01 Jul 1993

Three-Body Distorted-Wave Born Approximation for Electron-Atom Ionization

Stephenie J. Jones

Don H. Madison
Missouri University of Science and Technology, madison@mst.edu

Achim Franz

P. L. Altick

Recommended Citation

S. J. Jones et al., "Three-Body Distorted-Wave Born Approximation for Electron-Atom Ionization," *Physical Review A - Atomic, Molecular, and Optical Physics*, vol. 48, no. 1, pp. R22-R25, American Physical Society (APS), Jul 1993.
The definitive version is available at https://doi.org/10.1103/PhysRevA.48.R22

RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 48, NUMBER 1 JULY 1993

Three-body distorted-wave Born approximation for electron-atom ionization

S. Jones and D. H. Madison
Laboratory for Atomic and Molecular Research, University of Missouri–Rolla, Rolla, Missouri 65401

A. Franz and P. L. Altick
Physics Department, University of Nevada–Reno, Reno, Nevada 89557
(Received 28 December 1992)

We report a theoretical calculation for electron-impact ionization of atoms that includes short-range electron-atom effects for wave functions that satisfy the exact asymptotic boundary conditions. Results of this theory, which we label as the three-body distorted-wave Born approximation, are compared with experiment and other theories for ionization of hydrogen and helium for incident-electron energies from 4 to 18 times the ionization energy.

PACS number(s): 34.80.Dp

The problem of electron-atom ionization has attracted intense interest in the literature for more than a decade. Several experimental groups have examined this problem, and as a result there is now a large body of measurements available for different geometries and for incident energies ranging from near threshold to several keV. The challenge to theorists has been to develop a theory capable of explaining these observations. For energies greater than about six times the ionization energy, several different approaches are in reasonable agreement with the existing data. Particularly noteworthy are the eikonal-Born series calculations of Byron, Joachain, and Piraux [1], the second-order Coulomb-Born calculations of Srivastava and Sharma [2], the pseudostate close-coupling calculations of Curran and Walters [3], and the work of Brauner, Briggs, and Klar [4], which will be described below. None of these theories, however, is in agreement with the asymmetric coplanar measurements for lower energies.

Brauner, Briggs, and Klar [4] (hereafter to be referred to as BBK) performed the first, we believe, calculation for electron-atom ionization using a final-state wave function that satisfied the asymptotic three-body Schrödinger equation exactly. A major limitation of the BBK work lies in the fact that analytic plane waves were used for the incident electron and analytic Coulomb waves were used for the two final-state electrons. Wave functions of this type cannot properly take into account short-range effects between continuum electrons and the atom, particularly for scattering from atoms heavier than hydrogen. Since the BBK work, there has been considerable interest in developing a theory that includes short-range effects for wave functions that satisfy the exact asymptotic boundary conditions. Here we report such a theory.

Our starting point is the standard distorted-wave Born approximation (DWBA) amplitude for direct scattering [Ref. [5], Eq. (17.54)],

$$f_{\rm DWBA}=\langle \chi_a^-(\mathbf{r}_0)\chi_b^-(\mathbf{r}_1)|V_i-U_i|\psi_i(\mathbf{r}_1)\chi_i^+(\mathbf{r}_0)\rangle \ . \tag{1}$$

In Eq. (1), ψ_i is the initial target wave function, χ_i is the initial-state distorted wave that is generated from the static potential of the atom, U_i, and the interaction between the incident electron and the atom is V_i [taking hydrogen as an example, $V_i=-1/r_0+1/r_{01}$ and $U_i=\langle \psi_i(\mathbf{r}_1)|V_i|\psi_i(\mathbf{r}_1)\rangle$]. The final-state distorted waves χ_a and χ_b are generated in the static field of the ion. For helium, ψ_i is the Hartree-Fock wave function of Froese-Fisher [6], and this wave function is used to calculate the static potentials for both the atom and the ion. The primary strength of the standard DWBA approach lies in the fact that short-range effects between the continuum electrons and the atom or ion are properly taken into account. On the other hand, the primary weakness of the DWBA lies in the fact that final-state electron-electron correlation is contained only to first order. This interaction is just what BBK incorporated into their final-state wave function by adding and extending the form of a phase factor first written down by Redmond (see Ref. [7]). With the addition of this factor (the correlation factor) the BBK wave function becomes an asymptotic solution of the three-body Schrödinger equation. Following the work of Franz and Altick [8], the correlation factor,

