PRAMANA — journal of physics
© Indian Academy of Sciences
Vol. 58, No. 4
April 2002
pp. 647–656

(e, 3e) Test on e–e correlations in helium

M K SRIVASTAVA* and KSHAMATA MUKTAVAT
Department of Physics, Indian Institute of Technology, Roorkee 247 667, India
*Present address: S.I.E.T., Dulehra Marg, Modipuram, Meerut 250 110, India
Email: mksrafph@rurkiu.ernet.in; muktadph@rurkiu.ernet.in

MS received 10 August 2001; revised 26 November 2001

Abstract. The angular variations of the five-fold differential cross section obtained by using different wave functions of helium are compared with experimental data. It is found that in the coplanar geometry two kinematical arrangements, (i) equal energy sharing between the two ejected electrons with one of them ejected along the momentum transfer direction and the other along varying direction and (ii) the Bethe ridge condition with fixed sum of ejected electron energies and varying angle between them, are very sensitive to e–e correlations contained in the target wave function. This comparison has been used to show that open-shell class of wave functions better incorporate e–e correlations than the closed-shell class.

Keywords. Electron–electron correlation; differential cross section.

PACS Nos 34.50.Fa; 34.80.Dp

1. Introduction

One of the main aims of (e, 3e) studies initiated and pioneered by Lahmam-Bennani and co-workers about ten years ago was to investigate electron–electron correlation in the target. The angular distribution of the five-fold differential cross section (FDCS) in the kinematically fully determined initial and final states carries that information. Earlier experiments [1,2] were performed on Kr and Ar and that prompted theoretical (e, 3e) studies on these systems. The interpretation of the results in a (e, 3e) process and extraction of correlation information is however made quite difficult by several complicating factors. One of the factors relates to the mechanism of double ionization: (i) the shake-off (SO) in which the projectile is assumed to interact only once with the target and ejects one of the target electrons. The ejection of the other target electron is caused only by their mutual correlation in the initial state and the relaxation of the residual ion after the first ejection. (ii) a two-step (TS1) process in which the incident particle ejects one target electron which then interacts with and ejects the second one and (iii) another two-step (TS2) process in which the incident particle interacts successively with the target electrons and ejects them one by one. A proper accounting of e–e correlation in the final state which contains three electrons in the field of the residual ion and eliminating its influence on FDCS angular distribution is another complicating factor. Then, there are complications due to the multielectronic structure of the target and the residual ion. In order to better understand the process, several (e, 3e) studies have been done on helium [3–15]. Helium is the simplest target for (e, 3e) with no internal core and the residual He^{+2} ion is a bare nucleus and so there are no complications due to the multielectronic structure of the residual ion in the final channel. The details of the angular distribution of FDCS have been analyzed in the coplanar geometry with symmetric and asymmetric energy sharing between the ejected electrons and in the Bethe ridge kinematics and have also been compared with (γ, 2e) process. The calculations have been done at large incident energy $E_0 \sim 5$ keV, very small scattering angle and low ejected electron energies corresponding to the measurements of Lahmam-Bennani and co-workers.

Recent experiments [12–14] on helium have given a new dimension to (e, 3e) studies. A fairly large number of wave functions have been proposed over the years to describe the ground state of helium. It is now possible for the first time, due to the availability of (e, 3e) data, to '(e, 3e) test' them for internal electron–electron correlations and assess their suitability. These wave functions have been used in calculating various macroscopic quantities such as dielectric and magnetic susceptibility, Van der Waals constant etc. and in various studies such as elastic scattering, inelastic scattering, single ionization, etc. The results are found to be essentially similar and the experimental data is not able to lead to any preference for one choice over the other [16]. This is understandable since the results depend on the density distribution or single electron momentum distribution. The criteria for the choice of the wave function therefore has been simple analytic structure for ease in calculations, easier interpretation, largest binding energy and satisfying electron–nucleus and electron–electron cusp conditions.

$$\left(\frac{1}{\phi_0}\frac{\partial\phi_0}{\partial r_1}\right)_{r_1\to 0} = \left(\frac{1}{\phi_0}\frac{\partial\phi_0}{\partial r_2}\right)_{r_2\to 0} = -Z, \tag{1}$$

$$\left(\frac{1}{\phi_0}\frac{\partial\phi_0}{\partial r_{12}}\right)_{r_{12}\to 0} = \frac{1}{2}. \tag{2}$$

