Slow convergence of the Born approximation for electron-atom ionization

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It is usually assumed that the first-Born approximation for electron-atom ionization becomes valid for the fully differential cross section at sufficiently high impact energies, at least for asymmetric collisions where the projectile suffers only a small energy loss and is scattered by a small angle. Here we investigate this assumption quantitatively for ionization of hydrogen atoms. We find that convergence of the Born approximation to the correct nonrelativistic result is generally achieved only at energies where relativistic effects start to become important. Consequently, the assumption that the Born approximation becomes valid for high energy is inaccurate, since by the time it converges, nonrelativistic scattering theory is not valid.

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Ehrhardt *et al.* [1] argued some years ago that agreement between the first-Born approximation (FBA) and experiment for integrated (total) ionization cross sections is an inadequate test of the FBA, and that it is important to consider instead the fully differential cross section (FDCS). Although it is known that neglect of final-state Coulomb interactions will cause a slow convergence of the FBA to the correct result [1–3], no explicit demonstration showing convergence of the FDCS in the FBA has, to our knowledge, ever been given. Here we explicitly demonstrate convergence of the FBA for electron-impact ionization of atomic hydrogen by comparison with CDW-EIS (continuum distorted wave with eikonal initial state) calculations. For this comparison, we chose impact speeds ranging from a few atomic units to half the speed of light. (We study the convergence of the FBA within the framework of nonrelativistic scattering theory; in order to show that the FBA actually does converge, we need to consider impact speeds that exceed the range of validity of the nonrelativistic Schrödinger equation.)

The CDW-EIS approximation [4,5] goes beyond the FBA by incorporating projectile-target correlation (two-center effects) in the system wave functions both initially and finally. The FBA will give accurate results only when this correlation becomes negligible. For asymmetric collisions, where the projectile suffers only a small energy loss and is scattered by a small angle, initial-state correlation is already fairly weak at an impact energy of 250 eV [6]. Correlation in the final state, however, remains important up to much higher energies [1–3].

The CDW-EIS approximation provides accurate solutions of the nonrelativistic scattering problem over the entire range of impact energies considered here. In fact, CDW-EIS is in quantitative agreement with absolute measurements [7] at the lowest impact energy (250 eV) considered [8]. The approximation improves, of course, with increasing impact energy and, since we do not use partial-wave expansions, our numerical accuracy also improves with increasing impact energy.

Since the uncertainty of the absolute measurements at 250 eV is rather large (15% for the overall normalization and 10% for the internormalization of data points), it is important to have a second check on the accuracy of the CDW-EIS approximation. This is provided by the convergent close-coupling (CCC) calculations of Bray [9] (these are the calculations that were labeled "CCC99" in Ref. [6]). It was found that the two very different approaches, CDW-EIS and CCC, predict nearly identical results at 250 eV [6]. As a result, we are quite confident of the accuracy of the CDW-EIS *model* for impact energies above 250 eV.

An expression for the FDCS was given by Bethe [10] more than 70 years ago,

$$\sigma(\hat{\mathbf{v}}_1\hat{\mathbf{v}}_2,E_2)=(2\pi)^4\frac{v_1v_2}{v_0}|T_{fi}|^2 \tag{1}$$

(atomic units are used here, and throughout this paper, except where stated otherwise and unit vectors are denoted by a "hat," i.e., $\hat{\mathbf{x}}=\mathbf{x}/x$, where $x=|\mathbf{x}|$). Here E_2 is the energy of the ejected electron and $\mathbf{v}_0$, $\mathbf{v}_1$, and $\mathbf{v}_2$ are the velocities of the incident, scattered, and ejected electrons, respectively (electron exchange is negligible for the asymmetric collisions considered here). The flux factor in Eq. (1) is for continuum waves normalized to a δ function in momentum space.

In the FBA [10–12], the transition amplitude T_{fi} in Eq. (1) is a function of $\mathbf{v}_2$ and $\mathbf{q}$, where $\mathbf{q}=\mathbf{v}_0-\mathbf{v}_1$ is the momentum transferred from the projectile to the target atom. If $\hat{\mathbf{q}}$ is chosen as the quantization axis, then for a given $|\mathbf{q}|$, the only dependence of the FBA on the impact energy is the factor v_1/v_0 in Eq. (1) [1,11,12]. Then, scaling the FDCS (1) by the factor v_0/v_1 makes the FBA independent of impact energy, and provides a convenient way to study the convergence of the FBA.

