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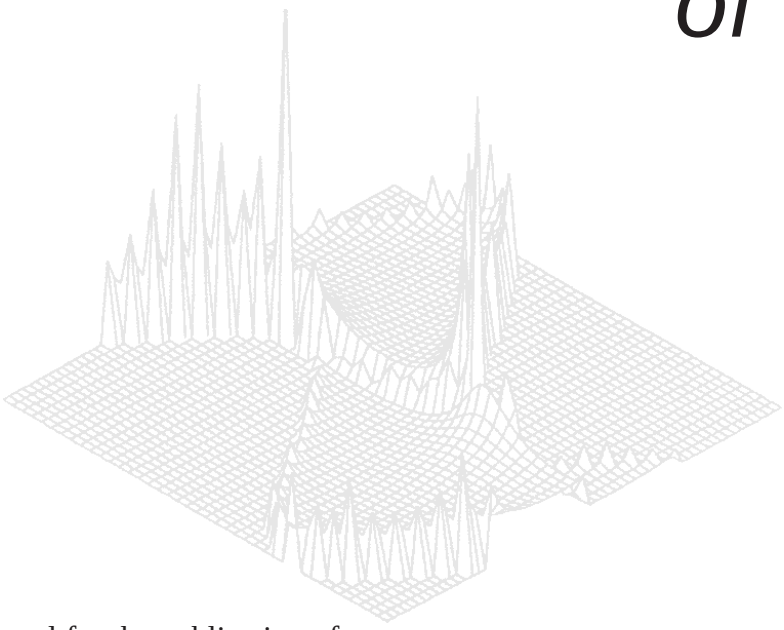

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Helium Double Photoionisation: An Accurate Solution of a Three-body Coulomb Problem*

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Abstract

We present here the solution of the helium double photoionisation problem by the convergent close-coupling (CCC) method. This method allows us to obtain the most detailed description of the double photoionisation process in the form of the fully resolved triply differential cross section (TDCS). The accuracy of our model is tested by calculating the TDCS in the three different forms of the electromagnetic operator which produces essentially identical results. We compare our calculation with the most accurate experimental and theoretical data available to date.

1. Introduction

The three-body break up of a charged system is one of the most fundamental and still intriguing problems of atomic collision physics. The helium double photoionisation is the simplest example of the three-body Coulomb break up and, as such, it attracts considerable interest from experimental and theoretical atomic physicists. The most detailed description of the helium double photoionisation, known also as the $(\gamma, 2e)$ reaction, can be obtained in the form of the fully-resolved triply differential cross section (TDCS) which gives the probability of detecting the two photoelectrons with fully determined kinematics. Considerable effort has been made to obtain this quantity experimentally. A large number of synchrotron-based experiments have been performed to measure the TDCS by observing the angular correlation of the two photoelectrons escaping with fixed energies. The first measurement was reported by Schwarzkopf *et al.* (1993*a*) who chose the symmetric energy sharing $E_1 = E_2 = 10$ eV and a simple geometry in which one of the two emitted electrons was directed along the major polarisation axis of the elliptically polarised light. The angular distribution of the second photoelectron in the polarisation plane was detected. Later, a number of similar experiments were reported at slightly different geometries with both equal ($E_1 = E_2 = 5, 10$ eV) and unequal ($E_1 = 5$ eV, $E_2 = 47{\cdot}9$ eV) energy sharing (Schwarzkopf 1995; Schwarzkopf *et al.* 1993*b*, 1994*b*). Common to all these experiments, performed at the BESSY storage ring (Berlin, Germany), was detection

* Dedicated to Professor Erich Weigold on the occasion of his sixtieth birthday.

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of the two photoelectrons in the plane perpendicular to the direction of the photon. This experimental set up is illustrated in Fig. 1. An attempt has been made to normalise the TDCS. The absolute data reported by Schwarzkopf and Schmidt (1995) were later revised upwards by a factor of two (Schwarzkopf and Schmidt 1996; Schmidt *et al.* 1996).

