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A Generalized Sturmian Treatment of $(e, 3e)$ Processes Described as a Three-Body Coulomb Problem

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Abstract The double ionization of helium by high energy electron impact is investigated. The pure four-body Coulomb problem may be reduced to a three-body one in accordance with the use of the first Born approximation. Even within this frame, major unexplained discrepancies subsist between several theoretical descriptions, and with available absolute experimental data. In this contribution we discuss an alternative formulation which allows to tackle the problem with a different methodology, the generalized Sturmian approach. We discuss some issues associated to the convergence of the calculated cross sections.

1 Introduction

It has been stated that the three-body Coulomb problem has been solved numerically, the proof being given through calculations of the single ionization [$(e, 2e)$ process] of hydrogen by electron impact [1]. Several numerical recipes like the Convergent-Close-Coupling [2], the Exterior-Complex-Scaling [3], the J-matrix [4], among others, managed with great success to numerically approach the solution of the problem. A similar success is also obtained when the same methods are applied to the double ionization of helium by photon impact [$(\gamma, 2e)$ process]. Except in some minor details, it can be said that these methods agree remarkably well with each other, and with the experimental observations.

However, for the double ionization of helium by impact of high energy electrons, the $(e, 3e)$ process, the same is not observed. When dealing with high energy projectiles the four-body problem corresponding to the $(e, 3e)$ process can be reduced to a three-body one. This reduction can be related to the First Born Approximation, within which no method is able to satisfactorily reproduce the absolute experimental data of the Orsay group [5, 6]. In addition, those numerical methods—which are in such beautiful agreement for $(e, 2e)$ and $(\gamma, 2e)$ processes—do not agree with each other when applied to the $(e, 3e)$ case [7]. In some sense, this brings some doubts on whether the three-body problem can be considered as solved in all cases.

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The aim of this contribution is to continue with the work initiated in [8] where only the total angular momentum $L = 0$ case (Temkin–Poet model) was considered. Here we present part of our studies on the convergence of the three-body function (any L) for the physical process ($e, 3e$) on helium produced by high energy electron impact. We use a generalized Sturmian approach [9] to solve a scattering driven equation and investigate how many partial waves L (and the number of partial waves pairs associated to the two ejected electrons) are necessary to reach convergence for the scattering solution. After sketching the formulation of the three-body scattering problem, we briefly present the methodology implemented with Generalized Sturmian Functions (GSF). We then present, for the first time, single differential cross sections (SDCS) for double ionization of helium induced by high energy electron impact, calculated with several total angular momenta.

2 Formulation of the Three-Body Coulomb Scattering Problem

From a theoretical point of view, the description of a ($e, 3e$) process on helium requires the solution of a pure four-body Coulomb problem. However, a reduction to a three-body one can be performed in the case of high energy projectiles. In the Orsay experiment, for example, the incident projectile possesses an energy of 5,599 eV and leaves the collision region with 5,500 eV. The fivefold differential cross sections (FDSCS)—within the first Born approximation—for two ionized electrons escaping with energy E_2 and E_3 (momenta k_2 and k_3 , respectively), and in the solid angles $d\Omega_2$ and $d\Omega_3$, is defined as [10]

$$\frac{d^5\sigma}{d\Omega_2 d\Omega_3 d\Omega_f dE_2 dE_3} = (2\pi)^4 \frac{k_f k_2 k_3}{k_i} \left| \frac{4\pi}{q^2} \langle \Psi_f^- | W | \Psi_0 \rangle \right|^2, \quad (1)$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ is the momentum transferred to the target by the projectile with initial and final momenta \mathbf{k}_i and \mathbf{k}_f , respectively. W contains the Fourier transform of the interaction between the projectile and the three target particles. Only three-body wave functions are required in Eq. (1): Ψ_0 representing the initial helium ground state, and a double continuum Ψ_f^- describing the two ejected electrons in the presence of the residual target ion ($Z = 2$ for helium).

In [8], it was shown that the First Born Approximation may be obtained by solving a driven equation for a scattering function possessing, to first order, all the information about the collision problem. The sought after scattering function, with outgoing behavior (+), solves the inhomogeneous equation

$$\left[-\frac{1}{2}\nabla_2^2 - \frac{1}{2}\nabla_3^2 - \frac{Z}{r_2} - \frac{Z}{r_3} + \frac{1}{r_{23}} - E_2 - E_3 \right] \Psi_{sc}^+(\mathbf{r}_2, \mathbf{r}_3) = \frac{1}{(2\pi)^3} \frac{4\pi}{q^2} \left(-Z + e^{i\mathbf{q}\cdot\mathbf{r}_2} + e^{i\mathbf{q}\cdot\mathbf{r}_3} \right) \Psi_0(\mathbf{r}_2, \mathbf{r}_3). \quad (2)$$

The transition amplitude obtained from the asymptotic limit of the first order solution Ψ_{sc}^+ is shown to be equivalent to the familiar First Born Approximation [8] [see Eq. (1) above].

