Converged cross-section results for double photoionization of helium atoms in hyperspherical partial wave theory at 6 eV above threshold

J. N. Das,[1,*] K. Chakrabarti,[2] and S. Paul[1]

[1]*Department of Applied Mathematics, University College of Science, 92 Acharya Prafulla Chandra Road, Calcutta 700 009, India*

[2]*Department of Mathematics, Scottish Church College, 1 & 3 Urquhart Square, Calcutta 700 006, India*

(Received 30 December 2003; published 2 April 2004)

Here we report a set of converged cross-section results for double photoionization of helium atoms obtained in the hyperspherical partial wave theory for equal energy sharing kinematics at 6 eV energy above threshold. The calculated cross section results are generally in excellent agreement with the absolute measured results of Dörner *et al.* [Phys. Rev. **57**, 1074 (1998)].

DOI: 10.1103/PhysRevA.69.044702 PACS number(s): 32.80.Fb

Double photoionization problems of helium atoms continue to attract wide attention of theoreticians as well as experimentalists, since these are among the most fundamental problems of atomic physics, which still present challenges towards their full understanding. Study of triple differential cross sections (TDCS) for this problem is most important since this offers the most stringent tests for theories to explain the experimental results. At present there exist absolute measured TDCS results of several groups for different photon energies −0.1 eV and 0.2 eV [1], 1 eV [2], 6 eV [2], and 20 eV [2,3], above threshold. However there are many more observed results which are not absolute but are only relative (see, for example, [4–9] and references therein). On the theoretical side there exist the results of older theories such as 3C theory [10], 2SC theory [11,12], and the Wannier theory [13]. Wannier theory gives good qualitative description at 6 eV excess energy but fails at higher energies. For a review of all these one may look to the review paper by Briggs and Schmidt [14]. For information regarding difficulties of these theories the paper by Lucey *et al.* [15] may be consulted. More recent theories are the convergent close coupling (CCC) theory [16], the hyperspherical $\mathcal{R}$-matrix theory with semiclassical outgoing waves (HRM-SOW) [17], and the time dependent close-coupling (TDCC) theory [18]. These have wider applicability. But except for the CCC theory the others have been tested only in a small number of problems. Another high level theory is the hyperspherical partial wave (HPW) theory suggested by one of the present authors [19] in the context of electron hydrogen atom ionization collisions and has already been applied for this problem [20]. Later this theory has been applied for double photoionization also [21,22] with considerable success and the results were found to be practically "gauge" independent. There it was applied for 20 eV and 40 eV excess photon energies only. Here, in our present calculation, we focus attention to lower energies for which the asymptotic domain recedes to far larger distances. So for our present study at 6 eV excess energy we made a much larger scale calculation to obtain converged cross-section results for equal energy sharing geometries.

Hyperspherical partial wave theory, in the context of double photoionization, has been described in detail in Ref. [21] and in outline in Ref. [22]. Here we only touch upon certain points for ready understanding of the present work.

The *T*-matrix elements for the double photoionization, in dipole approximation, which is sufficiently accurate here, is given by

$$T_{fi} = \langle \Psi_f^{(-)} | V | \Phi_i \rangle. \tag{1}$$

Here $\Phi_i(\vec{r}_1,\vec{r}_2)$ is the initial-state helium atom ground-state wave function, for which a 20-term Hylleraas-type wave function of Hart and Herzberg [24] is accurate enough in the present context. Since our results are practically "gauge" independent we choose here the velocity gauge in which V is given by

$$V = \vec{\epsilon} \cdot (\vec{\boldsymbol{\nabla}}_1 + \vec{\boldsymbol{\nabla}}_2), \tag{2}$$

where $\vec{\epsilon}$ represents the photon polarization direction. So for accurate cross-section results one needs only to use, in addition, a final-state two-particle continuum wave function which is sufficiently accurate. Such a wave function may be calculated in the HPW theory.