Different kinematics were used by the group working at the Super-ACO storage ring (Orsay, France) (Lablanquie *et al.* 1995; Mazeau *et al.* 1996; Malegat *et al.* 1997). These experiments were performed with linearly polarised light and one of the electrons directed along the polarisation vector of the photon. The second electron was detected in the plane formed by the polarisation vector and the momentum of the photon, also shown in Fig. 1. Following the convention of Malegat *et al.* (1997) we refer to this experimental set-up as the coplanar geometry. In contrast, the BESSY kinematical arrangement is referred to as the perpendicular geometry.

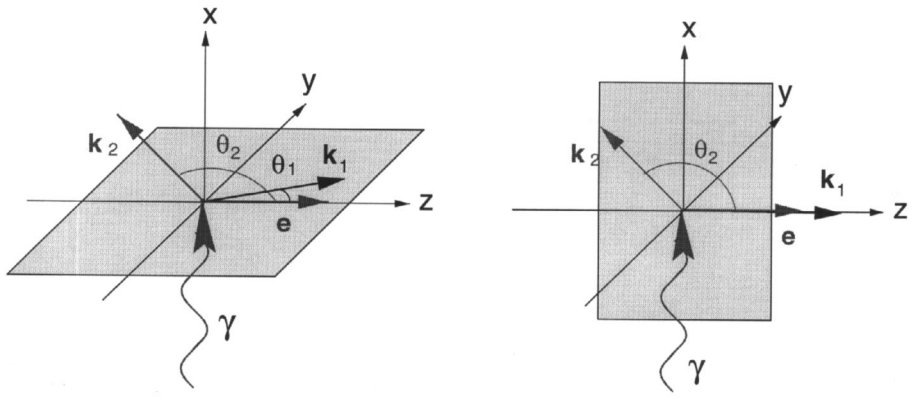

Fig. 1. Alignment of the photoelectron momenta $\boldsymbol{k}_1$, $\boldsymbol{k}_2$, and polarisation vector of the photon e. *Left:* perpendicular geometry used at BESSY. *Right:* coplanar geometry used at Super-ACO.

A different set of experimental data was reported by Dawber *et al.* (1995). They obtained the TDCS at photon energies very close to the double photoionisation threshold $E_1 + E_2 = 0{\cdot}6$, 1 and 2 eV both for equal and unequal energy sharing. Although their data were not absolute, all the TDCS were obtained with the same normalisation constant. This allowed a study of the departure from the Wannier regime of photoionisation with increasing photon energy.

An alternative way of studying helium double photoionisation was used by Dörner *et al.* (1996, 1997). Instead of detecting in coincidence the two outgoing electrons they studied the correlated motion of the He^{2+} ion and one of the photoelectrons. With this technique they were able to obtain the fully resolved double photoionisation cross sections within a 4π solid angle at energies 1–80 eV above the threshold.

From the point of view of theory, calculation of the fully resolved double photoionisation presents the most challenging task and requires a detailed account of all aspects of the electron–electron and electron–ion interactions. Following the pioneering work of Schwarzkopf *et al.* (1993*a*) various theoretical models have

been tried to calculate the helium double photoionisation TDCS. Maulbetsch and Briggs (1993*a*, 1993*b*) employed a three-body Coulomb (3C) correlated final-state wave function. Alternatively, Pont and Shakeshaft (1995*b*, 1996) described the final state as a product of two screened Coulomb (2SC) wave functions employing effective charges. The shape of the TDCS obtained in early experiments by Schwarzkopf *et al.* (1993*a*, 1994*b*) was reproduced very well both by the 2SC (Pont and Shakeshaft 1995*a*) and the 3C (Maulbetsch and Briggs 1993*a*; Schwarzkopf *et al.* 1994*b*) theories. The phenomenological fourth-order Wannier theory of Feagin (1996) reproduced very accurately shapes of the TDCS at photon energies up to 20 eV above the threshold (Dorner *et al.* 1997), but does not yield correct absolute values.

The 3C and 2SC theories (Maulbetsch *et al.* 1995) were also used to reproduce the experimental results obtained in the coplanar geometry by Lablanquie *et al.* (1995). The conclusion was that the two theories were close to each other and both in disagreement with the experiment. Later Mazeau *et al.* (1996) reported another set of measurements in the coplanar geometry with improved statistics. Comparison with the theory seemed to be more favourable (Huetz 1997).

