Projectile Atomic-Number Dependence for K-Shell Hole Production*

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An accurate numerical calculation of the projectile atomic-number dependence for K-shell hole production by Coulomb excitation has been carried out through the two leading terms in the plane-wave Born series. The calculation is restricted to velocities where the projectile is slower than the target K-shell electron, but fast enough that Coulomb deflection of the projectile is negligible. Agreement is found with experiments.

In this Letter we report on an accurate numerical calculation which shows that the dependence of K-shell hole-production cross sections on projectile atomic number, Z_p, at low velocity as experimentally determined is well reproduced by a simple independent-particle model for the atom. The importance of this result is that once the Z_p dependence of the cross section is established, the ratio of the absolute cross section to the Born cross section is known. This offers the intriguing possibility of a two-step calculation which for the first time would allow accurate absolute ionization cross-section calculations for many-electron atoms. Firstly all the sophistication of a configuration-interaction calculation[1] would be used to get the Born cross section, and then the ratio calculation used to give the absolute cross section.

In the past few years a series of experiments[2-4] on K-shell hole production with projectiles of different atomic number but moving at the same velocity, v, have provided a severe test for approximation methods.[5-7] The plane-wave Born series develops the cross section as a series in Z_p:

$$\sigma(Z_p) = \alpha Z_p^2[1 + Z_p \rho + O(Z_p^2)]. \quad (1)$$

The αZ_p^2 term is the usual first Born term, and the Z_p^3 term arises from interference between the first and second Born terms in the amplitude. The first Born, the Glauber, and the Cheshire (distorted wave) approximations fail to fit the data.[7] In a recent paper[8] it has been shown how to improve these standard treatments so that now theory and experiment do agree, but the method will not work unless the velocity of the projectile is greater than the velocity of the target electron. The calculation described here is accurate in the lower velocity region. In principle we can raise the energy of applicability of the method so we can join onto the high-velocity regime, though we have not yet done so.

If we wish to treat the K-shell vacancy production beyond the first Born approximation it is essential to understand the role the other electrons play in refilling the K-shell hole or providing holes in the Fermi sea for K-shell electron deposition.

It has been shown[9] that in the approximation of an independent-particle model description of the atom to get the total K-shell hole-production cross section excluding charge transfer, one simply calculates twice the cross section for a single electron to be lifted above the Fermi sea as if there were no other atomic electrons in interaction with the projectile. We then have to find the wave function ψ of a single-electron atom being perturbed by a time-dependent interaction,[7] where

$$i\hbar(\partial/\partial t)\psi = [H_e + V]\psi, \quad (2)$$

$$H_e = -\frac{\hbar^2}{2m_e}\nabla_r^2 - \frac{Z_n e^2}{r} + V_s(r) + I_K, \quad (3)$$

$$V = Z_p e^2/R - Z_p e^2/|\vec{\mathrm{R}} - \vec{\mathrm{r}}|, \quad (4)$$

and

$$\vec{\mathrm{R}} = (\vec{\mathrm{B}}, Z) = (\vec{\mathrm{B}}, vt).$$

Here $\vec{\mathrm{B}}$ is the impact parameter of the projectile moving with constant velocity, v, along the z axis past an atom, atomic number Z_n. The nucleus of the atom is assumed to remain at rest at the origin of coordinates. Initially, at $Z = -\infty$, $\psi = \chi_0(r)$. Here $\chi_0(r)$ is the K-shell ground target wave function and I_K is the K-shell ionization energy. $V_s(r)$ is the so-called screening potential, which accounts for the difference between the effective potential seen by the electron and the hydrogenic potential $-Z_n e^2/r$. The repulsive term $Z_p e^2/R$ is included for numerical convenience. As we are treating the projectile as following a constant-velocity classical path this term cannot affect the cross section calculated.[7]

If one is prepared to neglect $V_s(r)$ (as we shall

here) then this is a hydrogenic problem and it would seem reasonable that one could apply all the work done on proton-hydrogen codes to analyze the data. While this is undoubtedly true, proton-hydrogen codes[10,11] are very sophisticated, and time-consuming to run. We therefore sought a simpler procedure to take as much advantage as possible of the fact that, unlike the proton-hydrogen problem, here Z_p is much less than Z_n.

(1) We ignored all processes involving charge transfer[12] of the electron to the projectile. This is justified if the projectile charge is much less than that of the atom. It is incorrect for proton-hydrogen.

