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Low-energy electron-impact ionization of helium

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We present a combined experimental and theoretical study of 32.6-eV electron-impact ionization of helium. The measured absolute coplanar triply differential cross sections are in the equal-energy-sharing ($E_A=E_B=4$ eV) kinematical region, and have been obtained in the fixed θ_A, fixed $\theta_B-\theta_A$, and symmetric geometries. The convergent close-coupling calculations are in excellent agreement with experiment. [S1050-2947(98)50905-5]

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In recent times substantial progress has been made in the field of electron-impact ionization. Since the work of Brauner, Briggs, and Klar [1] there has been a rapid increase in general interest and variety of theoretical approaches. These include methods evolved from consideration of the three-body boundary conditions [1–4], methods that have apparently inappropriate boundary conditions such as close-coupling [5–8] and distorted-wave [9] approaches, and methods that avoid the need for the three-body boundary conditions using time-dependent [10,11] and time-independent [12] techniques.

The theoretical developments during this decade have at times been quite surprising and unexpected. For example, the separation of the theoretical results into shapes that agree with experiment, and magnitudes that do not, is particularly remarkable. The process of experimental normalization is very difficult in the case of differential ionization cross sections, and there exist substantial discrepancies between some sets of measurements, while still obtaining similar angular profiles. This is understandable, but much less so in the case of theory.

The latest victim of this disturbing situation has been the convergent close-coupling (CCC) approach to ionization [7,8]. While this method was able to describe the angular profiles to an unprecedented accuracy in the case of 64.6-eV e-He equal-energy-sharing triply differential cross sections (TDCS), the theory was found to be a factor of almost 2 lower than experiment [13]. Comparison with doubly differential cross sections (DDCS) showed a disturbing increase in this factor as the ionization threshold was approached [14]. Application to low-energy e-H ionization showed that this factor can be as large as 7 [15].

The problem with the absolute values arising in the theory of Brauner, Briggs, and Klar, often denoted by 3C due to existence of three Coulomb phases, is now well understood and resolved. The dynamical screening (DS3C) approach of Berakdar and Briggs [2] yields accurate absolute values where 3C does not. Indeed, Berakdar [16] showed that DS3C obtains accurate total ionization cross sections (TICS) and the associated spin asymmetries in e-H ionization. This is a most exciting and welcome development. However, the CCC theory also obtains accurate TICS and yet still yields differential ionization cross sections substantially lower than experiment in the equal-energy-sharing kinematical region.

The aim of this Rapid Communication is to present absolute near-threshold ionization data and show how the problem with the CCC theory may be resolved. We present a set of 32.6-eV e-He absolute equal-energy-sharing ($E_A=E_B=4$ eV) TDCS measurements that thoroughly test the CCC theory angular and absolute values at the lowest energy to date. The step function in the singly differential cross section (SDCS) hypothesis for the model problem [17] is applied in the present real case in order to obtain an estimate of the true SDCS. This in turn is used to specify the factor by which the CCC results need to be multiplied. We argue that this leads to a very accurate estimate of the absolute values in the near-threshold region.

The details of experimental apparatus and method of normalization have been given elsewhere [18–20]. Given the occasional substantial discrepancy in the absolute experimental values determined via various techniques we give a short summary of the method used here. The crucial part is that we use an ion detector and measure the ion rate, which is then combined with the very accurate data for the total ionization cross section of Shah *et al.* [21], to yield the product of the target density n, the rate of primary electrons N_e, and the gas-electron overlap length l. Avoidance of measuring these quantities separately is what makes our technique, in our view, particularly reliable. The remaining quantities necessary for the determination of the absolute values may be either accurately measured or inferred by comparison with appropriate experiment or calculation; see Refs. [14,13] for more detail.

The details of the CCC theory for electron-helium scattering have been given by Fursa and Bray [22] and extended to ionization by Bray and Fursa [8]. Briefly, the total wave function is expanded in a set of N square-integrable pseudostates obtained by diagonalizing the target Hamiltonian in an explicitly antisymmetric two-electron Laguerre basis assuming the frozen-core model [22]. We rely on the property of the Laguerre bases that by simply increasing N we ap-

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proach ''completeness'' in the expansion of the unsymmetrized total wave function. However, for any finite N such expansions ensure that only the projectile-space electron is allowed to escape to infinity. In other words, the boundary conditions are suited to inelastic scattering and not to true ionization. In the close-coupling (CC) approach we associate ionization with excitation of the positive-energy L^2 pseudostates.

