ISSN 1512-1461

UDC 539.1

THE ELECTRON-IMPACT DOUBLE IONIZATION OF HELIUM: DYNAMICAL VARIATIONAL TREATMENT

A. Dorn[1], Z.S. Machavariani[2]

[1] Max Planck Institute for Nuclear Physics, Saupfercheckweg 1, 69117 Heidelberg, Germany
[2] Department of Exact and Natural Sciences, Tbilisi State University, Chavchavadze Avenue 3, 0179 Tbilisi, Georgia

Abstract. *Two-electron emission from an atom is considered. Based on the Hulth´en-Kohn dynamical variational principle the effective charge seen by the ejected electrons are determined for a certain type of trial wave functions. Validity of the elaborated approach is assessed by calculating fully differential cross section (FDCS) for electron-impact double ionization of helium. The relatively small momentum transfer (q = 0.5 a.u.) at 2 keV impact energy and equal energy sharing between ejected electrons (5eV, 10eV, 20eV) provides reasonable kinematical conditions for application of the First Born Approximation (FBA). The calculated five fold differential cross section (FDCS) is in reasonable agreement with the corresponding experimental observations.*

Keyword: Ionization, Cross section, Variation.

Introduction

The study of the single and double ionization processes of atoms and molecules by collisions with electrons or positrons is of great interest in astrophysics, plasma physics and radiation physics and also in other sciences such as life science. Such processes are fundamental to the understanding of the mechanism of multiple ionizations and of the role of electron correlation. The double ionization of helium is the most interesting case for the theory because in addition to the projectile only two electrons interact with the nucleus. In order to explore the details of the reaction mechanisms the most suitable experiments are those which detect in coincidence all three electrons present in the final state. These so-called (e, 3e) experiments are very difficult to perform due to the low count rates involved but are now possible due to the progress in the techniques of multi-particle detection [1-10].

The main difficulty which arises in the theoretical study of single and multiple ionization of atoms by electron impact is related to the solution of the many-body problem. Several sophisticated methods such as exterior complex scaling [11], time dependant close coupling [12], convergent close coupling [13], *R*-Matrix theory [14] and the 3C model [15] have been elaborated. These theories were mostly successful in predicting cross sections for the ionization of hydrogen or helium but encounter some problems describing double ionization of helium [16,17]. Recently in [18] it was shown that the second Born approximation was needed for describing the experimental observations on double ionization of helium by 600-700 eV electron impact. This has been proved further in [19] showing that at the intermediate energy (640 eV) the second Born approximation works quite well for the double ionization of helium by using the closure approximation with particular values of the average excitation energy $\bar{w}$. The big shift of the binary peak found experimentally in [18] is well reproduced showing that the TS2 mechanism is very important in this case. A comprehensive review of double ionization processes is given in [20].

The most frequently the used methods consider the electrons that are involved in the ionization process as independent particles. The total wavefunction is represented as an antisymmetrized product of one-electron wavefunctions. The elaborated approaches can be

ISSN 1512-1461

derived into two main groups which are briefly presented hereafter. In the first one, the electron or electrons ejected from a target are described by the Coulomb continuum wavefunctions with the charge unity for single ionization, and with the charge of a residual ion for multiple ionization. In the second one, each of the active electrons is considered as a particle moving in the effective Coulomb field created by the nucleus of a target together with the other electrons involved in the ionization process. This Coulomb potential is described by an effective nuclear charge experienced by the ejected electrons. So in the first group the screening effects are perfectly ignored while in the second one these effects are taken into account.

Different methods have been employed to estimate the variable charges characterizing the effective Coulomb field. For double ionization a simple empirical method has been suggested in [21] and the effective charges experienced by the two outgoing electrons have been estimated. In [22] the total potential is represented in terms of two-body interactions and then the asymptotic relation between momentum and position vectors of the outgoing electrons is used. This approach has been employed in [23] with a modified derivation of the effective charges which are chosen to satisfy the physical situations in certain limiting configuration of the outgoing electrons and to interpolate them smoothly.

Perhaps the most well-known variational approximation in quantum mechanics is the Ritz method to obtain approximate energy levels of bound quantum systems [24]. Utilization of the variational principle for continuum spectrum problems has been done later. For the simplest one dimensional problem relevant to the continuum spectrum the variation method initially was formulated by Hulthen [25]. Independently, Tamm [26,27] formulated the variation method in a form close to Hulthen's result. In the same period Kohn [28,29] enlarged the method for the generalized scattering problems. The first works where a dynamical variation method has been proposed for studying the electron-hydrogen atom collision reaction belong to Su-Shu-Huang [30-32]. Later, Massey and Moiseiwitsch [33] significantly improved the results of Su-Shu-Huang. They treated the inelastic processes in electron hydrogen atomic [34] and electron helium atomic collision reactions [35]. The results achieved during the further years have been collected and discussed in a well known monograph of Mott and Massey [36].

The aim of this study is to show how it is possible by use of the Hulthen-Kohn variational method for calculating the scattering amplitude [37-39] to introduce the effective charges seen by the ejected electrons in electron-impact double ionization of helium and using these effective charges to calculate the corresponding FCDSs. We treat each of the ejected electrons as a particle moving in an effective field created by the nucleus of the target together with another ejected electron. The novelty of such a treatment is that the effective charges seen by the ejected electrons are determined by the Hulthen-Kohn dynamical variational principle. Recently the same method was successfully applied for electron-impact single ionization of hydrogen [40]. Unless otherwise indicated, atomic units are used throughout the paper.