$$C(\mathbf{r}_0,\mathbf{r}_1)=\exp[-i\alpha\ln(\kappa\rho+\boldsymbol{\kappa}\cdot\boldsymbol{\rho})] \ , \tag{2}$$

where $\boldsymbol{\kappa}=(\mathbf{k}_a-\mathbf{k}_b)/2$, $\alpha=1/(2\kappa)$, $\boldsymbol{\rho}=\mathbf{r}_0-\mathbf{r}_1$, and $\mathbf{k}_a$ ($\mathbf{k}_b$) is the wave vector for electron a (b), has been decomposed into partial waves so that it can be folded into the standard distorted-wave formalism. The scattering amplitude with the asymptotically exact final state is given by

$$f_{\rm 3DWBA}=\langle \chi_a^-(\mathbf{r}_0)\chi_b^-(\mathbf{r}_1)C(\mathbf{r}_0,\mathbf{r}_1)|V_i-U_i|\psi_i(\mathbf{r}_1)\chi_i^+(\mathbf{r}_0)\rangle \ . \tag{3}$$

The final-state wave function in Eq. (3) is a two-center, three-body wave function, so we call the present approach the three-body distorted-wave Born approximation (3DWBA). Since we consider kinematics with highly unequal final-state energies, exchange between electrons is ignored. Consequently, the triply differential cross section (TDCS) is given by

$$\frac{d^3\sigma}{d\Omega_a d\Omega_b dE_b} = \frac{(2\pi)^4}{E_i} N|f|^2 , \qquad (4)$$

where $N=1$ for hydrogen and $N=2$ for helium. The flux factor in Eq. (4) is for continuum wave functions normalized to a δ function in energy.

To summarize, in the BBK calculation, plane waves were used for the incident electron, Coulomb waves were used for the two final-state electrons, and a Coulomb-wave phase was used for the correlation factor, which asymptotically becomes the same as the present correlation factor, Eq. (2). In the 3DWBA, the incident electron is described by a distorted wave calculated in the field of a neutral atom, while the two final-state wave functions are distorted waves calculated in the field of the final-state ion. The important difference between the BBK and present wave functions lies in the fact that the present wave functions include short-range effects of screening by the atomic electrons while the BBK wave functions do not. For the case of hydrogen, the present final-state wave functions χ_a and χ_b are the same as those used by BBK.

We compare the 3DWBA with other theories, and with experiment, in Figs. 1–3. Extensive absolute measurements have been performed in Kaiserslautern for ionization of hydrogen [9] and helium [10,11] in coplanar asymmetric geometry (92 sets of data are available). Each set is for a given incident energy with the energy and angle of the faster final-state electron fixed, while the slower final-state electron is observed for all accessible angles in the scattering plane. In addition, relative data have been taken for 54.4-eV ionization of hydrogen [12]. We have selected, for presentation in this Rapid Communication, the two sets for each incident energy that correspond to the minimum and maximum momentum transfer ($q=|\mathbf{k}_i-\mathbf{k}_a|$) to the atom. In Figs. 2 and 3, these two cases are shown side-by-side with the smaller q case to the left. We adopt the convention that the angle of observation for the slower final-state electron is measured clockwise from the forward beam direction from 0° to 360°, while the angle of the faster electron is measured counterclockwise. In the angular distribution of the

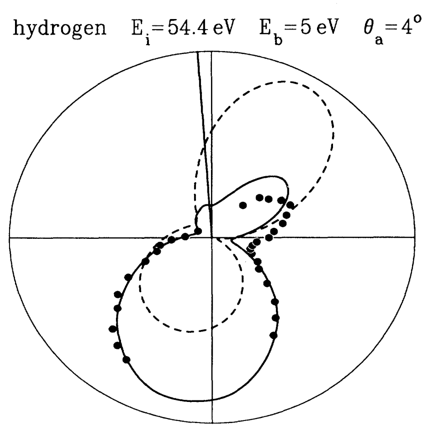

FIG. 1. Effect of the postcollision interaction for 54.4-eV ionization of hydrogen. The incident electron originates from the bottom of the graph along the vertical axis. The faster final-state electron is observed at 4° along the thick line drawn to the left of this axis. The TDCS for each angle of observation for the slower (5 eV) electron is shown in polar form, with the radius of the large circle corresponding to 3.6 a.u. [$a_0^2/(\mathrm{sr}^2\,\mathrm{hartree})$]. The solid circles are relative measurements of Schlemmer *et al.* [12] matched to the 3DWBA at one point. Theories: solid line, 3DWBA; dashed line, DWBA.