In this theory one uses hyperspherical coordinates $(R,\alpha,\theta_1,\phi_1,\theta_2,\phi_2)=(R,\omega)$, where $R=\sqrt{r_1^2+r_2^2}$, $\alpha=\arctan(r_2/r_1)$, and the other angular coordinates (θ_1,ϕ_1) and (θ_2,ϕ_2) are related to the position vectors $\vec{r}_1=(r_1,\theta_1,\phi_1)$ and $\vec{r}_2=(r_2,\theta_2,\phi_2)$ of the outgoing electrons having momenta $\vec{p}_a=(p_a,\theta_a,\phi_a)$ and $\vec{p}_b=(p_b,\theta_b,\phi_b)$ together defined by $(P,\alpha_0,\theta_a,\phi_a,\theta_b,\phi_b)=(P,\omega_0)$, where $P=\sqrt{p_a^2+p_b^2}$ and $\alpha_0=\arctan(r_b/r_a)$.

Since the final state $\Psi_f^{(-)}$ has the symmetry corresponding to $L=1$, $S=0$, $\pi=\text{odd}$, $\Psi_f^{(-)}$ has the expansion in terms of hyperspherical harmonics Φ_N with expansions $f_N(R)$, where N stands for the triplet (l_1,l_2,n), as

$$\Psi_f^{(-)}(R,\omega) = \sqrt{\frac{2}{\pi}}\sum_N \frac{f_N(R)}{\rho^{\frac{5}{2}}}\Phi_N(\omega), \tag{3}$$

where $\rho=PR$.

*Email address: jndas@cucc.ernet.in

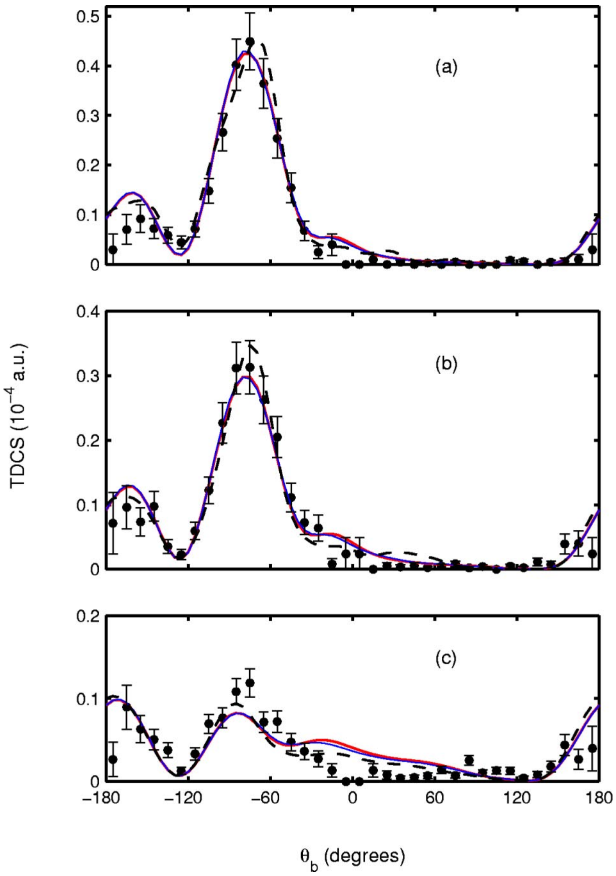

FIG. 1. Averaged TDCS results for equal energy sharing double photoionization of the helium atom at 6 eV excess energy, for θ_a in $[45°,65°]$, (a) for ϕ_{ab} in $[0°,20°]$, (b) for ϕ_{ab} in $[20°,45°]$, and (c) ϕ_{ab} in $[45°,90°]$ in the present calculation. Theory: thick curve, 150 channels; thin curve, 100 channels; dashed curve, 75 channels. Experiment: Dörner *et al.* [2].