Determination of the absolute TDCS appeared to be even a more difficult task both for theory and experiment. Firstly, it became obvious that the 3C calculation in various forms of the electromagnetic operator (length and velocity) gave results deviating in magnitude by a factor of 10. The 2SC calculation was reported only in the velocity form and fell right in between the length and velocity 3C results. Secondly, the existing absolute experimental data (Schwarzkopf and Schmidt 1995) were found inconsistent with a well established total double photoionisation cross section σ^{2+}. It forced Schwarzkopf *et al.* to revise their values upwards by a factor of two (Schwarzkopf and Schmidt 1996; Schmidt *et al.* 1996).

As it follows from the above discussion the problem of helium double photoionisation is far from a final solution and more theoretical work is still needed to produce an accurate and gauge-independent reliable absolute TDCS. In this paper we report on the first application of the convergent close-coupling (CCC) method to the calculation of helium double photoionisation TDCS. The method has been demonstrated to produce accurate integrated double photoionisation cross sections over a wide range of photon energies (Kheifets and Bray 1996). After an improvement had been made to the description of the helium atom correlated ground state by employing a 14-term Hylleraas ground state, the integrated cross sections calculated in the three gauges of the electromagnetic interaction, length, velocity and acceleration, became practically identical from threshold to 1 keV (Kheifets and Bray 1998). This development makes the CCC method a strong contender to produce an accurate and reliable absolute TDCS.

The paper is organised as follows. In Section 2 we present the CCC formalism as applied to the double photoionisation problem. In Section 3 we give the results in the form of the absolute TDCS for various experimental geometries and make a comparison with the data and other calculations. In conclusion we discuss possible extensions of the present theory.

2. Formalism

We treat the double photoionisation as a two step process. The first is the full absorption of the photon energy by one electron. The second is the interaction

of this electron with the helium nucleus and the remaining electron. We require an accurate description of the initial and final states of the target. For the initial state we choose a 14-term Hylleraas expansion. For the final state we use a close-coupling expansion to obtain the wave function corresponding to electron-impact excitation and ionisation of the He^+ ion. The part corresponding to ionisation is identified with double photoionisation. The excitation part corresponds to single photoionisation with excitation of the remaining electron.

The convergent close-coupling (CCC) method was first introduced by (Bray and Stelbovics 1992) for the e–H scattering problem. The first indication that it may be applied to ionisation problems came from the reproduction of the e–H total ionisation cross section (TICS) and spin asymmetry (Bray and Stelbovics 1993). Indeed, it has been successfully applied to the calculation of differential e–H ionisation (Bray *et al.* 1994). In the present case we are interested in e–He^+ ionisation, and the CCC method has already demonstrated the ability to obtain accurate TICS in this case (Bray *et al.* 1993). The details of the CCC theory and applications for electron scattering on one-electron targets have been given by (Bray and Stelbovics 1995). Briefly, the total wave function is expanded in a set of N square-integrable target states obtained by diagonalising the target Hamiltonian in an orthogonal Laguerre basis. The negative-energy states approximate the full target discrete spectrum, while the discrete positive-energy states provide an integration rule over the true target continuum. Ionisation is identified with the excitation of the positive-energy target states. The close-coupling equations are formed and solved for the T-matrix using momentum space techniques outlined by (McCarthy and Stelbovics 1983).

The fully differential cross section of helium double photoionisation resolved with respect to the solid angles of the two photoelectrons and the energy can be written, using the standard partial wave expansion, as

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2\, dE_2} = \frac{8\pi^2}{\omega c}\left|\sum_{l_1 l_2}(-i)^{l_1+l_2} e^{i[\delta_{l_1}(k_1)+\delta_{l_2}(k_2)]} D_{l_1 l_2}(k_1 k_2)\right.$$

$$\left. \times \sum_{m_1 m_2} Y_{l_1 m_1}(\hat{k}_1) Y^*_{l_2 m_2}(\hat{k}_2)(-1)^{m_2} \begin{pmatrix} l_1 & 1 & l_2 \\ m_1 & 0 & -m_2 \end{pmatrix}\right|^2 . \quad (1)$$