Theory

The total Hamiltonian of the electron-helium atom system can be represented as

$$\hat{H} = -\frac{1}{2}\Delta + \hat{H}_0(\vec{r}_1, \vec{r}_2) + \hat{V}, \tag{1}$$

where the kinetic energy operator of the incident electron is $\Delta/2$, $\hat{H}_0$ is a Hamiltonian describing helium atom before and after ionization and $\hat{V} = -Z/r + 1/|\vec{r} - \vec{r}_1| + 1/|\vec{r} - \vec{r}_2|$ represents the interaction between the incident electron and helium. $\vec{r}$ and $\vec{r}_1, \vec{r}_2$ are the position vectors for the incident and the two target electrons respectively. Z is the charge of the alpha particle.

As for discrete energy levels, the dynamical variational principle is based on the variation of a functional. For wave vectors $\vec{k}_0, \vec{k}_s$ and $\vec{k}_a, \vec{k}_b$ corresponding to the incident, scattered and two

ISSN 1512-1461

ejected electrons, respectively, the functional describing the double ionization process is given by [29–31]

$$\tilde{L} = \iiint \Psi_f\left(-\vec{n}_s, \vec{r}, \vec{r}_1, \vec{r}_2\right)\left(\hat{H} - E\right)\Psi_i\left(\vec{n}_0, \vec{r}, \vec{r}_1, \vec{r}_2\right) d\vec{r} d\vec{r}_1 d\vec{r}_2 \tag{2}$$

Here Ψ_f and Ψ_i are the wave functions of the colliding system in the initial and final states, respectively, E is the total energy and $\vec{n}_0, \vec{n}_s$ are the unit vectors directed along wave vectors $\vec{k}_0$ and $\vec{k}_s$. Wavefunctions Ψ_f and Ψ_i are the exact eigenfunctions of Hamiltonian (1).

When $\vec{r}_1$ tends toward infinity, Ψ_f and Ψ_i have the proper asymptotic form corresponding to the process under consideration [38]

$$\Psi_i \approx \frac{e^{i\vec{k}_0\vec{r}}}{(2\pi)^{3/2}}\left[\Phi_i\left(\vec{r}_1, \vec{r}_2\right) + \sum_j F_{ij}\left(\vec{n}_0, \vec{n}\right)\Phi_j\left(\vec{r}_1, \vec{r}_2\right)\frac{e^{ik_j r}}{r} + \int F_{i\varepsilon}\left(\vec{n}_0, \vec{n}\right)\Phi_\varepsilon\left(\vec{r}_1, \vec{r}_2\right)\frac{e^{ik_\varepsilon r}}{r} d\varepsilon\right], \tag{3a}$$

$$\Psi_f \approx \frac{e^{-i\vec{k}_s\vec{r}}}{(2\pi)^{3/2}}\left[\Phi_f\left(\vec{r}_1, \vec{r}_2\right) + \sum_j F_{fj}\left(-\vec{n}_s, \vec{n}\right)\Phi_j^*\left(\vec{r}_1, \vec{r}_2\right)\frac{e^{ik_j r}}{r} + \int F_{f\varepsilon}\left(-\vec{n}_s, \vec{n}\right)\Phi_\varepsilon^*\left(\vec{r}_1, \vec{r}_2\right)\frac{e^{ik_\varepsilon r}}{r} d\varepsilon.\right] \tag{3b}$$

In (3) $\Phi_j(\vec{r}_1, \vec{r}_2)$ and $\Phi_s(\vec{r}_1, \vec{r}_2)$ represent the wave functions to the discrete and to the continuum spectrum of Hamiltonian $\hat{H}_0$. Equation (3a) shows that Ψ_i is the sum of the plane wave propagating in the $\vec{n}_i$ direction and of the outgoing spherical waves whose amplitude in the $\vec{n}$-direction are $F_{ij}\left(\vec{n}_0, \vec{n}\right)$ and $F_{i\varepsilon}\left(\vec{n}_0, \vec{n}\right)$. Similarly, equation (3b) shows that Ψ_f is the sum of the plane wave propagating in the $-\vec{n}_s$-direction and of the outgoing spherical waves with amplitudes $F_{fj}\left(-\vec{n}_s, \vec{n}\right)$ and $F_{f\varepsilon}\left(-\vec{n}_s, \vec{n}\right)$. In asymptotic representation (3) the possibility of exchange between the scattered and ejected electrons is neglected. Inclusion of the exchange effects into the calculating scheme requires consideration of the additional asymptotic forms with the exchange amplitudes [37].

The integral in (2) has to be convergent. When the wave functions vary in (2), the convergence of the integral can be achieved if wave vector $\vec{k}_0$ changes simultaneously when changing $\Phi_i\left(\vec{r}_1, \vec{r}_2\right)$, so that condition

$$\iint \Phi_i\left(\vec{r}_1, \vec{r}_2\right)\hat{H}_0\Phi_i\left(\vec{r}_1, \vec{r}_2\right) d\vec{r}_1 d\vec{r}_2 + \frac{k_0^2}{2} = E \tag{4}$$

will be fulfilled [35]. In that case, the divergent terms will vanish in the integrand in (2).

