Differential Cross Sections for Electron Capture in High-Energy Proton-Atom Collisions*

Yehuda B. Band
Argonne National Laboratory, Argonne, Illinois 60439
(Received 11 June 1976)

Various high-energy calculations of proton–multielectron-atom differential capture cross sections are compared with each other (and with the data on p + Ar K-shell capture). The proton-core interaction, including screening from the core electrons, is found to affect significantly the differential cross sections. I speculate that final-state interactions of the hydrogen atom with the target electrons of large atomic targets play a significant role in capture events and are in part responsible for the poor agreement with the Ar data.

In a recent experiment, Cocke *et al.*[1] measured the differential total capture cross section, $d\sigma_{\text{tot}}/d\Omega$, of K-shell Ar electrons by 6-MeV protons. Differential cross-section data of this type for high-energy capture collisions by point projectiles provide a critical test of rearrangement theories. The data in the above experiment were compared with calculations based upon several high-energy approximations and the theoretical results did not agree with the data. These calculations were based upon a first-order perturbation theory (FOPT) which (a) contained the interaction potential between the proton and the active electron but omitted the interaction potential between the proton and the residual Ar core [known as the Oppenheimer-Brinkman-Kramers (OBK) approximation], (b) also included the proton-Ar nucleus interaction (Z_B/R, where Z_B is target nuclear charge) which can couple the initial and final states, and (c) included a proton-core interaction of the form $1/R$ (R^{-1} FOPT), thereby accounting in some fashion for electron screening for large R. The latter calculations[2] have met with some success in determining the integrated capture cross sections. The OBK approximation, when multiplied by factors, obtained empirically[3] or from p + H capture taking into account the proton-core interaction,[4] also seems to reproduce experimental trends for total charge capture cross sections.[5]

The purpose of this paper is to report the results of full FOPT calculations for high-energy capture cross sections from multielectron atoms. Besides the usual questions concerning the criteria for validity of FOPT for charge-capture collisions[2,6] and the effects of nonorthogonality corrections upon FOPT[6] (and higher-order perturbation theory terms), there are two crucial points which must be considered: the full inclusion of the proton-core interaction in FOPT, thus taking into account the screening due to the distribution of the atomic electrons, and the unsolved problem of determining the effect of the remaining electrons of the target atom upon the electron bound to the proton once capture has occurred. The latter effect should serve to ionize the hydrogen atom as a result of its final-state interactions with the outer-shell electrons, thus reducing the charge-capture cross section. For p + Ar K-shell capture there is no reason to suppose that this effect is negligible, but in p + He capture collisions, it may not be important. Given the agreement of the Born calculations and experiment for ionization of inner-shell electrons when the FOPT criteria are satisfied,[7] I attempt to apply FOPT to the capture collisions.

Using the coordinate system introduced in the first paper of Ref. 6, I let A denote the proton and B denote the target core. The full FOPT amplitude for capture (including nonorthogonality corrections) is given by

$$T_{fi} = \frac{\langle f|V_{Ae}+V_{AB}|i\rangle - \langle f|i\rangle\langle i|V_{Ae}+V_{AB}|i\rangle}{1-|\langle f|i\rangle|^2}, \tag{1}$$

where

$$|i\rangle = (2\pi)^{-3/2}\exp(i\vec{k}_i\cdot\vec{R}_A')\varphi_i(\vec{r}_B),$$

$$|f\rangle = (2\pi)^{-3/2}\exp(-i\vec{k}_f\cdot\vec{R}_B')\varphi_f(\vec{r}_A),$$

$V_{Ae} = -r_A^{-1}$, and V_{AB} is the interaction potential between the proton and the remaining core of the target atom given by

$$V_{AB}(R) = \prod_{k=1}^{Z_B-1}\int d^3r_k\,\psi_f^*(\{r_k\})\left(\frac{Z_B}{R} - \sum_{j=1}^{Z_B-1}\frac{1}{|R-r_j|}\right)\psi_i(\{r_k\}). \tag{2}$$