Here ω is the photon energy and $c \simeq 137$ is the speed of light in atomic units. The z axis is directed along the polarisation vector of the photon. The quantity $D_{l_1 l_2}(k_1 k_2)$ is the reduced dipole matrix element which is stripped of its angular dependence. We write

$$e^{i[\delta_{l_1}+\delta_{l_2}]} D_{l_1 l_2}(k_1 k_2) \approx e^{i[\delta_{l_1}(Z=1)+\delta_{l_2}(Z=2)]} D_{l_1 l_2}(k_1 n_2) \langle l_2 k_2 \parallel l_2 n_2 \rangle , \quad (2)$$

where $\langle l_2 k_2 \parallel l_2 n_2 \rangle$ is the overlap between the pseudostate of energy $\epsilon_{n_2 l_2}$ and the true Coulomb state radial wave function of the same energy ($k_2^2/2 = \epsilon_{n_2 l_2}$). The derivation of this approximation is similar to that given by (Bray and Fursa 1996) for electron-impact differential ionisation. The Coulomb radial orbitals

are normalised on energy in Ry as $\langle lk \parallel lk_1\rangle = \delta(k^2 - k_1^2)$. The pseudostate radial orbitals are a linear combination of the Laguerre square-integrable basis,

$$\langle r \parallel nl\rangle = \left(\frac{\mu_l (n-1)!}{(2l+1+n)!}\right)^{\frac{1}{2}} (\mu_l r)^{l+1} \exp(-\mu_l r/2) L_{n-1}^{2l+2}(\mu_l r)\,, \tag{3}$$

where the $L_{n-1}^{2l+2}(\mu_l r)$ are the associated Laguerre polynomials, and n ranges from 1 to the basis size N_l. The constant μ_l is arbitrary and is chosen so that sufficiently many true discrete He^+ eigenstates were accurately described, and to ensure that for each l_2 there was one n_2 such that $\epsilon_{n_2 l_2} = k_2^2/2 = E_2$ in (2). For He^+ we typically have $\mu_l \approx 1{\cdot}7 \pm 0{\cdot}3$.

The dipole matrix element is calculated by integrating the first-order dipole matrix with the dipole singlet T-matrix of the e–He^+ scattering system:

$$D_{l_1 l_2}(k_1 n_2) = \sum_{nl\lambda} \int k^2 dk \frac{\langle lk\,\lambda n \parallel T_{J=1,S=0} \parallel l_1 k_1\, l_2 n_2\rangle}{E - k^2/2 - \epsilon_{\lambda n} + i0}\; d_{l\lambda}(kn)\,. \tag{4}$$

The first-order dipole matrix is obtained as a transition amplitude of the dipole operator between the correlated ground state and the final state containing one continuum Coulomb wave and one discrete pseudostate:

$$\begin{aligned} d_{l\,l\pm1}(kn) = (-1)^{l_>} \sqrt{l_>} \langle lk\,(l\pm1)n || \omega\,(r_1 \delta_{(l\pm1)L} + r_2 \delta_{lL}) || \\ \times \sum_L (2L+1)^{-1} \Phi_L(r_1 r_2)\rangle\,, \end{aligned} \tag{5}$$

where $l_>$ the is greater of l and $l \pm 1$. Here the radial part of the dipole operator is taken in the length form. It can be also expressed in the velocity form $\partial/\partial r$ or the acceleration form $2/(\omega r)^2$.

We describe the correlated ground state by a 14-term Hylleraas expansion over the powers of $u = r_{12}$, $s = r_1 + r_2$ and $t = r_1 - r_2$ (Chandrasekhar and Herzberg 1955) in which the angular dependence is then reduced to the sum of Legendre polynomials:

$$\Phi(\boldsymbol{r}_1 \boldsymbol{r}_2) = N e^{-zs} \sum_{n=1}^{14} a_n s^{\alpha_n} t^{\beta_n} u^{\gamma_n} = \sum_L \Phi_L(r_1 r_2) P_L(\theta_{12})\,. \tag{6}$$

Expression (5) becomes separable after Φ_L is expanded over the Slater functions $F_l(r_1, r_2) = r_<^l / r_>^{l+1}$, where $r_<$ and $r_>$ are the lesser and the greater of r_1 and r_2 respectively.