Let us now consider variation of functional (2) conditioned by such variations of wave functions Ψ_f and Ψ_i that maintain unchanged the asymptotic form of the wave functions and change the amplitudes. Taking into account that Ψ_f and Ψ_i are the exact eigenfunctions of $\hat{H}$ we obtain

$$\delta\tilde{L}\left(\vec{n}_0, -\vec{n}_s\right) = -\frac{1}{2}\iiint\left[\Psi_f\Delta\left(\delta\Psi_i\right) - \delta\Psi_i\Delta\left(\Psi_f\right)\right] d\vec{r}_1 d\vec{r}_2 d\vec{r} \tag{5}$$

The integral in the right side of equation (5), containing Laplacians can be transformed into a surface integral by Green's theorem. Consequently,

$$\delta\tilde{L}\left(\vec{n}_0, -\vec{n}_s\right) = -\frac{1}{2}\int_S\iint\left[\Psi_f\frac{\partial}{\partial r}\left(\delta\Psi_i\right) - \delta\Psi_i\frac{\partial}{\partial r}\left(\Psi_f\right)\right] dS d\vec{r}_1 d\vec{r}_2 \tag{6}$$

ISSN 1512-1461

In (6), the integration is carried out over the surface *S* of a sphere the center of which is located at the origin of coordinates and the radius of which *r* is so large that wave functions Ψ_f and Ψ_i get their asymptotic form on the surface of the sphere.

Substituting asymptotic wave functions (3) into (6) and calculating the corresponding integrals as it is done in [37,39] we come to the following condition

$$\delta\tilde{L}\left(\vec{n}_0,-\vec{n}_s\right)=\frac{1}{4\pi^2}\left[F_{if}\left(\vec{n}_0,\vec{n}_s\right)-F_{fi}\left(-\vec{n}_s,-\vec{n}_0\right)+\delta F_{if}\left(\vec{n}_0,\vec{n}_s\right)\right]. \quad (7)$$

According to the reciprocity property of the amplitude [37], the first and second terms are equal in the right hand side of equation (7). Taking this into account we obtain that the variation of functional $\delta\tilde{L}\left(\vec{n}_0,-\vec{n}_s\right)$ is proportional to the variation of the amplitude: $\delta\tilde{L}\left(\vec{n}_0,-\vec{n}_s\right)=\left(2\pi\right)^{-1/2}\delta F_{if}\left(\vec{n}_0,\vec{n}_s\right)$. The latter equation can be rewritten as

$$\delta L\left(\vec{n}_0,-\vec{n}_s\right)=0 \quad (8a)$$

where

$$L\left(\vec{n}_0,-\vec{n}_s\right)=F_{if}\left(\vec{n}_0,\vec{n}_s\right)-4\pi^2\tilde{L}\left(\vec{n}_0,-\vec{n}_s\right). \quad (8b)$$

It follows from (8a) that $L\left(\vec{n}_0,-\vec{n}_s\right)$ is stationary with respect to small variations of wave functions Ψ_f and Ψ_i in the neighborhood of correct ones. Therefore, functional $L\left(\vec{n}_0,-\vec{n}_s\right)$ can be expected to be relatively insensitive to the precise shape of the wave functions, and the use of reasonable trial functions $\Psi_i^{(t)}$ and $\Psi_f^{(t)}$ leads to a good approximation for $L\left(\vec{n}_0,-\vec{n}_s\right)$

$$L\left(\vec{n}_0,-\vec{n}_s\right)\approx L^{(t)}\left(\vec{n}_0,-\vec{n}_s\right)=F_{if}{}^{(t)}\left(\vec{n}_0,\vec{n}_s\right)-4\pi^2\tilde{L}^{(t)}\left(\vec{n}_0,-\vec{n}_s\right). \quad (9)$$

The amplitude is determined to be equal to functional $L\left(\vec{n}_0,-\vec{n}_s\right)$ [35–37]. In that case we have

$$F_{if}\left(\vec{n}_0,\vec{n}_s\right)=F_{if}{}^{(t)}\left(\vec{n}_0,-\vec{n}_s\right)-4\pi^2\iiint\Psi_f^{(t)}\left(-\vec{n}_s,\vec{r}_1,\vec{r}_2,\vec{r}\right)\left(\hat{H}-E\right)\Psi_i^{(t)}\left(\vec{n}_0,\vec{r}_1,\vec{r}_2,\vec{r}\right)d\vec{r}d\vec{r}_1d\vec{r}_2. \quad (10)$$

The cross section and the trial functions

In the present work, we treat the double ionization within the FBA by using a 2CWG model [41-42]. In this model, the two ejected electrons are described in terms of Coulomb waves together with a Gamow factor to take into account the repulsion between them whereas plane waves are used for treating the incident and the scattered electrons. It was then shown that introducing the Gamow factor into the cross section calculations allowed reproducing the dominant angular behavior of the differential cross sections [43]. Among the Shake-off (SO), Two step1 (TS1) and Two step2 (TS2) double ionization mechanisms the (SO) mechanism which consists in a single ionization of one of the target electrons - the other one being simply ejected due to the relaxation is considered only.

The FDCS for double ionization of helium by electron impact is given by

$$\sigma^{(5)}=\frac{\mathrm{d}^5\sigma}{\mathrm{d}\Omega_a\mathrm{d}\Omega_b\mathrm{d}\Omega_s\mathrm{d}E_a\mathrm{d}E_b}=\frac{k_sk_ak_b}{k_i}\left|f_{if}\right|^2$$

where $\mathrm{d}\Omega_a\mathrm{d}\Omega_b\mathrm{d}\Omega_s$ denote, respectively, the elements of solid angles for the scattered and the ejected electrons *a* and *b* whereas the energy intervals of the ejected electrons are represented by $\mathrm{d}E_a$ and $\mathrm{d}E_b$. f_{if} is the transition amplitude and in general is determined by (10).