The predominant majority of all fast singly ionizing collisions involve asymmetric energy partitioning and small momentum transfer to the target [7]. As a result, the usual way of studying the FDCS at intermediate and higher energies is to fix the scattering angle of the projectile at a small angle and look at the angular distributions of slow ejected electrons. Usually, only electrons ejected into the scattering plane defined by $\mathbf{v}_0$ and $\mathbf{v}_1$ are considered. For sufficiently high impact energy, the following behavior is then observed for ionization of *s* states. In the angular distribution of the ejected electrons, two peaks are found—a binary peak in the direction of $\mathbf{q}$ and a recoil peak in the opposite direction, in

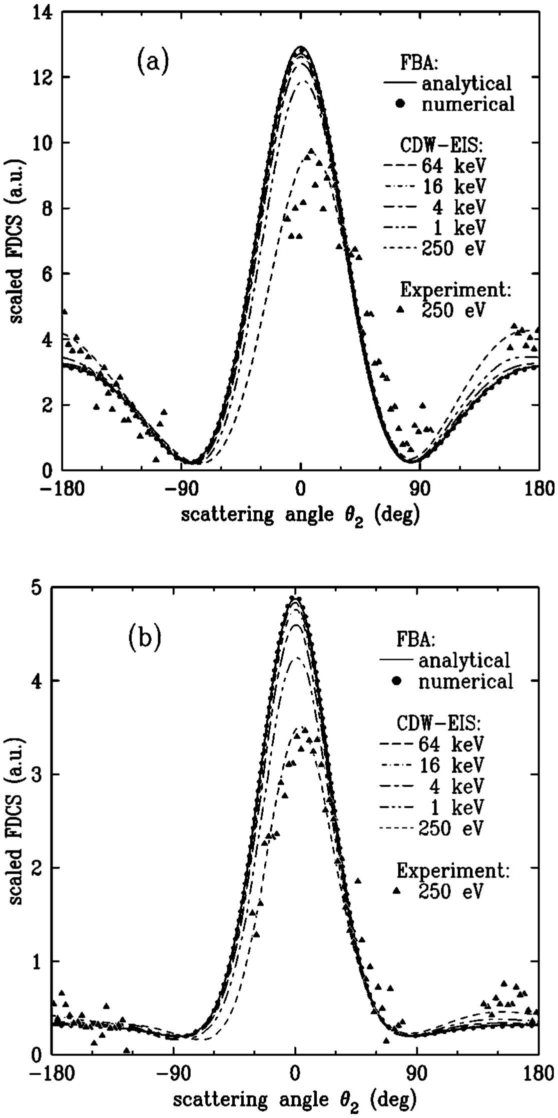

FIG. 1. Scattering-plane fully differential cross sections (FDCS's) for electron-impact ionization of atomic hydrogen. The ionized electron has an energy of 5 eV and is scattered, relative to the direction of the momentum transfer vector **q**, by the angle θ_2 (θ_2 is negative if both outgoing electrons emerge on the same side of **q**). The cross sections have been scaled as described in the text. The first-Born approximation (FBA) yields the same scaled cross section for all impact energies. Here we have calculated the FBA using both the analytical formula and six-dimensional numerical quadrature. Curves labeled by impact energy are CDW-EIS predictions. Solid triangles are absolute measurements of Ehrhardt *et al.* [7] at 250 eV, multiplied by 0.88 as recommended in Ref. [8]. The magnitude of **q** is (a) 0.2737 or (b) 0.6087 (a.u.).

accordance with the FBA. As the impact energy is lowered, however, the positions of the peaks shift to larger angles between the two outgoing electrons as a result of the final-state Coulomb interactions neglected in the FBA (which also strongly influence the magnitudes of both peaks) [1–3]. For impact energies below about 100 eV, initial-state projectile-target Coulomb interactions become strong and, in particular, significantly affect the height and position of the recoil peak [5,6].

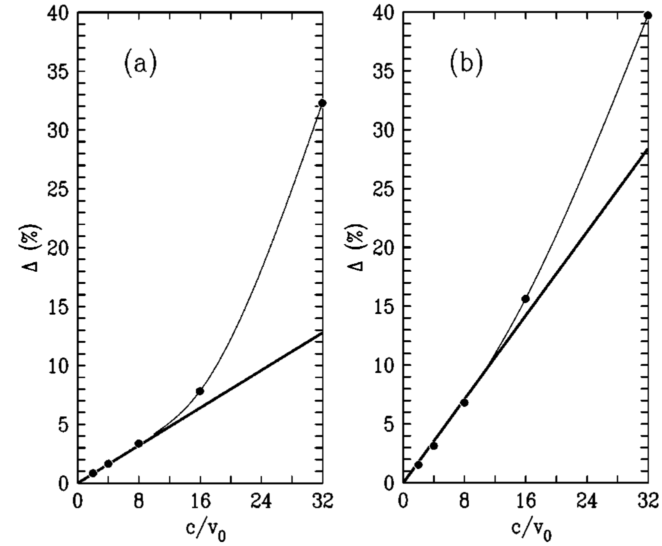

FIG. 2. The magnitude Δ (solid circles) of the fractional difference (expressed here as a percentage difference) between CDW-EIS and FBA for the height of the binary peak for the impact speeds v_0 considered in Fig. 1. For $c/v_0 \approx 2$, 4, 8, 16, and 32 (c is the speed of light), the impact energies are 64, 16, 4, 1, and 0.25 keV, respectively. The thick straight line corresponds to $\Delta = 2q/v_0$ and the thin solid curve is to guide the eye. The momentum transfer q is (a) 0.2737 or (b) 0.6087 (a.u.).

