

**Valence-electron correlation in the double  $K$ -shell photoionization of atomic beryllium**

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(Received 30 January 2017; published 27 June 2017)

We extended the multiconfiguration Hartree-Fock (MCHF) + effective charge (EFC) method for double photoionization of atoms and investigated the effect of valence-electron correlation in the double  $K$ -shell photoionization of atomic beryllium. We used the MCHF method, which accounts for electron correlations, to calculate the initial-state wave function. The wave functions for the two continuum electrons in the final state are calculated in the angle-dependent EFC approximation. The actual interaction potential between the two final-state continuum electrons is approximated by the EFC, which is determined variationally. We studied the effect of valence shell electron correlation on the  $K$ -shell double photoionization of beryllium for both equal and unequal sharing of excess photon energies at four fixed scattered electron directions in order to study the effects near the double  $K$ -shell ionization threshold. We found considerable effect of valence shell correlation in the triple-differential cross section for double photoionization of the beryllium atom at each of the excess photon energies.

DOI: [10.1103/PhysRevA.95.063423](https://doi.org/10.1103/PhysRevA.95.063423)**I. INTRODUCTION**

There is a great interest recently in both the  $K$ -shell and valence shell double photoionization of atoms. A large number of investigations have been carried out, both experimentally and theoretically, to study the electron correlation between the two electrons ionized by a single photon in helium and heliumlike atoms. Very recently a few studies have been made for double photoionization of electrons in atoms with more than two-electron targets. These studies required the consideration of electron correlation between the electrons which are ionized and also between the other electrons in the target. Sometimes these electrons are inner and outer with respect to the electrons which are to be ionized. In those cases electron correlations between the ionized electrons and the other electrons are quite different. Recently double photoionization of atomic beryllium has been investigated with several nonperturbative *ab initio* methods. In most cases double photoionization of valence electrons has been made keeping the inner electrons frozen. It is found that electron correlation among the active electrons and the core electrons is very important and must be treated carefully and accurately. Kheifets and Bray [1] performed triple-differential cross sections (TDCSs) of double photoionization (DPI) of valence shell electrons of the beryllium atom using convergent close-coupling approximation. Colgan and Pindzola [2] calculated the integral, energy, and angle differential cross sections for double photoionization of valence shell electrons using time-dependent close-coupling method. Citrini *et al.* [3] calculated double photoionization of valence shell electrons of the beryllium atom using hyperspherical R-matrix method with semiclassical outgoing continuum wave function. Yip *et al.* [4] also calculated the TDCS of double photoionization of valence shell electrons of atomic beryllium using the hybrid approach. Their results compare well with other accurate calculations. Very recently investigators started considering double  $K$ -shell photoionization of multielectron closed-shell targets like beryllium. The  $K$ -shell double photoionization of alkaline-

earth atoms has been performed by Kheifets *et al.* [5] using the convergent close-coupling approximation from threshold to the nonrelativistic limit of infinite photon energy. They calculated the total cross section of the double  $K$ -shell photoionization. They calculated the double to single photoionization ratios for Mg and Ca and compared with experimental values. In particular, they investigated the effect of electron correlation in the ground and doubly ionized final states. Yip *et al.* [6] investigated theoretically the TDCS following the double photoionization of  $K$ -shell electrons in atomic beryllium using a hybrid approach. This approach combines both orbital and grid based representations of the Hamiltonian.

So far, most of the calculations did not consider the effect of electron correlation due to the valence shell electrons on the  $K$ -shell DPI cross section. In this paper we are interested in considering the valence-electron correlation on the  $K$ -shell double photoionization of atomic beryllium using the multiconfiguration Hartree-Fock (MCHF) approximation for the initial state and effective charge (EFC) approximation for the final continuum state. The TDCS of the He atom was investigated by us previously [7] at a photon energy 30 eV for sharing of excess energy equally by the two final-state continuum electrons using our extended MCHF+EFC approximations. The results were very encouraging. In the present investigation it is found that in both equal and unequal sharing of excess photon energy the TDCS calculated using the MCHF+EFC approximations shows considerable effect of electron correlation of the valence shell electrons on the double  $K$ -shell photoionization of atomic beryllium. Calculations are performed for various geometries, emission angles, and energy sharing to test the merit of MCHF+EFC approximations.

