PHYSICAL REVIEW A VOLUME 56, NUMBER 2 AUGUST 1997

Strong interference effects in the triple differential cross section of neutral-atom targets

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(Received 2 December 1996; revised manuscript received 29 April 1997)

Recently a striking structure has been observed experimentally in the ionization of helium in symmetric out-of-plane geometry. We will show that this structure, a very sharp dip, is well represented in a distorted-wave Born approximation calculation and that it is the result of a strong interference effect between incident and final channel distorted waves. We have located similar structures in other targets, in particular Li$(2s)$, Ar$(2s)$, and Ne$(2s)$. No such structure was found for hydrogenic targets. For Ar$(2p)$ and Ne$(2p)$ targets we predict that such interference effects will be masked by the different behavior of the magnetic sublevels. [S1050-2947(97)06308-7]

PACS number(s): 34.80.Dp

I. INTRODUCTION

The study of $(e,2e)$ processes on helium at impact energies of 100 eV and below has yielded a wealth of experimental data and has contributed greatly to the understanding of the Coulomb few-body problem. The great advantage of coincidence measurements is that one can manipulate the geometry of the experiment to study delicate processes that yield striking structures in a particular arrangement, but are largely masked by stronger effects in virtually all other setups. Quite recently Murray [1] identified a very strong structure in the ionization of helium at an impact energy of 64.6 eV in a very specific out-of-plane geometry. In this paper we will show that this structure is well represented in a distorted-wave Born approximation (DWBA) calculation and we will interpret it as an interference, that is to say a pure quantum, effect. We predict that similar structures will be present in the triple differential cross section (TDCS) for some targets but not for others.

II. THE IONIZATION OF HELIUM

It will be helpful to fix our notation and to define the geometries used. In Fig. 1 we show the collision geometry. We assume that an electron, wave vector $\mathbf{k}_0$, is incident on a target and two electrons $\mathbf{k}_1$ and $\mathbf{k}_2$ are collected in coincidence. Let ψ define the angle of the incident electron with respect to the plane defined by $\mathbf{k}_1$ and $\mathbf{k}_2$ and let ϑ_{12} be the angle between the electrons. We take our origin at the target and our z axis to lie in the direction of the projection of the incident vector on the detectors plane. The two exiting electrons will be detected at angles ϑ_1 and ϑ_2 right and left of this z axis, i.e., $\vartheta_1+\vartheta_2=\vartheta_{12}$. If $\psi=0°$ we will describe the arrangement as being coplanar, if $\psi=90°$, perpendicular, and out of plane otherwise. We describe it as a symmetric measurement if $\vartheta_1=\vartheta_2=\vartheta_{12}/2=:\ \vartheta$ and $|\mathbf{k}_1|=|\mathbf{k}_2|$.

Murray and his collaborators [1,2] reported results on helium in symmetric perpendicular plane geometry at impact energies ranging from 44.6 to 104.6 eV. Excellent agreement with experiment was achieved by Whelan *et al.* [3] who used a distorted-wave Born approximation. The TDCS is given for an arbitrary atomic target by

$$\frac{d^3\sigma^{\mathrm{DWBA}}}{d\Omega_1 d\Omega_2 d\epsilon}=2(2\pi)^4\frac{k_1k_2}{k_0}\sum_{m_b}\,[|f_{m_b}|^2+|g_{m_b}|^2 -\mathrm{Re}(f^*_{m_b}g_{m_b})], \tag{1}$$

where

$$f_{m_b}=\left\langle \chi^-(\mathbf{k}_1,\mathbf{r}_1)\chi^-(\mathbf{k}_2,\mathbf{r}_2)\left|\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\right|\chi^+(\mathbf{k}_0,\mathbf{r}_1)\phi_{m_b}(\mathbf{r}_2)\right\rangle, \tag{2}$$

$$g_{m_b}=\left\langle \chi^-(\mathbf{k}_1,\mathbf{r}_2)\chi^-(\mathbf{k}_2,\mathbf{r}_1)\left|\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\right|\chi^+(\mathbf{k}_0,\mathbf{r}_1)\phi_{m_b}(\mathbf{r}_2)\right\rangle. \tag{3}$$

m_b denotes the magnetic sublevels of the target wave function. In the case of helium $m_b=0$ and the wave function $\phi_{m_b}(\mathbf{r}_2)$ was taken from Ref. [4]. The distorted-wave χ^+ was generated in the static-exchange potential of the atom, the distorted waves χ^- were each generated in the static exchange potential of the ion and each orthogonalized to ϕ. Exchange was included using the spin-singlet local exchange approximation of Furness and McCarthy [5] for the final states and the closed-shell equivalent for the incident electron.