In the choice of target states we have freedom to choose the maximum orbital angular momentum $\ell_{\max}$, and for each $\ell \leq \ell_{\max}$ and spin $s=0,1$, the number of states $N_{\ell s}$. The total number of states N is then the sum of all $N_{\ell s}$. The size of the computational problem is governed by the number of channels, with an ℓ-state generating $\ell+1$ number of channels. For this reason we are severely restricted in the value of $\ell_{\max}$. Thanks to the unitarity of the CC formalism, we find that this is not a major practical problem. In the case of 20-eV outgoing electrons ($E_0=64.6$ eV) taking $\ell_{\max}=5$ was sufficient to obtain convergence in angular distributions [13].

Having defined the N target-space states the CC equations are solved at the specified total energy E. Upon solution we obtain scattering amplitudes $f^N_{n\ell s}$ for all open positive-energy $\epsilon_{n\ell s}, n \leq N_{\ell s}$ states. The continuum normalization and Coulomb phase are restored by multiplying $f^N_{n\ell s}$ by the overlap of the associated pseudostate and the true continuum function of same energy $\epsilon_{n\ell s}$. For a derivation of this procedure see Ref. [8]. The amplitudes are then interpolated on to the continuous energy scale $f_{\ell s}(\epsilon)$ with $0<\epsilon<E$.

Fundamentally, the CCC approach treats the electrons as being distinguishable, with antisymmetry being built into the potentials. Though the physics on either side of $E/2$ is identical we obtain highly asymmetric results. In fact for $\epsilon \ll E/2$ the amplitudes are such that $|f^N_{\ell s}(\epsilon)|^2 \gg |f^N_{\ell s}(E-\epsilon)|^2$. The step-function hypothesis [17] states that the latter amplitude should be zero for infinite N, with all of the physics being contained in the energy region $0 \leq \epsilon \leq E/2$. For finite N, however, we combine incoherently the theoretically distinguishable amplitudes on either side of $E/2$. For an example of coherent and incoherent summation in the case of 20-eV outgoing electrons see Bray *et al.* [13].

So how can the CCC theory be too low in the equal-energy-sharing kinematical region and what can be done about it? The answer lies in the SDCS as calculated by the CCC theory. Figure 8 of Röder *et al.* [14] shows that the CCC theory yields unphysical oscillations in the SDCS, with the equal-energy-sharing point becoming increasingly below the experiment as the incident energy is reduced. Bray [17] suggested that this problem may be remedied should the true SDCS be well-modeled by a quadratic function. This assumption is particularly valid at low energies, where the true SDCS is expected to be relatively flat (maybe even a little convex [23]), and so is determined to a large extent simply by the TICS. Thus, we obtain two SDCS from the CCC theory: one directly from the excitation of the positive-energy pseudostates [24] and the other from the CCC estimate of the TICS. The former is incorrect due to the inability of a finite basis expansion to approximate a step function, though due to unitarity yields the correct TICS upon integration. The latter SDCS is likely to be accurate, particularly

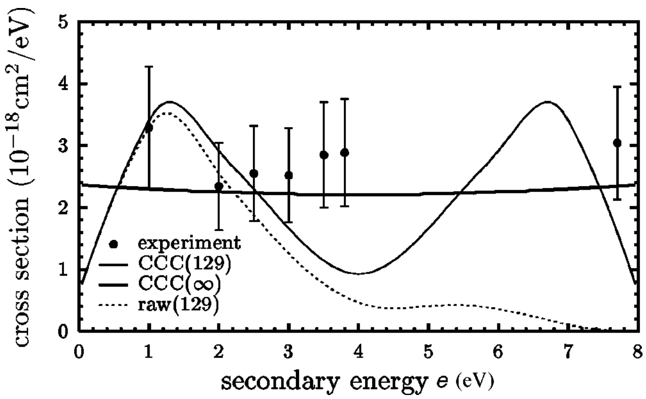

FIG. 1. The 32.6-eV e-He singly differential ionization cross section. The CCC(129) curve is obtained by summing the raw(129) results on either side of $E/2=4$ eV. The CCC(∞) is similarly obtained from the step-function estimate (see text) raw(∞), which takes the values of CCC(∞) for $e \leq 4$ and zero for $e>4$. The ratio between CCC(∞) and CCC(129) at $e=4$ eV is 2.3.

close to threshold, and may be used to renormalize the directly obtained CCC results by multiplying them by the ratio of the two SDCS at the required energy.

To illustrate these ideas we present experiment and theory for 32.6-eV electron-impact ionization of the ground state of helium in the equal-energy-sharing kinematical region. The CCC calculations have been performed using a total of 129 states. These consist of $15-\ell$ states for each $\ell \leq 4$ and spin $s=0,1$, with the exception of ^3S states (14 are taken, as there is no 1^3S). The Laguerre exponential fall-offs are taken to be much the same and adjusted ($\lambda_\ell \approx 1.25 \pm 0.12$) so that one pseudostate, for each target symmetry, has an energy near 4 eV, thus reducing the uncertainty due to interpolation [8].

