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Comments

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Universal cross sections for *K*-shell ionization by low-velocity protons: Importance of relativistic and energy-loss effects

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Recent data reported by Zander and Andrews for *K*-shell ionization of $_{22}$Ti, $_{26}$Fe, $_{28}$Ni, and $_{30}$Zn by 60–150-keV protons are reanalyzed in terms of the ECPSSR theory of Brandt and Lapicki. The ECPSSR approach takes into account the energy-loss effect (E) as well as the Coulomb deflection (C), perturbed-stationary state (PSS), and relativistic (R) effects. Agreement between theory and experiment is improved, and the remaining discrepancies are partially attributed to inaccuracies of the wave functions utilized in the calculation of inner-shell ionization cross sections.

When $Z_1 \ll Z_2$, inner-shell ionization of a target atom of atomic number Z_2 by a projectile of atomic number Z_1 occurs predominately via removal of an inner-shell electron to the target atom continuum (direct ionization). Electron capture then contributes insignificantly to the ionization, and thus the predictions of perturbative-in-Z_1/Z_2 theories of direct ionization can be tested through comparison with measured ionization cross sections. We present such a comparison with the recently reported data[1] for *K*-shell ionization of the $Z_2 = 22$, 26, 28, and 30 elements by 60-150-keV protons ($Z_1 = 1$). These ionization cross sections were inferred from x-ray production measurements using Krause's fluorescence yields.[2]

Since 100-keV protons have velocities v_1 which are smaller than the *K*-shell electron orbital velocities, v_{2K}, in the target atoms considered, they are referred to as low-velocity protons. The variable $\xi_K = v_1/\frac{1}{2}v_{2K}\theta_K$, which characterizes the collision (θ_K is the ratio of the observed binding energy to its screened hydrogenic value $\frac{1}{2}v_{2K}^2$ with $v_{2K} = Z_{2K}$ and $Z_{2K} = Z_2 - 0.3$), is less than 1. In fact, at these low velocities, $\xi_K < 0.3$, so that in the standard plane-wave Born approximation (PWBA),

$$\sigma_K^{\mathrm{PWBA}}(\xi_K, \theta_K) = (\sigma_{0K}/\theta_K)F_K(\xi_K, \theta_K)\,, \tag{1}$$

with $\sigma_{0K} \equiv 8\pi Z_1^2/Z_{2K}^4$ in atomic units, the dimensionless function F_K starts to depend *solely* on ξ_K as[3]

$$F_K(\xi_K, \theta_K) = (2^9/45)\xi_K^8/(1 + 1.72\xi_K^2)^4\,. \tag{2}$$

The PWBA cross sections scaled by σ_{0K}/θ_K are given by Eq. (2) and, as such, they become a universal function of a single variable for all collision systems.

The curve in Fig. 1 represents Eq. (2) and is compared with σ_K^{EXPT} of Ref. 1 divided by σ_{0K}/θ_K of Eq. (1). Clearly, and as has been noted often in the literature before, these PWBA cross sections *overestimate* the experimental values by as much as two orders of magnitude in the low-velocity regime. This perturbative approach is strictly valid when $Z_1/Z_2 \to 0$.

Over the years, the New York University group of Brandt and his co-workers has developed a theory that proved to be in much better agreement with experiment than the PWBA.[3-8] This theory evolved as it successively included the effects that were inherently not accounted for in the standard PWBA. Originally, only the Coulomb deflection (C) and binding effects were incorporated into the theory.[3,4] The binding and polarization effects were then introduced in a perturbed-stationary state (PSS) approach[5] so that the theory was referred to as the CPSS theory.[6] The CPSS cross sections were cast in terms of Eq. (1) as

$$\sigma_K^{\mathrm{CPSS}} = 9E_{10}(\pi\, dq_{0K}\zeta_K)\sigma_K^{\mathrm{PWBA}}(\xi_K/\zeta_K, \zeta_K\theta_K)\,, \tag{3}$$

where the $9E_{10}$ and ζ_K factors accounted for the Coulomb deflection (C) and PSS effects, respectively. As shown by the open symbols in Fig. 2, the data divided by $\sigma_{0K}9E_{10}(\pi\, dq_{0K}\zeta_K)/\zeta_K\theta_K$ and plotted versus ξ_K/ζ_K are indeed in much better agreement with the universal function F_K than in Fig. 1. Yet the CPSS cross sections still overestimate σ_K^{EXPT} in the low-velocity regime by as much as a factor of 4.

