15]. He proposed the separable trial function:

$$\varphi_{\mathrm{Plu}}(r_1,r_2,r_{12}) = N_\mathrm{p}\psi_{\mathrm{unc}}(r_1,r_2)\,\mathrm{e}^{-i\kappa_{12}r_{12}} \times F\left[1-i\frac{1}{2\kappa_{12}},2,2i\kappa_{12}r_{12}\right] \tag{6}$$

as the solution of the first three terms of Eq. (5) with the energy E defined by $E_1 = E_2 = -Z^2/2$ and $E_{12} = \kappa_{12}^2$. In the definition of φ_{Plu} the energies E_1 and E_2 are negative, while the E_{12} is positive.

The Pluvinage function satisfies the Kato cusp conditions [16]. A wave function satisfying these conditions properly diagonalizes the three-body Coulomb Schrödinger equation, Eq. (5), at the coalescence points where the Coulomb potential diverges. The parameter κ_{12} is chosen variationally to approximately diagonalize the Coulomb interactions in the He Hamiltonian. Pluvinage obtained $\kappa_{12} = 0.41$ for He, but the method was used more recently in other atomic systems [4,17].

At this point we should emphasize that the Pluvinage function (6) does not include radial correlation [18]: there is not any explicit dependence on the coordinates r_1 and r_2 in ψ_{corr}. Then, the Pluvinage function as well as the functions defined by Ancarani et al. [19] only present angular correlation. We note

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[1] In the few following equations, N_L represents a normalization factor for each function ϕ_L, while L is an acronym to label each one of the different initial states.