At energies above 100 eV the DWBA as defined in Eq. (1) also gave excellent agreement in coplanar symmetric geometry (see Refs. [6–8]), however, for energies of 50 eV and below agreement was very poor. This disagreement prompted Whelan *et al.* [9] to suggest that it would be valuable to carry out a series of measurements relating the coplanar symmetric geometry of Rösel *et al.* [8] with the perpendicular plane geometry of Murray *et al.* [2]. Murray [1] did this and while rotating the plane came across a deep minimum in the TDCS for an impact energy of 64.6 eV and $\psi=67.5°$, which is the subject of this paper. A full discussion of the TDCS for all gun angles ψ will be given elsewhere [10]. Here we only remark that there is quite some evidence that the shape of the TDCS in the coplanar case is the result

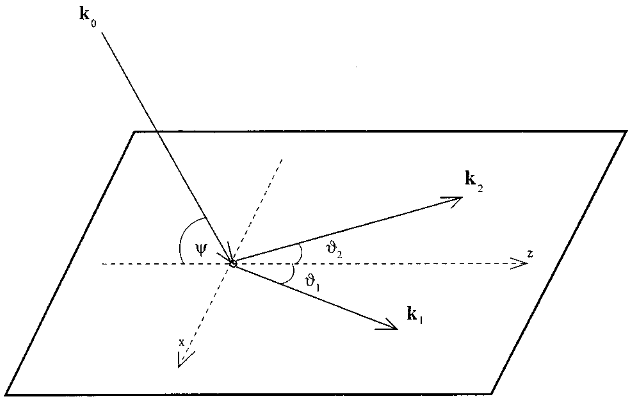

FIG. 1. Shown is the general setup for an $(e,2e)$ experiment. $\mathbf{k}_0$, $\mathbf{k}_1$, and $\mathbf{k}_2$ denote the incident and two outgoing electrons. ψ denotes the angle by which the incident electron gun is raised out of plane.

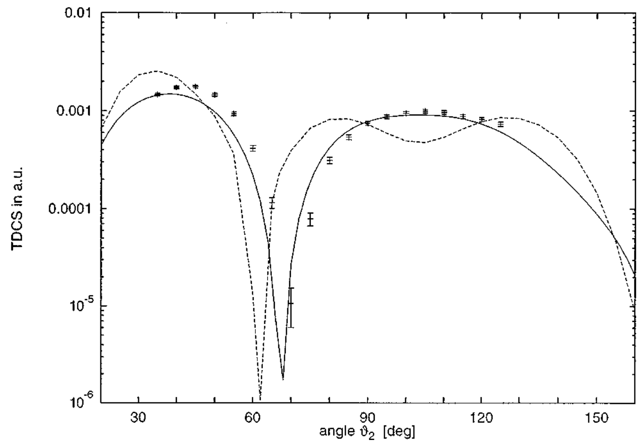

FIG. 2. TDCS for helium in symmetric equal energy sharing geometry at an impact energy of 64.6 eV. Electron gun raised to ψ=67.5°. Shown are DWBA+M_{ee} (solid curve) compared with the Berakdar and Briggs results (dashed-dotted line).

of a delicate interplay between three-body effects in the incident and final channels (see Refs. [3] and [11–14]) while in the perpendicular plane the three-body effects tend to enhance existing structures and not to interfere. For the spherical case we are interested in here, the deep minimum observed has a different origin.

In order to see how such a structure can arise we made a number of calculations. Firstly we performed a DWBA calculation, as defined by Eqs. (1)–(3), then we considered a number of model calculations, i.e., (i) a plane wave in the incident channel but distorted waves for the two outgoing electrons; (ii) plane waves for the outgoing but a distorted wave for the incident electron. The results of these two model calculations are shown in the figures for all atoms considered here. A sharp dip is only found when we have distorted waves in both the incident and final channels. The dip is thus clearly an interference effect and only exists when we allow for elastic scattering from the atom in the incident channel and from the ion in the final channel. It should be emphasized that we have not allowed for either the polarization of the target or postcollisional interaction in the final state. We may to some extent allow for the latter by the inclusion of a multiplicative factor in the TDCS, i.e.,