In Fig. 1, we compare FBA and CDW-EIS for electron-impact ionization of H(1s) for $E_2 = 5\,\mathrm{eV}$ and for $q \approx 0.27$ a.u. [Fig. 1(a)] and $q \approx 0.61$ a.u. [Fig. 1(b)] (the two cases where absolute measurements are available at 250 eV impact energy). Impact energies range from 250 eV to 64 keV and all cross sections (including the measurements) have been multiplied by v_0/v_1. Thus the solid curve in each part of Fig. 1 is what the FBA predicts for *any* impact energy. On the other hand, the scaled CDW-EIS cross sections, which are in quantitative agreement with the absolute measurements at 250 eV [7], approach the FBA only slowly with increasing impact energy.

In terms of the speed of light $c \approx 137$ (a.u.), the impact speeds v_0 are approximately $c/32$, $c/16$, $c/8$, $c/4$, and $c/2$ for the impact energies of 0.25, 1, 4, 16, and 64 (keV) in Fig. 1. Since relativistic corrections are $O(v_0^2/c^2)$ [13], they should be significant for the two highest speeds (on the order of 25% for $c/2$ and 6% for $c/4$, but only 2% for $c/8$).

Although the FBA results were obtained using the well-known analytical formula, the CDW-EIS results were obtained numerically; hence there is numerical error associated with the CDW-EIS calculations. We can get a good estimate of our numerical uncertainty by calculating the FBA using the same numerical procedure (six-dimensional numerical quadrature) that was used for CDW-EIS. Ordinarily, the FBA would not provide a robust error estimate for CDW-EIS; however, for the high energies considered here, the effects of correlation on the wave functions vary slowly and do not significantly affect the values of the numerical parameters needed to converge the six-dimensional quadrature. Comparing the analytical and fully numerical FBA results (Fig. 1), we find that our numerical error is about 1% (it does not exceed 1.5% at any angle and is less than 1.0% at the peaks).

To further quantify our discussion on the convergence of the FBA, we introduce the quantity

$$\Delta \equiv \frac{|\sigma_{(\text{CDW-EIS})} - \sigma_{(\text{FBA})}|}{\sigma_{(\text{CDW-EIS})}}.$$

Here $\sigma_{(\text{CDW-EIS})}$ is the FDCS for CDW-EIS at the binary-peak maximum and $\sigma_{(\text{FBA})}$ is the same for the FBA (for internal consistency, we use the numerically evaluated FBA to calculate Δ). It can be seen from Fig. 1 that Δ is proportional to q and inversely proportional to v_0 for the higher energies (each time v_0 is doubled for a given q, the difference between CDW-EIS and FBA is halved; while, for a given v_0, the fractional difference for $q \approx 0.6$ a.u. is about twice as large as for $q \approx 0.3$ a.u.). This makes sense because it is known that the FBA becomes valid in the (nonphysical) limit $q \rightarrow 0$ [14] and because the "strength" of the final-state Coulomb interactions neglected in the FBA is determined by the magnitude of their Sommerfeld parameters, i.e.,

$$\frac{1}{|\mathbf{v}_1 - \mathbf{v}_2|} + \frac{1}{|\mathbf{v}_1|} \approx \frac{2}{v_0}$$

for asymmetric collisions.

In Fig. 2, the calculated Δ for the energies considered in Fig. 1 are plotted as solid circles and the straight line corresponds to $\Delta = 2q/v_0$. Clearly,

$$\Delta \approx 2q/v_0 \quad \text{for } v_0 \gg 1 \text{ a.u.}$$

(for the lower energies, Δ diverges from $2q/v_0$ as the FBA further loses validity). As a result, if an accuracy of 1% in the FBA is desired for $q = 0.5$ a.u., an impact speed of 100 a.u. is required. Thus, although the FBA does converge to the correct nonrelativistic result for high enough energy, by the time it converges, relativistic effects are important.

In conclusion, we have explicitly demonstrated convergence of the Bethe-Born theory for the fully differential cross section for electron-impact ionization of atomic hydrogen in coplanar asymmetric geometry. Convergence of the FBA to the correct nonrelativistic result is generally achieved only at speeds where relativistic effects start to become important. Consequently, if a highly accurate representation of experiment is desired, the nonrelativistic FBA will not be valid at any energy. This slow convergence of the FBA is a consequence of neglecting long-range Coulomb interactions in the final state [1–3]. For a given impact speed v_0 and momentum transfer q, the magnitude of the fractional error in the FBA for the height of the binary peak is approximately given by $2q/v_0$ provided $v_0 \gg 1$ a.u.

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