In Fig. 1 we give the experimental estimate of the SDCS [14] as well as the present CCC calculations. The raw(129) results are obtained directly from the excitation of the positive-energy pseudostates. It is this SDCS that we expect will tend to a step-function raw(∞) result as the number of states goes to infinity. The integral of the raw(129) results yields a TICS (8.9×10^{-18} cm^2), which is consistent with the accurate measurements of Shah *et al.* [21] ($9.2\pm0.3 \times10^{-18}$ cm^2), and which is used to estimate the raw(∞) results by assuming that the true SDCS is almost flat. The presented CCC(129) and CCC(∞) results have been obtained by summing the corresponding raw results on either side of $E/2$, and yield twice the TICS upon integration. Comparison of the CCC(∞) and the CCC(129) SDCS indicates that sometimes the obtained CCC(129) ionization results will be too big and sometimes too small. In particular, at $e=4$ eV the CCC(129) results for the SDCS, DDCS, and TDCS need to be multiplied by 2.3. This factor is the ratio of the CCC(∞) and CCC(129) SDCS at $e=4$, and we expect to yield magnitudes to an accuracy of $\pm10\%$.

Having worked out the factor by which the CCC(129) results need to be multiplied we turn to comparison with experiment for the TDCS. In Fig. 2 we look at the fixed θ_A geometry. We use the convenient coplanar geometry convention that positive and negative θ are on either side of the initial electron beam, which defines the Z axis. We see excellent agreement between the CCC(129) calculations with experiment, when the former have been multiplied by 2.3

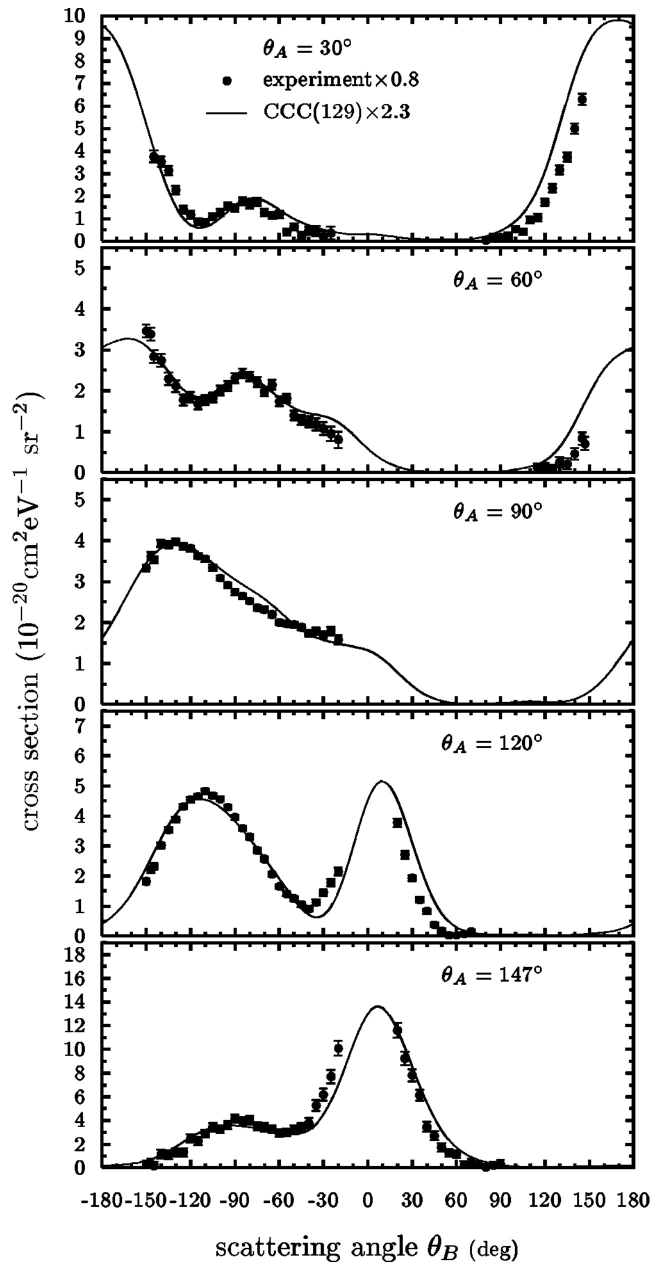

FIG. 2. The measured and calculated 32.6-eV e-He coplanar equal-energy-sharing TDCS in the specified fixed θ_A geometry. The CCC results have been multiplied by the factor 2.3, obtained from Fig. 1. The experimentally normalized measurements, with an uncertainty of $\pm 25\%$, have been multiplied by 0.8 to obtain best visual fit with theory, and hence made consistent with the CCC(∞) SDCS at $e=4$ of Fig. 1.

and the latter by 0.8. The 20% reduction of experiment is within the $\pm 25\%$ absolute value determination uncertainty, and ensures that the reduced mean values are consistent with the TICS, unlike previously found [14]. The same quality of agreement is found in the case of the fixed $\theta_B - \theta_A$ geometry, presented in Fig. 3, and the symmetric geometry, presented in Fig. 4. Agreement with such a diverse set of measurements suggests that the CCC theory yields correct TDCS in the entire (θ_A, θ_B) plane, a truly remarkable result given the asymmetric treatment of the two 4-eV electrons.