After integration over the angular variables in (1) one gets the single-differential cross section (SDCS):

$$\frac{d\sigma(E_2)}{dE_2} = \frac{8\pi^2 \omega}{3c} \sum_{l_2 = l_1 \pm 1} |D_{l_1 l_2}(k_1 n_2)|^2 \frac{1}{2\sqrt{E_2}}\,. \tag{7}$$

This cross section corresponds to the energy $E_1 = E - E_2$ with $E_2 = \epsilon_{n_2 l_2}$ for some pseudostate n_2 and every l_2. Variation of the Laguerre exponential fall-off for each l_2 allows this for one value of E_2. To define the SDCS for all $0 \leq E_2 \leq E$ we form the SDCS for each l_2 by interpolation onto a common energy grid and then sum over all l_2, see Bray and Fursa (1995) for detail.

The total double photoionisation cross section is then obtained by energy integration:

$$\sigma^{2+} \approx \sum_{nl:\epsilon_{nl}>0} \sigma_{nl} \approx \int_0^E dE_2 \frac{d\sigma(E_2)}{dE_2}\,, \tag{8}$$

where σ_{nl} is the cross section for photoexcitation of the nl pseudostate of energy ϵ_{nl}. The integral above is from 0 to E because in the close-coupling formalism electron flux is distributed between all pseudostates with energy $\epsilon_{nl} < E$. We find that we do not obtain convergence in the SDCS with increasing Laguerre bases N_l here, or even in model problems (Bray 1997). We suspect that as $N_l \to \infty$ the SDCS, as obtained from (7), tends to a step function since it tends to 0 for $E_2 > E/2$. This is a systematic problem associated with the finite basis close-coupling formalism and likely stems from the incorrect boundary conditions for the ionisation processes. In finite calculations there is non-zero electron flux for $E_2 > E/2$, though usually very small. Thus, in making a comparison with experiment we combine incoherently amplitudes corresponding to the theoretically distinct process for E_2 and $E - E_2$. We choose the incoherent combination as this is imposed in the integral (total). In practice, for substantially asymmetric energy-sharing kinematics, only one amplitude contributes. For equal energy-sharing we always obtain two cross sections, of similar magnitude, which are then summed. Examples of these two cross sections and a coherent combination in the case of (e, 2e) has been given by (Bray *et al.* 1997).

3. Results and Discussion

To test the CCC theory outlined in the previous section we performed a number of calculations which correspond to the perpendicular geometry used in the BESSY experiments. By chosing this geometry we test our method against the best established set of experimental and theoretical data.

The CCC calculations have been carried out using the following parameters. We included $N_{l_2} = 17 - l_2$ states for $0 \leq l_2 \leq 4$ in all calculations presented here. For each l_2 the Laguerre exponential fall-off factors have been varied to ensure that one of the positive energy pseudostates had the energy (E_2) of one of the detected electrons. By doing so we avoided interpolation of the complex amplitudes when calculating the TDCS using (1). The total double photoionisation cross section σ^{2+} is obtained by summing the cross sections for excitation of the positive-energy pseudostates (8). The contribution from the true discrete eigenstates is projected out from this cross section. The total double photoionisation cross section σ^{2+} is almost identical in the three gauges of the electromagnetic operator. It agrees well with experiment (Kheifets and Bray 1998), and therefore can be used to estimate the true SDCS. In this estimate we are assisted by the theoretical results of Pont and Shakeshaft (1995*a*) and the experiment of Wehlitz *et al.*. The SDCS