**II. THEORY****Triple-differential cross sections**

In atomic units the triple-differential cross section for double photoionization of atoms is defined by

$$\frac{d^3\sigma}{dE_2 d\Omega_1 d\Omega_2} = 4\pi^2 \alpha k_1 k_2 \omega |\langle \Psi_f^- | T | \Psi_i^+ \rangle|^2 \quad (1)$$

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where  $\omega$  is the photon energy and  $\alpha$  is the fine-structure constant. The momenta  $k_1$  and  $k_2$  are related to kinetic energy  $E_i = \frac{k_i^2}{2}$  of the  $i$ th continuum electron in the final state. The dipole operator  $T$  for double photoionization of the atom is given by

$$T = \hat{\epsilon} \cdot (\vec{r}_1 + \vec{r}_2) \quad (2)$$

in the length form and

$$T = \frac{1}{i\omega} \hat{\epsilon} \cdot (\vec{\nabla}_1 + \vec{\nabla}_2) \quad (3)$$

in the velocity form.

The wave functions  $\Psi_i^+$  and  $\Psi_f^-$  represent the initial and final states, respectively. The initial state is described by the orbital and spin angular momenta  $L_0$  and  $S_0$ , respectively. The final-state wave function is characterized by the orbital and spin angular momenta  $L_c$  and  $S_c$  of the  $(N-2)$  electrons of the core ion and by the momenta  $\vec{k}_1$  and  $\vec{k}_2$  and orbital angular momenta  $l_1$  and  $l_2$  of the two continuum electrons. Using the partial wave representation of the two final-state continuum electron wave functions, we expand the initial-state  $\Psi_i^+$  and the final-state  $\Psi_f^-$  wave functions in terms of the antisymmetrized,  $LS$  coupled wave function for the  $N$ -electron system. The TDCS for double photoionization of the atom then reduces to

$$\sigma^{(3)} = \frac{4\pi^2\alpha\omega}{[L_0]} |A(\hat{k}_1\hat{k}_2)|^2 \quad (4)$$

where

$$\begin{aligned} A(\hat{k}_1\hat{k}_2) &= \sum_{l_1 l_2} \sum_{m_1 m_2} (-i)^{l_1+l_2} e^{i(\sigma_1+\delta_1+\sigma_2+\delta_2)} \\ &\times \begin{pmatrix} l_1 & 1 & l_2 \\ m_1 & 0 & -m_2 \end{pmatrix} \\ &\times Y_{l_1 m_1}(\theta_1, \phi_1) (-1)^{m_2} Y_{l_2 m_2}^*(\theta_2, \phi_2) \langle \psi_f \| T \| \psi_i \rangle \end{aligned}$$

where  $\langle \psi_f \| T \| \psi_i \rangle$  is the reduced dipole matrix element and  $[x] = (2x+1)$ .

### III. COMPUTATIONAL PROCEDURE

#### A. Initial state

The initial state, the ground state of atomic beryllium, is calculated in the MCHF approximation, which accounts for electron correlation. The MCHF method can identify configurations which are important for electron correlation through mixing coefficients of the configurations used in the MCHF expansion of the wave function. In the present case, we expanded the initial-state bound beryllium wave function in terms of excited-state configurations of the same symmetry in the  $LS$  coupling approximation. The excited orbitals and mixing coefficients are calculated completely *ab initio* by solving the Schrödinger equation in the form of radial coupled integro-differential equations completely numerically and self-consistently [8] through the configuration interaction procedure. The calculation converged very well. Using the  $2s$  and  $2p$  orbitals from the initial-state wave function we calculated the energy of the correlated valence shell ( $C_1 2s^2 + C_2 2p^2$ ) configuration expansion. The values of the mixing coefficients are found to be  $C_1 = 0.937483$  and