The presented excellent quality of agreement between theory and experiment in angular distributions is comparable

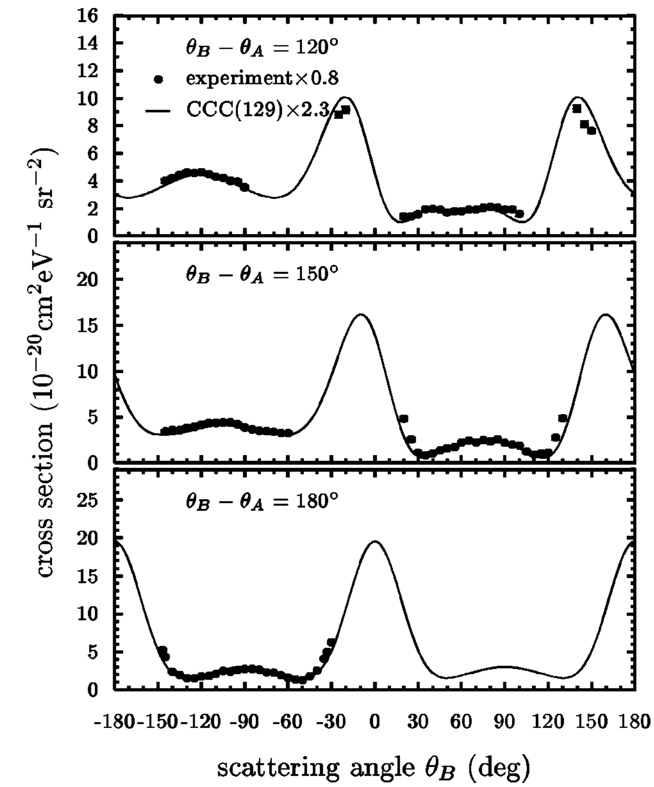

FIG. 3. As for Fig. 2, except for the indicated constant $\theta_B - \theta_A$ geometry.

to that in the case of 64.6-eV incident electrons [13]. The angular agreement suggests that the uncertainty in the theoretical absolute values depends only on the uncertainty associated with estimating the true SDCS from the TICS. In the present case we estimate this uncertainty to be $\pm 10\%$, which is an improvement on initially being $2.3/0.8 \approx 2.9$ too low [14], or the initial experimental uncertainty of $\pm 25\%$. Since it has been shown that the CCC theory is able to predict correct e-H TICS to within 1 eV of the ionization threshold [25], the present prescription is practical to at least this energy. If we also obtain shape agreement with experiment of similar quality as we have here, then we will be able to predict absolute values in the near-threshold region to say $\pm 10\%$ instead of being up to 100% too low [15].

We are also confident of being able to accurately estimate the true SDCS from the TICS, correctly obtained in the CCC

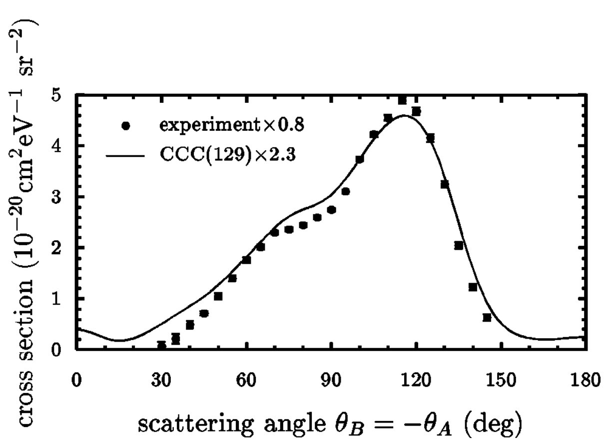

FIG. 4. As for Fig. 2 except for the symmetric geometry.

theory, even in the intermediate energy range (note that by 100 eV there are no problems [26]). In this case we take advantage of the following observation. For targets with a large ionization threshold the SDCS at $e=0$ varies very slowly with E. In other words, the magnitude of the cross section depends primarily on the interaction of the very slow electron with the residual ion, and is largely independent of the energy of the outgoing much faster electron. In the case of e-He ionization the SDCS at $e=0$ can be supposed to be constant from threshold to 100 eV incident energy [14] (maybe even to 600 eV [8]). This fixes the quadratic estimate of the true SDCS, and recovers the factor of 1.8 at 64.6 eV [13]. These considerations are currently under investigation.

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