These wave functions may be put in three broad groups: (i) Hartree–Fock wave function [17], its analytical fit by Byron–Joachain [18], Hylleraas zero order wave function and a recent one by Bhattacharyya *et al* [19]. These are sometimes called closed-shell (CS) type. (ii) Hylleraas higher order wave functions, those due to Silvermann *et al* [20], Mires [21], Srivastava and Bhaduri [22], Wu [23], Joachain and Vanderpoorten [24] and a recent one by Sech *et al* [25]. These are classified as open-shell (OS) type. (iii) Third group contains wave functions that are based on Feshbach–Rubinow [26,27] model, one due to Abott and Maslen [28] and another due to Tripathi *et al* [29]. The wave functions in the third group are a bit complicated and hence have not been used in any calculation. The Silvermann wave function [20], one-parameter Slater wave function and a Hylleraas-type wave function [30] have been used earlier [11,13,15]. In the present study we choose one wave function from the first group and the other from the second group and apply the (e, 3e) test. The former is closed-shell type and the latter is open-shell type.

2. Theory

We consider events in which fast electrons having energy E_0 are incident on helium and are inelastically scattered with energy E_a into the solid angle $d\Omega_a$ in the direction (θ_a, Φ_a)

and eject both the target electrons with low energies E_b and E_c into the solid angles $\mathrm{d}\Omega_b$ and $\mathrm{d}\Omega_c$ in the directions (θ_b, θ_b) and (θ_c, Φ_c) respectively. The FDCS for this process is given by

$$\frac{\mathrm{d}^5\sigma}{\mathrm{d}E_a \mathrm{d}E_b \mathrm{d}\Omega_a \mathrm{d}\Omega_b \mathrm{d}\Omega_c} = \frac{k_a k_b k_c}{k_0} |F|^2, \tag{3}$$

where $\vec{k}_0$, $\vec{k}_a$, $\vec{k}_b$ and $\vec{k}_c$ are the momenta of the incident, scattered and ejected electrons respectively and F is the ionization amplitude. The energy–momentum conservation leads to

$$E_0 = E_a + E_b + E_c + I, \tag{4}$$

$$\vec{k}_0 - \vec{k}_a = \vec{q} = \vec{k}_b + \vec{k}_c + \vec{k}_r, \tag{5}$$

where I, $\vec{k}_r$ and $\vec{q}$ are the double ionization threshold energy, recoil momentum of the residual ion and momentum transfer by the incident electron to the target respectively. The amplitude F in the second born approximation which incorporates the SO and TS2 processes is given by

$$F = F_{\mathrm{B1}} + F_{\mathrm{B2}}, \tag{6}$$

where

$$\begin{aligned} F_{\mathrm{B1}} = &-\frac{1}{2\pi} \int (\phi_f^*(r_1, r_2) - S^* \phi_0^*(r_1, r_2)) \mathrm{e}^{-\mathrm{i}\vec{k}_a \cdot \vec{r}_0} \left(-\frac{2}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}} \right) \\ &\times \phi_0(r_1, r_2) \mathrm{e}^{\mathrm{i}\vec{k}_0 \cdot \vec{r}_0} \, \mathrm{d}\vec{r}_0 \, \mathrm{d}\vec{r}_1 \, \mathrm{d}\vec{r}_2 \end{aligned} \tag{7}$$

$$\begin{aligned} F_{\mathrm{B2}} = &\frac{1}{8\pi^4} \int \frac{\mathrm{d}\vec{q}'}{(q'^2 - k_0^2 + 2\bar{\omega} - \mathrm{i}\varepsilon)} \\ &\times \left\langle \{\phi_f(\vec{r}_1, \vec{r}_2) - S\phi_0(\vec{r}_1, \vec{r}_2)\} \mathrm{e}^{\mathrm{i}\vec{k}_a \cdot \vec{r}'_0} \middle| \left(-\frac{2}{r'_0} + \frac{1}{r'_{01}} + \frac{1}{r'_{02}} \right) \middle| \mathrm{e}^{\mathrm{i}\vec{q}' \cdot \vec{r}'_0} \right\rangle \\ &\times \left\langle \mathrm{e}^{\mathrm{i}\vec{q}' \cdot \vec{r}_0} \middle| \left(-\frac{2}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}} \right) \middle| \phi_0(r_1, r_2) \mathrm{e}^{\mathrm{i}\vec{k}_0 \cdot \vec{r}_0} \right\rangle \end{aligned} \tag{8}$$