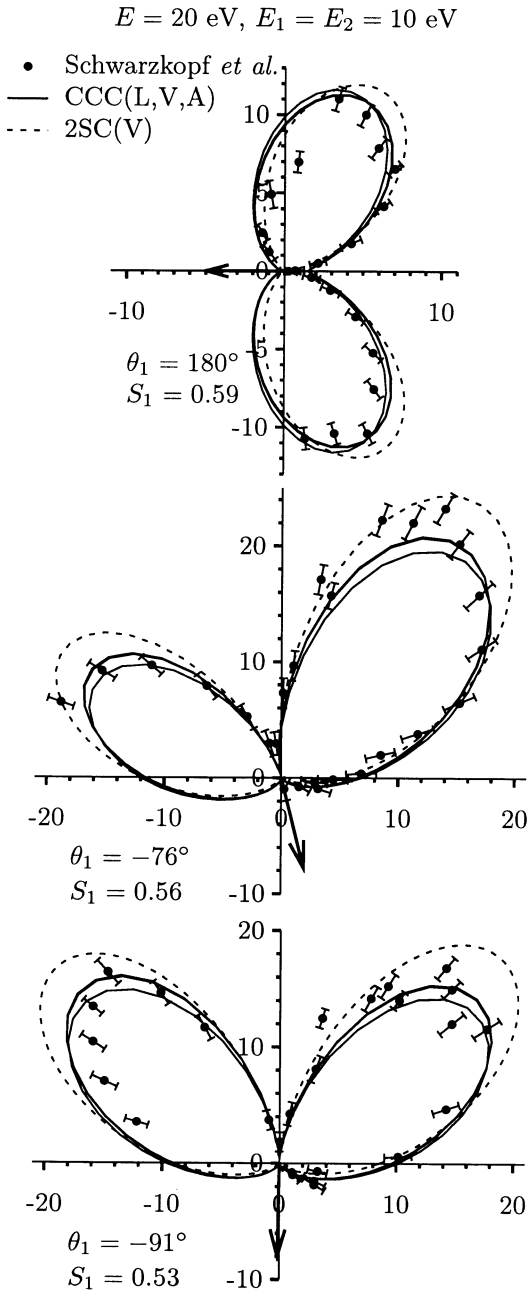

Fig. 2. Triply differential cross sections for photon-impact double ionisation of the ground state of helium. One of the detectors is positioned to receive electrons with energy $E_1 = E - E_2$ at fixed θ_1 indicated by arrow. The other electron, of energy E_2 is detected in coincidence on the full circular angular range. The $\theta_1 = 180°$ measurement is absolute (Schwarzkopf and Schmidt 1995, 1996), others are all relative (Schwarzkopf *et al.* 1993*b*; Schwarzkopf 1995), and have been normalised by best visual fit to both the present CCC (see text) and the 2SC calculations of Pont and Shakeshaft (1995*b*) and Shakeshaft (1997).

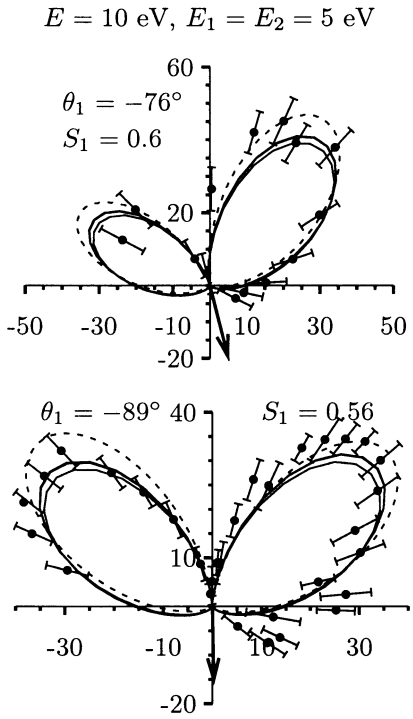

Fig. 3. Theory and relative experiment as for Fig. 2, except for the energies indicated.

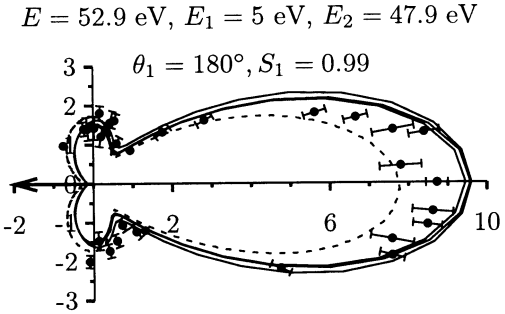

Fig. 4. Theory and relative experiment (Schwarzkopf *et al.* 1994*b*) as for Fig. 2, except for the energies indicated.