(2) We diagonalized the target Hamiltonian H_e in a truncated basis set, $u_j^l(r)$, giving a set of states χ_λ as a linear combination of the u's with eigenvalues W_λ. This allows specific representation of the rapidly oscillating part of the time dependence of the interaction potential[13] V_I, defined by

$$\langle\lambda|V_I|\lambda'\rangle = \exp(iH_eZ/\hbar v)\langle\lambda|V|\lambda'\rangle\exp(-iH_eZ/\hbar v) = \exp[i(W_\lambda - W_{\lambda'})Z/\hbar v]\langle\lambda|V|\lambda'\rangle. \quad (5)$$

(3) We calculated only the first two terms in the Born series for the K-shell hole production cross section.[14]

With these restrictions one has to evaluate

$$\sigma_K = 4\pi(Z_pe^2/\hbar v)^2\int_0^\infty B\,dB\sum_\lambda\left|\int_{-\infty}^{\infty}\langle\lambda|V_I|0\rangle dZ\right|^2$$
$$-4\pi i(Z_pe^2/\hbar v)^3\int_0^\infty B\,dB\sum_{\lambda,\lambda'}\{[\int_{-\infty}^{\infty}\langle\lambda|V_I|\lambda'\rangle^* dZ\int_{-\infty}^{Z}\langle\lambda'|V_I|0\rangle^* dZ'][\int_{-\infty}^{\infty}\langle\lambda|V_I|0\rangle dZ] - \text{c.c.}\}. \quad (6)$$

Here the sum on λ' is taken over all states in our basis but λ runs over unoccupied states only. The basis set used contained functions with radial part of the form[11]

$$u_j^l = r^l\exp\{-c_lr/a_n[1-\epsilon\exp(i\varphi_j)]\}. \quad (7)$$

Here a_n is the Bohr radius for a hydrogenic atom of nuclear charge Z_n. The φ_j are taken equally spaced between 0 and 2π, and c_l is a constant depending on the orbital angular momentum. For s states c_0 was 1 and for p states we tried c_l as 1.5. We took ϵ ranging from 0.5 to 0.9. It was ensured that at least the hydrogenic ground state and the occupied excited states were well represented.

The above basis, which is complete, has been studied extensively for the proton-hydrogen problem.[11] It allows a tremendous simplification in the calculation of the matrix elements of the potential as opposed to a Slater-type basis because each matrix element has exactly the same form for different λ's. In addition, the neglect of charge exchange has the important consequence that the matrix elements of the potential are independent of the energy of the projectile. Further they depend only on the variable R (as opposed to R and B), apart from quickly calculable terms like Z/R. This means we can calculate the matrix elements of our potential once and for all and store them in a one-variable array in the computer without taking too much space. Of course, this is only true if a small number of mesh points are needed to obtain convergence of the integrals. In this regard a special numerical problem is posed by the oscillatory integrands; the oscillations become more severe as $Z_ne^2/\hbar v$ becomes large. To handle this problem the integrals were divided up into a sum of integrals over subintervals. Then to evaluate the resulting subinterval integrals, which are of the form

$$\int_{t_n}^{t_{n+2}}\exp(i\lambda t)f(t)\,dt,$$

we approximated $f(t)$ on the subinterval by a parabola and then did the resulting integral exactly.[15] Care was taken to handle properly the long-range parts of the potential matrix elements. For these calculations convergence was obtained with an integration mesh of thirty to sixty points. Without this device 400 points are typically needed, rendering the storage problem impossible. On an IBM 360/65 it takes approximately 3 to 4 min to evaluate the potentials and then approximately 1 to 2 min to calculate ρ at each velocity. This is two orders of magnitude faster than normal proton-hydrogen codes.[10]

In the present calculation only s and p states were included. This restricts the maximum projectile velocity at which our calculations apply. The approximate velocity at which d and higher angular momentum states can be neglected was estimated by using methods similar to those of Merzbacher and Lewis[16] and of Khandelwal[17] to calculate the contribution to the first Born cross section from s, p, and all angular momentum final states. In our calculations we kept nine s

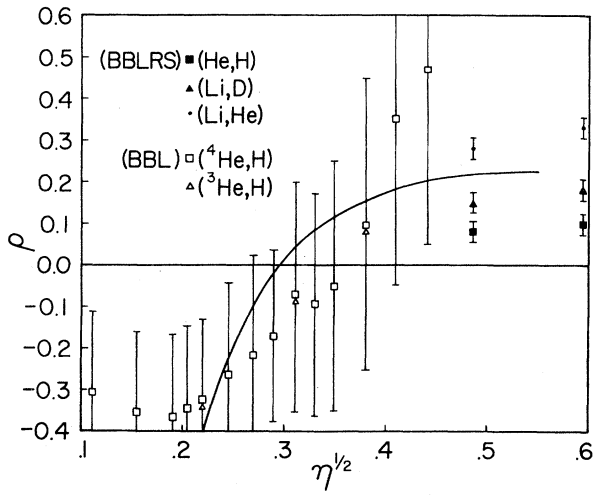

FIG. 1. Cross-section ratio ρ for Al as a function of $\eta^{1/2}$. BBLRS is the first paper in Ref. 2; BBL is the second. The symbols in parentheses give the projectile pairs from which the ratio was determined.