$$S = \int \phi_0^*(\vec{r}_1, \vec{r}_2) \phi_f(\vec{r}_1, \vec{r}_2) \mathrm{d}\vec{r}_1 \, \mathrm{d}\vec{r}_2 \tag{9}$$

$$\phi_f(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left\{ \mathrm{e}^{\mathrm{i}\vec{k}_b \cdot \vec{r}_1} \mathrm{e}^{\mathrm{i}\vec{k}_c \cdot \vec{r}_2} C(\vec{k}_b, \vec{k}_c, \vec{r}_1, \vec{r}_2) + \mathrm{e}^{\mathrm{i}\vec{k}_b \cdot \vec{r}_2} \mathrm{e}^{\mathrm{i}\vec{k}_c \cdot \vec{r}_1} C(\vec{k}_b, \vec{k}_c, \vec{r}_2, \vec{r}_1) \right\} \tag{10}$$

$$C(\vec{k}_b, \vec{k}_c, \vec{r}_1, \vec{r}_2) = N_1 F_1(\mathrm{i}\alpha_b, 1, -\mathrm{i}(k_b r_1 + \vec{k}_b \cdot \vec{r}_1))_1 F_1(\mathrm{i}\alpha_c, 1, -\mathrm{i}(k_c r_2 + \vec{k}_c \cdot \vec{r}_2)) \tag{11}$$

$$N = (2\pi)^{-3} \mathrm{e}^{-\pi\alpha_b/2}\Gamma(1-\mathrm{i}\alpha_b)\mathrm{e}^{-\pi\alpha_c/2}\Gamma(1-\mathrm{i}\alpha_c)\mathrm{e}^{-\pi\alpha_{bc}/2}\Gamma(1-\mathrm{i}\alpha_{bc}) \tag{12}$$

$$\alpha_b = -Z_b/k_b, \quad \alpha_c = -Z_c/k_c \quad \text{and} \quad \alpha_{bc} = Z_{bc}/2k_{bc}. \tag{13}$$

Here $\vec{r}_0$, $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of incident and bound electrons with respect to the nucleus and $r_{0i} = |\vec{r}_0 - \vec{r}_i|$, $r'_{0i} = |\vec{r}'_0 - \vec{r}_i|$. ϕ_f is the symmetrized product of Coulomb wave functions corresponding to the two ejected electrons with Gamow factor and S is the overlap of ϕ_f with the target wave function ϕ_0. The wave function ϕ_f and the target initial state wave function ϕ_0 are eigenstates of the same hamiltonian and so their overlap S must vanish. However, ϕ_f here is only an approximate wave function and this overlap does not vanish. ϕ_f has therefore been Schimdt orthogonalized with respect to ϕ_0 to enforce this requirement. The excitations of the intermediate states have been approximated by an average excitation energy $\bar{\omega}$ (= 2 a.u.) and sum over them has been carried out by closure following Byron and Joachain [31]. The use of average excitation energy $\bar{\omega}$ has been in vogue since 1973 [31]. The choice of $\bar{\omega}$ has been varied over the range 0.7–1.3 times the threshold for the process. The results are however not very sensitive to its value. α_b, α_c and α_{bc} are effective momentum-dependent Sommerfeld parameters and $\vec{k}_{bc}$ is momentum conjugate to $\vec{r}_{12} (= \vec{r}_1 - \vec{r}_2)$. The effective charges Z_b, Z_c and Z_{bc} are given by [32]

$$Z_{b,c} = Z + \frac{Z}{2}\frac{k_{b,c}}{k_a} - \frac{k_{b,c}}{|\vec{k}_a - \vec{k}_{b,c}|} \tag{14}$$

$$Z_{bc} = 1. \tag{15}$$

The integration over the co-ordinates of the incident electron in eqs (7) and (8) is performed by using Bethe Integral

$$\int \frac{\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_0}}{r_{01}} \mathrm{d}\vec{r}_0 = \frac{4\pi}{q^2} \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_1}. \tag{16}$$