According to the above mentioned description of the scattered and ejected electrons the initial state trial function can be represented as $\Psi_i^{(t)}=e^{i\vec{k}_0\vec{r}}\Big/\left(2\pi\right)^{3/2}\Phi_i^{(t)}\left(\vec{r}_1,\vec{r}_2\right)$. Here $\Phi_i^{(t)}\left(\vec{r}_1,\vec{r}_2\right)$

ISSN 1512-1461

is the wavefunction for the initially bounded helium atom and is represented by a Hylleraas-type accurate wavefunction [44]

$$\Phi_i^{(t)}\left(\vec{r}_1,\vec{r}_2\right)=C_i\left(e^{-\alpha r_1-\beta r_2}+e^{-\alpha r_2-\beta r_1}\right)\left[1+\gamma r_{12}\right] \tag{11}$$

C_i being the normalization factor and r_{12} the electron-electron distance, $\alpha=2.2077$, $\beta=1.4368$, $\gamma=0.2934$. The energy of the initial state given by this function is $E=-2.901419\,\text{a.u.}$ This energy is 99,94% of the energy given by more sophisticated correlated wavefunction (see the 14th row of the table I in [45]) which is used in a recent treatment of double ionization of helium by electron and positron impact [19]. Therefore, wavefunction (11) on one hand reasonably treats the radial as well as the angular correlations between target electrons and on the other hand significantly facilitates the calculation of the matrix element. We also use a wavefunction which only includes the radial correlation (the wavefunction (11) with $\alpha=2.1832$, $\beta=1.1885$ and $\gamma=0$). The energy of the initial state given by this wavefunction is $E=-2.875661\,\text{a.u.}$

As final state trial function one can choose $\Psi_f^{(t)}=e^{i\vec{k}_s\vec{r}}/(2\pi)^{3/2}\,\Phi_f^{(t)\perp}\left(\vec{r}_1,\vec{r}_2\right)$ where the approximate BBK wavefunction [46] in its general orthogonalized form with respect to initial state trial wavefunction $\Phi_i^{(t)}\left(\vec{r}_1,\vec{r}_2\right)$ is such that

$$\Phi_f^{(t)\perp}\left(\vec{r}_1,\vec{r}_2\right)=\Phi_f^{(t)}\left(\vec{r}_1,\vec{r}_2\right)-\left\langle\Phi_f^{(t)}\middle|\Phi_i^{(t)}\right\rangle\Phi_i^{(t)}\left(\vec{r}_1,\vec{r}_2\right), \tag{12}$$

$$\Phi_f^{(t)}\left(\vec{r}_1,\vec{r}_2\right)=\frac{1}{\sqrt{2}}\left[\Psi_c^-\left(\vec{k}_a,\vec{r}_1\right)\Psi_c^-\left(\vec{k}_b,\vec{r}_2\right)+\Psi_c^-\left(\vec{k}_b,\vec{r}_1\right)\Psi_c^-\left(\vec{k}_a,\vec{r}_2\right)\right]\varphi\left(\left|\vec{k}_a-\vec{k}_b\right|\right), \tag{13}$$

and repulsive Gamov factor

$$\varphi\left(\left|\vec{k}_a-\vec{k}_b\right|\right)=e^{-\pi/2\left|\vec{k}_a-\vec{k}_b\right|}\Gamma\left(1-i/\left|\vec{k}_a-\vec{k}_b\right|\right). \tag{14}$$

$\Psi_c^-\left(\vec{k}_e,\vec{r}\right)$ is the hydrogen-like exact wavefunction for the continuum state

$$\Psi_c^-\left(\vec{k}_\mu,\vec{r}_i\right)=\frac{1}{(2\pi)^{3/2}}\exp\left(i\vec{k}_\mu\vec{r}_i\right)\Gamma\left(1-i\eta_{\mu i}\right)\exp\left(-\pi\eta_{\mu i}/2\right){}_1F_1\left(i\eta_{\mu i},1,-i\left(\vec{k}_\mu\vec{r}_i+k_\mu r_i\right)\right), \tag{15}$$

normalized to the three dimensional delta function in momentum space with $\eta_{\mu i}=Z_i/k_\mu$ $\mu=a,b\quad i=1,2$. Z_i are the effective charges seen by the ejected electrons.

Substituting the trial wave functions $\Psi_i^{(t)}$ and $\Psi_f^{(t)}$ determined by use of (11) and (12) into (10) and taking into account equation (4), we obtain for the transition amplitude

$$\begin{aligned}F_{if}\left(\vec{n}_0,\vec{n}_s\right)\equiv f_{B1}=-(2\pi)^2\left\langle\Phi_f^{(t)\perp}\left(\vec{r}_1,\vec{r}_2\right)\middle|\exp\left(i\vec{q}\vec{r}_1\right)+\right.\\ \left.+\exp\left(i\vec{q}\vec{r}_2\right)\middle|\Phi_i^{(t)}\left(\vec{r}_1,\vec{r}_2\right)\right\rangle\end{aligned} \tag{16}$$

This is just the FBA for double ionization of helium by electron impact.