One difficult issue related to the Coulomb three-body problem is to impose on the solution, in the Ω_0 region where all three particles are far from each other, the Peterkop-type asymptotic behavior [11]

$$\Psi_{sc}^+(\mathbf{r}_2, \mathbf{r}_3) \longrightarrow A(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_3, \alpha) \frac{e^{iK\rho - i\gamma(\omega_5)\ln(2K\rho)}}{\rho^{5/2}}, \quad (3)$$

where $K = \sqrt{2(E_2 + E_3)}$ defines the hyper-momentum, $\rho = \sqrt{r_2^2 + r_3^2}$ the hyper-radius, $\alpha = \tan^{-1}(r_3/r_2)$ the hyperangle; the hyperspherical Sommerfeld parameter $\gamma(\omega_5)$ depends on the angular coordinates $\omega_5 = \{\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_3, \alpha\}$ [9, 12]. The coefficient $A(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_3, \alpha)$ is proportional to the transition amplitude [13].

3 Methodology

Our main goal is to solve the three-body differential equation (2) within a generalized Sturmian approach. As the scattering problem is notoriously difficult both from a theoretical and a numerical implementation point of view, we have started first to investigate the asymptotic issue on one hand, and the use of adequate basis sets, on the other, within two S -wave scattering models [8, 12]. Both deal with three-body break-up processes, and contain most of the difficulties encountered in real three-body scattering problem, e.g., non-separability in the electrons' spherical coordinates and Coulombic asymptotic behavior.

Very recently we have solved Eq. (2) but within an S -wave model [8]. To do so we used a generalized Sturmian approach in two independent numerical implementations, one using spherical [14] and the other hyperspherical [15,16] coordinates. Since the two yielded a remarkable mutual agreement, it allowed us to test convergence issues such as the size of the computational domain and the number of partial waves to be included. From our ab initio solution, the transition amplitude was extracted, and SDCS were calculated. They can be taken as benchmark values to test other numerical methods in a previously unexplored energy domain. To test more deeply the methodology we implemented also an hyperspherical S -wave model and we solved it both numerically and analytically [12,17]. The Sturmian approach resulted to be very accurate and robust even at very large distances where all the particles are far away from each other.

Both investigations have been helpful in understanding the difficulties associated to the theoretical/numerical description of the real $(e, 3e)$ process. Going beyond S -wave models, we have now tackled the physical problem (2) and present here some preliminary results obtained with spherical GSF. For a given total angular momentum L and projection M , we propose for a three-body wave function the following Configuration Interaction expansion

$$\Psi(\mathbf{r}_2, \mathbf{r}_3) = \sum_{LMl_2l_3} \sum_{n_2=1}^{N_2} \sum_{n_3=1}^{N_3} a_{n_2n_3}^{LMl_2l_3} \mathcal{A} \frac{S_{n_2l_2}(r_2)}{r_2} \frac{S_{n_3l_3}(r_3)}{r_3} \mathcal{Y}_{l_2l_3}^{LM}(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_3) \quad (4)$$

where $a_{n_2n_3}^{LMl_2l_3}$ are the expansion coefficients, \mathcal{A} is the symmetrization operator that accounts for the exchange of the particles, and $\mathcal{Y}_{l_2l_3}^{LM}$ are coupled spherical harmonics (see [9] for more details). For convenience we use the same expansion (4) for the helium target bound state $\Psi_0(\mathbf{r}_2, \mathbf{r}_3)$ with $L = M = 0$, and for the final double continuum $\Psi_{sc}^+(\mathbf{r}_2, \mathbf{r}_3)$ (any L) describing the ejected electrons. For the latter, outgoing behavior is imposed on each two-body GSF $S_{nl}(r)$ while for the bound state exponentially decaying behavior is taken. The method has been applied successfully [9] for three-body bound states and scattering problems including $(e, 2e)$ and $(\gamma, 2e)$ processes. Although using spherical coordinates basis functions, expansion (4) succeeds in building up the expected hyperspherical wave front (3) of the scattering wave function. The calculation of the flux

$$F = \frac{1}{2i} \left(\Psi_{sc}^{+*}(\mathbf{r}_2, \mathbf{r}_3) \frac{\partial \Psi_{sc}^+(\mathbf{r}_2, \mathbf{r}_3)}{\partial \rho} - \Psi_{sc}^+(\mathbf{r}_2, \mathbf{r}_3) \frac{\partial \Psi_{sc}^{+*}(\mathbf{r}_2, \mathbf{r}_3)}{\partial \rho} \right) \quad (5)$$

leads, as shown in [11,13], directly to the transition amplitude and thus to the cross section.