$C_2 = 0.3480287$ . This shows that the  $2p^2$  configuration of the doubly charged ion mixes very strongly with the parent  $2s^2$  configuration. The calculated  $K$ -shell ionization potential is found to be 320.11 eV. This agrees well with the result obtained by Yip *et al.* [6] (320.6 eV) and also by Mitnik and Miraglia [9] (319.2 eV).

#### B. Final state

In the final state, there are two continuum electrons. These two continuum electrons correlate very strongly. To determine the effect of electron correlation the effective charge approximation is used. In the effective charge approximation, the exact Coulomb interaction between the two continuum electrons in the final state is approximated by a variationally determined angle dependent screening potential arising due to the mutual screening of the nucleus by the ejected electrons. This screening effect can be taken into account in terms of effective charge of the nucleus which satisfy proper asymptotic boundary conditions. The two effective screening charges  $\Delta_1$  and  $\Delta_2$  which determine the screening potential for the two continuum electrons are obtained by the condition [10–13]

$$\frac{Z_T - \Delta_1}{k_1} + \frac{Z_T - \Delta_2}{k_2} = \frac{Z_T}{k_1} + \frac{Z_T}{k_2} - \frac{1}{\vec{k}_1 - \vec{k}_2} \quad (5)$$

where  $Z_T$  is the net asymptotic charge of the ionized target. The effective screening charges which satisfy the above relation are obtained as [10–13]

$$\Delta_i = \frac{(\vec{k}_i \cdot \vec{k}_{ij}) k_i}{k_{ij}^3} \quad (i = 1, 2) \quad (6)$$

where  $\vec{k}_{ij} = \vec{k}_i - \vec{k}_j$  and  $j \neq i$ , with  $k_{ij} = |\vec{k}_{ij}|$ .

The set of radial functions  $P_i(r), i = 1, \dots, m$  describing the target, which is obtained from the MCHF bound-state calculations for the core ion, is kept fixed. The set of radial functions describing the continuum orbitals is determined variationally. These radial functions are the solutions of the integro-differential equations of the form [14]

$$\begin{aligned} &\left[ \frac{d^2}{dr^2} + \frac{2Z}{r} - \frac{l_i(l_i+1)}{r^2} \right] P_i(r) \\ &= \frac{2}{r} [Y_i(r)P_i(r) + X_i(r) + I_i(r)] + \sum_{i'} \epsilon_{ii'} P_{i'}(r), \quad (7) \end{aligned}$$

which has the same form as the Hartree-Fock equation for a singly occupied orbital of a bound-state system, the only difference being the specified binding energy  $\epsilon_{ii} = \frac{k_i^2}{2}$ , the effective charge  $Z = Z_T - \Delta_i$ , and the boundary condition at infinity.

In this equation  $\frac{2}{r} Y_i(r)$  is a part of the direct potential,  $\frac{2}{r} X_i(r)$  is the exchange function, and  $\frac{2}{r} I_i(r)$  represents terms arising from interactions between the configurations. The off-diagonal energy parameter  $\epsilon_{ii'}$  is related to Lagrange multipliers that ensure orthogonality between the continuum and the bound electrons of the target having the same symmetry. These operators have their usual meanings as for bound-state problems.

