Semiclassical-quantal approach to the near-threshold ionization of hydrogen

N. C. Deb and D. S. F. Crothers
Theoretical and Computational Physics Research Division, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom

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A recent improved version of the semiclassical-quantal approach has been applied to the e^--H near-threshold ionization for $\theta_{12}=180°$ geometry. It is found, that unlike other sophisticated theoretical methods such as distorted wave theory or convergent close-coupling calculation, the present relatively simpler approach produces correct behavior and numerical values for the triple-differential cross sections. We compare our results with recent absolute measurements and accurate numerical calculations at 2 eV and 4 eV above the threshold at constant θ_{12} geometry.

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Although considerable attention has been focused on $(e,2e)$ studies in e^--H scattering, the overall situation is far from complete specially in the near-threshold region. While the sophisticated theories such as convergent close-coupling (CCC) calculations [1,2] or theories based on distorted-wave (DW) formalism [3–6] have had some success in predicting the correct behavior of the angular distributions, their results close to the threshold show large quantitative disagreement ranging from a factor of 2 to 7 for the CCC theory and by a factor of 10 to 27 for certain variants of DW theory. Based on an exterior-complex-scaling (ECS) procedure, McCurdy and co-workers [7,8] were spectacularly successful in describing accurate total and differential cross sections for the e^--H scattering. This gigantic numerical effort involves an enormous amount of supercomputing time and their results down to 4 eV above the threshold and upwards at constant θ_{12} geometry are now available. Comparison of these results [7,8] with recent measurements [9,10] show excellent agreement.

There has been some criticism of the CCC calculations that they do not satisfy the symmetrization postulate and represent incoherent combinations of amplitudes on either side of $E/2$, E being the excess energy above the threshold. To address these criticisms Bray [11] introduced a step-function hypothesis that the ionization amplitude beyond the $E/2$ is identically zero. However, this hypothesis is yet to be proved analytically. A detailed analysis in this regard has been presented by Rescigno *et al.* [12]. The CCC angular behavior of the triple-differential cross sections (TDCS) even close to the threshold show good qualitative agreement with the measurement [9]. Recently Bray [13] has successfully shown that the "raw" CCC amplitudes are now purported to converge to exactly half the correct value at $E/2$. This makes the CCC results better in the sense that it no longer requires arbitrary scaling constants to compare with measurement [9]. Nevertheless, a factor of 2 or so still remains to be unexplained for the near-threshold results. In our present calculation we shall compare the most recent CCC results obtained from them [14]. We note that the measurements are absolute only at 2 eV and 4 eV and at remaining energies they are relative measurements normalized to the distorted partial-wave (DPW) calculation of Pan and Starace [6]. A host of other variants of distorted wave approximations [3–5] has been applied to the e^--H ionization with reasonably good description of the triple-differential cross section but preferentially in the high-energy region (at least not close to the ionization threshold). Among the distorted-wave calculations the method of Pan and Starace [6] represented the best agreement of the TDCS with the measurement [9] close to the threshold. While the DPW results at 4 eV above the threshold show very good agreement both qualitatively and quantitatively with the absolute measurement [9], the results are off by a factor of 2 at 2 eV above the threshold. Therefore, we are still in search of a technique that can produce correct angular distributions and numerical values of the TDCS close to the threshold. In what follows, we shall demonstrate that a recently reported improved version [15,16] of the semiclassical-quantal treatment of Crothers [17] can provide just such a reasonably accurate technique for the electron impact ionization of atomic hydrogen.

The direct amplitude for the electron impact ionization of atomic hydrogen is given by

$$f(\hat{\mathbf{k}}_1,\hat{\mathbf{k}}_2)\simeq\frac{2i}{\pi}\int \Psi_f^{-}{}^*(\mathbf{r}_1,\mathbf{r}_2)\left[\frac{1}{r_{12}}-\frac{1}{r_1}\right]e^{i\mathbf{k}_0\cdot\mathbf{r}_1}\varphi(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2, \tag{1}$$

where $\varphi(\mathbf{r}_2)$ is the ground state of hydrogen atom, $\Psi_f^{-}{}^*(\mathbf{r}_1,\mathbf{r}_2)$ the final-state wave function for the two outgoing electrons with momenta $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_0$ being the momentum of the incident electron. Energy conservation demands that $k_0^2/2-\epsilon_I=k_1^2/2+k_2^2/2$ with ϵ_I the ionization threshold of atomic hydrogen (13.6 eV). In equation (1) $\mathbf{r}_1$ and $\mathbf{r}_2$ are the projectile and atomic electron coordinates with respect to the bare nucleus.

Since in the final channel the wave function for the two outgoing electrons is independent of the target we can use the same final-state wave function used in our recent calculations [15,16] for ionization of atomic helium. The uniform semiclassical wave function $\Psi_f^{-}{}^*(\mathbf{r}_1,\mathbf{r}_2)$ in the final channel for the two outgoing electrons was first obtained [17] by solving the corresponding equation in hyperspherical coordinates and is given by

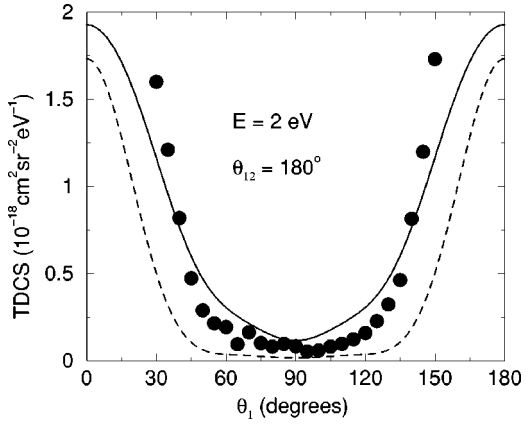

FIG. 1. TDCS in the constant geometry of $\theta_{12}=\pi$ at $E=2$ eV above threshold. Filled circles: measurement [9], dashed lines: CCC results [14], and solid line: present results.