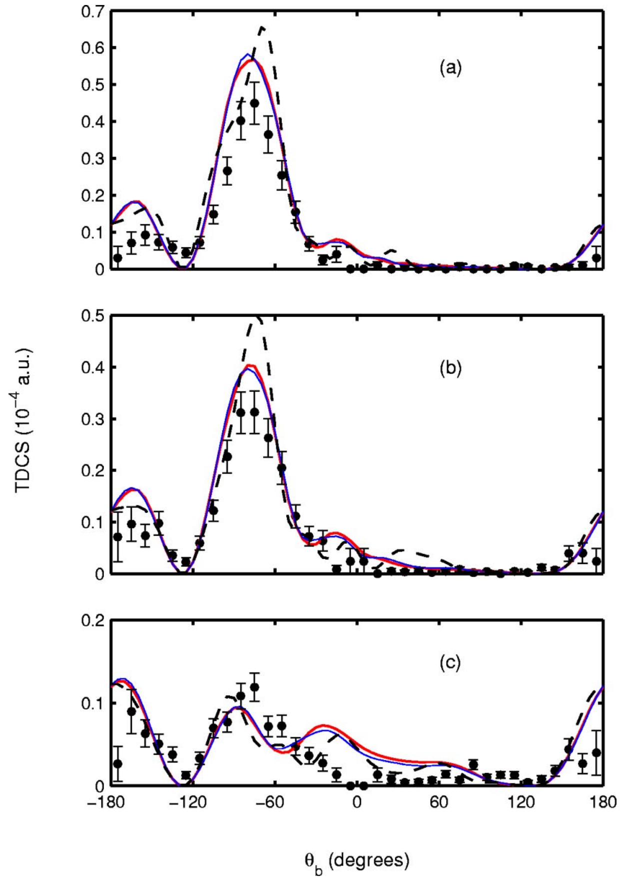

FIG. 2. TDCS results (at midpoints of angular domains) for equal energy sharing double photoionization of the helium atom at 6 eV excess energy. Here θ_a=52.5° and (a) ϕ_{ab}=10°, (b) ϕ_{ab}=32.5°, and (c) ϕ_{ab}=67.5° for the present calculation. Theory: thick curve, 150 channels; thin curve, 100 channels; dashed curve, 75 channels. Experiment: Dörner *et al.* [2].

The functions f_N's satisfy a single infinite coupled set of differential equations, in place of an infinity of such equations for electron-hydrogen atom ionization collisions, given by

$$\left[\frac{d^2}{dR^2}+P^2-\frac{\nu_N(\nu_N+1)}{R^2}\right]f_N+\sum_{N'}\frac{2P\alpha_{NN'}}{R}f_{N'}=0. \quad (4)$$

Here $\alpha_{NN'}$ are the charge matrix elements and N's are all allowed sets of (l_1,l_2,n) triplets with $l_2=l_1+1$ and l_1, n taking independently the values $0,1,2\cdots$, etc., l_1, l_2 being the angular momenta of the individual electrons and n's are the orders of the Jacobi polynomials. We truncate the number of equations in Eq. (4) to some N_{mx} numbers in N_{mx} number of variables f_N's for approximate numerical solutions. We call the number N_{mx} the channel number. Here we did the calculations with 50, 75, 100, and 150 channels.

Now the equations f_N's are to be solved from the origin to a point R_∞ in the far asymptotic domain. The equations have been solved as in Ref. [21] over $[0,R_\infty]$, first over an interval $(0,\Delta)$ using a seven point difference scheme [21] in steps of h=0.05 a.u. Then from Δ onwards up to R_∞, Taylor's expansion method has been used in steps of h'=0.1 a.u., including some 15–20 terms in the expansion, stabilizing frequently [23]. Finally at R_∞ we obtain an asymptotic series solution [20] suitably expanding in sine and cosine terms multiplied by inverse powers of ρ, until the series gets converged. The solution which starts with values 0 at origin is suitably matched at points Δ and R_∞.

