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Semi-Classical Approach to Inner-Shell Ionization

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Semi-Classical Approach to Inner-Shell Ionization[1]

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A semi-classical calculation of atomic ionization depends upon the trajectory of the projectile. In the past, it has been customary to assume that the projectile passes the atom in a straight line. We have investigated this assumption by calculating realistic trajectories for heavy projectiles scattered from Hartree-Fock atomic potentials. We have also examined the experimental procedure of correlating impact parameters with projectile scattering angles using Rutherford scattering. It was found that this procedure is inaccurate for the lower projectile energies.

INDEX DESCRIPTORS: Semi-classical Theory, Inner-Shell Ionization, trajectories, impact parameters.

The problem of atomic inner-shell ionization by heavy particle bombardment has recently received a great deal of attention in the literature[1,2]. Experimental work in this area has been performed primarily by converted nuclear physicists who have measured total ionization cross sections by observing the emitted x-rays or Auger electrons[2]. These experiments have been adequately explained using the Plane Wave Born Approximation (PWBA)[3,2].

Quite recently, however, experimentalists have measured differential cross sections by observing the angular deflection of the heavy projectile. In the analysis of these experiments, it was assumed that the deflection of the projectile is caused primarily by elastic scattering in the atomic field and that the atomic field is Columbic. As a result, the angle of deflection may be directly related to an impact parameter for the collision using Rutherford scattering. The corresponding theoretical differential cross sections have been obtained using the Semi-Classical Approach (SCA)[5,6]. In this theory the impinging particle is treated classically while the target atom is treated quantum mechanically. Such a theory can be justified for high energy, heavy projectiles by noting that the collision is of such a short duration that the projectile follows an essentially classical trajectory. Due to the complexity of a SCA calculation, it has been customary to choose the trajectory of the projectile to be a straight line. Such a procedure has given satisfactory agreement with experiment for high energy projectiles passing the atom at large impact parameters[6]. However, recent experiments at smaller impact parameters have not agreed well with the straight-line SCA theory[7,8].

The purpose of this paper is to demonstrate: (1) that the disagreement between the small impact parameter experiments and straight-line SCA theory does not necessarily represent a deficiency in the SCA theory since realistic classical trajectories would be highly non-linear and (2) that the experimental procedure of relating angles of deflection to impact parameters using a Coulombic potential is inaccurate in certain angular and energy ranges. To achieve this end, we examine the collision problem using the SCA theory. However, instead of using non-realistic or approximate atomic potentials, classical trajectories are calculated using the best available numerical Hartree-Fock[9] atomic potentials.

THEORY

In the SCA theory, the ionization probability can be shown to be [10]

$$I(p) = -ize^2\hbar^{-1}\int_{-\infty}^{\infty} \langle \Psi_f(\vec{r}) | [\vec{R}(t) - \vec{r}]^{-1} | \Psi_i(\vec{r}) \rangle \exp(i\omega_{fi} t)\, dt$$

where Ψ_f and Ψ_i are the final and initial states of the atom, $\vec{R}(t)$ is the position of the projectile at any time (impact parameter dependent), ω_{fi} is the energy transferred in units of $\hbar$ and p is the impact parameter. Equation 1 depends upon the trajectory of the projectile and can be evaluated easily only for straight line trajectories. Therefore, SCA ionization probabilities are typically evaluated using straight line trajectories.

The two equations that may be used for calculating the trajectory of the projectile are the conservation of energy equation

$$m(\dot{r}^2 + r^2\dot{\theta}^2) + V(r) = E_o, \qquad (2)$$

and the conservation of angular momentum equation

$$mr^2\dot{\theta} = J = b(mE_o)^{1/2}, \qquad (3)$$

where m is the mass of the projectile, V(r) is the atomic potential, E_o is the total energy of the projectile, J is the angular momentum, and a dot indicates a derivative with respect to time. Atomic units are used in these equations. (energy in Rydbergs, distance in Bohr radii.) Substituting Eq. (3) into Eq. (2) yields

$$m(\dot{r}^2 + E_o m^{-1} b^2 r^{-2}) + V(r) = E_o. \qquad (4)$$

Equation 4 may then be integrated to obtain time (t) as a function of r

$$t = \pm \int_a^r m^{-1/2} [E_o(1 - b^2 r^{-2}) - V(r)]^{-1/2} dr. \qquad (5)$$

Here we have set t=0 at the distance of closest approach (a). In this equation the ± symbol distinguishes between events that occur before the projectile reaches the distance of closest approach (−) and after the projectile leaves the distance of closest approach (+).