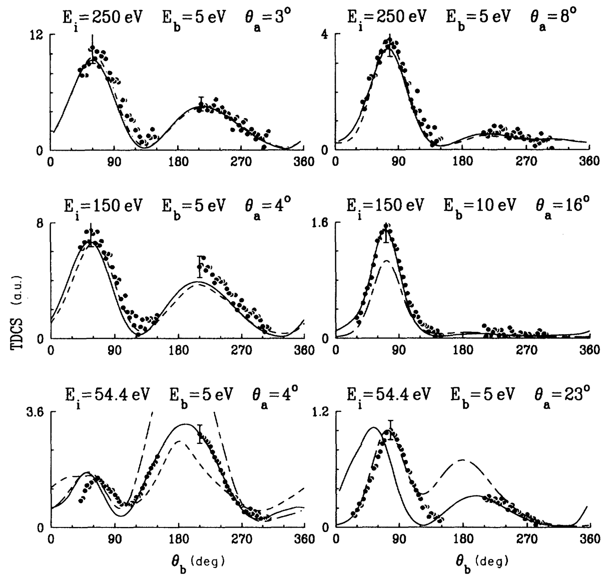

FIG. 2. TDCS for electron-impact ionization of hydrogen. The solid circles are the absolute experimental results of Ehrhardt *et al.* [9], except for 54.4-eV incident energy, where relative data from Schlemmer *et al.* [12] are shown matched to the 3DWBA at one point. Theories: solid line, 3DWBA; dot-dashed line, EBS; long dash–short dash line, BBK; dashed line, PSCC.

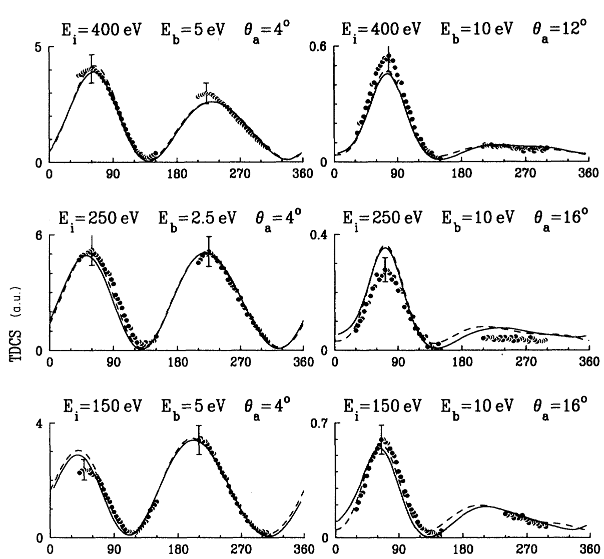

FIG. 3. TDCS for electron-impact ionization of helium. The solid circles are the absolute experimental results of Schlemmer *et al.* [11]. Theories: solid line, 3DWBA; dashed line, CB2.

slower electron two peaks are typically found, the small-angle "binary" peak usually positioned near the direction of the momentum transfer **q**, and the large-angle "recoil peak" approximately positioned at $-\mathbf{q}$.

Before making a detailed comparison with other theories, we first consider the effects of the correlation factor. Correlation between the two out-going electrons will be strongest for small incident energies and small momentum transfer. Thus, in Fig. 1, we compare the 3DWBA and the DWBA for an incident energy (E_i) of 54.4 eV, with the scattering angle of the faster electron (θ_a) fixed at 4°. The energy of the slower electron (E_b) is 5 eV. Recall that the only difference between these two theories is the inclusion of the correlation factor in the 3DWBA. Clearly, electron-electron repulsion in the final state is responsible for the huge "recoil" peak, and the 3DWBA is in significantly better agreement with experiment than the DWBA.

Results for ionization of hydrogen are presented in Fig. 2 for energies between 54 and 250 eV. Here the 3DWBA cross sections are compared with experiment, the BBK results, the eikonal-Born series (EBS) calculations [1], and the pseudostate close-coupling (PSCC) results [3]. For 250 eV (18 times the ionization potential), the 3DWBA, EBS, and PSCC calculations all predict very similar results, which are in good agreement with experiment. The EBS is not shown for the larger momentum transfer, since it would be essentially indistinguishable from the 3DWBA. For 150 eV, the 3DWBA, EBS, and PSCC results remain very similar (PSCC results are displayed for the small-q case) and the 3DWBA is in reasonable accord with experiment for both the large-q and small-q cases. The BBK, on the other hand, significantly underestimates the magnitude of the binary peak for the large-q case. Since short-range effects are not very important for fast electrons, the crucial difference between the 3DWBA and BBK (for this case) lies in the correlation function. These results suggest that just using the asymptotic form, Eq. (2), is preferable to using the form of the correlation factor employed by BBK, especially for larger q and lower energy.

