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Double photoionization of helium atoms at 1 eV above threshold

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Abstract. An ab initio calculation of triple differential cross-section for double photoionization of helium atoms are presented for a very low energy of just 1 eV above threshold in the equal energy sharing kinematics. We have used hyperspherical partial wave theory together with a Numerov difference scheme in place of other schemes used in our earlier works. The results are in excellent qualitative agreement with the measurements of Dörner et al. [Phys. Rev. A **57**, 1074 (1998)].

PACS. 32.80.Fb Photoionization of atoms and ions

1 Introduction

For double photoionization of helium atoms very close to threshold, absolute measured cross-section results have been reported by Dörner et al. [1] at incident photon energies of 1 eV and 6 eV above threshold. However, to the best of our knowledge, for such low energies theoretical results of successful theories like hyperspherical R-matrix theory with semiclassical outgoing waves (HRM-SOW) [2], the time depending close coupling (TDCC) theory [4] and the convergent close coupling (CCC) theory [5] are not yet known.

Maulbetsch et al. [6] calculated the double photoionization triple differential cross-section (TDCS) at incident photon energies 0.6 eV, 1 eV and 20 eV above threshold for different energy sharing and linearly polarized light (with different degrees of polarization characterized by the Stokes parameter S_1) and obtained good agreement with the experiments. They used two different methods to compute the photoionization TDCS which, however, did not seem to agree with each other with respect to absolute values even though they obtained good qualitative agreement with the experiments. For low incident photon energies, there are also the theoretical analysis of Huetz et al. [7] and Wannier description of Feagin [8], which need fitting with experimental results. Calculations following Huetz et al. need a Gaussian fitting of a correlation function and in the Wannier analysis certain parametrization is needed. These situations encouraged us to undertake the present calculation in the hyperspherical partial wave (HPW) theory [9–11] for the present problem. The HPW theory has already been applied successfully for the double photoionization of helium at 20eV [9], 20 eV and 40 eV [10] and 6 eV [11] excess energies. Here we undertake HPW calculation at 1 eV excess energy which needs special considerations.

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2 Hyperspherical partial wave theory

Hyperspherical partial wave theory for the calculation of three-particle (nucleus and two electrons) scattering state has been described in detail in the context of electron-hydrogen ionization problems in [12–14] and outlined in several other publications, particularly in the context of double photoionization of helium atom in [9]. We therefore present here only the essentials. In the double photoionization calculation the scattering cross-sections are calculated from the T-matrix element given by

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

where $\Psi_f^{(-)}$ is the final three-particle scattering state with incoming boundary condition, Φ_i is the initial ground state wave function and V is the interaction term which, in the velocity gauge, is given by

$$V = \boldsymbol{\epsilon} \cdot (\nabla_1 + \nabla_2). \tag{2}$$

The final scattering state, which is singlet with odd parity and total angular momentum L = 1 ($^1\mathrm{P}^o$ symmetry), is expanded 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 $\rho = PR$ and ϕ_N are hyperspherical harmonics which are a symmetrized product of normalized Jacobi

polynomials $P_n^{l_1 l_2}$ and coupled angular momentum eigenfunctions $\mathcal{Y}_{l_1 l_2}^{LM}$ [12]. The index N denotes the triplet (n, l_1, l_2), l_1, l_2 being the angular momenta of the outgoing electrons, n is the order of the Jacobi polynomial in the hyperspherical harmonics $\phi_N(\omega)$ and M is the projection of the total angular momentum L. Denoting the coordinates of the two outgoing electrons by $\mathbf{r}_1 = (r_1, \theta_1, \phi_1)$ and $\mathbf{r}_2 = (r_2, \theta_2, \phi_2)$, the hyperspherical coordinates are (R, ω) where the hyperradius R is defined by $R = \sqrt{r_1^2 + r_2^2}$ and ω denotes the collection of five angular coordinates $(\alpha, \theta_1, \phi_1, \theta_2, \phi_2)$, $\alpha = \arctan(r_2/r_1)$ being the hyperspherical angle. The corresponding quantities for the two outgoing electron momenta $\mathbf{p}_1 = (p_1, \theta_1, \phi_1)$ and $\mathbf{p}_2 = (p_2, \theta_2, \phi_2)$ are (P, ω_0) with $P = \sqrt{(p_1^2 + p_2^2)}$, $\omega_0 = (\alpha_0, \theta_1, \phi_1, \theta_2, \phi_2)$, $\alpha_0 = \arctan(p_2/p_1)$.