In the single channel case, the radial function  $P_i(r)$  satisfies the boundary conditions

$$P_i(r) \underset{r \rightarrow 0}{\rightarrow} r^{l+1}, \quad P_i(r) \underset{r \rightarrow +\infty}{\rightarrow} \sqrt{\frac{2}{\pi k_i}} \sin\left(k_i r - \frac{l_i \pi}{2} + \delta_l\right)$$

if the target is an atom and

$$P_i(r) \underset{r \rightarrow +\infty}{\rightarrow} \sqrt{\frac{2}{\pi k_i}} \sin\left(k_i r - \frac{l_i \pi}{2} + \frac{q}{k_i} \ln 2k_i r + \sigma_l + \delta_l\right)$$

if the target is an ion. Here  $\sigma_l = \arg[\Gamma(l_i + 1 - \frac{iq}{k_i})]$  is the Coulomb phase shift, and  $q = Z - N$  is the net charge of the ion.

The wave function for each of the final-state continuum electrons in the effective charge approximation is calculated using multiconfiguration Hartree-Fock method [14] for bound and continuum electrons at each relative angle between the two continuum electrons ejected at equal and unequal energies for the angular momentum  $l = 0-6$  for the partial wave  $LS = {}^1P$ . Since effective charges are angle dependent, the wave function of the continuum electrons in the final state is also dependent on relative angle between the two continuum electrons.

The integro-differential equation (7) is solved numerically by the iterative method similar to the bound-state problem. The self-consistent field procedure is applied to compute the continuum wave functions. The continuum radial function is normalized by fitting the computational values at two adjacent points to the regular and irregular Bessel or Coulomb functions depending on the target as soon as the region is reached where the direct and exchange potentials are vanishingly small. This may be at a considerably smaller value of  $r$  than the asymptotic form represented by the boundary conditions specified above.

The continuum electron wave functions are calculated with and without valence shell correlation to compare the effect of valence shell electron correlation in the TDCS of double  $K$ -shell photoionization. Also in each of these cases the continuum electron wave function is made orthogonal to the bound orbitals of the  $Be^+$  ion having the same angular momentum. The description of this method was reported earlier [14].

## IV. RESULTS AND DISCUSSION

### A. TDCS results at equal energy sharing of excess photon energies

In this paper, we calculated TDCSs for double photoionization of  $K$ -shell  $1s^2$  electrons of the beryllium atom with and without valence shell correlation to determine the effect of valence shell electron correlation. As already mentioned the initial-state wave function is calculated using the MCHF approximation where electron correlation is fully accounted for completely *ab initio*. The effective charge approximation is used to describe the final-state continuum electron wave function as a function of relative angle between the two final-state continuum electrons with and without valence shell electron correlation. It should be mentioned that we calculated the continuum electron wave functions in the potential of valence shell correlation ( $C_1 2s^2 + C_2 2p^2$ ) and without the valence shell correlation  $2s^2$ .