From observation of the symmetrized plane wave, expanded in hyperspherical harmonics [19], all the unknown coefficients of $\Psi_f^{(-)}$ are determined completely. Finally T-matrix element is calculated from Eq. (1), and then the triple differential cross section is given by

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1}=\frac{2\pi^2 p_a p_b}{\omega_i}|T_{fi}|^2. \quad (5)$$

In our present calculation for 6 eV excess energy we made a very large scale computation with asymptotic range parameter R_∞ chosen as 2000 a.u., with as many channels as 150. Thus in our calculations we have included (l_1,l_2,n) triplets up to (14, 15, 9). Actually we increased the number of channels, taking values 50, 75, 100, and 150. In the figures we present results for N_{mx}=75,100, and 150 only.

The TDCS cross-section results have been averaged over the angular openings corresponding to observations. Thus for results presented in Fig. 1(a) we averaged over $(40°,65°)$ for θ_a, the polar angle measured from the photon polarization direction and over $(0°,20°)$ for ϕ_{ab}, the azimuthal angular difference of the electrons, corresponding to the observations of Dörner *et al.* [2], presented in their Fig. 13(d). Similarly for the results presented in Figs. 1(b) and 1(c) we averaged over the same angular domain for θ_a but over $(20°,45°)$ and $(45°,90°)$, respectively, for ϕ_{ab}. Results obtained in this way have been compared with the corresponding measured results of Dörner *et al.* It may be mentioned here that regarding the angular opening corresponding to the other polar angle θ_b, nothing is stated in the work of Dörner *et al.* So we could not make any averaging corresponding to this variable. In averaging we made calculations at 5° intervals both for θ_a and for ϕ_{ab}. Thus for results presented in Fig. 1(a) we calculated altogether $6\times 5=30$ sets of results and averaged over these. Similarly for Fig. 1(b) we calculated $6\times 6=36$ sets of results for averaging and for Fig. 1(c) we calculated $6\times 10=60$ sets of results for averaging. Next we consider comparison of our results with those of measured results of Dörner *et al.* The results, shown in Figs. 1(a) and 1(b) are in excellent agreement with the measured values. However for the results presented in Fig. 1(c), although there is generally agreement, there are some differences as well. Our results show some undulation around −25°, but no such thing is shown in the experimental results. Now in this case the angular opening is significantly large. As a result there may be some uncertainty in the averaging process. Moreover the theoretical results corresponding to the extremity $\phi_{ab}=90°$ has a double peak structure, symmetric about $\theta_b=0°$ and that even for $\phi_{ab}=67.5°$, the midpoint value, there is a prominent peak as is shown in Fig. 2(c) around −25°. Thus the structure shown in the calculated curve, i.e., in Fig. 1(c) is not very unreasonable. In any case this is only a disturbing feature of the present results. So further theoretical and, possibly, experimental results are necessary to resolve the problem. We also present results corresponding to midpoint for θ_a and ϕ_{ab} intervals in Fig. 2. These results are also generally in agreement with the experimental values except that the results are about 30% larger. Only in Fig. 2(c) there are some significant differences. Here the peak height at −25° is further enhanced. It may be mentioned here that we could not compare with other theoretical results like those of CCC, HRM-SOW or TDCC theories for these kinematic conditions since such results are not available in the literature.

Now we conclude with the remarks that for the kinematical conditions considered, with equal energy sharing, the calculations have practically converged with 100 channels. As is shown in the figures, the 100-channel and 150-channel results are practically indistinguishable. It may be mentioned here that our results are *ab initio* and there is no scaling parameter. For unequal energy sharing kinematics larger size calculations may be necessary for converged results. Such calculations are not possible with the present computational resources available to us.

Here it may be mentioned that our present computations have been done on Pentium-IV PC's with 512 MB RAM and 2.6 GHz clock speed. A 150 channels computation took about 12 h time for a single run.