At the distance of closest approach, conservation of energy and angular momentum requires

$$mu_o^2 = mu^2 + V(a), \qquad (6)$$

and

$$mu_o b = mua, \qquad (7)$$

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where u_o is the initial projectile velocity and u is the velocity at the distance of closest approach. Eqns. (6) and (7) may be rearranged to obtain

$$1 - b^2 a^{-2} \doteq V(a)/E_o . \tag{8}$$

An examination of this relationship reveals that the integrand of Eqn. (5) has a pole at a distance of closest approach. Therefore the interval of integration containing the distance of closest approach represents a special numerical problem that must be treated separately. It is well known that as r approaches zero, the Coulomb and Hartree-Fock potentials become identical. Therefore, for r near a, the distance of closest approach, (which is close to 0), the actual Hartree-Fock potential may be well represented by a Coulomb term plus a correction term. Consequently for r near a,

$$V(r) = a_1 E_o r^{-1} + a_2 E_o r^{-2} , \tag{9}$$

where a_1 and a_2 can be found by numerically fitting to the atomic potential. If the atomic potential were exactly a coulomb potential $a_1 E_o$ would be twice the nuclear charge and a_2 would be zero. A relationship for t close to the distance of closest approach may be obtained by substituting Eqn. (9) into (5).

$$t = \pm \int_a^r rm^{-1/2} [E_o r^2 + E_o b - a_1 E_o r - a_2 E_o]^{-1/2} dr. \tag{10}$$

This integral is a known convergent integral.

For r further away from the distance of closest approach, the integration may be done numerically using Simpson's three point integration technique.

The same methods may be used to find the angular deflection of the projectile as a function of r

$$\theta = \theta_o + b(E_o/m)^{1/2} \int_{t(r_o)}^{t} [r(t)]^{-2} dt. \tag{11}$$

where θ_o is the angle of approach subtended when the projectile enters the atomic field at r_o.

RESULTS

We have calculated classical trajectories for protons impinging upon a titanium target atom. In these calculations we have used both a realistic numerical Hartree-Fock potential and a Coulombic potential to approximate the actual atomic potential V(r). Typical results for classical trajectories are presented in the first four figures for various impact parameters and proton energies.

Figure 1 contains trajectories for 5 KeV incident protons at various impact parameters. The impact parameters are given in atomic units. The solid curves are trajectories obtained using the numerical Hartree-Fock potential and the dashed curves were obtained using a Coulombic potential. It is to be noted that there is a significant difference between the Coulombic and Hartree-Fock trajectories for the larger impact parameters. At the smaller impact parameters, the two trajectories approach each other. This is to be expected since, for small impact parameters, the projectile penetrates closer to the nucleus where the actual atomic potential is more Coulombic.

Figure 2 contains a similar plot for a proton energy of 10 KeV. From this figure it can be seen that a 10 KeV proton is not deflected as much as a 5 KeV proton, but the trajectories are still high non-linear. As in the previous figure, there is a measurable difference between the trajectories obtained from the Coulombic and Hartree-Fock potentials. Figure 3 contains the trajectories of a 100 KeV proton scattered at two impact parameters. Here again the trajectories are highly non-linear, but more closely resemble a straight line than in the two previous figures. At this projectile energy, no detectable difference between scattering by the Coulombic and Hartree-Fock potentials is found.

The final trajectory plot (Figure 4) is for a 1 MeV proton incident on Titanium again at two impact parameters. For a projectile with this energy and impinging at the larger of the two impact parameters, the trajectory is approximately a straight line. However, the trajectory for a proton impinging at the smaller impact parameter varies significantly from a straight line.

