Deflection effects in inner-shell ionization*

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Recently a method of calculating inner-shell ionization has been formulated in which Hartree-Fock wave functions are employed and all terms in the Born series retained. Results have so far been presented only in the energy region where projectile deflection effects are of little importance. In this paper it is shown how the time-dependent problem can be solved just as conveniently for hyperbolic classical projectile paths that result from the nuclear repulsion. The method is applied to the impact-parameter dependence of K-shell ionization by protons on copper in the energy range 0.5 to 2 MeV. Excellent agreement is found at the lower energy with experiments of Andersen *et al.* Poorer agreement is obtained in the higher-energy regime.

I. INTRODUCTION

Until recently inner-shell vacancy production had been investigated only in a series of convenient approximation schemes: the plane-wave Born (PWBA),[1] the semiclassical (SCA),[2] the binary encounter (BEA),[3] the Glauber,[4] the Brinkman-Kramers approximation (BK),[5] and so on. Basbas *et al.*[6] have presented a semiquantitative theory which corrects the SCA and have shown that large and important effects are present due to increased binding and polarization. In some recent papers,[7] three of the present authors have demonstrated the feasibility of solving the time-dependent Schrödinger equation numerically by expanding the wave function in a truncated set of Hilbert basis states centered about the target atom. This method is primarily designed for processes with projectile atomic numbers much less than the target atomic number. Charge transfer channels are not included as intermediate states, and charge transfer itself, as a final state, is not included as a mechanism for K-shell hole production.

In all our work so far we have considered the projectile as moving with constant speed in a straight-line path. In this paper we show that it is straightforward to remove this restriction and allow the projectile to travel on a classical trajectory. We consider the deflecting force to be just that of the mutual Coulomb repulsion between the two nuclei involved. Coulomb deflection effects have been considered in Ref. 2 in the Born approximation for hydrogenic models. Here all orders of the Born series are treated. The atom is allowed to ionize into single-electron states treated in the Hartree-Fock approximation. We keep s, p, and d angular momentum states. A U-matrix approach[7] is used to integrate out the Schrödinger equation.

This method is briefly reviewed in the next section, and in Sec. III the results of an application to analysis of recent experiments[8] for large-angle scattering of protons on copper is given.

II. THE METHOD

Our method for solving the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi_I}{\partial t} = V_I \Psi_I \ , \tag{1}$$

where

$$V_I = Z_p e^2 \exp\left(\frac{iH_e t}{\hbar}\right)\left[\frac{1}{R(t)} - \frac{1}{|\vec{\mathbf{R}}(t) - \vec{\mathbf{r}}|}\right] \times \exp\left(-\frac{iH_e t}{\hbar}\right) \tag{2}$$

and

$$H_e = -\frac{\hbar^2}{2m_e}\nabla_r^2 + V_{HF} + I_K \tag{3}$$

has been described in detail elsewhere[7] and we limit ourselves here to only the briefest review. We first diagonalize the Hartree-Fock Hamiltonian H_e on a finite set of Hilbert basis vectors $U_i(\vec{\mathbf{r}})$. This produces a set of eigenfunctions of PH_eP, $u_\lambda(\vec{\mathbf{r}})$. Here P is the projection operator onto our basis set and

$$u_\lambda(\vec{\mathbf{r}}) = Y_L^M(\theta, \phi)\sum_{i=1}^{N_L} a_i^\lambda r^L \exp[-(c_L/\epsilon_i)r] \ . \tag{4}$$

The complex numbers ϵ_i are chosen to represent most conveniently and accurately the occupied bound states of the atom, together with the continuum states important at the projectile energies to be considered.

We now write

$$\Psi_I(t_3) = U(t_3, t_1)\Psi_I(t_1) \simeq \exp\left(-\frac{i}{\hbar}\int_{t_1}^{t_3} V_I \, dt\right)\Psi_I(t_1) \ . \tag{5}$$

Here Ψ_I and V_I are a vector and matrix, respectively, in the u_λ representation; e.g.,

$$V_I = \langle u_\lambda | \exp[i(\lambda - \lambda')t/\hbar] \, V | u_{\lambda'} \rangle \ . \tag{6}$$

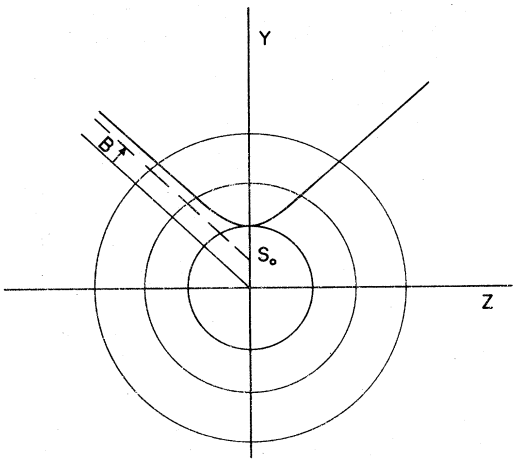

FIG. 1. Coordinate system used in the present calculation. The hyperbolic classical trajectory is shown. B is the impact parameter and S_0 the distance of closest approach. The circles represent the values of R for which the potential matrix elements are precomputed and stored.