Equation for the effective charges

The effective charges seen by the ejected electrons can be determined from the stationary property of the amplitude. Considering Z_i as variational parameters, the stationary condition (8a) yields equation $dF_{if}\left(\vec{n}_0,\vec{n}_s\right)/dZ_i=0\;i=1,2$ (i = 1, 2) to find the effective charges. Thus in our treatment we assume that the bound electrons experience the charges determined according to the equation (11), whereas the ejected electrons see the effective charges determined from the stationary property (8a).

ISSN 1512-1461

The transition amplitude defined by equation (16) is a complex quantity. Therefore, condition $dF_{if}\left(\vec{n}_0,\vec{n}_s\right)/dZ_i = 0$ gives four equations for two Z_i. Generally speaking, four equations cannot be satisfied by only two variables. This disadvantage can be removed by (i) stipulating that $F_{if}(\vec{n}_{0,}\vec{n}_s)$ as well as its complex conjugate value $F_{if}^{*}(\vec{n}_{0,}\vec{n}_s)$ are not equal to zero and by (ii) taking the sum of two terms, where one is $dF_{if}\left(\vec{n}_0,\vec{n}_s\right)/dZ_i = 0$ multiplied by $F_{if}^{*}(\vec{n}_{0,}\vec{n}_s)$ and another is $dF_{if}^{*}\left(\vec{n}_0,\vec{n}_s\right)/dZ_i = 0$ multiplied by $F_{if}(\vec{n}_{0,}\vec{n}_s)$. In this way, we obtain two equations for one unknown effective charge Z_i

$$\frac{d\left|F_{if}\left(\vec{n}_0,\vec{n}_s\right)\right|^2}{dZ_i} = 0 \tag{17}$$

Equation (17) contains the kinematical variables. Hence, this equation determines the momentum-dependent, dynamically-screened effective charges which are experienced by the two ejected electrons.

Results and discussion

We focus on a scattering geometry with highly asymmetric energy sharing between the scattered and two ejected electrons. In this case the possibility of exchange between the scattered and two ejected electrons can be neglected.

Figure 1 shows FDCS for a projectile electron energy 2 keV and equal energy sharing between ejected electrons $E_a = E_b = 5eV, 10eV, 20eV$ [5]. The momentum transfer is $q = 0.5\text{au}$. This momentum transfer _ belongs to the so-called intermediate regime between the dipole regime for $q << 1$ and impulsive regime for $q >> 1$. The momentum vectors of the ionized electrons are lying in the plane defined by incoming and outgoing projectile momenta, so-called coplanar scattering geometry.

As both ejected electrons have the same energy, _ symmetry with respect to exchange $\sigma^{(5)}(\theta 1, \theta 2) = \sigma^{(5)}(\theta 2, \theta 1)$ is present and the diagonal line $\theta 1 = \theta 2$ is, in all cases, a line of reflection symmetry of the cross section. We also observe that the regions on the plots which correspond to nearly parallel ejection of the two electrons give very small FDCS values, which is physically reasonable because of Coulomb repulsion. This is ensured by the presence of the Gamow factor (14). The orthogonality of the final state function is conserved due to equation (12) but the norm is destroyed because of the presence of the Gamow factor, and thus the results cannot be considered as absolute. In the same time also the experimental data are not on an absolute scale. Therefore, the comparison between experiment and theory can only concern the structure of the cross section pattern. We observe that all theoretical curves reveal the symmetry around the momentum transfer direction (for the sake of clarity see perpendicular lines in lower left panel of the figure 1. The pink dot in the color electronic version corresponds to the momentum transfer direction) which is the well known feature of the first Born theory. The well pronounced two peak structure of the FDCS along with all kinematical conditions is well explained in the dipole regime by the binary and recoil maxima [10].