can be assumed flat for the photon energies considered of 89 eV ($E = 10$) and 99 eV ($E = 20$). The TDCS is then rescaled by the ratio (≈ 2) of this SDCS and the SDCS obtained via (7) at $E_2 = E_1 = E/2$. At the other photon energy considered of 132 eV ($E = 53$) the existing experimental data are for the asymmetric energy-sharing conditions. Here we estimate the true SDCS by assuming that it is well-described by a quadratic, with the three coefficients determined by the following requirements: (1) the symmetry about $E/2$, (2) the integral must yield σ^{2+}, and (3) by matching to the calculated SDCS at $E_2 = 0$ (the boundary condition problem is least here). The result agrees with the SDCS prediction of Pont and Shakeshaft (1995*a*) at $E/2$ and yields the same result at the detected electron energy as the original SDCS, and so no rescaling is performed.

In Figs 2–4 we present a comparison of the CCC calculations, in the three gauges, with the available measurements in the perpendicular geometry from the BESSY group and the velocity-gauge 2SC calculations of Pont and Shakeshaft (1995*b*). We see that there is excellent agreement between the theories and experiment. The agreement between the CCC three gauges for the TDCS has no parallel in the previous theoretical work. What is also remarkable is the agreement between the CCC and 2SC theories. Since both theories have similar SDCS, the angular and magnitude agreement presented suggests that the two theories are likely to yield similar results over the full phase-space of the two electrons. Given the diverse origin of the CCC and 2SC approaches such good agreement gives us great confidence in the accuracy of the two theories for this problem. The strength of the CCC method is that it has the capacity to obtain accurate, essentially gauge-independent TDCS from near threshold to 1 keV photon energies.

However, the news is not all good. As mentioned in the Introduction the measurements of Lablanquie *et al.* (1995) in the coplanar geometry were found to be in disagreement with the 3C and 2SC calculations of Pont *et al.* (1996). We attempted to resolve this controversy by applying the CCC method here also. Preliminary investigation suggests much closer agreement to the 2SC theory than the experimental data. We shall investigate this problem in more detail. In addition, we are looking forward to applying the CCC theory to the absolute measurements reported by Dörner *et al.* (1997) and the near-threshold measurements of Dawber *et al.* (1995).

4. Conclusion

We have demonstrated a unique capacity of the CCC method to produce an absolute TDCS for the helium double photoionisation over a wide range of energies. The internal consistency of the calculation in the three gauges of the electromagnetic interaction and its remarkable agreement with experiment makes us quite confident that the helium double photoionisation problem can be eventually solved.

As an obvious extension of the present theory we consider the application of the CCC method to the double photoionisation of other two-electron atoms such as Be, Mg, Ca. Our formalism can also be easily adopted to describe the electron impact double ionisation under the condition of high incident energy when the projectile can be regarded as a structureless probe. In this case the dipole electromagnetic operator is simply replaced by the Born operator and the rest of the formalism remains unchanged.

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References

Bray, I. (1997). *Phys. Rev. Lett.* **78**, 4721.
Bray, I., and Fursa, D. V. (1995). *J. Phys.* B **28**, L435.