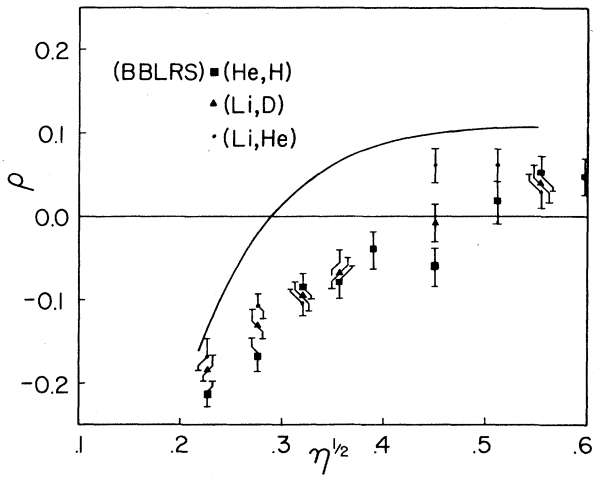

FIG. 2. Cross section ratio for Ni, as in Fig. 1.

and eighteen p states. To establish the convergence of our results with respect to change in the basis we used up to 11 s and 28 p states, and also did calculations with different choices of φ_j, ϵ, and c_l. The change was less than 2%. As an additional check on the representation of the continuum by the basis sets, we showed that they gave good agreement (less than 2% error) with the exact s and p first Born ionization calculations.

In our hydrogenlike model the results simply scale from one target atom to the other. The appropriate variable $\eta^{1/2}=\hbar v/Z_n e^2$ is the ratio of the velocity of the projectile to the velocity of the K-shell electron. It can be seen from Eqs. (1) and (6) that ρ is a function of η divided by Z_n. The only other effect in our calculations when the target atom is changed is that the number of occupied states to be excluded as final states changes. This effect was included but is a small one, especially at the higher projectile velocities at which our results are reported.

The low-energy limit on our method is the fact we have ignored any bending that the projectile path suffers as a result of nuclear repulsion and that only the two leading terms in the Born series have been retained.

In Figs. 1–3 we show our theoretical and experimental results for aluminum, nickel, and carbon, respectively. We extracted ρ from the experiments under the assumption that

$$Z_p'^2\sigma(Z_p)/Z_p^2\sigma(Z_p')=[1+Z_p\rho]/[1+Z_p'\rho]. \quad (8)$$

The agreement is excellent for Al, good for Ni, and fair for C. It confirms the physical picture given in Ref. 2 of two competing effects: increased binding and polarization. The increased discrepancy for carbon might be due to neglect of charge transfer. But it is not clear that including this would make matters better. Within the Brinkman-Kramers approximation[18] the Z_p dependence at *high velocities* is Z_p^5. The addition of such a term to $\sigma(Z_p)$ would certainly increase the discrepancy. One could argue, however, that the high-energy estimate is not reliable here. Only a calculation including charge transfer will settle the matter. Another possible explanation is that higher-order terms in the Born series,

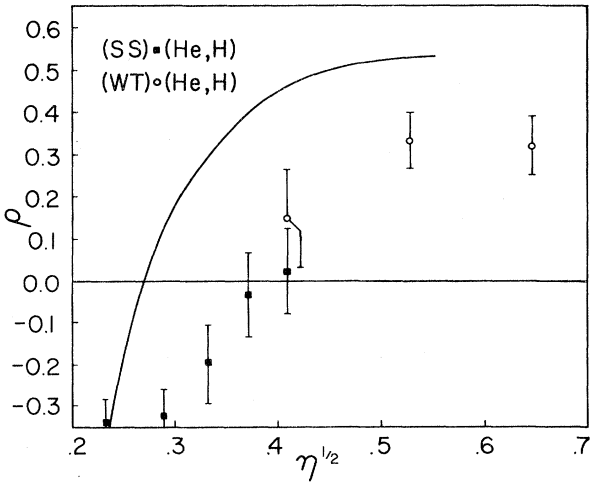

FIG. 3. Cross section ratio for C, as in Fig. 1. SS is Ref. 3; WT is Ref. 4.

neglected here, are important at the comparatively low velocities for C. In any case it is clear that the simple scaling law given by the hydrogenic model is breaking down somewhat as it does not fit both aluminum and nickel. It is straightforward to diagonalize a Hartree-Fock Hamiltonian rather than a hydrogenic one and this will be done next to see if this changes the Z_n dependence. A Hartree-Fock calculation will indeed be essential for higher-shell ionization calculations where the wave functions are much more sensitive to $V_s(r)$. Nevertheless, the agreement with experiment is impressive considering the simplicity of the approach. A real promise is held out that reliable absolute cross sections can soon be calculated including both effects of configuration interaction and higher-order Born terms.

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