This leads to

$$F_{\mathrm{B1}} = -\frac{2}{q^2}\int (\phi_f^*(r_1,r_2) - S^*\phi_0^*(r_1,r_2))(-2 + \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_1} + \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_2})\phi_0(r_1,r_2)\mathrm{d}\vec{r}_1\mathrm{d}\vec{r}_2 \tag{17}$$

and

$$F_{\mathrm{B2}} = \frac{2}{\pi^2}\int \frac{\mathrm{d}\vec{q}'}{q_i^2 q_f^2 (q'^2 - k_0^2 + 2\bar{\omega} - \mathrm{i}\varepsilon)} \Big\langle \{\phi_f(\vec{r}_1,\vec{r}_2) - S\phi_0(\vec{r}_1,\vec{r}_2)\} \\ \times \Big| (-2 + \mathrm{e}^{\mathrm{i}\vec{q}_f\cdot\vec{r}_1} + \mathrm{e}^{\mathrm{i}\vec{q}_f\cdot\vec{r}_2})(-2 + \mathrm{e}^{\mathrm{i}\vec{q}_i\cdot\vec{r}_1} + \mathrm{e}^{\mathrm{i}\vec{q}_i\cdot\vec{r}_2}) \Big| \phi_0(r_1,r_2) \Big\rangle \tag{18}$$

where $\vec{q}_i = \vec{k}_0 - \vec{q}'$ and $\vec{q}_f = \vec{q}' - \vec{k}_a$.

The evaluation of F_{B1} and F_{B2} now involves standard Nordseick integral [33] and the second Born term has been calculated by following the method of Srivastava and Sharma [34]. Atomic units have been used in all the calculations.

3. Results and discussion

The present study is in two parts. We compare the angular variation of FDCS obtained by using different wave functions with the experimental data and then look for kinematical arrangements where the differences in the results show up most prominently. For the first part, the ground state wave functions ϕ_0 of helium have been taken to be the one given by Byron and Joachain [18] (BJ) as a representative of CS class

$$\phi_0(\vec{r}_1,\vec{r}_2) = u(\vec{r}_1)u(\vec{r}_2)$$
$$u(r) = \gamma_1 \mathrm{e}^{-\beta_1 r} + \gamma_2 \mathrm{e}^{-\beta_2 r}$$
$$\gamma_1 = 2.60505, \quad \beta_1 = 1.41$$
$$\gamma_2 = 2.08144, \quad \beta_2 = 2.61$$

and by Silvermann *et al* [20] (SPM) as a representative of OS class

$$\phi_0(\vec{r}_1,\vec{r}_2) = N_0(\mathrm{e}^{-\eta_1 r_1}\mathrm{e}^{-\eta_2 r_2} + \mathrm{e}^{-\eta_1 r_2}\mathrm{e}^{-\eta_2 r_1})$$
$$\eta_1 = 2.17, \quad \eta_2 = 1.21 \quad \text{and} \quad N_0 = 0.718.$$