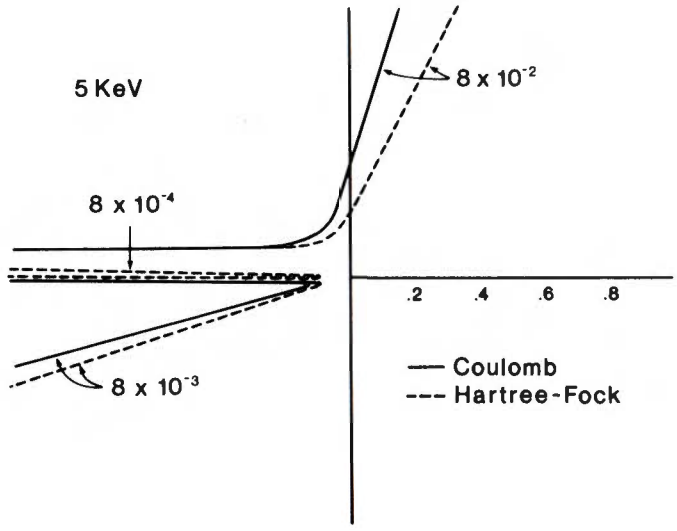

Figure 1. Classical trajectories for 5 KeV protons scattered from titanium. The solid curve was calculated using a Hartree-Fock atomic potential and the dashed curve was calculated using a Columbic potential. The impact parameter for the collision is given for each set of curves. For an impact parameter of 8 x 10^{-4}, the two curves coincide.

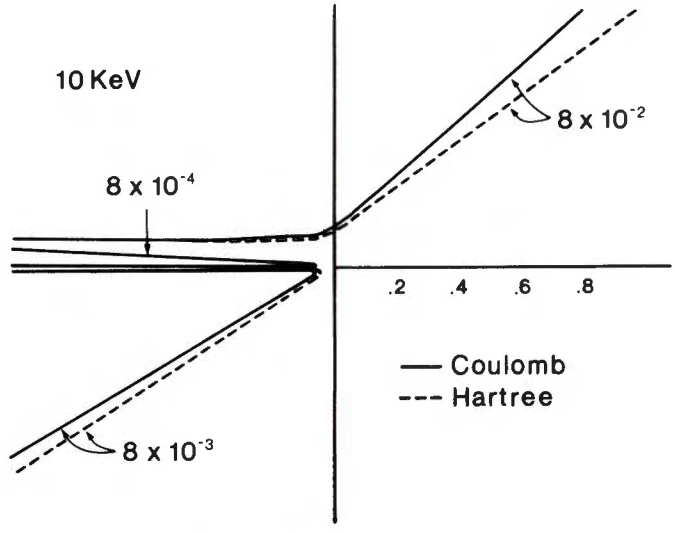

Figure 2. Same as Fig. 1 except here the proton energy is 10 KeV.

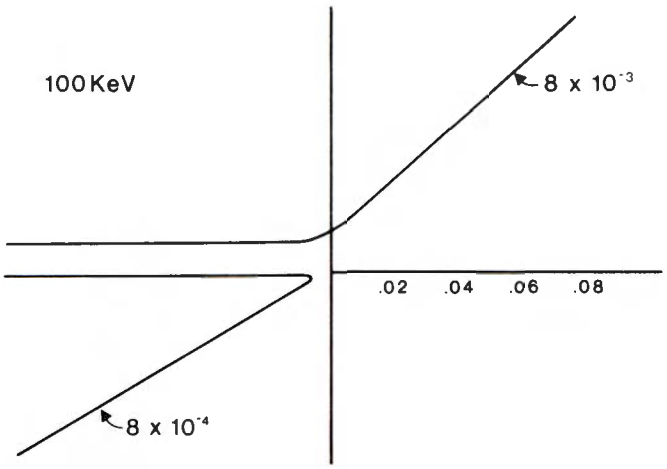

Figure 3. Same as Fig. 1 except here the proton energy is 100 KeV. The curve calculated using the Coulombic potential coincides with the curve calculated using the Hartree-Fock potential at these impact parameters.

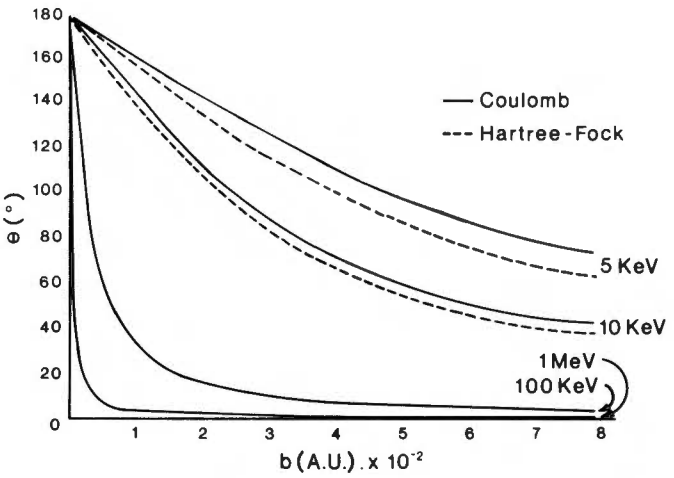

Figure 5. Angular deflections of protons scattered from titanium as a function of impact parameter. The solid curve was obtained using a Hartree-Fock atomic potential and the dashed curve was calculated using a Coulombic potential. For the higher proton energies, the two curves coincide.