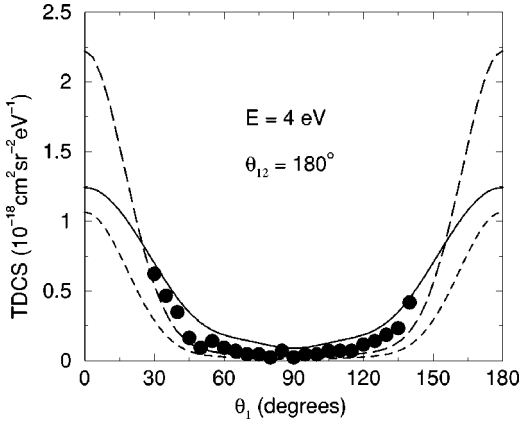

FIG. 2. Same as Fig. 1 but for $E=4$ eV and long-dashed line represents ECS results [8].

$$\Psi_f^{-}{}^{*}=\frac{c^{1/2}E^{m_{12}/2}u_1^{1/2}}{\tilde{\omega}^{1/2}\rho^{5/2}\sin\alpha\cos\alpha}\delta(\hat{\mathbf{k}}_1-\hat{\mathbf{r}}_1)\,\delta(\hat{\mathbf{k}}_2-\hat{\mathbf{r}}_2)\times\exp\left(\frac{4i}{(8Z_0\rho)^{1/2}}(\Delta\theta_{12})^{-2}\right)\exp\left[-i\left(S_0+\frac{1}{2}S_1(\Delta\alpha)^2+\frac{1}{8}S_2(\Delta\theta_{12})^2+\frac{\pi}{4}\right)-(\text{conjugate})\right]. \tag{2}$$

The presence of the term $\delta(\hat{\mathbf{k}}_1-\hat{\mathbf{r}}_1)\,\delta(\hat{\mathbf{k}}_2-\hat{\mathbf{r}}_2)$ in Eq. (2) is necessary to ensure that the two electrons have specific directions asymptotically and to project out the required outgoing scattering amplitude. Various constants and expressions for the classical action variables S_0, S_1, and S_2 in Eq. (2) are are all given in our recent calculation [16]. The wave function in Eq. (2) includes both radial and angular correlation through the hyperspherical coordinates $\alpha=\tan^{-1}(r_2/r_1)$ and $\theta_{12}=\cos^{-1}(\hat{\mathbf{r}}_1\cdot\hat{\mathbf{r}}_2)$, respectively. The classical action was expanded in a Taylor series around the Wannier ridge angles $\alpha=\pi/4$ and $\theta_{12}=\pi$ and terms through second order were retained. This wave function is then used to evaluate the direct amplitude in Eq. (1). The α integration in the hyperspherical space has been evaluated by using the method of stationary phase/steepest descent, the point of stationary phase being given naturally enough by $\alpha=\pi/4$, the saddle point. The remaining integrations are done numerically using Gauss-Lobatto quadrature. The exchange amplitude is obtained from the direct amplitude by interchanging θ_1 and θ_2 made by the two outgoing electrons with the incident beam direction.

In Fig. 1 we compare our TDCS results at 2 eV excess energy (15.6 eV incident electron energy) with corresponding absolute measurement of Röder *et al.* [9] and the CCC results [14]. All the results are in the constant geometry of $\theta_{12}=\pi$. Our results show good agreement with the measurement for the angular region $40°<\theta_1<140°$. Outside this region our results tend to deviate from the measured values that are strongly peaked in the forward or backward directions. It is to be noted here that at this energy the experimental uncertainty is 35%. The CCC results at this energy as shown in the combined experiment-theory paper [9] demonstrated better agreement only after being scaled up by a factor of 7. The apparent deviation of our results at the forward or backward angles was also noted earlier [15,16] for the ionization of helium.

Figure 2 shows a comparison of the TDCS results at 4 eV excess energy in the present calculation, unscaled CCC results [14], the absolute measurement [9], and the results of ECS calculation [8]. Note that the experimental uncertainty at this energy is as large as 40%. The agreement of the present as well as CCC results with the measurement [9] is similar to that of the 2 eV excess energy case. The ECS results [8] show the best agreement with the measurement [9] and tend to peak strongly in the forward and backward direction. From both figures we note that the present and CCC results show similar behavior in the extreme forward or backward directions. It is interesting to note from Figs. 1 and 2 that the present results are higher than both CCC and ECS results in the trough region while at the forward and backward angles the present results are lower than ECS results but higher than CCC results. This will make the integrated cross sections under the curves closer to the ECS results. The DPW results [6], as presented by Röder *et al.* [9], are no better and no worse than ours, in comparison with CCC [14], ECS [18], and the experimental results [9]. In the absence of any experimental data at these angles, it is difficult to judge the accuracy of any theoretical results although ECS results [18] are more likely to be accurate.

In conclusion, we have demonstrated that the present relatively much simpler semiclassical-quantal approach can provide a reasonably good description of the TDCS for the electron-hydrogen ionization process. The present method is far less time consuming than the large multistate CCC calculation or the giant numerical ECS technique. However, the present method may have its own limitation in that the final-state wave function for the two outgoing electrons is based on a Wannier model and therefore may not be suitable either

for the angles far away from the ridge angles or for the energy far above the threshold. Here we report our results only at a constant geometry of $\theta_{12}=\pi$. Results at other geometries will be reported elsewhere.

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