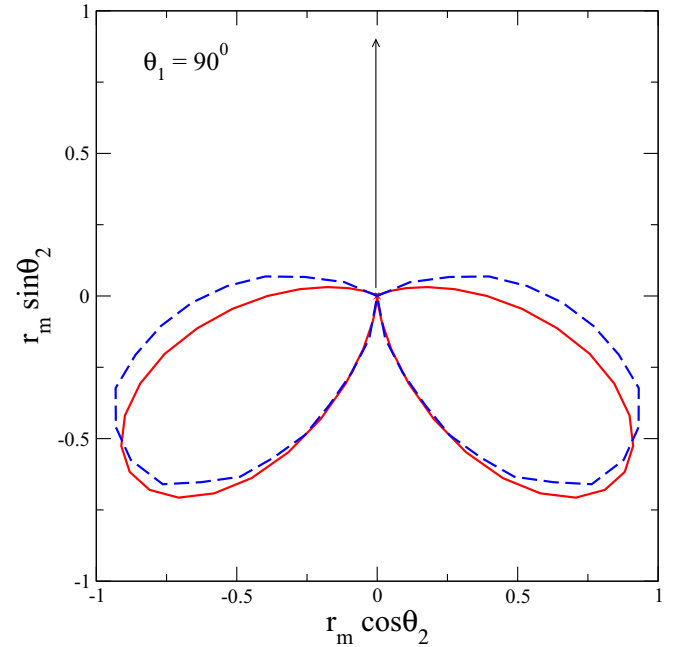


FIG. 1. The triple-differential cross sections are shown for double photoionization of  $K$ -shell electrons of beryllium for excess energy 79.4 eV shared equally by the two continuum electrons at fixed  $\theta_1 = 90^\circ$  as a function of  $\theta_2$  in degrees. The solid curve shows our results while the dashed curve is that of Yip *et al.* [6]. The scaled length of the unit maximum measures the magnitude of the cross section. The scaling factor of the present results is  $r_m = 1.888$  and that of Yip *et al.* is  $r_m = 0.26$  in units of  $b eV^{-1}$ .

In order to establish the accuracy of the present method we calculated and compared, in Fig. 1, the TDCS at excess energy 79.4 eV shared equally by the two continuum electrons at fixed  $\theta_1 = 90^\circ$  with those calculated by Yip *et al.* [6]. Comparison shows that the present results are in good qualitative agreement.

Figure 2 presents a comparison of the present TDCS velocity results with (solid curve) and without (dotted curve) valence shell electron correlation at 40 eV excess photon energy shared equally by the two continuum electrons. The results are shown for four fixed directions of  $\theta_1$ . The two curves are qualitatively similar but quantitatively the results without the valence shell electron correlation (dotted curve) are larger than those with valence shell correlation (solid curve) for each fixed direction of  $\theta_1$ . As mentioned earlier, the valence shell electrons in  $2s^2$  configuration of  $Be^{2+}$  configuration mix strongly with  $2p^2$  configuration of  $Be^{2+}$  configuration of the same symmetry.

It should be mentioned that there is a gauge dependence between the length and velocity forms of the present results. The reason for this is described in detail in our previous paper [7]. The results presented in this paper are in the velocity form and are more reliable than the length results. In Fig. 3 we compared the length and the velocity forms of TDCS results for 40 eV excess photon energy shared equally by the two continuum electrons at fixed  $\theta_1 = 90^\circ$  as a function of  $\theta_2$ .

In Fig. 4 we compare the triple-differential cross section for double photoionization of  $K$ -shell electrons at 10 eV

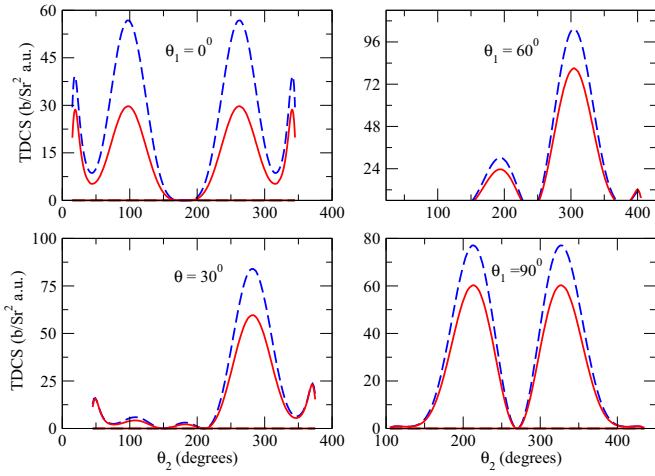


FIG. 2. Comparison of triple-differential cross sections for double photoionization of  $K$ -shell electrons of beryllium with (solid curve) and without (dotted curve) valence shell electrons correlation. The excess photon energy considered is 40 eV shared equally by the two continuum electrons. The results are shown for four different fixed directions of  $\theta_1$ .

low excess photon energy close to threshold shared equally by the two ionized  $K$ -shell electrons for four fixed different directions of  $\theta_1$ . The results are shown with and without valence shell electron correlation. The cross sections with and without valence shell correlation are quite similar but different from those with four times larger excess photon energy. Again the magnitude of the cross section with valence shell correlation is relatively smaller than that without the valence shell correlation. Comparison of cross sections at low excess energy close to threshold appears relatively more pronounced and quantitatively different in magnitude than the cross sections at larger energy.