This disagreement becomes even more drastic when a relativistic description of the K-shell electron is made; the cross sections based on relativistic wave functions are larger than the nonrelativistic cross sections of Eqs. (1) and (3). In the CPSSR theory,[7] the relativistic effect is incorporated through an appropriate increase of ξ_K to ξ_K^R. Thus in the CPSSR approach, the open symbols are shifted horizontally to the right in Fig. 2 and are drawn as the crossed symbols which are even further away from the universal curve F_K vs ξ_K^R/ζ_K.

In the most recent development, the CPSSR theory has been modified to account for the energy-loss effect (E).[8] This effect was incorporated *both* in the PWBA cross sections, in terms of which $\sigma_K^{\mathrm{CPSSR}}$ are cast, and in the argument of the Coulomb-deflection factor. In the standard PWBA, cross sections are evaluated with approximate values of the minimum and maximum momentum transfers; they are obtained under the assumption that Δ_K defined as the energy loss divided by the kinetic energy of the projectile in the center-of-mass system, is negligible. The EPWBA cross sections evaluated with the exact limits for the momentum transfer are smaller than the standard PWBA cross sections. An analytical function $f_K(z)=\sigma_K^{\mathrm{EPWBA}}/\sigma_K^{\mathrm{PWBA}}<1$, with $z\equiv(1-\Delta_K)^{1/2}$, was derived in Ref. 8. Also in this reference, the energy-loss effect was incorporated into the Coulomb-deflection factor; the argument of the $9E_{10}$ factor, $\pi d q_{0K}$, was simply increased to $\pi d q_{0K} 2/z \times (1+z)$. This led to a further decrease of the ionization cross sections due to the finite energy-loss effect via smaller values of the $9E_{10}$ function. Finally then, the K-shell ionization cross section in the ECPSSR theory, with $z_K\equiv(1-\zeta_K\Delta_K)^{1/2}$, can be written as[8]

$$\sigma_K^{\mathrm{ECPSSR}}=9E_{10}[\pi\, d q_{0K}\,\zeta_K 2/z_K(1+z_K)]\; f_K(z_K)\sigma_K^{\mathrm{PWBA}}(\xi_K^R/\zeta_K,\zeta_K\theta_K)\,. \tag{4}$$

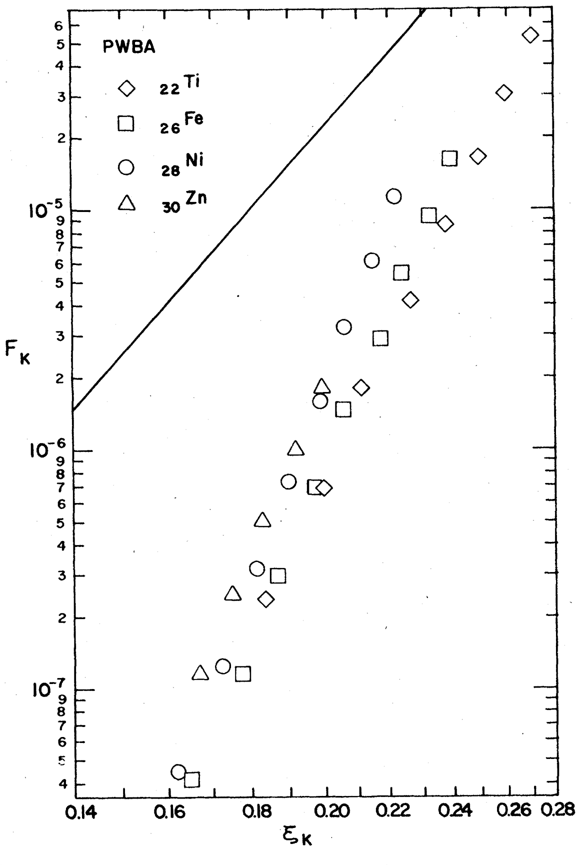

FIG. 1. Comparison of experimental and theoretical values for the universal function F_K of Eq. (2) according to the plane-wave Born approximation.

