Theoretical study of the (e,3e) double ionization of the K and L shells of beryllium by fast electrons

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Abstract. The production of Be²⁺(1s²) and hollow Be²⁺(2s²) in an (e,3e) collision between an electron and neutral Beryllium is studied theoretically. The variations of the fully differential cross sections (FDCS) of the two ionisation cases in terms of incident and ejection energies and detection angles are analysed. Aiming to probe electron-electron correlation, compact analytical wave correlated Jastrow functions satisfying Kato’s cusp conditions are used for the four-electron Be initial state as well as for the two-electron Be²⁺ final states. The two ejected electrons are described by 3C correlated functions.

1. Introduction
Recently we have developed [1] an all electron procedure for the determination of the fully differential cross section for the (e,3e) ionization of the four electron Beryllium target, which is, since few years, the subject of increasing interest for the fundamental aspects of its electronic structure [2-4] and its behavior in inelastic collisions in one hand, and its role in applied physics on the other hand, such as in the study of erosion effects in the fusion device in ITER [5].

Most of the works on beryllium or its ions concern the photo-excitation or photo-ionization. Among the most recent ones, we can quote S. Hasegawa and al [6] for the observation of K-shell and L-shell hollow beryllium atom, using a Dirac-Fock calculation to identify the configuration of the peaks. In the same domain, F. Yoshida and al [7] have observed many new auto-ionizing resonance peaks of the Be²⁺ and Be⁴⁺ spectra, by the inner-shell photo-excitation of the Rydberg series. A. S. Kheifets and I. Bray have applied the CCC approach to the photo-double-ionization of beryllium, using the frozen-core model [8] and the triple ionization of beryllium by the double shake-off model respectively [9].

The aim of this paper is to probe electron-electron correlation by studying the variation of the fully differential cross section of the double ionization of the L and K shells by applying an all electron procedure for different wave functions describing the initial neutral target and the final fundamental Be²⁺(1s²) and doubly excited metastable Be²⁺(2s²) state. As the correlation in the neutral beryllium between the 1s and 2s electrons is supposed to be very weak, we will not discuss here the double ionization channel in which one electron is ionized from the L and other from the K shell leaving the residual ion in the Be²⁺(1s2s) state. Atomic units are used throughout, unless otherwise indicated.
2. Theory

We are concerned by the collision of a fast electron with a 4-electron atomic system. Our approach to the (e,3e) double ionization of such targets is presented in our recent paper [1], where the fully differential cross section is given by

$$\sigma = \frac{d^4\sigma}{d\Omega_i d\Omega_f d^2k_i d^2k_f} = (2\pi)^2 \frac{k_i k_f}{k_i^2} |T_{s1}|^2$$

In the first Born approach, the transition matrix element is given by

$$T_{s1} = \langle \Psi_f | V | \Psi_i \rangle,$$

where $$\Psi_i$$ and $$\Psi_f$$ are respectively the initial and final wave functions. The potential seen by the incident electron is given by

$$V = -\frac{Z}{r_o} + \frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} + \frac{1}{r_4},$$

with $$r_o$$, the distance of the incident electron from the nucleus, and $$r_n$$, its distance from the atomic electrons. Considering that the total spin is conserved in the process, we can have two possible values between the five electrons. The initial and final states will therefore be given by the following five electron Slater determinants

$$\Psi_i \left( S = \frac{1}{2}, M_s = + \frac{1}{2} \right) = |\chi, \sigma, \phi, \phi, \phi\rangle,$$

$$\Psi_f \left( S = \frac{1}{2}, M_s = + \frac{1}{2} \right) = \frac{1}{\sqrt{2}} \left\{ |\chi, \sigma, \phi, \phi, \phi\rangle - |\chi, \sigma, \phi, \phi, \phi\rangle \right\}$$

This satisfies the condition $$\hat{S}^2 \psi_{s,f} = \frac{1}{2} (-1 + 1) \Psi_{s,f}$$ and takes into account all the possible exchanges between the five electrons.

Using individual spin orthogonality, and neglecting exchange between the projectile electron and the atomic ones in the case of fast incidence, the transition matrix element can be expressed in terms of four direct matrix elements designated by $$f_i$$.

$$T_{s1} = \sqrt{2} \left[ f_1 + f_2 - f_3 - f_4 \right]$$

More, in the relatively high incident energy domain, studied in this paper, we have observed that only the two first integrals $$f_1$$ and $$f_2$$ contribute with a significant manner. Their expressions are given by simple products of wave functions

$$f_i = \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 \chi' (\vec{k}_i, \vec{r}_i) \psi_{k_f'} (\vec{r}_i, \vec{r}_i) \xi (\vec{k}_i, \vec{r}_i, \vec{k}_i, \vec{r}_i) [V] \chi (\vec{k}_i, \vec{r}_i) \Phi (\vec{r}_i, \vec{r}_i, \vec{r}_i, \vec{r}_i)$$

$$f_2 = \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 \chi' (\vec{k}_i, \vec{r}_i) \psi_{k_f'} (\vec{r}_i, \vec{r}_i) \xi (\vec{k}_i, \vec{r}_i, \vec{k}_i, \vec{r}_i) [V] \chi (\vec{k}_i, \vec{r}_i) \Phi (\vec{r}_i, \vec{r}_i, \vec{r}_i, \vec{r}_i)$$

