Ionization of K-shell electrons by highly relativistic protons

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(Received 17 August 1987)

A comparative study of three recent theoretical formalisms by Anholt, Scofield, Becker, and coworkers for K-shell ionization by highly relativistic protons has been carried out. The importance of the spin-flip mechanism is emphasized. It is concluded that in the analysis of such inner-shell ionization processes, an accurate description of the projectile-target interaction is of much more significance than the accuracy of the wave functions of the atomic electrons.

Ever since the availability of high-energy heavy-ion sources, considerable theoretical and experimental effort has been made to study the relativistic effect in the ionization process of medium-heavy and heavy atoms by such projectiles.[1] In particular, an important experiment was carried out by Anholt *et al.*[2] on the K-vacancy production by protons of 4.88 GeV obtained from the Lawrence Berkeley Laboratory bevatron. Their analysis showed that, in addition to the ordinary Coulomb interaction between the projectile proton and the K electron, the transverse and the spin-flip effects contribute significantly in such a process.[2,3] Nevertheless, in these theoretical analyses, the K electron has been treated only semirelativistically by using Darwin wave functions for their description. One is therefore tempted to improve the comparison between theory and experiment by introducing a fully relativistic description of the inner-shell electrons. In an earlier analysis using only the Coulomb (longitudinal photon) interaction, Anholt had pointed out that the results show a very minor difference when Dirac-Hartree-Fock (DHF) or Dirac-hydrogenic- (DH-) type wave functions are used to describe the K electron.[4] However, one should expect appreciable improvement with these relativistic wave functions over Schrödinger- or Darwin-type wave functions for heavy target elements. In this paper, we shall present a comparative study of Anholt's calculation with the calculations using DHF-type wave functions in the plane-wave Born approximation (PWBA) and the DH-type wave function in the semiclassical approximation (SCA) formalism and shall conclude that an accurate description of the projectile-target interaction is far more important than improving the accuracy of the wave functions being used.

In order to make the discussion self-contained, let us briefly review Anholt's[3] formalism. By employing the PWBA and including the direct Coulomb interaction (longitudinal photons), the retardation effect (transverse photons), the spin-flip effect caused by the change of the spin of the atomic electron while being ionized, and describing the K electron using semirelativistic Darwin functions, Anholt obtained the total ionization cross section in the form

$$\sigma_K=\frac{8\pi Z_1^2}{\eta_K Z^4}\sum_{W_{\min}}^{\infty} d^2dW\sum_{Q_{\min}}^{\infty}\frac{dQ}{Q^2}\left[F_K+\frac{(\beta Z\alpha)^2(1-Q_{\min}/Q)}{(1-\beta^2Q_{\min}/Q)^2}(G_K+\tfrac{1}{4}QF_K)\right], \quad (1)$$

where

$$d^2=[1+(Z\alpha/2)^2]^{-1}[1+(W-1)(Z\alpha/2)^2]^{-1},$$

$$Q_{\min}=W^2/4\eta_K,$$

$$W_{\min}=\theta_K=2U_K/Z^2,$$

$$\eta_K=v^2/Z^2,$$

$$Z=Z_2-0.3,$$

and U_K is the K-electron binding energy, v is the projectile velocity, Z_1 is the projectile charge, Z is the target charge, F_K and G_K are essentially the nonrelativistic matrix elements using hydrogenic Schrödinger wave functions and can be expressed as

$$F_K=(3Q+W)QA_3,$$

$$G_K=\tfrac{1}{4}WA_2,$$

with

$$A_n=\frac{2^7\exp\{-2/k\tan^{-1}[2k/(Q+1-k^2)]\}}{3[1-\exp(-2\pi/k)][(Q-k^2+1)^2+4k^2]^n},$$

and

$$k=(W-1)^{1/2}.$$

While comparing with the data from the 4.88-GeV proton experiment, Anholt has very clearly shown the importance of the transverse and spin-flip effects. In particular, it is to be noted that while the transverse effect is important for highly relativistic incident protons for all target elements, the spin-flip effect is particularly significant for heavy target atoms. Of course, an improvement in Anholt's work can be made by replacing the Darwin wave functions by DHR- or DH-type wave functions to make the analysis fully relativistic.

In order to obtain results using DHF-type wave functions in the PWBA approach, one can use Scofield's theory,[5] who had formulated the K-shell ionization problem in a fully relativistic approach for incident *electrons* without including the exchange effects. Since at such high energies the exchange effect between the incident and the target electrons can be neglected,[6] Scofield's formalism can be applied as well to the case of incident *protons*. Expressing in terms of four-currents, the differential cross section in Scofield's formalism can be expressed as

$$\frac{d\sigma_k}{d\Omega}=\left[\frac{2e^2p'}{pq^4}\right]\sum_{\mu,\nu}\left[p_\mu p'_\nu+p'_\mu p_\nu+\frac{g_{\mu\nu}q^2}{2}\right]J^\mu J^{\nu *}\;, \tag{2}$$

where p and p' are the four-momenta of the incident and outgoing proton and q is the four-momentum transferred to the K electron, respectively. The large parentheses inside the summation sign signifies the *unpolarized* incident proton current and

$$J^\mu = e\langle \psi_b e^{i\mathbf{q}\cdot\mathbf{r}}\gamma^\mu \psi_a\rangle$$

signifies the transition current of the atomic electron. By using the vector multipole-expansion technique, Scofield had worked out all the matrix elements in terms of the 3-j and 6-j symbols and the radial integrals of the DHF-type wave functions. It should be pointed out that since Eq. (2) uses unpolarized proton current, Scofield's formalism does not incorporate the spin-flip interaction.