The radial wave functions f_N then satisfy a single infinite coupled set of differential equations [9]

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

where $\alpha_{NN'}$ are the matrix elements of the full three-body interaction potential in the basis $\phi_N(\omega)$ and $\nu_N = 2n + l_1 + l_2 + 3/2$.

3 Calculations

In this calculation, the number of functions and the corresponding number of equations in equation (4) are truncated to N_{mx} numbers. Each N identifies a possible *channel* and here we present results for 100 and 150 channels. The set of equations (4) have to be solved accurately over a domain $[0, R_\infty]$, where the point R_∞ is in the far asymptotic domain. As in our earlier calculations we divide the interval $[0, R_\infty]$ into two subintervals $[0, \Delta]$ and $(\Delta, R_\infty]$. In (Δ, R_∞) we solve the equations by Taylor's expansion method. We also need solutions at R_∞ and beyond and this is done by suitable expansion of each f_N in inverse power of ρ with suitable sine and cosine factors as in our earlier calculations [9].

Solution over $[0, \Delta]$ is the most difficult part. Here we use Numerov difference scheme with three, five and seven-point schemes respectively for one-point, two-point and three or more points away from the boundaries $R = 0$ and $R = \Delta$. These schemes appear to be more stable and somewhat more accurate than the scheme we used earlier [5]. The Numerov three-point, five-point and seven-point difference formulas we have used here are respectively the following:

$$f_N(R_{k-1}) - 2f_N(R_k) + f_N(R_{k+1}) = \frac{h^2}{12}\left[f_N^{"}(R_{k-1}) + 10f_N^{"}(R_k) + f_N^{"}(R_{k+1})\right], \tag{5}$$

$$f_N(R_{k-2}) - 16f_N(R_{k-1}) + 30f_N(R_k) - 16f_N(R_{k+1}) + f_N(R_{k+2}) = \frac{2h^2}{15}[f_N^{"}(R_{k-2}) - 4f_N^{"}(R_{k-1}) - 84f_N^{"}(R_k) - 4f_N^{"}(R_{k+1}) + f_N^{"}(R_{k+2})], \tag{6}$$

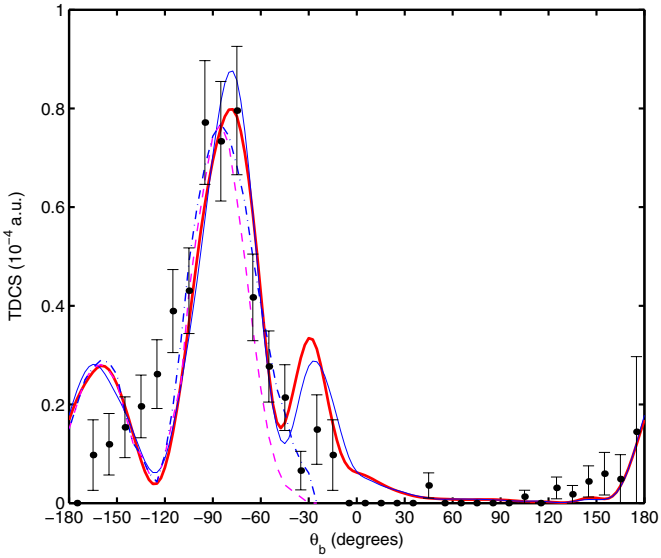

Fig. 1. (Color online) TDCS against scattering angle θ_b (horizontal axis) for equal energy sharing double photo ionization of the helium atom at 1 eV excess energy, averaged over [45°, 65°] for θ_a and over [0°, 20°] for ϕ_{ab}. Theory: thick curve - 150 channels, thin curve - 100 channels; dashed curve - fourth order Wannier calculation with parameterization, dash dotted curve - fit with a Gaussian correlation. Experiment: Dörner et al. [1].