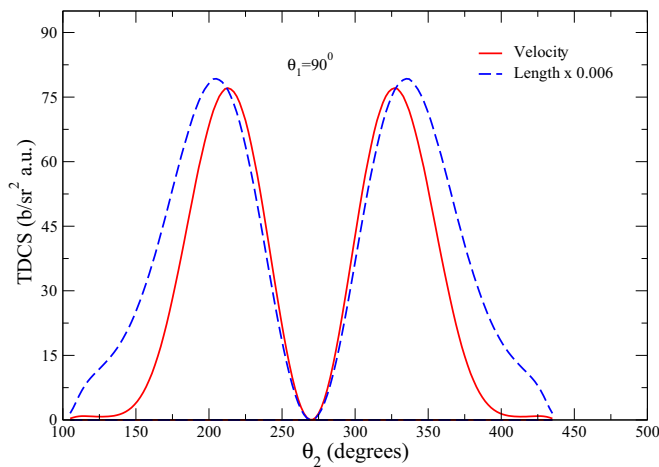


FIG. 3. Comparison of length and velocity forms of the triple-differential cross sections for double photoionization of  $K$ -shell electrons of beryllium with velocity form (solid curve) and length form (dotted curve) for excess photon energy 40 eV shared equally by the two continuum electrons at fixed  $\theta_1 = 90^\circ$ .

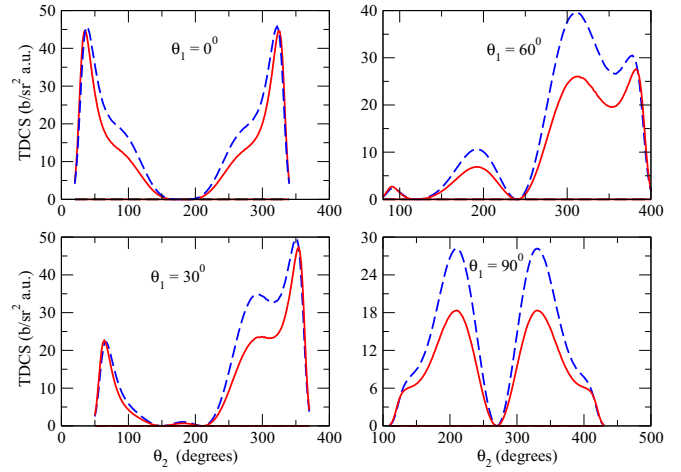


FIG. 4. Same as Fig. 2, but for excess energy 10 eV shared equally by the two continuum electrons.

**B. TDCS results at unequal sharing of excess photon energies**

In Fig. 5, we present the cross sections for double photoionization of  $1s^2$  core electrons with and without valence shell correlation for excess energy  $E = 40$  eV. This excess energy is shared unequally  $E_1 = 4$  eV and  $E_2 = 36$  eV by the two continuum electrons. Again, the magnitude of the cross sections without the valence shell correlation is relatively larger than that with the valence shell correlation. Also it is observed that the qualitative behavior of the cross sections is more or less similar at this excess energy with equal and unequal sharing of excess energy by the two continuum electrons.

The cross sections for double photoionization of  $K$ -shell electrons with and without valence shell correlation are displayed in Fig. 6 for excess energy  $E = 10$  eV shared unequally,  $E_1 = 1$  eV and  $E_2 = 9$  eV, between the two continuum electrons. The cross sections are larger in magnitude without the valence shell electron correlation relative to the case with valence shell correlation. Also at this low unequal energy sharing the cross sections are more distinct in their