$$\frac{d^3\sigma}{d\Omega_2 d\Omega_2 dE}=M_{ee}\frac{d^3\sigma^{\rm DWBA}}{d\Omega_1 d\Omega_2 dE}, \tag{4}$$

where $d^3\sigma^{\rm DWBA}/d\Omega_1 d\Omega_2 dE$ is given by Eq. (1) and the M_{ee} factor is that introduced by Ward and Macek [15], i.e.,

$$M_{ee}=N_{ee}|{}_1F_1(-i\nu_3,1,-2k_3 r_{3\rm ave})|^2, \tag{5}$$

where

$$N_{ee}=\frac{\gamma}{e^{\gamma}-1}, \quad \text{with} \quad \gamma=\frac{2\pi}{|\mathbf{k}_1-\mathbf{k}_2|} \tag{6}$$

and

$$\nu_3=-\frac{1}{|\mathbf{k}_1-\mathbf{k}_2|}. \tag{7}$$

The parameter $r_{3\rm ave}$ is given by

$$r_{3\rm ave}=\frac{\pi^2}{16\epsilon}\left(1+\frac{0.627}{\pi}\sqrt{\epsilon}\ln\epsilon\right)^2, \tag{8}$$

where ϵ is the total energy of the two exiting electrons.

The Gamov factor N_{ee}, defined in Eq. (6) above, has been used to represent the final-state electron-electron interaction in a number of calculations [3,11,14,16]. The Gamov factor was first used in the theory of alpha decay and is intimately related to the normalization of the Coulomb function; it plays an interesting role in the Brauner-Briggs-Klar approximation of Ref. [17] where it corresponds to the Coulomb normalization of the third wave function, i.e., the electron-electron wave function, in the zero energy limit. The problem with it is that it does not represent well the absolute size of the cross section at very low energies. It predicts a yield that goes to zero exponentially as the impact energy approaches threshold in direct contradiction to the power law predicted by Wannier [18]. N_{ee} does very well at predicting the shape of the TDCS over a wide range of geometries and kinematics [3,11,13,14]. The M_{ee} factor is chosen to give the Wannier behavior near threshold. There is little difference between the shapes of the TDCS with the M_{ee} or N_{ee} factors, but we use the former rather than the latter since it gives a better normalization.

In Fig. 2 we compare calculations of DWBA+M_{ee} and the experimental data of Murray, together with the calculation of Berakdar and Briggs [19], which we will discuss below. We note that the DWBA, DWBA+M_{ee}, and the Berakdar and Briggs [19] calculations all agree with respect to absolute size. Murray [1] normalized his data with respect to the absolute coplanar value of Gélébart and Tweed [20]. This value was later scaled down by the Brest group [21] and the latest results from the Brest-Kaiserslautern collaboration have suggested that it may be necessary to reduce it even further [22]. The experimental determination of absolute cross sections is an extremely delicate and difficult task, and very slight differences in the setup can produce very large errors ([23,24]). We have used a normalization of the Murray data consistent with the new preliminary results of the Brest-Kaiserslautern experiments and which gives the best agreement with DWBA+ M_{ee} over all geometries, i.e., not just

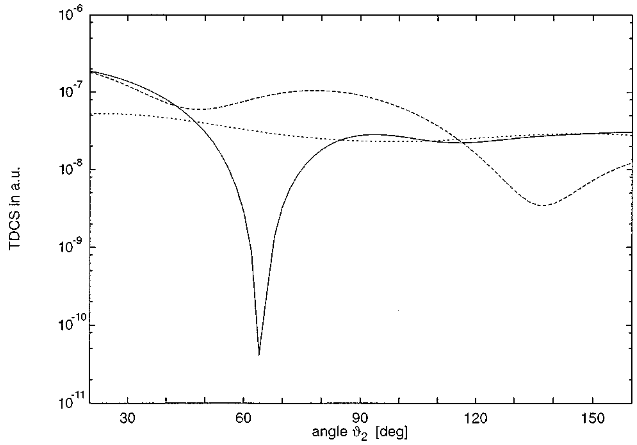

FIG. 3. TDCS for neon($1s$) in symmetric equal energy sharing geometry at an impact energy of 2170.2 eV. Electron gun raised to ψ=72.5°. Shown are DWBA (solid curve), DWBA with incoming plane wave (long-dashed curve), DWBA with outgoing plane waves (short-dashed curve). All calculations include the M_{ee} factor.