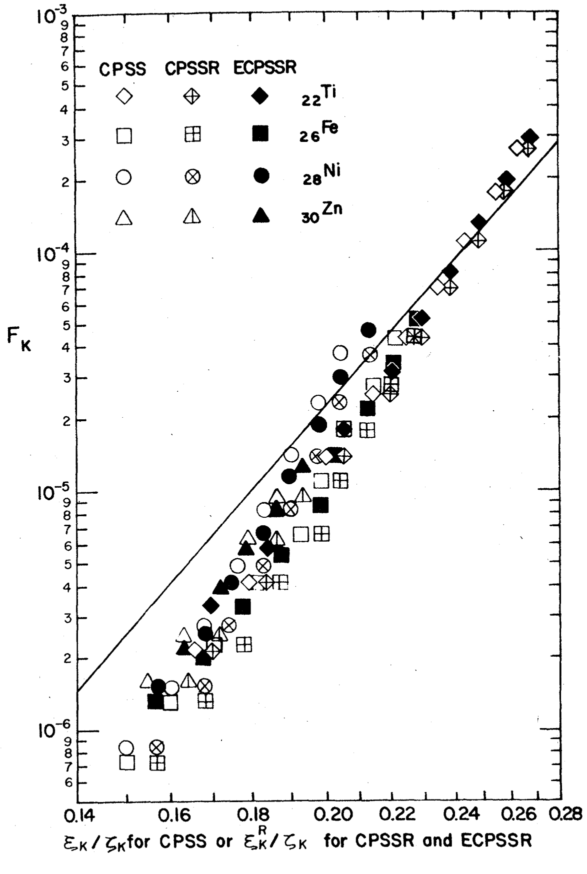

FIG. 2. Comparison of experimental and theoretical values for the universal function F_K of Eq. (2) according to the CPSS, CPSSR, and ECPSSR of Refs. 6, 7, and 8, respectively.

As a result of the energy-loss effect, the crossed symbols are shifted upward by a factor of $9E_{10}(\pi\, dq_{0K}\,\zeta_K)/\{9E_{10}[\pi\, dq_{0K}\,\zeta_K 2/z_K(1+z_K)]f_K(z_K)\}$ in Fig. 2, and they are drawn as the closed symbols closer to the universal curve F_K than the points obtained in the CPSSR theory.

Judging from the agreement between the experiment and the theory, Fig. 2 demonstrates that the theory developed at New York University[3-8] is not only superior to the PWBA, but also apparently converges to a best formulation as one considers subsequent steps in its evolution. The agreement of the CPSS approach with data is somewhat accidental; for the collision systems under consideration, the increase of the ionization cross sections due to the relativistic effect is to a large extent offset by their decrease due to the energy-loss effect. The remaining disagreement between the ECPSSR theory and the analyzed data, which is as much as a factor of 2, could be viewed as the sole result of an as yet unaccounted effect in the theory.

We would like to caution the reader, however, about the hazards of such a hasty conclusion. X-ray production cross sections, reported by various authors for *identical* collision systems, often differ from each other by as much as a factor of 2; disagreement of this magnitude between theoretical predictions and a single data set may likely result from erroneous measurements. A meaningful assessment of a theory on this level of resolution can only be made through comparison with a sufficiently large data base. Such a comparison is made by Brandt and Lapicki.[8] Based on some 2300 measured ionization cross sections, which were inferred from K-shell x-ray production cross sections by protons ($Z_1 = 1$) in targets covering the range $10 \leqslant Z_2 \leqslant 92$ and which included the data presently analyzed, they concluded that the ECPSSR theory agrees on the average with experiment to within ±10%. This remaining discrepancy was statistically significant and attributed to the quality of wave functions employed in calculations of inner-shell ionization cross sections.

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[1] A. R. Zander and M. C. Andrews III, Phys. Rev. A 20, 1484 (1979).

[2] M. O. Krause, J. Phys. Chem. Ref. Data 8, 307 (1979).

[3] W. Brandt and G. Lapicki, Phys. Rev. A 10, 474 (1974).

[4] W. Brandt, R. Laubert, and I. Sellin, Phys. Lett. 21, 518 (1966); Phys. Rev. 151, 56 (1966); G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973).

[5] G. Basbas, W. Brandt, and R. H. Ritchie, Phys. Rev. A 7, 1971 (1973).

[6] G. Lapicki, Ph.D. thesis, New York University, New York, 1975 (unpublished); G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 17, 1655 (1978).

[7] W. Brandt and G. Lapicki, Phys. Rev. A 20, 465 (1979).

[8] W. Brandt and G. Lapicki, Phys. Rev. A 23, 1717 (1981).