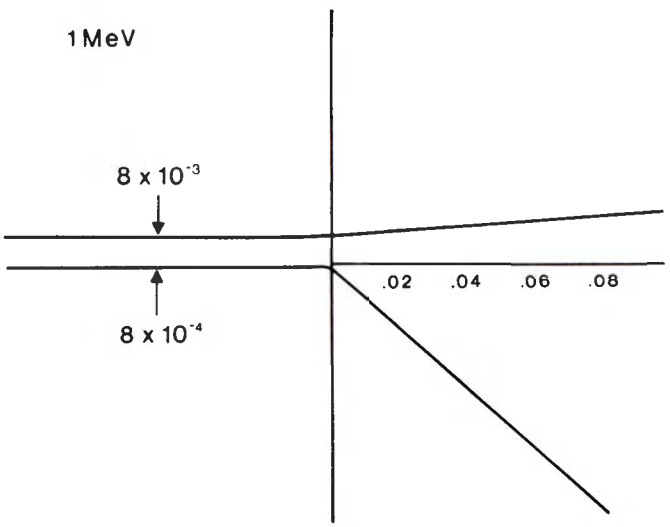

Figure 4. Same as Fig. 3 except here the proton energy is 1 MeV.

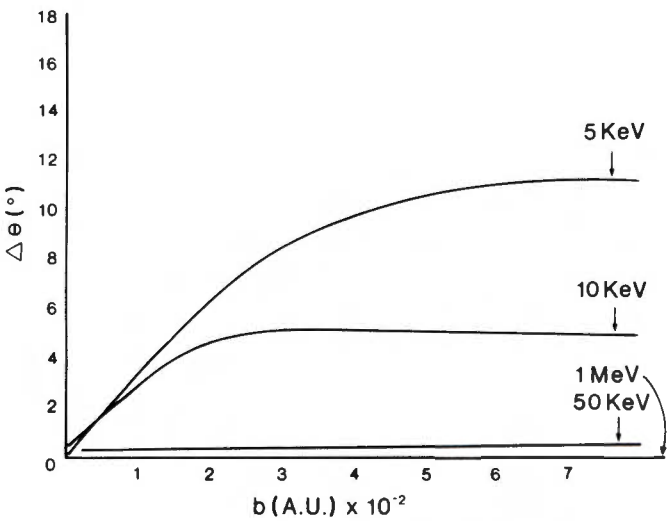

Figure 6. Difference between Coulombic and Hartree-Fock scattering angles as a function of impact parameter for various incident proton energies.

The final two figures present results for the calculation of angular deflections. Figure 5 contains the angular deflection of protons scattered by titanium for proton energies between 5 KeV and 1 MeV. The solid curves were obtained using the Hartree-Fock potential and the dashed curves were obtained using a Coulombic potential. The two cures are identical for proton energies of 100 KeV and 1 MeV. The experimental procedure of relating impact parameters to angular deflections using Rutherford scattering will be accurate only when the two curves coincide. As may be seen from the figure, this procedure will yield incorrect impact parameters for the lower proton energies.

In figure 6, we have plotted the difference between the Coulombic and Hartree-Fock scattering angles as a function of impact parameter. When this difference is zero, the proton will be scattered into the same angle by both the Hartree-Fock and Coulombic potentials. As can be seen from the figure, this difference becomes as large as 12° for 5 KeV protons which is appreciably larger than the resolution of most experimental detectors.

CONCLUSION

The results of these calculations contain implications for both the theoretician and the experimentalist. For the theoretician, it is seen that the classical trajectories are highly non-linear at these small impact parameters. Since the ionization probability is largest at the small impact parameters, it is necessary to use realistic trajectories in a SCA calculation. It is not surprising that the customary straight-line trajectory calculations do not agree well with experiment in this range of impact parameters. We would conclude that much improved agreement with experiment would be obtained if a SCA calculation would be performed using Hartree-Fock trajectories. That particular problem will be studied in the near future by the present research group.

For the experimentalist, the present results indicate that it is inaccurate to use Coulombic potentials to correlate impact parameters with scattering angles for low projectile energies. At the lower energies, the best trajectories are obtained using a Hartree-Fock atomic potential and a correlation between scattering angle and impact parameter should be obtained from numerical results such as those presented in figure 5.

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