Here, $$\vec{k}_i$$, $$\vec{k}_i$$, $$\vec{k}_i$$, and $$\vec{k}_i$$ represent respectively the wave vectors of the incident, scattered and ejected electrons. For neutral targets, and for high incidence energy (>1000eV) we will consider a plane wave description $$\chi(k, \vec{r}) = (2\pi)^{-\frac{1}{2}} e^{i\vec{k} \cdot \vec{r}}$$ for the incident electron. Integrating over $$\vec{r}_0$$ permits us to put the above integral in the form:

$$f_1 = \int d\vec{r} d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 \psi_{k_f'} (\vec{r}_i, \vec{r}_i) \xi (\vec{k}_i, \vec{r}_i, \vec{k}_i, \vec{r}_i) \left[ -4 + e^{i\vec{k}_i \cdot \vec{r}_i} + e^{i\vec{k}_i \cdot \vec{r}_i} + e^{i\vec{k}_i \cdot \vec{r}_i} + e^{i\vec{k}_i \cdot \vec{r}_i} \right] \Phi (\vec{r}_i, \vec{r}_i, \vec{r}_i, \vec{r}_i)$$

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Where \( \vec{K} = \vec{k}_1 - \vec{k}_2 \) represents the momentum transferred by the projectile to the target. The advantage of this approach is that, we can express the fully differential cross section in terms of wave functions \( \psi_{12\alpha\beta}(\vec{r}_1, \vec{r}_2) \), \( \varphi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4) \) and \( \Phi(\vec{r}_1, \vec{r}_2, k, \vec{r}_3) \) in which, we have no permutations or spin coordinates. We must also underline here, that in the limit of small momentum transfer an analogy can be found between the dipole transition matrix element of \((\gamma, 2e)\) and that of \((e,3e)\).

The two slow ejected electrons, which constitute a double continuum, will be described by a 3C wave function \([10]\) given by:

\[
\varphi(\vec{k}_1, \vec{k}_2, \vec{r}_1, \vec{r}_2) = M e^{i\vec{k}_1 \cdot \vec{r}_1} e^{i\vec{k}_2 \cdot \vec{r}_2} \Psi(\vec{r}_1, \vec{r}_2),
\]

with \( \Psi(\vec{r}_1, \vec{r}_2) = \prod_{j=1}^{3} F_1[i\alpha_j, 1----------i(\vec{k}_{1j} + \vec{k}_{2j}, \vec{r}_j), F_2[i\alpha_{12}, 1----------i(\vec{k}_{12}, \vec{r}_{12})] \), and the constant

\[
M = (2\pi)^{-3} e^{-\frac{\pi}{2}(\alpha_1 + \alpha_2 + \alpha_{12})} \Gamma(1 - i\alpha_1) \Gamma(1 - i\alpha_2) \Gamma(1 - i\alpha_{12}),
\]

\( \alpha_i = -\frac{z_{\alpha_i}}{|k_i|}, \quad \alpha_2 = -\frac{z_{\alpha_2}}{|k_2|}, \quad \alpha_{12} = \frac{1}{2|k_{12}|} \),

\( \vec{k}_{12} = \frac{1}{2}(\vec{k}_1 - \vec{k}_2) \) and \( z_{\alpha} = 2 \) the asymptotic charge.

The bound state functions of the 2-electron residual ion in its fundamental as well as in its doubly excited states, and the 4-electron neutral Beryllium are constructed by orbitals of the form:

\[
\varphi(\vec{r}) J(\vec{r}_1, \vec{r}_2),
\]

where the function \( \varphi(\vec{r}) \) describes the independent movement of an electron in the nucleus field, and the so-called Jastrow term \( J(\vec{r}_1, \vec{r}_2) \), given by

\[
J(\vec{r}_1, \vec{r}_2) = \exp \left\{ \sum_i \ln \left[ \cosh(\lambda r_i) \right] + \sum_{i<j} \frac{cr_{ij}}{1 + br_{ij}} \right\},
\]

which gives accurate description of the electronic correlations and respects the asymptotical cusp conditions. The full expressions of the functions are given in \([1]\).

3. Results

In what follows we will present some particular variations of the fully differential cross section (FDCS) for several kinematical situations in terms of the incident or ejection energy values, and the scattering and ejection angles. Although the \((e,3e)\) reaction is a purely quantum phenomenon, we will try nevertheless to analyze our results semi-classically to point out the mechanisms of the double ionization process, to test the validity of our theory and to bring guidance for experiments.