ISSN 1512-1461

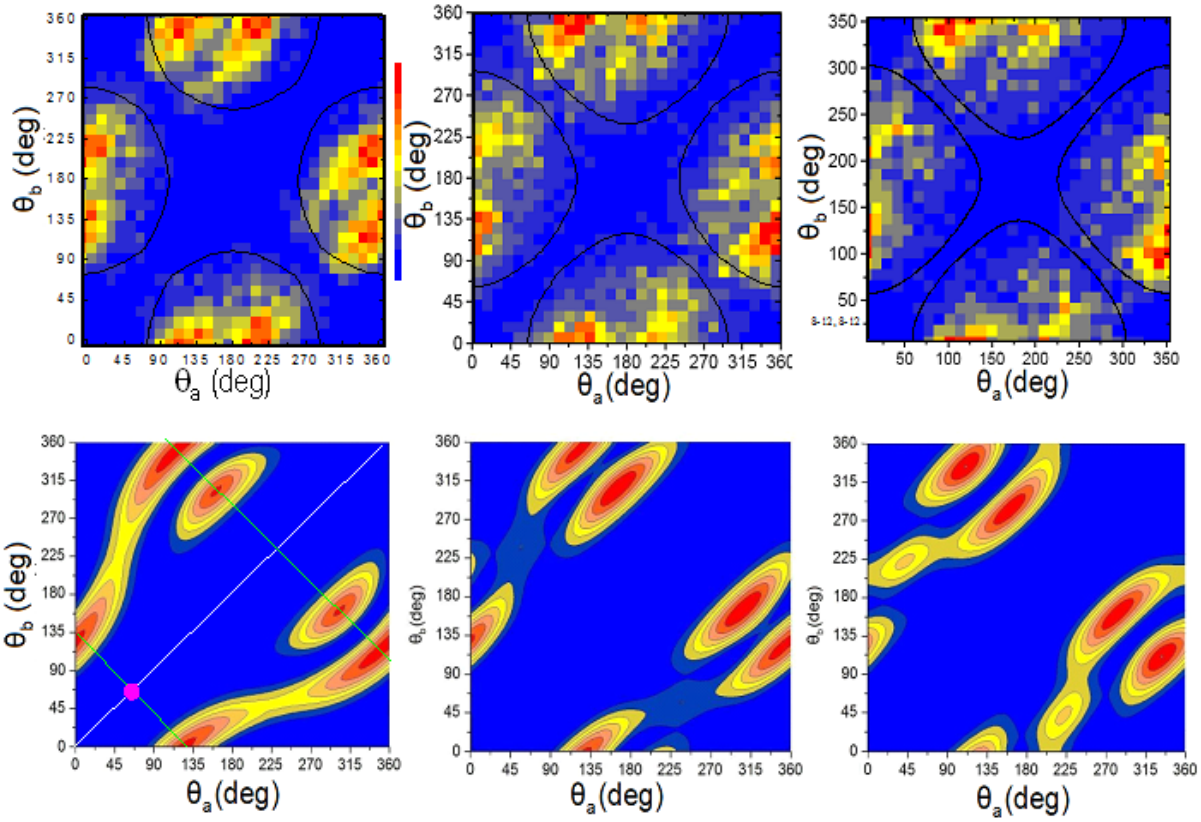

Figure 1: Contour plot for FDCS for projectile electron energy 2 keV and equal energy sharing between ejected electrons. The momentum transfer $q = 0.5\text{au}$. First column $E_a = E_b = 5eV$, second column $E_a = E_b = 10eV$ third column $E_a = E_b = 20eV$. Upper panel's row represents the experiment from [5]. Here due to the detector deadtime only the angular ranges inside the solid circular lines have full detection efficiency. Lower panel's row represents the present results. Pink dot corresponds to momentum transfer direction. Mutually perpendicular lines are the symmetry lines of FBA.

In figure 2 we present the calculation with fixed nuclear charge Z=2 seen by the ejected electrons. Upper panels correspond to the case when γ=0 in formula (11) meaning that only radial correlation between target electrons are kept in the initial state wavefunction. Lower panels show the results when γ≠0 and thus radial as well as the angular correlations between target electrons are taken into account in the initial wavefunction. The final double continuum state wavefunction remains the same as in the previous case. As it is clear from figure 2 the main characteristic features of the FDCS are kept. But if we look at the ratio of binary and recoil peaks heights we see that in the cases $E_a = E_b = 10eV, 20eV$ this ratio reveals better agreement with the experimental observation when angular correlation between target electrons are taken into account (second and third lower panels in figure 2) rather than in case of only radial correlation (second and third upper panels in figure 2). In case of $E_a = E_b = 5eV$ the situation is just an opposite. The calculation of the FDCS with the effective charges seen by the ejected electrons described above improves the ratio_ of the binary and recoil peaks heights towards the experimental observation for $E_a = E_b = 5eV$ ejected electrons energies, but underestimates this ratio for $E_a = E_b = 10eV, 20eV$ energies (see the lower row in figure 1). It has