The authors are grateful to Reinhardt Dörner for providing the experimental results in electronic form. K.C. acknowledges support from the University Grants Commission, New Delhi, in the form of a Minor Research Project No. F.PSW-035/02/(ERO). S.P. is grateful to CSIR for providing financial support.

[1] A. Huetz and J. Mazeau, Phys. Rev. Lett. **85**, 530 (2000).
[2] R. Dörner *et al.*, Phys. Rev. A **57**, 1074 (1998).
[3] H. Bräuning *et al.*, J. Phys. B **31**, 5149 (1998).
[4] G. Dawber, L. Avaldi, A. G. McConkey, H. Rojas, M. A. MacDonald, and G. C. King, J. Phys. B **28**, L271 (1995).
[5] O. Schwarzkopf *et al.*, J. Phys. IV **3**, 169 (1993); O. Schwarzkopf and V. Schmidt, J. Phys. B **28**, 2847 (1995).
[6] P. Lablanquie, J. Mazeau, L. Andric, P. Selles, and A. Huetz, Phys. Rev. Lett. **74**, 2192 (1995).
[7] S. Cvejanović, J. P. Wightman, T. J. Reddish, F. Maulbetsch, M. A. MacDonald, A. S. Khiefets, and I. Bray, J. Phys. B **33**, 265 (2000).
[8] P. Bolognesi, R. Camilloni, M. Coreno, G. Turri, J. Berakdar, A. S. Kheifets, and L. Avaldi, J. Phys. B **34**, 3193 (2001).
[9] C. Dawson, S. Cvejanović, D. P. Seccombe, T. J. Reddish, F. Maulbetsch, A. Huetz, J. Mazeau, and A. S. Kheifets, J. Phys. B **34**, L525 (2001).
[10] F. Maulbetsch and J. S. Briggs, J. Phys. B **26**, 1679 (1993).
[11] M. Pont and R. Shakeshaft, Phys. Rev. A **51**, R2676 (1995).
[12] M. Pont, R. Shakeshaft, F. Maulbetsch, and J. S. Briggs, Phys. Rev. A **53**, 3671 (1996).
[13] J. M. Feagin, J. Phys. B **28**, 1495 (1995); **29**, L551 (1996).
[14] J. S. Briggs and V. Schmidt, J. Phys. B **33**, R1 (2000).
[15] S. P. Lucey, J. Rasch, C. T. Whelan, and H. R. J. Walters, J. Phys. B **31**, 1237 (1998).
[16] A. S. Kheifets and I. Bray, J. Phys. B **31**, L447 (1998); Phys. Rev. A **58**, 4501 (1998); Phys. Rev. Lett. **81**, 4588 (1998); Phys. Rev. A **62**, 065402 (2000).
[17] L. Malegat, P. Selles, and A. K. Kazansky, Phys. Rev. A **60**, 3667 (1999); Phys. Rev. Lett. **85**, 4450 (2000); P. Selles, L. Malegat, and A. K. Kazansky, Phys. Rev. A **65**, 032711 (2002).
[18] J. Colgan, M. S. Pindzola, and F. Robicheaux, J. Phys. B **34**, L457 (2001).
[19] J. N. Das, Pramana, J. Phys. **50**, 53 (1998).
[20] J. N. Das, S. Paul, and K. Chakrabarti, Phys. Rev. A **67**, 042717 (2003).
[21] J. N. Das, K. Chakrabarti, and S. Paul, J. Phys. B **36**, 2707 (2003).
[22] J. N. Das, K. Chakrabarti, and S. Paul, Phys. Lett. A **316**, 400 (2003).
[23] B. H. Choi and K. T. Tang, J. Chem. Phys. **63**, 1775 (1975).
[24] J. F. Hart and G. Herzberg, Phys. Rev. **106**, 79 (1957).