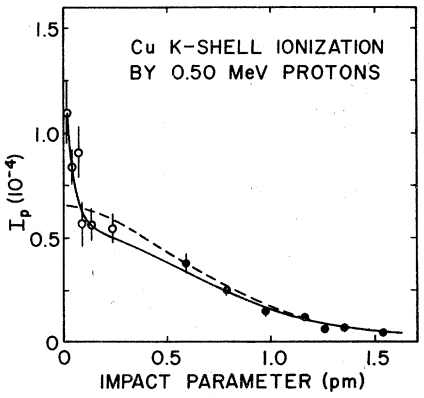

FIG. 2. Impact-parameter dependence of the K-shell ionization probability I_p for 0.5-MeV protons on copper. The experimental points are from Ref. 8. The solid and dashed curves are the present calculations with and without the Coulomb deflection.

The U matrix propagates the wave function from time t_1 to time t_3. To obtain Ψ_I at $t=\infty$, we take a product of U matrices. We use time-reversal symmetry to relate $U(+\infty, -\infty)$ to $U(\infty, 0)$ and hence save a factor of 2 in computational effort.[7] We typically keep up to the fourth power in V_I in expanding out the exponential in Eq. (5). The time-step interval is mainly governed by the convergence properties of the integral to be exponentiated. For the lowest projectile energies presented here, up to 150 points were used to establish convergence.

The difficulty with the problem is the oscillation of the integral V_I as a function of time. Our procedure is to store $\langle\lambda|V|\lambda'\rangle$, the potential matrix element, as a function of R on a set of predetermined points. We then integrate over three consecutive points in time by assuming $\langle\lambda|V|\lambda'\rangle$ is quadratic in time. As the speed of the method depends on the ability to store in the computer a set of elements $\langle\lambda|V|\lambda'\rangle$ to be used for all impact parameters, the procedure when $\vec{\mathbf{R}}(t)$ describes a hyperbolic path needs some clarification. In Fig. 1, we illustrate our method. We calculate the matrix elements as a function of $\vec{\mathbf{R}}(t)$ so that we have them (apart from quickly calculable terms such as Z/R, Y/R, etc.) available on the representative circles shown. We next chose an impact parameter B by requiring that it lead to a distance of closest approach S_0 which is equal to the radius of the smallest of the circles. This is given by

$$B=[S_0^2-(2Z_p/\eta)(m_e/m_p)S_0]^{1/2}\,. \tag{7}$$

Here Z_p is the atomic number of the projectile, m_e/m_p is the ratio of the mass of the electron to that of the projectile, and $\eta^{1/2}$ $(=\hbar v_p/Z_n e^2)$ is the ratio of the initial projectile velocity v_p to the K-shell electron velocity. The units of S_0 and B are a_0/Z_n.

Having calculated B we next determine the eccentricity of the projectile path, ϵ, from

$$\epsilon=\frac{1+(B/S_0)^2}{1-(B/S_0)^2}\,. \tag{8}$$

We have three parametric equations in Ω,[9] for R, Z, and Y, i.e.,

$$\begin{aligned} R&=S_0(\epsilon\cosh\Omega+1)/(\epsilon+1)\,,\\ Z&=S_0\sinh\Omega\,[(\epsilon-1)/(\epsilon+1)]^{1/2}\,,\\ Y&=S_0(\cosh\Omega+\epsilon)/(\epsilon+1)\,. \end{aligned} \tag{9}$$

We use the first of these equations to calculate Ω such that R is one of our predetermined circles. With this Ω we then obtain Z and Y. Finally we obtain the time at which the projectile path intersected the particular circle by using

$$t=S_0(\epsilon\sinh\Omega+\Omega)/[(\epsilon+1)v_p]. \tag{10}$$

Here v_p is the initial velocity of the projectile.

We start this procedure for $R=S_0$ and integrate out, three points at a time, until our largest circle (typically 400 a_0/Z_n) is reached. Note the symmetry in time about the Y axis.

The method is repeated, choosing larger values of S_0 each time, until we have mapped out the complete impact-parameter dependence of the U matrix.