Figure 1a shows the variation of FDCS with the angle of ejection θ_c at an incident energy $E_0 = 5599$ eV, scattering angle $\theta_a = 0.45°$ and ejected electron energies $E_b = E_c = 10$ eV. One of the electrons say b, is assumed to be ejected along the momentum transfer direction, $\theta_b = \theta_q = 319°$. The theoretical results are compared with the absolute experimental data of Lahmam-Bennani [13] in the angular range $27° \leq \theta_c \leq 153°$. The emphasis here is on the qualitative features and shape comparison of FDCS. Therefore different scaling factors for SPM and BJ results are used in different kinematics to make their magnitudes comparable to the data for the sake of clarity. The angular variation of the SPM results is in pretty good agreement with the experimental data. The overall normalization has been adjusted to fit the data at $\theta_c \sim 100°$. The BJ results are qualitatively very different. There is a small peak in the central region where the data point to a minimum. The results (not shown here) with the Hartree–Fock and Hylleraas first order wave functions are more or less identical to those with BJ wave function. The CS wave functions thus fail to reproduce the angular variation of FDCS in this kinematics. Another feature of the results is that the peak at $\sim 260°$ is larger than the peak at $\sim 100°$, the second Born approximation increases the former and decreases the latter over the first Born values. But this feature cannot be confirmed in the absence of data over the whole range of θ_c. Figures 1b and 1c show the results when the electron b is ejected opposite to the momentum transfer direction and almost perpendicular to it $(\theta_b = 221°)$ respectively. In both of these cases, it is difficult to choose between BJ and SPM results. The agreement with the experimental data is equally good for both. Figure 2a shows the SPM and BJ results at $E_0 = 1099$ eV, $\theta_a = 1.1°$, $E_b = E_c = 10$ eV along with the relative experimental data of Lahmam-Bennani [35]. The agreement with the experimental data is not very good here, though the SPM results do show a minimum as indicated by the data. The BJ results are again very different. Figures 2b and 2c show the results when the electron b is ejected at fixed angles of 189° and 97° respectively with the momentum transfer direction. Here again there is nothing much to choose between BJ and SPM results.

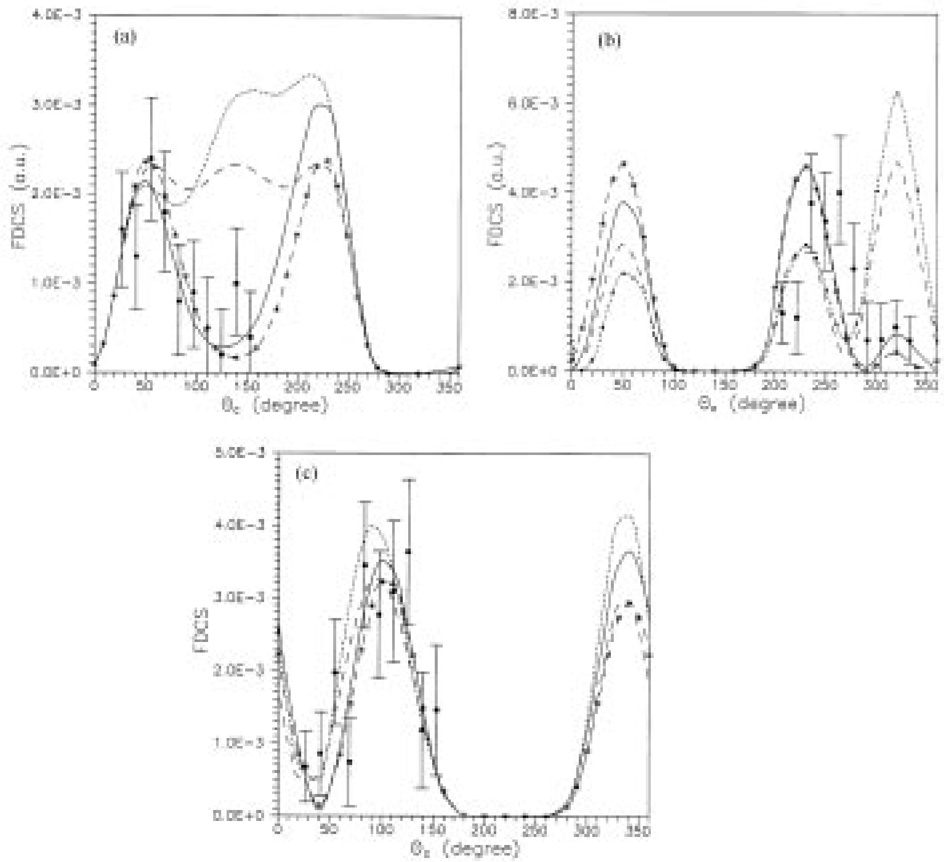

Figure 1. (**a**) FDCS plotted against θ_c. $E_0 = 5599$ eV, $E_b = E_c = 10$ eV, $\theta_a = 0.45°$. The direction of the other ejected electron $\theta_b = \theta_q = 319°$, θ_q is the momentum transfer direction. The dashed line with stars and the solid line are respectively first Born (B1) and second Born (B2) results with SPM wave function for He. The long dashed line and the short dashed line represent respectively B1 and B2 results with BJ wave function for He. A factor 200 is multiplied to the results with BJ and a factor 120 is multiplied to the results with SPM to compare with the experimental data. (**b**) Same as figure 1a, but for $\theta_b = 139°$. A factor 400 is multiplied to the BJ results and a factor 308 is multiplied to the SPM results to compare with the experimental data. (**c**) Same as figure 1a, but for $\theta_b = 221°$. A factor 200 is multiplied to the BJ results and a factor 110 is multiplied to the SPM results to compare with the experimental data.