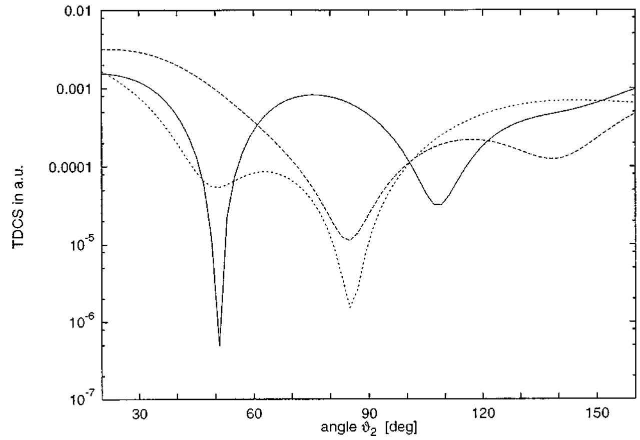

FIG. 4. TDCS for neon($2s$) in symmetric equal energy sharing geometry at an impact energy of 110.5 eV. Electron gun raised to ψ=42°. Shown are DWBA (solid curve), DWBA with incoming plane wave (long-dashed curve), and DWBA with outgoing plane waves (short-dashed curve). All calculations include the M_{ee} factor.

the present out-of-plane case. We remark that many theories can predict reasonable shapes for the TDCS in a range of geometries ([17,19], our own work) but differ wildly in absolute size. It is now the case, in our view, that only absolute cross sections can discriminate between the models especially when final-state Coulomb interactions are important. We strongly encourage our experimental colleagues to focus their attention on this very difficult problem.

The correlated final-state approach of Berakdar and Briggs [19] starts from the TDCS given by

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE}=(2\pi)^4\frac{k_1k_2}{k_0}\langle\Psi_f^-|V_i|\Phi_i\rangle, \tag{9}$$

where the initial asymptotic wave function is given by

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}_0\cdot\mathbf{r}_1}\phi(\mathbf{r}_2,\mathbf{r}_3) \tag{10}$$

and $\phi(\mathbf{r}_2,\mathbf{r}_3)$ represents the He($1s$) bound state (see Ref. [19] for more details).

Berakdar and Briggs [19] then approximate the exact wave function Ψ_f^- by

$$\begin{aligned}\Psi_f^-(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\approx&\frac{1}{(2\pi)^3}e^{i\mathbf{k}_1\cdot\mathbf{r}_1}e^{i\mathbf{k}_2\cdot\mathbf{r}_2}\phi^{+1}(\mathbf{r}_3)\\&\times\prod_j N_j\,{}_1F_1(i\alpha_j(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_{12}),1,\\&-i(k_jr_j+\mathbf{k}_j\cdot\mathbf{r}_j))\end{aligned} \tag{11}$$

where $N_j=e^{\alpha_j\pi/2}\Gamma(1+i\alpha_j)$. The momentum $\mathbf{k}_{12}$ is defined as $\mathbf{k}_{12}=(\mathbf{k}_1-\mathbf{k}_2)/2$ and its conjugate coordinate as $\mathbf{r}_{12}=(\mathbf{r}_1-\mathbf{r}_2)/2$. $\phi^{+1}(\mathbf{r}_3)$ is the hydrogenic wave function with charge $Z=2$. The parameters α_j are Sommerfeld parameters and are defined in Ref. [19].

The initial channel interaction potential in Eq. (9) is taken to be

$$V_i=\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{2}{\mathbf{r}_1}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_3|}. \tag{12}$$

Due to the fact that this potential consists of three terms, one has to add three complex amplitudes, which need to cancel to produce the dip. Since the third term represents interaction with the remaining target ''spectator'' electron, Berakdar and Briggs [19] argued that such a dip could not be observed in a hydrogen target. We note that the Berakdar and Briggs [19] approximation proceeds through its ansatz given by Eq. (11) and places strong emphasis on including the asymptotic three-body interactions. Our calculation on the other hand includes postcollisional interaction (PCI) effects only through the M_{ee} factor, in the region of the dip the M_{ee} factor has only a marginal effect, which inclines us to the view that PCI is not significant in this region. The DWBA calculation does, however, take into account the elastic scattering of the incident and exciting electrons in the field of the atom and the ion. Thus the role of the spectator electron is automatically included to all orders in this part of the calculation. In order to test for the significance of the spectator electron we performed DWBA calculations on H and He^+. For hydrogen we found no evidence of a dip out of plane, nor could we find such a structure in He^+. However, it is possible to observe such a structure in an open-shell system such as Li($2s$) as shown in Fig. 7. Since the impact energy is very low (22.4 eV) it remains to be seen if this is actually a real effect and will not be swamped by polarization, which may be strong at this energy. There are also a number of differences. The dip occurs at a much higher ratio of impact to bound state energy, at about 4.15 and at a much larger angle ϑ. Furthermore since Li does contain extra electrons it would be interesting to see if a Berakdar and Briggs [19] style calculation would reproduce a dip in this case.