In ‘Figure 1a’ and ‘Figure 1b’ we present respectively the variations of the FDCS of the L and K shell double ionization of Beryllium, in terms of the energy of the projectile electron for a scattering angle of \(1^\circ\) and for equal energy sharing regime in opposite ejection directions, parallel to the momentum transfer. In spite of the fact that, this situation is not favorable, as shown below, it gives the possibility to do some interesting observations. Now, to explain the common behavior of the two curves, we can say that for the given fixed scattering angle the projectile should pass closer and closer to the target with increasing energy. In doing this, the projectile will first meet the L shell and ionize it. This happens, as shown on ‘Figure 1a’, around 1.5keV. Then it will meet the K shell and ionize it at around 11keV, shown on ‘Figure 1b’. As expected, it is also observed that, the ionization of the K shell is much less probable than that of the L shell, mainly because of the difference between the ionization potential of the two shells, in other words, because the core electrons are more tightly bound to the nucleus than are the valence electrons. This will be confirmed in all other situations studied in this paper.
Figure 1: The variation of the FDCS (in a.u.) as a function of $E_i$ (in keV) and for a fixed scattering angle $\theta_s = 1^\circ$, in the kinematics, $E_i = E_z = 10\text{eV}$, $\vec{k}_i = \vec{K}$, $\vec{k}_z = -\vec{k}_i$. (a) L-shell ionization, (b) K-shell ionization.

It is also interesting to consider another kinematical situation where the momentum vectors of the ejected electrons are orthogonal to each other, one of them being parallel to the momentum transfer. In varying the scattering angle, we observe on both ‘Figure 2a’ and ‘Figure 2b’ a typical structure with a maximum for the scattering angles for which in a particular energy value, the momentum transfer $\vec{K} = \vec{k}_i$. Now, as the momentum conservation condition imposes $\vec{K} = \vec{k}_i + \vec{k}_z + \vec{q}$, where $\vec{q}$ represents the recoil momentum of the ion, and $\vec{K} = \vec{k}_i$, so $\vec{k}_z = -\vec{q}$ at this particular scattering angle. This is classically the optimal condition, which is verified here by our results.

Figure 2: The variation of the FDCS (in a.u.) as a function of the scattering angle $\theta_s$, in the kinematics, $E_i = E_z = 15\text{eV}$, $\vec{k}_i = \vec{K}$, $\vec{k}_z \perp \vec{k}_i$. (a) L-shell ionization $E_i = 3\text{keV}$, (b) K-shell ionization $E_i = 11\text{keV}$.

In the simultaneous variation of the ejection energy values shown on the ‘Figure 3a’ and ‘Figure 3b’, we see that, the optimal ejection energy values for the valance L-shell will happen for the equal energy sharing regime around 10eV, while the optimal energy direction for the inner K-shell double ionization will also happen for equal energy sharing regime but around 40eV. This can be explained by the fact that the two K-shell electrons, being more tightly bound to the nucleus, will acquire more energy to escape.
Figure 3: The variation of the FDCS (in a.u.) as a function of ejection energies $E_1, E_2,$ in the kinematics $\theta_1 = 90^\circ, \theta_2 = 240^\circ.$ (a) L-shell ionization $E_i = 2 keV, \theta_i = 0.2^\circ,$ (b) K-shell ionization $E_i = 5 keV, \theta_i = 0.1^\circ.$

Let us now pass to the simultaneous variation of the FDCS with the ejection angles for both cases, shown on ‘Figure 4a’ and ‘Figure4b’ respectively. Here, we are in small scattering angle situation and the “island” structure observed is analogous to that of the $(\gamma, 2e)$ process, with the difference that the external islands are, as expected, more intense than the inner ones. We observe also, the two forbidden regions in the center of the graphs, around the directions $\theta_1 \approx \theta_2,$ and between the two islands for $\theta_2 \approx \theta_1 + 180^\circ.$

Figure 4: The variation of the FDCS (in a.u.) as a function of ejection angles $\theta_1, \theta_2,$ for equal asymptotic energies $E_1 = E_2 = 10 eV.$ (a) L-shell ionization $E_i = 500 eV, \theta_i = 0.2^\circ,$ (b) K-shell ionization $E_i = 5 keV, \theta_i = 0.1^\circ.$

Finally, we present in the ‘Figure 5’ the variation of the cross section of the L-shell double ionization of beryllium in terms of the ejection angle $\theta_j,$ for the same conditions as that of (e,3e) of helium given by B. Joulakian and C. Dal Cappello [11] (‘Figure 2’ page 3791), who applied a similar method with correlated initial and final functions. We observe that the magnitude of the FDCS for the beryllium is much larger than that of helium, which can be explained by the fact that the electrons of
the L shell are less tightly bound to the nucleus. Although the overall structures of the curves for the two atoms are quite similar, we observe differences in the positions of the two maxima and their mutual magnitudes. We must underline, that the ionization potential and consequently the momentum transfer vector are quite different for the two atoms, which could be one of the reasons of the existence of these differences.

4. Conclusion

We have performed an all electron first Born calculation of the fully differential cross section of the (e,3e) double ionization of the L and K shells of Beryllium using correlated wave functions for the description of the four electrons of the target and the two electrons of the residual ion and the double continuum of the two ejected electrons. The behavior of the variation of the FDCS, in terms of the geometry, the electron energy, scattering and ejection angles, is analyzed and commented. The analogies between ($\gamma,2e$) and (e,3e) is verified for very small scattering angles.

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