

## High-energy calculation of $K$ -shell ejection cross sections as a function of projectile charge\*

J. F. Reading and E. Fitchard

Cyclotron Institute and Physics Department, Texas A&M University, College Station, Texas 77843

(Received 5 July 1973; revised manuscript received 15 April 1974)

We present a high-energy calculation of the  $K$ -shell ejection cross section  $\sigma(Z_p)$  as a function of projectile charge  $Z_p$ . Charge-transfer effects are not included. The wave function for the heavy projectile is written as  $e^{i\vec{k}_0 \cdot \vec{R}} F(-in, 1, ik_e |\vec{R} - \vec{r}| - i\vec{k}_c \cdot (\vec{R} - \vec{r})) \Gamma(1+in) e^{-n\pi/2}$ , as opposed to the Glauber approximation  $e^{i\vec{k}_0 \cdot \vec{R}} \exp(-in \int_{-\infty}^Z dZ' |\vec{R} - \vec{r}'|^{-1})$ . These two approximations agree at large distances but differ as the electron and projectile approach closely to each other. A prediction is made that if  $T_m$  (the maximum classical energy an electron at rest may receive) is much greater than  $I_K$  then  $r_{12}$  will be less than unity. Here  $r_{12} = \sigma(Z_1)Z_2^2 / \sigma(Z_2)Z_1^2$ ,  $Z_1 > Z_2$ . Higher-energy experiments are needed to confirm this theoretical result.

### I. INTRODUCTION

The dependence of the  $K$ -shell ionization cross section  $\sigma(Z_p)$  on the charge of the projectile,  $Z_p$ , provides a severe testing ground for theoretical calculations.<sup>1</sup> For example, it has been demonstrated<sup>2,3</sup> that the Born<sup>4,5</sup> approximation is invalid for  $K$ -shell ionization in the high-energy region by measuring the ratio  $r_{12}$  where

$$r_{12} = \sigma(Z_1)Z_2^2 / \sigma(Z_2)Z_1^2, \quad Z_1 > Z_2.$$

In Figs. 1–3, the experimental points for this ratio are plotted for the  $K$ -shell ionization of carbon, copper, and titanium by  $\alpha$  particles and deuterons moving with the same velocity. This ratio should be unity if the Born approximation holds, in fact it differs appreciably from unity.

In this paper, we show that the same experiments indicate the inadequacy of the Glauber approximation,<sup>6</sup> but that the Cheshire approximation<sup>7</sup> improves matters. Further, both approximations are shown to predict that  $r_{12}$  should be less than unity at high energies, a fact as yet unconfirmed by experiment. It is our hope that this paper might encourage such experiments to be undertaken, as the energy needed for copper is only a few MeV higher than the experiments already performed.

We should say at the outset that none of our calculations include charge exchange directly, and so we have nothing to say yet about ionization processes in which the charge of the nucleus and the projectile are comparable.<sup>3,8</sup> Indeed, until we have understood the data with a comparatively weak probe of one or two electron charges, we would regard such an attempt as being too ambitious. It seems to us, from this work, that the most important problem to tackle is the correction of the Cheshire approximation to include binding to the atom.

Before we become submerged in mathematics, it might be advantageous to see what physical insight we can obtain from a quasiclassical description of ionization. An important quantity in this regard is the maximum classical energy an electron originally at rest can receive in a collision. We designate this energy  $T_m$ . In this notation, as throughout the paper, we follow Merzbacher and Lewis.<sup>4</sup> If  $T_m \ll I_K$ , the ionization energy, then only electrons moving towards the projectile can be ejected. Electrons with the highest components of velocity in the bound-state wave function  $\chi_0(r)$  are to be found near  $\vec{r}$  equal to zero. Similarly, in order for the projectile to turn the electron around, the distance between the projectile located at  $\vec{R}$  and the electron located at  $\vec{r}$  must be small. These two facts have as a consequence the fact that ejection only takes place for values of the impact parameter  $\vec{B}$  that are somewhat less than  $a_K$ , the radius of the  $K$  shell. Thus, the projectile finds itself attracting the electron closely towards the very nucleus it is trying to eject it from. This effect might be responsible for the fact that  $r_{12}$  is less than unity at low energies.<sup>1</sup>

As the energy of the projectile is increased so that  $T_m \approx I_K$ , the projectile need not approach the nucleus so closely. The fact that it attracts the electron towards it enhances the cross section as the density of the electron cloud is increased around the projectile.