In Fig. 2 we compare the calculation [19] with the DWBA+M_{ee} calculation. We see that the DWBA calculation is in better agreement with the experiments in that the calculation [19] has the location of the dip shifted somewhat to the left of the experiment and predicts an additional struc-

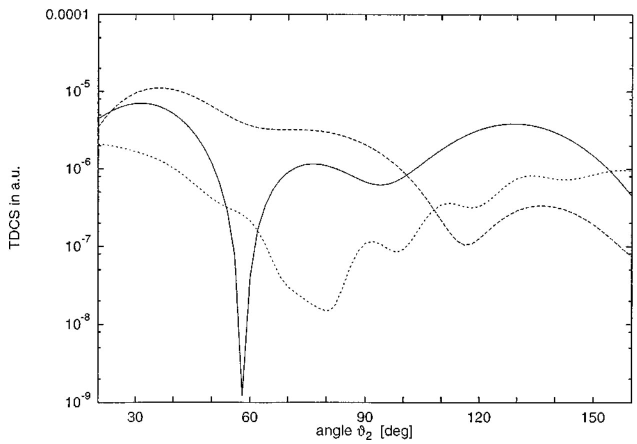

FIG. 5. TDCS for argon$(2s)$ in symmetric equal energy sharing geometry at an impact energy of 826.3 eV. Electron gun raised to ψ=50°. Shown are DWBA (solid curve), DWBA with incoming plane wave (long-dashed curve), and DWBA with outgoing plane waves (short-dashed curve). All calculations include the M_{ee} factor.

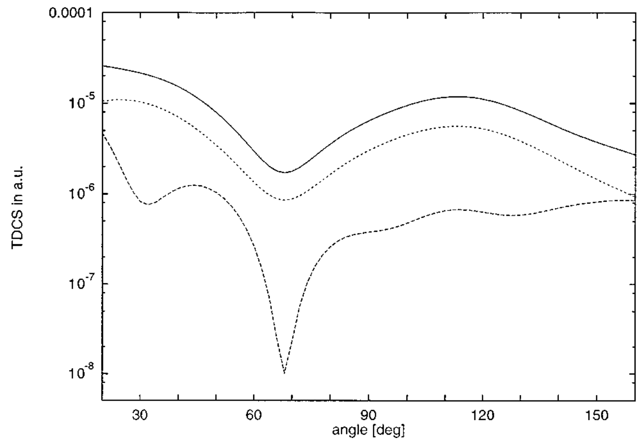

FIG. 6. TDCS for argon$(2p)$ in symmetric equal energy sharing geometry at an impact energy of 849 eV. Electron gun raised to ψ=47.5°. Shown are DWBA calculations for different magnetic sublevels: averaged over all sublevels (solid curve), and for the magnetic sublevel $m_b=0$ (long-dashed curve), $m_b=-1$ (short-dashed curve), the calculation for $m_b=+1$ is equal to the one for $m_b=-1$. All calculations include the M_{ee} factor.

ture at around 100°, which is neither in the DWBA calculations nor in the measurement.

It is of interest to see if such sharp interference effects are to be observed in other systems. We have performed calculations on Ne$(1s)$ at an impact energy of 2170.2 eV with ψ=72.5°, Ne$(2s)$ at an impact energy of 116.5 eV with ψ=40° and on Ar$(2s)$ at an impact energy of 826.3 eV with ψ=50° and predict that very strong interference structures should be observable (Figs. 3–5). Switching off any of the distorting potentials in either the initial or final channels causes the dip to disappear. There are a number of similarities between the atoms. This applies to the ratio of the impact to bound state energy, gun angle ψ and angle θ_2 at which the dips occur (see Table I).