ISSN 1512-1461

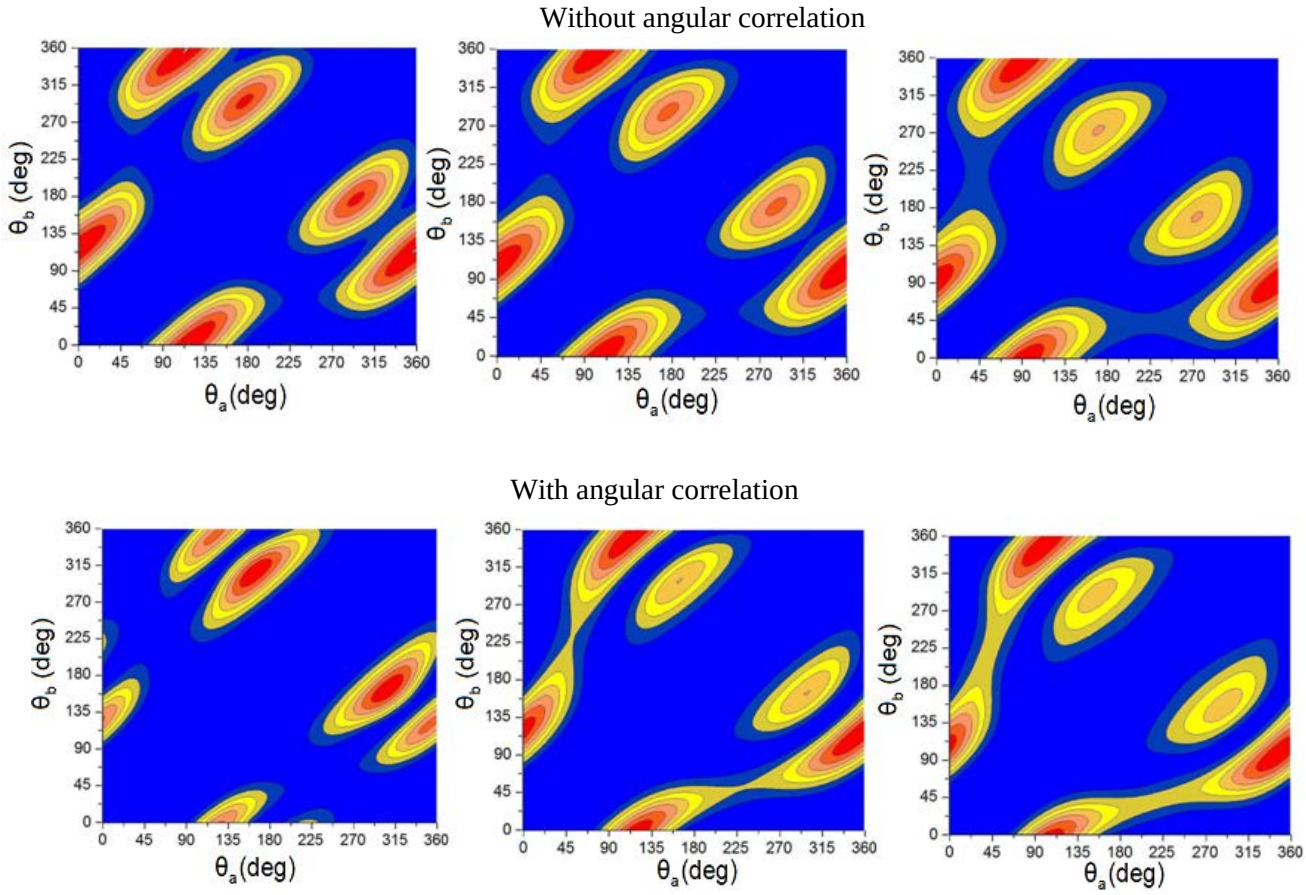

Figure 2: The kinematical conditions and panel's distributions are the same as in figure1. Upper panel's row represents the results obtained by use of γ=0 in formula (11). Lower panel's row represents the calculation with formula (11).

to be also mentioned that at $E_a = E_b = 20eV$ the calculation show relatively small back-to back emission pick ($\theta_a \approx 45^\circ, \theta_b \approx 225^\circ$ in the lower right panel of figure 1) which is not case for the calculation with fixed Z=2 nuclear charge and is in a good accordance with the experimental observation.

Of course there is still significant difference between experiment and theory. We attribute this disagreement to (i) incomplete description of the double ionization process even in this highly asymmetric energy sharing in the framework of the FBA. This is clearly demonstrated by the systematic shifting away of the recoil pick from the Born symmetry line in the experimental observation. This shift is often interpreted as a non-first Born effect. ii) very important issue is the correct choice of the initial and final state wavefunctions. Our choice of the wave functions was dictated by the facilitation of the task of calculation of FDCS. This is necessary because the finding of the roots of equation (17) is very time consuming numerical procedure. It is obvious that there is only one possibility to calculate FDCS analytically when only radial correlation between target electrons are taken into account in the initial state and 2C wavefunction with or without Gamov factor represents the final double continuum state. But in this case the results obtained by the above described method are very poor: the two-peak structure of the FDCS is replaced by only one very pronounced peak which has no physical significance. This result once again confirms the experience that a balanced treatment of correlation is necessary in initial and

ISSN 1512-1461

final states in order to achieve good results with approximate wavefunctions [23]. However, our interest here is the demonstration of the validity of the elaborated scheme of calculation of effective charges for double ionization processes. We clearly understand that facilitation of the trial wavefunctions can cause the loss of important physical effects. At this stage we only pretend that at least qualitative agreement with the experiment can be achieved by use of wavefunctions described above. But the advantage of the proposed method with respect to other methods is that the calculation scheme is based on rigorous mathematical method and can be considered as parameter-free method.

Finally, it is worthwhile to list some advantages of dynamical variational method for treatment of the electron impact double ionization process: i) the effective charges are introduced naturally as a variational parameters. ii) Determination of the effective charges is based on the exact quantum mechanical principle without any empirical assumptions.

Conclusion

In conclusion, a parameter-free method based on the application of the Hulth´en-Kohn variational principle for the transition amplitude has been developed and FDCSs have been calculated for electron-impact double ionization of the helium atom. The examination of the obtained results allows us to think, that the approach elaborated in the present work is easy for realization, it leads to the agreement with the experimental results and therefore, can be successfully used for the calculation of FDCS for electron-impact double ionization of multi-electronic atoms. Note that the additional calculations which should be carried out in this case are related with the calculation of the overlap integrals between the initial and final state wavefunctions of the spectator electrons.

Acknowledgments

ZSM would like to thank DAAD foundation for the financial support of this research. ZSM also thanks for hospitality of Max Plank Institute for Nuclear Physics in Heidelberg during the period of the project implementation. ZSM also thanks Prof. Alexander Dorn for hosting this project and Prof. Michael Schulz for interesting discussions.