4 Results

With our GSF numerical implementation we have solved Eq. (2) taking the coplanar experimental conditions of Lahmam-Bennani [5]: incident and scattered energy of $E_i = 5,599$ eV and $E_f = 5,500$ eV, respectively; the scattering angle was set at $\theta_f = 0.45^\circ$, yielding a small momentum transfer $q = 0.24$ a.u. Since the double ionization potential is about 2.9037 a.u. $\simeq 79$ eV, only $E_2 + E_3 = 20$ eV are to be shared by the two ejected electrons and one may define an energy fraction $0 < E_2/(E_2 + E_3) < 1$. In the experiments [5] the two electrons were detected with equal energy, i.e. $E_2 = E_3 = 10$ eV, and FDCS were measured.

The preliminary calculations presented here were obtained as follows. For the helium ground state Ψ_0 we used expansion (4) yielding an energy of -2.9027 a.u.; the accuracy of this value can be easily increased [9] but it is sufficient for our purposes. For the scattering wave function Ψ_{sc}^+ we have included in expansion (4) the first three total angular momenta: $L = 0$ (with pairs $(l_2, l_3) = (0, 0), (1, 1), (2, 2), (3, 3)$), $L = 1$ (with pairs $(l_2, l_3) = (0, 1), (1, 2), (2, 3), (3, 4)$), and $L = 2$ [with pairs $(l_2, l_3) = (0, 2), (1, 1), (2, 2), (1, 3)$]. The radial grid was set to 30 a.u. per radial coordinate. All these numerical values will be improved in a more advanced calculation. However, they suffice here to illustrate that the results converge and thus that our GSF method is viable to describe the double ionization process by electron impact.

Following the study presented in [8], we extract from the scattering wave function the transition amplitude $t_{LMl_1l_2}$ by evaluating it at large distances. Using the definitions given in [13], the full transition amplitude is calculated as the sum over the $\mathcal{Y}_{l_2l_3}^{LM}(\hat{\mathbf{r}}_2, \hat{\mathbf{r}}_3)$ where the $t_{LMl_1l_2}$ are the coefficients. For a given q value, we deduce thereafter a SDCS as a function of the two-electrons' energy sharing. Formally, the resulting SDCS should be independent of the hyper-radial coordinate [see Eq. (3)]; effectively, one evaluates it numerically at different values of ρ and then extrapolates the result to infinite distances [11,18]. One has to keep in mind that

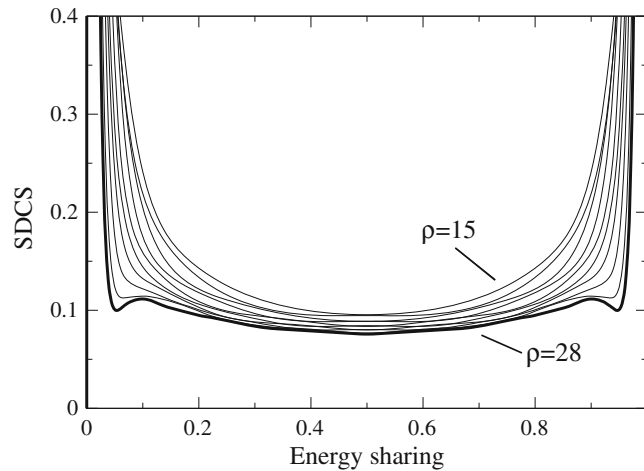


Fig. 1 Single differential cross section (in arbitrary units) as a function of the energy sharing fraction $E_2/(E_2 + E_3)$, calculated for two electrons ejected with a total energy of $E_2 + E_3 = 20$ eV and $q = 0.24$ a.u. We have included several pairs (l_2, l_3) corresponding to $L = 0, 1, 2$ (see text). The different curves correspond to the extraction at successively larger distances ρ , the thicker (bottom) curve being evaluated at 28 a.u.

the source term on the right-hand-side of the driven Eq. (2) includes the helium ground state and thus vanishes at distances of about 10 a.u.

In Fig. 1 we show the SDCS as a function of the energy sharing fraction $E_2/(E_2 + E_3)$. The 10 curves correspond to the evaluation at successively larger ρ values ranging from 15 to 28 a.u. (from top to bottom). Although 28 a.u. is still a small distance for a Coulomb three-body problem, one may appreciate from the figure how the SDCS starts to converge (thicker line).

5 Summary

We showed that the generalized Sturmian approach may be used, within a three-body framework, to study the electron impact double ionization of helium. A coupled expansion of two-body basis functions with outgoing boundary conditions is able to build up the double continuum hyperspherical front. Although proper convergence needs to be reached, our preliminary single differential cross sections indicate that physical results may be extracted from our numerical implementation of the GSF method. Fivefold differential cross sections will then also be extracted and compared with other theoretical results and with experimental data.

A comparison between spherical and hyperspherical Sturmian approaches applied to $(e, 3e)$ processes should be enriching. In both methodologies the scattering wave function is forced to have purely outgoing behavior at large values of ρ . This condition is built in the spherical approach, while it is more natural (intrinsic) in the case of the hyperspherical approach. It will be interesting to explore convergence advantages of one method with respect to the other.

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