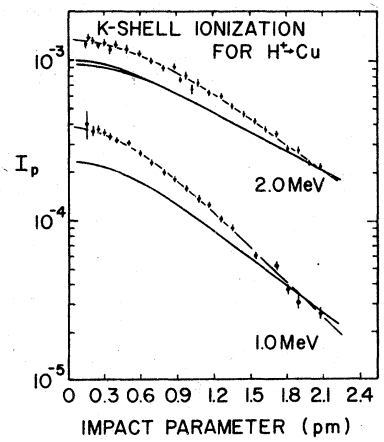

FIG. 3. Impact-parameter dependence of the K-shell ionization probability I_p for 1- and 2-MeV protons on copper. The experimental points are from Ref. 8. The solid curves are the present calculation. The lower curve is with our standard basis set ($5s, 12p, 15d$). The upper solid curve is with a larger basis set ($10s, 20p$, $15d$).

III. THE RESULTS

We applied the above method to the calculation of the "conventional" K-shell ionization probability for proton impact on a copper atom. What is really plotted in the figures is *twice* the ionization probability for a single-electron-atom calculation, i.e.,

$$I_p = 2\sum_{\lambda} |\langle \lambda | U | \mu \rangle|^2 . \tag{11}$$

Of course I_p can, in principle, be greater than unity. Here μ represents the ground state and the sum on λ is taken over all the unoccupied pseudostates.

The results for 0.5-MeV protons on copper are shown in Fig. 2 (solid curve) together with the same calculation where the mass of the projectile is set infinitely large (broken line), i.e., where no deflection occurs. The agreement with experiment[8] is remarkable. The larger peak at small impact parameters, interpreted by Anderson *et al.*[8] as an interference effect between the two "legs" of the deflected path, is very accurately reproduced. The calculation was carried out with a basis containing $5s$, $12p$, and $15d$ states.

In Fig. 3 we show the comparison of our calculations with 1-MeV and 2-MeV data also obtained by Andersen *et al.*[8] Though the slopes of the experimental and theoretical curve are similar, the absolute normalization is very different. Further, Andersen *et al.* cite an absolute total cross section at 2 MeV of 115 b, where our calculation gives 82 b. This particular cross section has been measured by other authors, where results of 96 ± 5 b[10] or 94 ± 7 b[11] are quoted. These latter two results are based on somewhat different fluorescent yields, 0.445 and 0.343, respectively.

In view of the discrepancy between our calculation and experiment at these higher energies, we did a more extensive calculation with $10s$, $20p$, and $15d$ states. Experience[7] in previous calculations has shown that very good convergence can only be obtained with this rather large basis. It is quite expensive to perform this calculation, and we did not repeat it at the other energies. But the change in the results should be considered as a typical numerical error present in the graphs shown. As can be seen from Fig. 3 from the upper solid curve, there is a small change in the cross section, mainly due in fact to a shift in the first Born term. At 2 MeV this gives a total cross section of 89 b. It is much too small a change to explain the discrepancy. We do note, however, that the difference between theory and experiment is no greater than the difference between the two experimental results reported.

In conclusion, the deflection effects can easily be incorporated in our method, reproducing the salient features of the impact-parameter dependence at low energies of inner-shell ionization. There are still descrepancies between absolute cross sections predicted theoretically and those measured experimentally.

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[1]E. Merzbacher and H. W. Lewis, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1958), Vol. 24, p. 166ff.

[2]J. Bang and J. M. Hansteen, K. Dan. Vidensk. Selsk. Mat-Fys. Medd. 31, No. 13 (1959); J. M. Hansteen and O. P. Mosebekk, Z. Phys. 234, 281 (1970).

[3]J. D. Garcia, Phys. Rev. A 1, 280 (1970); J. S. Hansen, *ibid.* 8, 822 (1973).

[4]J. F. Reading and E. Fitchard, Phys. Rev. A 10, 168 (1974).

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

[6]G. Basbas, W. Brandt, R. Laubert, A. Ratkowski, and A. Schwarzschild, Phys. Rev. Lett. 27, 171 (1971).

[7]J. F. Reading, A. L. Ford, and E. Fitchard, Phys. Rev. Lett. 36, 573 (1976); A. L. Ford, E. Fitchard, and J. F. Reading, Phys. Rev. A (to be published).

[8]J. U. Anderson, E. Laegsgaard, M. Lund, C. D. Moak,

L. Kocbach, J. Phys. B 9, 3247 (1976); J. U. Andersen, E. Laegsgaard, M. Lund, and C. D. Moak, Nucl. Instrum. Meth. 132, 507 (1976).
[9]K. A. Ter-Martirosyan, Zh. Eksp. Teor. Fiz. 22, 284 (1952).
[10]R. Akselsson and T. B. Johansson, Z. Phys. 266, 245 (1974).
[11]R. Lear and T. J. Gray, Phys. Rev. A 8, 2469 (1973).