It is interesting to see if similar interference structures can be observed in open-shell systems. Mathematically we are merely dealing with a six-dimensional integral over a highly oscillatory argument and as such destructive interference effects may yield very small values for certain cases. Indeed a pure DWBA calculation for hydrogen reveals a sharp dip in symmetric coplanar geometry at 29 eV. However, as we mentioned earlier, polarization effects are very important in the coplanar case and if we include these in our calculation the dip disappears, in contrast to the out-of-plane He case discussed here where the sharp dip persists in the presence of the very strong polarization potential of [3] (for more details see Ref. [24]).

Finally we look for such structures in closed-shell p-state targets such as Ar$(2p)$, Ne$(2p)$: no dip was found. However, if we look at the individual magnetic sublevels we see a slightly different behavior. Since the experiment cannot normally distinguish between the scattering of different bound state sublevels m_b one has to average over them, i.e., sum over all final channels in Eq. (1).

TABLE I. Similarities in the occurrence of the interference structure in different closed-shell atoms. First column: ratio of the impact (E_0) to bound state (E_b) energy; second column: gun-angle ψ; third column: angle at which the minimum of the dip occurs.

	E_0/E_b	ψ	ϑ_2
He$(1s)$	2.63	67.5°	68.0°
Ne$(1s)$	2.49	72.5°	64°
Ne$(2s)$	2.28	42°	51.0°
Ar$(2s)$	2.53	50°	58.0°

Figure 6 shows a DWBA calculation for Ar$(2p)$ that includes calculations for particular sublevels. It is interesting to see that the sublevel $m_b=0$ exhibits such a strong structure at the same ϑ_2 point; however, the sublevels $m_b=-1$ and $m_b=+1$ do not exhibit this structure so that a summation over all three sublevels lets the dip disappear.

III. CONCLUSION

We have demonstrated that the sharp dip observed by Murray [1] in symmetric out-of-plane geometry can be well

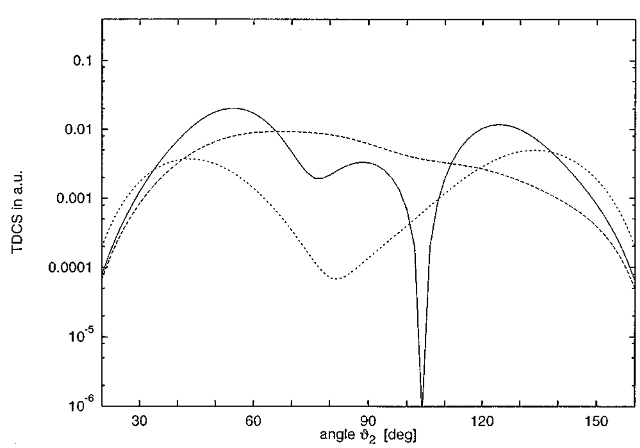

FIG. 7. TDCS for lithium$(2s)$ in symmetric equal energy sharing geometry at an impact energy of 22.4 eV. Electron gun raised to ψ=77.5°. Shown are DWBA (solid curve), DWBA with incoming plane wave (long-dashed curve), and DWBA with outgoing plane waves (short-dashed curve). All calculations include the M_{ee} factor.

represented in a distorted-wave Born approximation. The dip exists even in the simplest calculation of this type where neither polarization nor postcollisional electron-electron interaction is included. It is necessary to allow for elastic scattering of the incident electron from the atom and elastic scattering of the exiting electrons from the ion if this structure is to manifest itself. The DWBA calculations automatically include the effect of the spectator electron as well as the nucleus on these channels and it is impractical to try to separate them. Results of simpler calculations seem to indicate that both play a part and this is partially confirmed by the nonexistence of such a dip in hydrogenic systems.

We have predicted where similar structures are likely to be found for other atoms. Interference effects of this kind can only be sensibly interpreted in quantum mechanical terms and arise when we integrate over wave functions and as such are important to identify and study.

ACKNOWLEDGMENTS

We thank Jochen Röder and Amedé Pochat for communicating information of their absolute measurements prior to publication. We would also like to thank Joe Macek for discussion concerning the M_{ee} factor. We gratefully acknowledge financial support for this work from the British Council and DAAD (ARC), NATO through Grant No. CRG 950407 and the European Union (HCM CHRX-CT93-0350). J. R. would like to thank Wolfson College, Cambridge for financial support.

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