All the terms in (1) except $\langle f|V_{AB}|i\rangle$ are easily evaluated using $\vec{r}_A$ and $\vec{r}_B$ as the independent coordinates in performing the integrations.[6] The proton-core term can be reduced to

$$\langle f|V_{AB}|i\rangle = (2\pi)^{-3}\int d^3k\, \tilde{V}(\vec{k})\tilde{\varphi}_f^*(\vec{C}-\vec{k})\tilde{\varphi}_i(\vec{B}-\vec{k}), \quad (3)$$

where $\tilde{f}$ is the Fourier transform of f, i.e., $\tilde{f}(\vec{p}) = \int e^{i\vec{p}\cdot\vec{r}}f(\vec{r})d^3r$, $\vec{B}$ and $\vec{C}$ are mass-weighted linear combinations of $\vec{k}$ and $\vec{k}_f$, and the method proposed in the second paper of Ref. 6 may be employed to carry through the integration over $\vec{k}$. Using a Slater basis for the electronic wave functions of the target electrons, $V(\vec{k})$ can be analytically evaluated. For p + He capture the analytic expression for $V(\vec{k})$ using the variational wave function for helium[8] is simple to derive. For relatively large atoms, the procedure of calculating V_{AB} from accurate wave functions and then taking the Fourier transform of V_{AB} becomes tedious. For the level of accuracy warranted in FOPT, we may use a Thomas-Fermi or Thomas-Fermi-Dirac potential[9]

$$V_{AB}(R) = R^{-1}[Z_B - (Z_B - 1)\varphi(x)], \quad (4)$$

where $\varphi(x)$ is the Thomas screening function and $x = 2Z_B^{1/3}R/(3\pi/4)^{2/3} = R/\mu$. A good fit to φ is obtained by taking a linear combination of three exponentials

$$\varphi(x) = \sum_{j=1}^{3} c_j \exp(-a_j x),$$

where the values of c_j and a_j are obtained by a least-squares analysis,[9] and we obtain

$$V(k) = 4\pi\left((Z_B - 1)\sum_{j=1}^{3}\frac{c_j}{k^2 + (a_j/\mu)^2} + \frac{1}{k^2}\right). \quad (5)$$

Halpern and Law[10] have recently performed a rough calculation of the screening where they have approximated the first term in $V(k)$ by a constant times $\delta^3(k)$. Further details regarding the method of calculation may be obtained from Ref. 6.

Calculated differential capture cross sections are presented in Figs. 1 and 2 for p + He and p + Ar collisions for incident proton energies E_p = 300 keV and E_p = 6 MeV, respectively. The differential capture cross section for $p + \mathrm{He} \to \mathrm{H}(nlm) + \mathrm{He}^+(1s)$, summed over the $1s$, $2s$, $2p$, $3s$, and $3p$ states of hydrogen is plotted in Fig. 1. The cross section for capture into higher excited states is small. Figure 1 shows that for the larger scattering angles, the full FOPT cross sections are substantially greater than the R^{-1}-FOPT or the OBK results. For scattering at larger an-

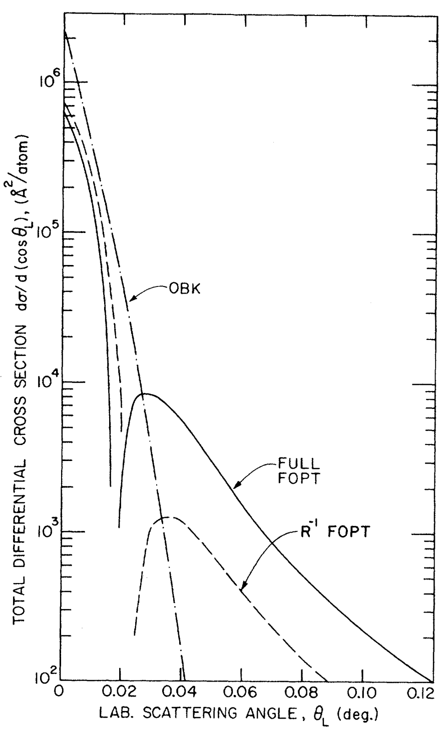

FIG. 1. Calculated differential capture cross sections $p + \mathrm{He} \to \sum_{nlm}\mathrm{H}(nlm) + \mathrm{He}^+(1s)$ for 300-keV incident protons. The solid curve is the full FOPT, the dashed curve is R^{-1} FOPT, and the dash-dotted curve is the OBK approximation.