As the energy is increased further,  $T_m > I_K$ , it is no longer necessary to have electrons moving towards the projectile to be ejected, and therefore the electrons need not closely approach the projectile either. However, they are still pulled in, and hence their density is decreased far from the projectile. This could suppress the cross section.

The Glauber approximation assumes that  $k_e |\vec{R} - \vec{r}|$

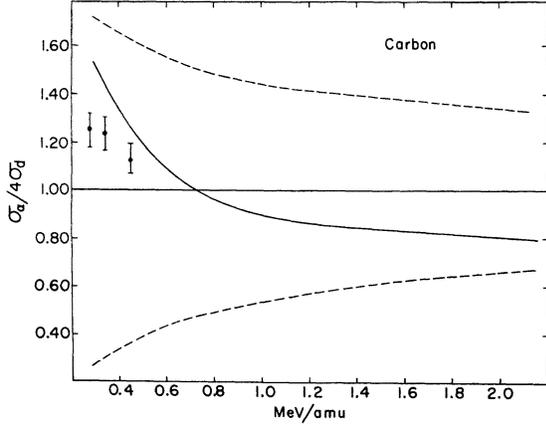


FIG. 1. Comparison of theoretical calculation for  $r_{12}$  with experimental data taken from Ref. 2 for  $\alpha$  and deuteron bombardment of carbon.

is large in the region of configuration space important to the cross section. Here

$$k_e = m_e v / \hbar,$$

where  $m_e$  is the electron mass. We shall designate by  $k$  the projectile's momentum,  $m_p v / \hbar$ . We might therefore expect the Glauber cross section to be reliable for  $T_m > I_K$ . We find that it does predict  $r_{12} < 1$ . As we lower the energy so that  $k_e |\vec{R} - \vec{r}| \sim 1$  is the region important for the cross section, we would expect the Cheshire approximation, which is designed to work for this region, to do better than the Glauber. It does predict  $r_{12} > 1$ . As we lower the energy still further, neither of the approximations should really work well, as they neglect the all important interaction of the electron with the nucleus *after* it interacts with the projectile. The experiments seem to confirm this.

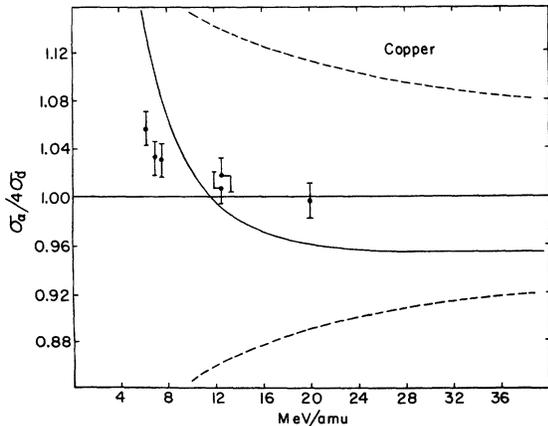


FIG. 2. Comparison of theoretical calculation for  $r_{12}$  with experimental data taken from Ref. 2 for  $\alpha$  and deuteron bombardment of copper.

We now return to mathematics. In Sec. II, we demonstrate a rather important theorem for this work, i.e., that the projectile nuclear interaction can be removed from the problem if one only wishes to calculate a total inelastic cross section in a high-energy approximation. In Sec. III we use this result to derive a rather simple result for the Glauber and Cheshire approximations. In Sec. IV we discuss the comparison with the experiments and the need to correct the Cheshire approximation to make further progress.

## II. REMOVING THE PROJECTILE NUCLEAR FORCE

In this section we demonstrate that it is possible to remove the projectile nuclear force for the calculation if one is only interested in calculating a total inelastic cross section in a small-angle high-energy approximation. This has an important consequence of rendering separable, and therefore tractable, the multidimensional integrals involved in the calculation.