For the much lower energy of 54.4 eV, the 3DWBA continues to be in qualitative agreement with the experimental data. Since these data are not absolute, they have been normalized to the 3DWBA for the small-momentum-transfer case. BBK results are a factor of 2.11 smaller than the 3DWBA at the binary peak for both the small- and large-q cases. As a result, the BBK is multiplied by this factor so that relative shapes can be more readily compared. While the 3DWBA is in good agreement with experiment for both the recoil peak and the ratio of the maximum binary-peak intensity to the maximum recoil-peak intensity for 54.4 eV, the location of the binary peak is shifted by about 20° from experiment. Neither the BBK nor the PSCC predict the qualitative shape of the experimental data at this energy.

In Fig. 3, results for ionization of helium are shown. Here, we have compared our calculations with the second-order Coulomb-Born (CB2) calculation of Srivastava and Sharma [2]. The CB2 calculation differs from the standard second Born theory in that the slower final-state electron is described by a distorted wave instead of a Coulomb wave. An examination of the figure reveals that the CB2 and present results are very similar for energies in this range. Since the electron-electron interaction is treated to all orders of perturbation theory in the present approach, but only to second order in the CB2, the agreement between these two theories indicates that third- and higher-order effects for the electron-electron interaction are small for incident energies greater than 150 eV. It is important to note that even for the relatively low incident energy of 150 eV (six times the ionization potential), both 3DWBA and CB2 are in good agreement with experiment. The fact that the two significantly different theories are in good agreement with each other but not with the absolute value of the experimental data for the large-q case at the relatively high energy of 250 eV is striking and difficult to explain. It should be noted, however, that these cross sections are quite small and thus more difficult to measure.

The present theoretical calculation for electron-atom ionization includes both the short-range effects for the electron-atom interactions and the proper asymptotic three-body final-state wave function. As a result, this work represents an important step forward in establishing a theory for electron-atom ionization that is capable of predicting accurate cross sections over a wide range of kinematics. It was found that the 3DWBA was in good agreement with the experimental data at incident energies of six times the ionization potential and higher. The primary weakness in the present work lies in the fact that the asymptotic form of the final-state electron-electron interaction is used. Consequently, events for which the short-range form of this interaction is important will not be accurately treated (low energy and small angular separations between the two electrons). The 20° shift in the binary peak for 54.4-eV scattering from hydrogen most likely stems from this problem. However, the present work demonstrates that the correlation factor given by Eq. (2) is evidently more appropriate than the one used by BBK since we find good agreement with the absolute experimental data, while the BBK results become significantly smaller than experiment with decreasing energy and increasing momentum transfer. Future work will center on the examination of different correlation factors that more realistically model the short-range electron-electron interaction while asymptotically being identical to the present correlation factor.

This work was sponsored by the National Science Foundation under Grants Nos. PHY-9209420 and 9116199.

[1] F. W. Byron, Jr., C. J. Joachain, and B. Piraux, J. Phys. B **18**, 3203 (1985).
[2] M. K. Srivastava and S. Sharma, Phys. Rev. A **37**, 628 (1988).
[3] E. P. Curran and H. R. J. Walters, J. Phys. B **20**, 337 (1987).
[4] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[5] C. J. Joachain, *Quantum Collision Theory,* 3rd ed. (North-Holland, Amsterdam, 1983), p. 449f.
[6] C. Froese-Fisher, Comput. Phys. Commun. **4**, 107 (1972).
[7] L. Rosenberg, Phys. Rev. D **8**, 1833 (1973).
[8] A. Franz and P. L. Altick, J. Phys. B **25**, 1577 (1992).
[9] H. Ehrhardt, K. Jung, G. Knoth, and P. Schlemmer, Z. Phys. D **1**, 3 (1986).
[10] K. Jung, R. Müller-Fiedler, P. Schlemmer, H. Ehrhardt, and H. Klar, J. Phys. B **18**, 2955 (1985).
[11] P. Schlemmer, M. K. Srivastava, T. Rösel, and H. Ehrhardt, J. Phys. B **24**, 2719 (1991).
[12] P. Schlemmer, T. Rösel, K. Jung, and H. Ehrhardt, J. Phys. B **22**, 2179 (1989).