The usefulness of the kinematics in figures 1a and 2a is expected. It corresponds to the most probable case when one of the electrons is emitted along the momentum transfer direction. The angular distribution of ejection of the other electron then depends on the correlation between the two.

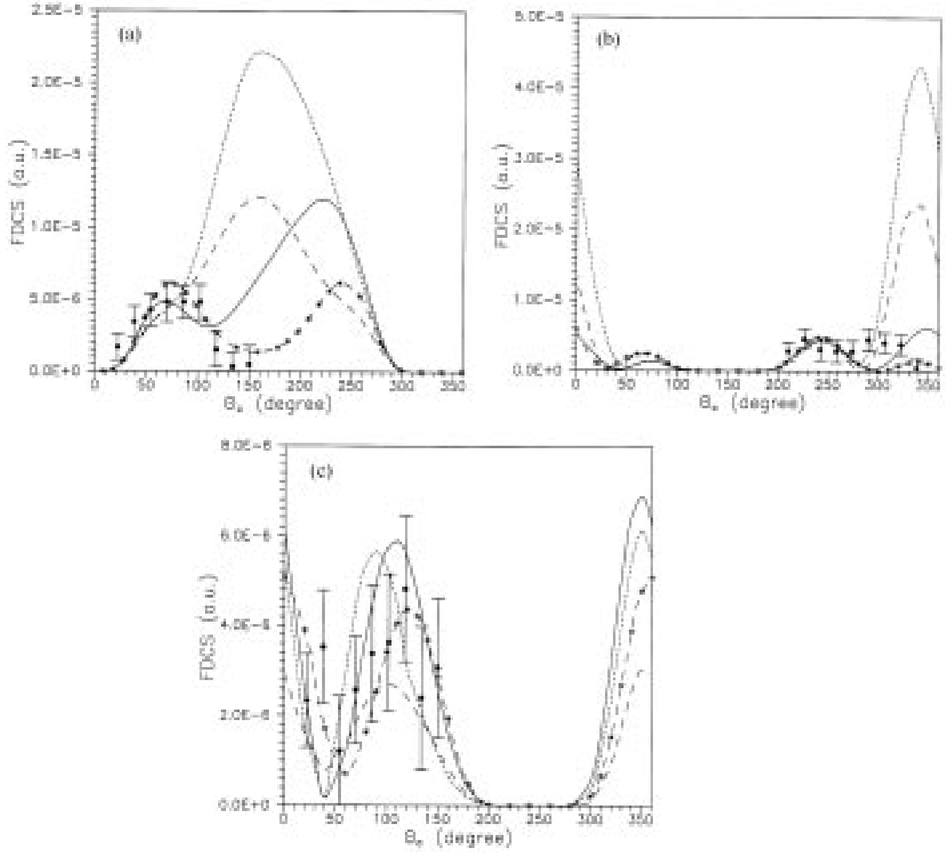

Figure 2. (**a**) Same as figure 1a, but for $E_0 = 1099$ eV, $\theta_a = 1.1°$ and $\theta_b = \theta_q = 338°$. Here, results are not multiplied by any factor. (**b**) Same as figure 1a, but for $E_0 = 1099$ eV, $\theta_a = 1.1°$ and $\theta_b = 150°$. Here, SPM results are not multiplied by any factor, but a factor 2 is multiplied to the BJ results to compare with the experimental data. (**c**) Same as figure 1a, but for $E_0 = 1099$ eV, $\theta_a = 1.1°$ and $\theta_b = 242°$. A factor 0.5 is multiplied to the BJ results and a factor 0.6 is multiplied to the SPM results to compare with the experimental data.