The Schrödinger equation describing a projectile scattering from a single electron bound to a nucleus fixed at the origin of coordinates is given by

$$\left( -\frac{\hbar^2}{2m_p} \nabla_R^2 - \frac{\hbar^2}{2m_e} \nabla_r^2 + U(r) + V(\vec{r}, \vec{R}) + W(R) + I_K \right) \psi = \frac{\hbar^2 k^2}{2m_p} \psi. \quad (1)$$

Following Glauber,<sup>6</sup> we substitute

$$\psi = e^{i\vec{k}_0 \cdot \vec{R}} S(\vec{r}, \vec{R}) \quad (2)$$

and neglecting a term  $(-\hbar^2 \nabla_R^2 / 2m_p)$ , we arrive at an equation for  $S$

$$\begin{aligned} i\hbar v \frac{\partial S(\vec{r}, \vec{R})}{\partial Z} &= \left( \frac{-\hbar^2}{2m_e} \nabla_r^2 + U(r) + V(\vec{r}, \vec{R}) \right. \\ &\quad \left. + W(R) + I_K \right) S(\vec{r}, \vec{R}) \\ &= (H_e + V + W) S. \end{aligned} \quad (3)$$

We thus have used the assumption that the mass of the projectile  $m_p$  is much greater than  $m_e$ .<sup>9</sup>

Our aim is to solve this equation as accurately as possible with the boundary condition that  $S(\vec{r}; \vec{B}, -\infty)$  is  $\chi_0(r)$ . We then substitute  $S(\vec{r}, \vec{R})$  into the equation for the inelastic scattering amplitude, i.e.,

$$\begin{aligned} f_{m,0}(q) &= -\frac{2m_p}{4\pi\hbar^2} \int e^{-i\vec{k}_m \cdot \vec{R}} \chi_m^*(r) [V(\vec{r}, \vec{R}) + W(R)] \\ &\quad \times e^{i\vec{k}_0 \cdot \vec{R}} S(\vec{r}, \vec{R}) d^3r d^3R. \end{aligned}$$

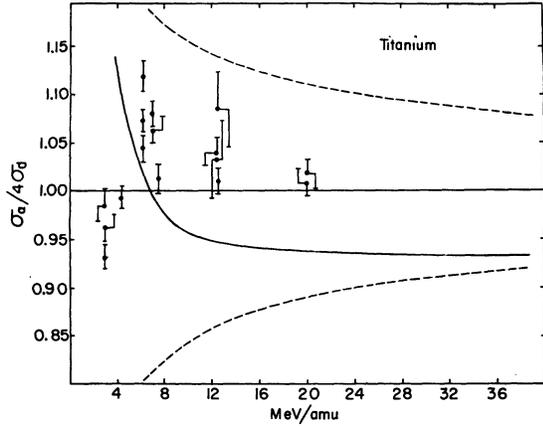


FIG. 3. Comparison of theoretical calculation for  $r_{12}$  with experimental data taken from Ref. 2 for titanium.

Here

$$\begin{aligned}\vec{q} &= \vec{k}_m - \vec{k}_0 \\ &\equiv (\vec{q}_b, q_z) \approx [2k \sin(\frac{1}{2}\theta), -(W_m + I_K)/\hbar v]\end{aligned}$$

and

$$k_m \approx k - (W_m + I_K)/\hbar v.$$

The excited atom has wave function  $\chi_m(r)$  and energy  $W_m$ .

In the Glauber approximation, one sets  $H_e(r)$  equal to zero, which allows one to write  $(V+W)S$  in Eq. (3) as a perfect differential in Eq. (4). One could now perform the  $Z$  integration if one were consistent in setting  $H_e$  equal to zero, as  $\vec{q} \cdot \vec{Z}$  would then be equal to zero. However, this latter approximation has the unfortunate consequence that now even the Born approximation is incorrect. This difficulty can be overcome by making  $\vec{q} \cdot \vec{Z}$  equal to zero by "redefining" the  $Z$  direction.<sup>10</sup> This approximation seems difficult to justify, especially at small angles, and is a large price to pay for one integration. Instead, we follow a method outlined by one of the present authors.<sup>9</sup> We write

$$S(\vec{r}, \vec{R}) = e^{-iH_e Z/\hbar v} S_I(\vec{r}, \vec{R}) \quad (5)$$

and then derive

$$\begin{aligned}i\hbar v \frac{\partial S_I(\vec{r}, \vec{R})}{\partial Z} &= e^{iH_e Z/\hbar v} V(\vec{r}, \vec{R}) \\ &\times e^{-iH_e Z/\hbar v} S_I + W(R) S_I.\end{aligned} \quad (6)$$