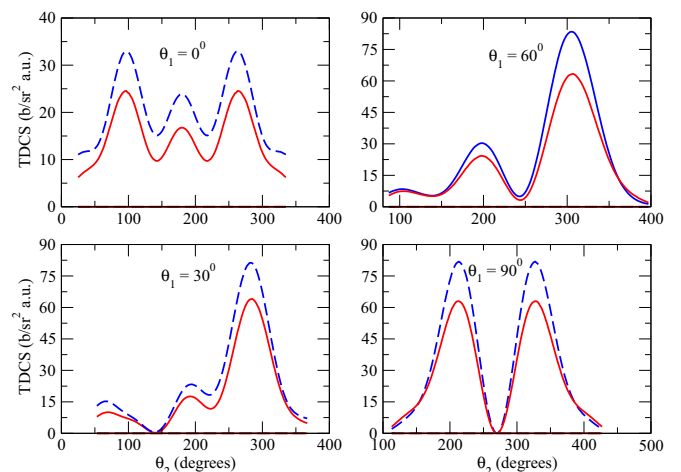


FIG. 5. Same as Fig. 2, but for excess photon energy 40 eV shared unequally  $E_1 = 4$  eV and  $E_2 = 36$  eV.

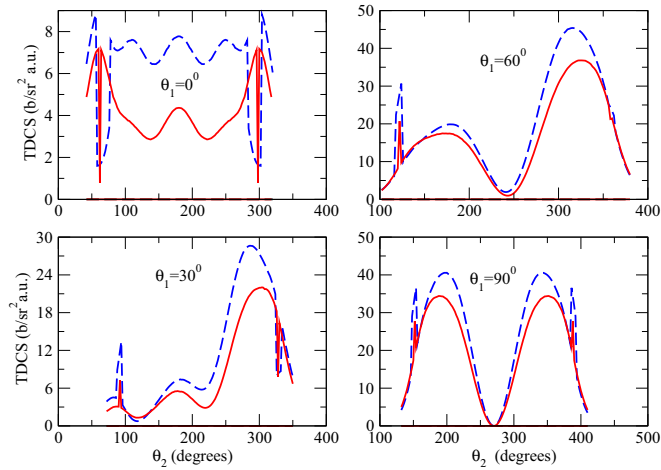


FIG. 6. Same as Fig. 2, but for excess photon energy 10 eV shared unequally  $E_1 = 1$  eV and  $E_2 = 9$  eV.

qualitative behavior compared to those at the higher energies and also at equal energy sharing. It is expected that at energies close to threshold, in particular at these unequal energies close to threshold, the cross sections show relatively more distinct features.

## V. CONCLUSION

We investigated the triple-differential cross sections for double photoionization of  $K$ -shell core electrons in the presence of uncorrelated and correlated valence shell electrons of

the beryllium atom. The initial state of beryllium is calculated in the MCHF approximation. The wave functions of the continuum electrons in the final state are calculated in the effective charge approximation. The final-state wave functions are calculated with valence shell correlation and also without valence shell correlation. It is found that the valence shell correlation effect of the final-state wave functions is very important and considerable. We calculated the cross section for double photoionization of core  $1s^2$  electrons with and without the valence shell electron correlation. We considered two distinct excess photon energies shared equally and unequally by the two final-state continuum electrons and investigated the cross sections at four fixed directions of  $\theta_1$ . Our investigation shows that the magnitude of the cross sections is larger without valence shell correlation whereas with the valence shell correlation the magnitude is smaller. The cross sections at low excess photon energy close to threshold are more distinct and informative than those at large excess energies. To our knowledge, there is no experimental result available for  $K$ -shell double photoionization of beryllium. We believe that the present theoretical investigation will stimulate interest for experimental measurement. Also there is no previous result on the calculation of TDCSs for DPI of  $K$ -shell electrons with the valence shell correlation. The present extended method is general and can be applied to consider core electron correlations in DPI of atoms.

## ACKNOWLEDGMENT

We express our gratitude to Prof. Robin Shakeshaft for useful discussions.

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