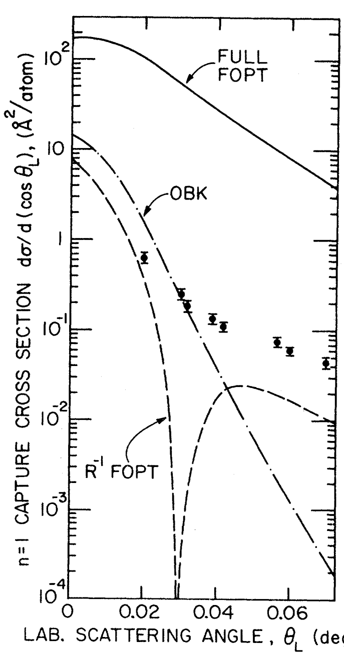

FIG. 2. Calculated differential cross sections for K-shell vacancy in $p + \mathrm{Ar} \to \mathrm{H}(1s) + \mathrm{Ar}^+$ with 6-MeV incident protons. The data are those of C. L. Cocke *et al.*

gles (smaller impact parameters) the full FOPT core interaction is considerably larger than R^{-1}, thus accounting for the order-of-magnitude larger cross section. For smaller scattering angles there is a cancellation between contributions from the attractive V_{Ae} potential and those from the repulsive V_{AB} potential. This cancellation is responsible for the dark angle in the full and R^{-1}-FOPT calculations of capture to s states. This cancellation significantly reduces the size of the integrated cross section from the OBK result and helps to satisfy the FOPT critieria better.[6] Capture cross sections for higher angular momentum states do not have a dark angle as a consequence of the filling of the dark angle for a given magnetic substate cross section, $d\sigma_{nlm}/d\Omega$, by the cross sections for other magnetic substates, but the excited states do not completely fill in the dark angle. Capture into $H(nlm) + He^{+}(n'l'm)$ may fill in the dark angle further.[4] The use of a six-parameter Hylleras He wave function[4] may further modify the angular distribution and fill in the dark angle. Experiments to measure this differential cross section are under way[11] and will provide a test of high-energy rearrangement theories.

Figure 2 shows that for $p + Ar$ collisions the full FOPT curve for ground-state capture has the same shape as the experimental data but is too large by two orders of magnitude. Note the absence of a dark angle. Capture into excited states does not significantly change the shape of the curve. There is no indication of a dark angle in the data, and the slope of the data points is considerably different from the OBK result. Comparing the full FOPT results to the other calculations indicates that a large part of the charge-capture amplitude results from capture within the Ar atom radius, and that it is therefore important to include the correct screening of the proton Ar-nucleus potential by the Ar electrons. The strong cancellation which gives rise to the dark angle in $p + He$ is no longer present in FOPT. The nonorthogonality terms in the full FOPT are small at this energy. Given the poor agreement with theory, one might *speculate* that the final-state interaction of the H atom with the outer electrons is responsible for the strong depletion of flux from the charge-capture channel. This flux would be redistributed in some fashion into the ionization channel for K-shell vacancy producing processes. In the forward peak where the full FOPT angular distribution is large, the depletion would be weakly dependent upon scattering angle, so that the shape of the cross section would remain unaltered. It is observed that the cross section for K-shell vacancy production is larger by several orders of magnitude than the K-shell capture cross section and therefore there is no inconsistency in speculating that the large capture cross section is converted into ionization by the final-state interactions, accounting for part (approximately $\frac{1}{5}$) of the flux into the large K-shell ionization channel.

It is my pleasure to thank Dr. M. Inokuti for helpful discussions.

*Work performed under the auspices of the U. S. Energy Research and Development Administration.

[1]C. L. Cocke, J. R. Macdonald, B. Curnutte, S. L. Varghese, and R. Randall, Phys. Rev. Lett. 36, 782 (1976).

[2]K. Omidvar, J. E. Golden, J. H. McGuire, and L. Weaver, Phys. Rev. A 13, 500 (1976).

[3]V. S. Nikolaev, Zh. Eksp. Teor. Fiz. 51, 1263 (1966) [Sov. Phys. JETP 24, 847 (1967)].

[4]R. A. Mapleton, *Theory of Charge Exchange* (Wiley, New York, 1972).

[5]J. R. Macdonald, C. L. Cocke, and W. W. Eidson, Phys. Rev. Lett. 32, 648 (1974).

[6]Y. B. Band, Phys. Rev. A 8, 243, 2857, 2866 (1973), and J. Phys. B 7, 2055 (1973), and Can. J. Phys. 53, 465 (1973).

[7]J. D. Garcia, R. J. Fortner, and T. M. Kavanaugh, Rev. Mod. Phys. 45, 111 (1973).

[8]H. A. Bethe and R. W. Jackiw, *Intermediate Quantum Mechanics* (Benjamin, New York, 1968), p. 83.

[9]R. A. Bonham and T. G. Strand, J. Chem. Phys. 39, 2200 (1963); S. C. Mukherjee, Indian J. Phys. 35, 165 (1961).

[10]A. M. Halpern and J. Law, Phys. Rev. A 12, 1776 (1975).

[11]C. L. Cocke and J. R. Macdonald, private communication.