Bray, I., and Fursa, D. V. (1996). *Phys. Rev.* A **54**, 2991.
Bray, I., and Stelbovics, A. T. (1992). *Phys. Rev.* A **46**, 6995.
Bray, I., and Stelbovics, A. T. (1993). *Phys. Rev. Lett.* **70**, 746.
Bray, I., and Stelbovics, A. T. (1995). *Adv. Atom. Mol. Phys.* **35**, 209.
Bray, I., Fursa, D. V., Röder, J., and Ehrhardt, H. (1997). *J. Phys.* B **30**, L101.
Bray, I., Konovalov, D. A., McCarthy, I. E., and Stelbovics, A. T. (1994). *Phys. Rev.* A **50**, R2818.
Bray, I., McCarthy, I. E., Wigley, J., and Stelbovics, A. T. (1993). *J. Phys.* B **26**, L831.
Chandrasekhar, S., and Herzberg, G. (1955). *Phys. Rev.* **98**, 1050.
Dawber, G., Avaldi, L., McConkey, A. G., Rojas, H., Macdonald, M. A., and King, G. C. (1995). *J. Phys.* B **28**, L271.
Dörner, R., Brauning, H., Feagin, J. M., Mergel, V., Jagutzki, O., Spielberger, L., Vogt, T., Khemliche, H., Prior, M. H., Ullrich, J., Cocke, C. L., and Schmidt-Böcking, H. (1997). *Phys. Rev.* A **57**, 1074.
Dörner, R., Feagin, J. M., Cocke, C. L., Brauning, H., Jagutzki, O., Jung, M., Kanter, E. P., Khemliche, H., Kravis, S., Mergel, V., Prior, M. H., Schmidt-Böcking, H., Spielberger, L., Ullrich, J., Unversagt, M., and Vogt, T. (1996). *Phys. Rev. Lett.* **77**, 1024.
Feagin, J. M. (1996). *J. Phys.* B **29**, L551.
Huetz, A. (1997). Private communication.
Kheifets, A., and Bray, I. (1996). *Phys. Rev.* A **54**, R995.
Kheifets, A., and Bray, I. (1998). *Phys. Rev.* A **57**, 2590.
Lablanquie, P., Mazeau, J., Andric, L., Selles, P., and Huetz, A. (1995). *Phys. Rev. Lett.* **74**, 2192.
McCarthy, I. E., and Stelbovics, A. T. (1983). *Phys. Rev.* A **28**, 2693.
Malegat, L., Selles, P., Lablanquie, P., Mazeau, J., and Huetz, A. (1997). *J. Phys.* B **30**, 263.
Maulbetsch, F., and Briggs, J. S. (1993*a*). *J. Phys.* B **26**, 1679.
Maulbetsch, F., and Briggs, J. S. (1993*b*). *J. Phys.* B **26**, L647.
Maulbetsch, F., Pont, M., Briggs, J. S., and Shakeshaft, R. (1995). *J. Phys.* B **28**, L341.
Mazeau, J., Andric, L., Jean, A., Lablanquie, P., Selles, P., and Huetz, A. (1996). *In* 'Atomic and Molecular Photoionisation' (Eds A. Yagishita and T. Sasaki), p. 31 (Universal Academy: Tokyo).
Pont, M., and Shakeshaft, R. (1995*a*). *J. Phys.* B **28**, L571.
Pont, M., and Shakeshaft, R. (1995*b*). *Phys. Rev.* A **51**, R2676.
Pont, M., and Shakeshaft, R. (1996). *Phys. Rev.* A **2**, 1448.
Pont, M., Shakeshaft, R., Maulbetsch, F., and Briggs, J. S. (1996). *Phys. Rev.* A **53**, 3671.
Schmidt, V., Schaphorst, S. J., Krassig, B., Schwarzkopf, O., and Scherer, N. (1996). *J. Elect. Spectrosc. Relat. Phenom.* **79**, 279.
Schwarzkopf, O. (1995). PhD thesis, Freiburg University.
Schwarzkopf, O., and Schmidt, V. (1995). *J. Phys.* B **28**, 2847.
Schwarzkopf, O., and Schmidt, V. (1996). *J. Phys.* B **29**, 1877.
Schwarzkopf, O., Krassig, B., Elmiger, J., and Schmidt, V. (1993*a*). *Phys. Rev. Lett.* **70**, 3008.
Schwarzkopf, O., Krassig, B., and Schmidt, V. (1993*b*). *J. Phys. (Paris)* C **3**, 169.
Schwarzkopf, O., Krassig, B., Schmidt, V., Maulbetsch, F., and Briggs, J. S. (1994*a*). *J. Phys.* B **27**, L347.
Schwarzkopf, O., Krassig, B., Schmidt, V., Maulbetsch, F., and Briggs, J. S. (1994*b*). *J. Phys.* B **27**, 4817.
Shakeshaft, R. (1997). Private communication.
Wehlitz, R., Heiser, F., Hemmers, O., Langer, B., Menzel, A., and Becker, U. (1991). *Phys. Rev. Lett.* **67**, 3764.

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