In Fig. 1 we have reproduced Anholt's data and his calculations with (solid line) and without (dashed line) the spin-flip effect, and have compared them with our numerical results obtained from Scofield's theory (dotted-dashed line). It is interesting to see that Scofield's results lie very close to Anholt's calculation when the spin-flip effect is not incorporated. Since Anholt's calculation, including the spin-flip effect, agrees better with the data, in spite of employing less accurate wave functions, we conclude that the accuracy in incorporating the relevant interaction is much more important than using more accurate atomic wave functions.

To further substantiate our observation, we plot in Fig. 2 Scofield's results (dotted-dashed line) for U as the target element for very high incident energies. We find that once again, Scofield's results are closer to those of Anholt without the spin-flip contribution. The difference between Anholt's calculation without the spin-flip effect and that of Scofield may be attributed to differences in the wave functions being used.

Quite recently, Becker and co-workers[7,8] in Germany have also tried to improve the comparison between Anholt's theory and experiment by replacing the Darwin wave functions with Coulomb-Dirac wave functions. They formulated the problem in the semiclassical approximation[7] and found that their numerical results lie about 10% below those of Anholt and hence further away from

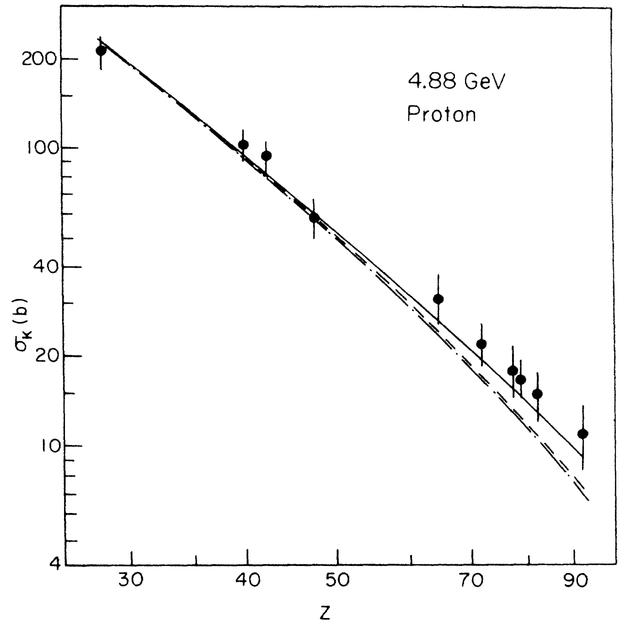

FIG. 1. K-shell ionization cross sections vs Z for 4.88-GeV protons. The solid and dashed lines show Anholt's results with and without the spin-flip term, respectively. The results of Scofield are shown by the dotted-dashed line.

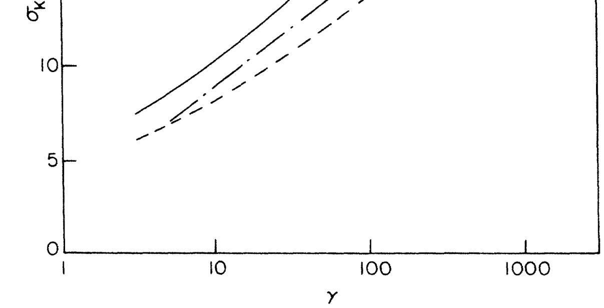

FIG. 2. K-shell ionization cross sections as a function of $\gamma=(1-v^2/c^2)^{-1/2}$. The solid and dashed curves show Anholt's results with and without the spin-flip term, respectively. The results of Scofield are shown by the dotted-dashed line.

the data. Becker, Grun, and Scheid[8] claimed that this 10% difference is in good agreement with estimate made by Anholt *et al.*[9] as the effect of the different wave functions. Nevertheless, we believe that the 10% effect discussed by Anholt *et al.* is completely unrelated to that noted in the work of Becker *et al.*, for Anholt *et al.* were referring to the comparison of results using different wave functions within the *same* PWBA quantum-mechanical formulation of the process, while the 10% discrepancy in the calculation of Becker *et al.* arises from the SCA formulation of the problem in which the "straight-line trajectories" have been assumed and hence the spin-flip effects are completely ignored as stated in their paper. Furthermore, the transverse-photon effect in the quantum-mechanical PWBA treatment is not completely equivalent to the Lienard-Wichert potential treatment in the SCA.[7,8] This explains to a certain extent why the results of Becker *et al.* deviate further from the experimental data though they use more accurate atomic wave functions. As a matter of fact, for heavier incident ions for which their approximation is more valid, their results lie closer to the data as can be seen from Fig. 1 of their paper for incident Ne ions.[8] As far as the SCA is concerned, it is accurate in low-energy regions where only the Coulomb interaction is important.[10]

From the above comparative study, we therefore conclude that in the analysis of such inner-shell ionization processes, an accurate description of the projectile-target interaction is of much more significance than the accuracy of the wave function of the atomic electron.

This work was partially supported by the National Aeronautics and Space Administration under Grant No. NAG 1577.

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[1]For a recent review, see, e.g., R. Anholt and H. Gould in *Advances in Atomic and Molecular Physics,* edited by D. Bates and B. Bederson (Academic, Orlando, 1986), Vol. 22.

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