and

$$2f_N(R_{k-3}) - 27f_N(R_{k-2}) + 270f_N(R_{k-1}) - 490f_N(R_k) + 270f_N(R_{k+1}) - 27f_N(R_{k+2}) + 2f_N(R_{k+3}) = \frac{69h^2}{140}\Big[-f_N^{"}(R_{k-3}) + 6f_N^{"}(R_{k-2}) - 15f_N^{"}(R_{k-1}) + \frac{8860}{23}f_N^{"}(R_k) - 15f_N^{"}(R_{k+1}) + 6f_N^{"}(R_{k+2}) - f_N^{"}(R_{k+3})\Big]. \tag{7}$$

For our present calculation in the equal energy sharing kinematics, we need at least a 100 channel calculation and a choice of R_∞ of about 2000 au for approximate convergence. Our results overestimate the experiment, which are in an absolute scale, nearly by a factor of two. We also carried out calculations for 150 channels and these are in close agreement with the 100 channel results as can be seen in Figure 1. Since at the low energy considered here fewer partial waves are expected to contribute, we conclude that convergence has probably been reached with respect to the number of channels. However, convergence in TDCS not only depends on the number of channels but also on the parameter R_∞ as shown by Malegat et al. [3]. We therefore anticipate that the higher value of our calculated TDCS is perhaps due lack of convergence with respect to this parameter. For full convergence one would need to increase this parameter to thousands of atomic units. Such calculations would require much more sophisticated and stable numerical techniques for propagating the radial wavefunction and better computational facilities than we can afford at present and hence are not attempted. Also for smooth

convergence, we had to cut short a few large eigenvalues of the charge matrix ($\alpha_{NN'}$).

The triple differential cross-section (TDCS) (actually a four-fold differential cross-section $d^4\sigma/d\cos\theta_a d\cos\theta_b d\phi_{ab} dE_a$) thus calculated, has been averaged for θ_a, the polar angle measured from photon polarization direction over the range $(40°, 65°)$ and for ϕ_{ab}, the azimuthal angular separation, over $(0°, 20°)$. In averaging for θ_a and ϕ_{ab} we made calculations at 2.5° intervals. We thus calculated altogether $11 \times 9 = 99$ sets of results and averaged over these. We also observed that for 100 and 150 channel calculations, the single differential cross-sections are about 50% higher than the experiments. Accordingly we multiplied our TDCS values by a factor 0.60 to get a fit with the experiments.

4 Results and discussion

We present our results in Figure 1. The absolute experimental results presented in Figure 1 are that of Dörner et al. [1] and correspond to linearly polarized light with Stokes parameter $S_1 = 0.99 \pm 0.01$. For this reason, we do not compare our results with those of Maulbetsch et al. [6] which are for a different value of S_1. In absence of theoretical results of other ab initio theories, we compare our results with the only available semi-empirical calculations presented in [1] following Huetz et al. [7] and Feagin [8]. In Figure 1 there is good overall agreement between our results and those of the experiment. The peak around $-90°$ is well represented by our theory as well as by the semi-empirical theories of Huetz et al. [7] and of Feagin [8]. The peak around $-25°$ is also well represented in our calculation though not by the semi-empirical calculations. There is also a third peak at about $-160°$ in our theoretical results as well as in semi-empirical calculations. Although such peaks exist at 6 eV and 20 eV excess energies in the experimental results, here no such peak in the experimental results developed. As for the other side of the plane of scattering our results agree well with the experimental results. It has been pointed out that the shape of the photoionization TDCS is governed by selection rules [15] (see also the excellent review article [16] by Briggs and Schmidt). For equal energy sharing kinematics, the $^1P^\circ$ character of the final state suppresses ejection of both electrons in the opposite direction. This is manifested by the deep minimum near $-50°$ in Figure 1.

5 Conclusion

We conclude that the results of our present calculation are in excellent qualitative agreement with the experiments and with other available theories at 1 eV excess energy for the equal energy sharing case. The third peak near $-160°$ predicted in our results and also in those of Huetz et al. and Feagin but not in the experiment may be worth noting. For fully converged results, perhaps a larger size calculation with a more accurate scheme for solving the relevant coupled set of radial equations may be needed.

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