ISSN 1512-1461

References

1. A. Lahmam-Bennani, C. Dupré, and A. Duguet, Phys. Rev. Lett. 63, (1989) 1582
2. I. Taouil, A. Lahmam-Bennani, A. Duguet, and L. Avaldi, Phys. Rev. Lett. 81, (1998) 4600
3. A. Dorn, R. Moshammer, C. Schroter, T.J.M. Zouros, W. Schmitt, H. Kollmus, R. Mann, J. Ullrich, Phys. Rev. Lett. 82 (1999) 2496.
4. A. Dorn, A. Kheifets, C.D. Schroter, B. Najjari, C. Hohr, R. Moshammer, J. Ullrich, Phys. Rev. A 65 (2002) 032709.
5. A. Dorn, A. Kheifets, C.D. Schroter, B. Najjari, C. Hohr, R. Moshammer, Phys. Rev. Lett. 86 (2001) 3755.
6. A Lahmam-Bennani1, A Duguet1, M N Gaboriaud, I Taouil, M Lecas, A Kheifets, J Berakdar and C Dal Cappello J. Phys. B: At. Mol. Opt. Phys. 34 (2001) 3073
7. A. Lahmam-Bennani, C.C. Jia, A. Duguet, L. Avaldi, J. Phys. B 35 (2002) L215.
8. A. Duguet, A. Lahmam-Bennani, M. Lecas, B. El Marji, Rev. Sci. Instrum. 69 (1998) 3524.
9. A. Kheifets, I. Bray, A. Lahmam-Bennani, A. Duguet, I. Taouil, J. Phys. B 32 (1999) 5047.
10. A. S. Kheifets Phys. Rev. A**69** (2004) 032712
11. Rescigno T N, Baertschy M, Isaacs W A and McCurdy C W 1999 *Science* **286** 2474
12. Colgan J and Pindzola M S 2006 Phys. Rev. A 74 012713
13. Bray I 2002 Phys. Rev.Lett. 89 273201
14. Reid R H G, Bartschat K and Raecker A 1998 J. Phys. B: At. Mol. Opt. Phys 31 563
15. M. Brauner, J.S. Briggs, H. Klar, J. Phys. B At. Mol. Opt. Phys. 22, 2265 (1989)
16. Dürr M, Dorn A, Ullrich J, Cao S P, Czasch A, Kheifets A S, G¨otz J R and Briggs J S 2007 Phys. Rev. Lett. 98 193201
17. Pindzola M S, Robicheaux F and Colgan J 2008 J. Phys. B: At. Mol. Opt. Phys 41 235202
18. Lahmam-Bennani A, Staicu-Casagrande E M, Naja A, Dal Cappello C and Bolognesi P 2010 J. Phys. B: At. Mol. Opt. Phys. 43 105201
19. C Dal Cappello, A Haddadou, F Menas and A C Roy J. Phys. B: At. Mol. Opt. Phys. **44** (2011) 015204
20. J. Berakdar, A. Lahmam-Bennani, C. Dal Cappello Physics Reports 374 (2003) 91
21. Berakdar J 1996 *Phys. Lett.* A 220 238; 1997 *Phys. Rev.* A 55 1994
22. Lahmam-Bennani A, Taouil I, Duguet A, Lecas M, Avaldy L and Beracdar J 1999 *Phys. Rev.* A59 3548
23. Götz J R, Walter M and Briggs J S 2005 *J. Phys. B: At. Mol. Opt. Phys.* 38 1569; 2006 *J. Phys. B: At. Mol. Opt. Phys.* 39 4365
24. Albert Messiah. Quantum Mechanics. Courier Dover Publications, 1999.
25. L. Hulthen. Kungl. Fys. Säll. Lund För., 14, 1, 1944
26. I. E. Tamm JETF 18, 337, 1948
27. I. E. Tamm JETF 19, 74, 1949
28. W. Kohn Phys. Rev. , 74**,** 1763, 1948
29. W. Kohn Phys. Rev. , 84**,** 495, 1951
30. Su-Shu-Huang. Phys. Rev. 75, 980; 76 447, 1948
31. Su-Shu-Huang. Phys. Rev. 76, 866 1949
32. Su-Shu-Huang. Phys. Rev. 78**,** 1878; 1949
33. H. S. W. Massey, B. L. Moiseiwitsch Proc. Roy. Soc. A205 483 1951
34. G. A. Erskine, H. S. W. Massey Proc. Roy. Soc. A212 521 1952
35. B. H. Brandsen, A. Dalgarno. Proc. Roy. Soc. A66 268 1953
36. N.F.Motta and H. S. W. Messay "The Theory of Atomic Collisions", Second Edition, Oxford, 1949
37. Yu.N. Demkov, Variational Principles in Collision Theory (Izdatelstvo Fiziko-Matematicheskoi Literaturi, Moscow, 1958) (in Russian)
38. C.J. Joachain, Quantum Collision Theory (North-Holland Publishing Company, Amsterdam, New York, 1979), Vol. 1
39. N.F. Mott, H.S.W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1965)
40. P. Defrance, T. Kereselidze,a, J. Lecointre, and Z.S. Machavariani Eur. Phys. J. D **64**, 303–310 (2011)
41. R El Mkhanter and C Dal Cappello J. Phys. B: At. Mol. Opt. Phys. **31** (1998) 301
42. Dal Cappello C, Hda H and Roy A C 1995 *Phys. Rev.* A **51** 3735
43. Ward S J and Macek J H 1994 *Phys. Rev. A* **49** 1049
44. R.G. Newton, *Scattering Theory of Waves and Particles* (New York, McGrow-Hill Book Company)
45. R. A. Bonham and D. A. Kohl J. Chem. Phys. 45, 2471 (1966)
46. Dal Cappello C, Joulakian B and Langlois J 1993 J. Phys. 3 125

Article received: 2015-04-16