Figures 3a and 3b show our results in the Bethe ridge kinematics. This kinematics corresponds to the situation where the recoil momentum $\vec{k}_r$ of the residual ion is zero. In this case, eqs (4) and (5) can be solved for given initial energy E_0, scattering angle θ_a (or momentum transfer $\vec{q}$) and scattering energy E_a to give E_b, E_c and angles θ_{bq} and θ_{cq} (ejection angles with respect to $\hat{q}$) for different values of θ_{bc}. At $\theta_{bc} = 180°$, the energetic of the two electrons is ejected along $\hat{q}$ and the other one in the opposite direction. At $\theta_{bc} = 180°$, BJ results are larger than SPM and decrease with decreasing θ_{bc} while SPM results increase with decreasing θ_{bc}. The variations of BJ and SPM with θ_{bc} are thus very different. This difference, however, cannot be used at present in the absence of experimental data to prefer one wave function over the other.

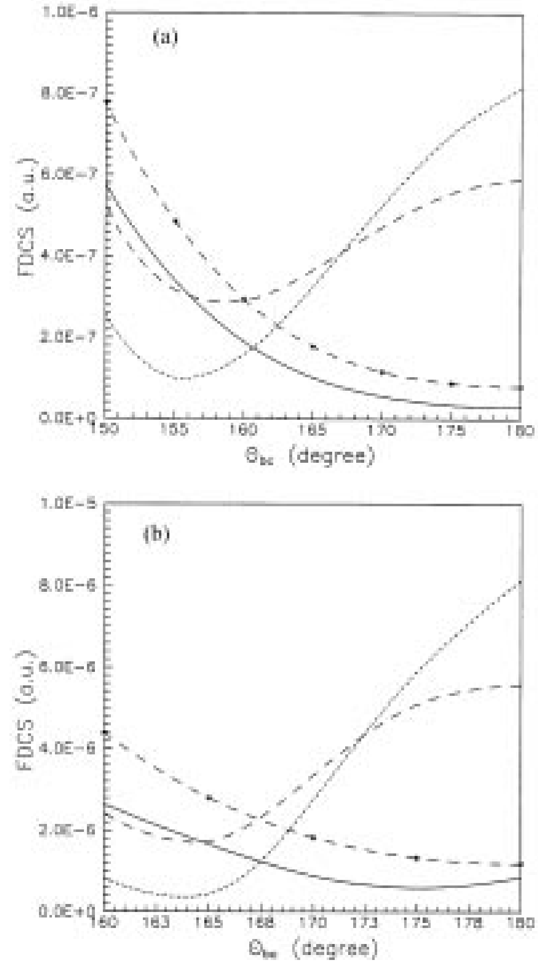

Figure 3. FDCS plotted against θ_{bc}. $E_0 = 5599$ eV, $\theta_a = 0.45°$. E_b, E_c, θ_b and θ_c are changed such that Bethe ridge condition $(\vec{k}_r = 0)$ is satisfied at all values of θ_{bc}. $E_b + E_c$ is fixed at (**a**) 4 eV and (**b**) 10 eV. The description of lines is same as in figure 1.

We thus find that in the coplanar geometry two kinematical arrangements: (i) equal energy sharing $E_b = E_c$ with one electron ejected along the momentum transfer direction and the other along the varying direction and (ii) the Bethe ridge condition with fixed $E_b + E_c$, are very sensitive to e–e correlations in the target and could be used to sort out different wave functions. The comparison of BJ and SPM results with the data clearly shows that OS class wave functions incorporate e–e correlations better than the CS class. Further sorting within the class depending on the e–e angular correlation is not possible till data is available over the whole range of θ_c and with better statistics.

These observations are expected to be model independent as the general qualitative shapes of FDCS obtained by using a correlated four-body final state or convergent close coupling formalism are grossly similar to the one obtained by using three-Coulomb wave method of Brauner, Briggs and Klar (BBK) [36]. Present choice of the final state wave function using effective charges and Gamow factor is an approximation to the BBK wave function [37] and has been found to lead to essentially identical results which differ only in the over-all magnitude [38–40].

Acknowledgements

This work was supported by the Department of Science and Technology (DST), Government of India. One of us (KM) would like to thank DST for providing a research fellowship during the period of this study. We are thankful to Prof. A Lahmam-Bennani for sending the experimental data before publication.

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