We can now write

$$\vec{q} \cdot \vec{R} = \vec{q}_b \cdot \vec{B} - H_e Z/\hbar v \quad (7)$$

in Eq. (4), where  $q_b$  is  $2k \sin(\frac{1}{2}\theta)$ . This is a small-angle approximation entirely consistent with the approximation that led to Eq. (3). This allows the

$Z$  integration to be performed exactly, giving

$$f_{m,0}(q_b) = \frac{k}{2\pi i} \int e^{-i\vec{q}_b \cdot \vec{B}} \chi_m^*(r) S_I(\vec{r}; \vec{B}, \infty) d^3r d^2B. \quad (8)$$

To find the total inelastic cross section  $\sigma_{m,0}$ , we now integrate  $|f|^2$  over  $\vec{q}_b$  and following Glauber,<sup>6</sup> arrive at

$$\sigma_{m,0} = \int d^2B \left| \int \chi_m^*(r) S_I(\vec{r}; \vec{B}, \infty) d^3r \right|^2. \quad (9)$$

We now note that from Eq. (6) that defining  $S_{MI}$  such that

$$S_I(\vec{r}; \vec{B}, Z) = S_{MI}(\vec{r}; \vec{B}, Z) \exp\left(\frac{-i}{\hbar v} \int^Z W(\vec{B}, Z') dZ'\right) \quad (10)$$

gives an equation

$$i\hbar v \frac{\partial S_{MI}}{\partial Z} = e^{iH_e Z/\hbar v} V(\vec{r}, \vec{R}) e^{-iH_e Z/\hbar v} S_{MI}. \quad (11)$$

If, for the time being, we assume that  $W$  is a short-range force, we can write

$$\begin{aligned}S_I(\vec{r}; \vec{B}, \infty) &= S_{MI}(\vec{r}; \vec{B}, \infty) \\ &\times \exp\left(\frac{-i}{\hbar v} \int_{-\infty}^{+\infty} W(\vec{B}, Z') dZ'\right)\end{aligned} \quad (12)$$

Substitution of  $S_I$  into Eq. (9) leads to

$$\sigma_{m,0} = \int d^2B \left| \int \chi_m^*(r) S_{MI}(\vec{r}; \vec{B}, \infty) d^3r \right|^2.$$

Thus the effect of  $W$ , if we assume it is short range, is merely to add a phase factor to the wave function which cancels when we calculate the total inelastic cross section.<sup>11</sup> We can therefore remove  $W(R)$  from the calculation entirely, and replace Eq. (4) by

$$\begin{aligned}f'_{m,0}(q) &= -\frac{2m_p}{4\pi\hbar^2} \int e^{-i\vec{q} \cdot \vec{R}} \chi_m^*(r) \\ &\times V(\vec{r}, \vec{R}) S_M(\vec{r}, \vec{R}) d^3r d^3R,\end{aligned} \quad (13)$$

where  $f'_{m,0}(q)$  is to be used only to calculate total cross sections. Here

$$i\hbar v \frac{\partial S_M(\vec{r}, \vec{R})}{\partial Z} = [H_e(r) + V(\vec{r}, \vec{R})] S_M(\vec{r}, \vec{R}), \quad (14)$$

and

$$S_M(\vec{r}, \vec{R}) = e^{-iH_e Z/\hbar v} S_{IM}(\vec{r}, \vec{R}). \quad (15)$$

It should be emphasized that we are not neglecting  $W(R)$  or the bending of the projectile that this force

produces. It is certainly incorrect to ignore  $W(R)$  if we wish to calculate  $f_{m,0}(\vec{q})$ , and we make no such claim. We merely point out that, in a consistent small-angle approximation, there is no need to include  $W(R)$  if one wishes to calculate the total cross section. This simplification allows tractable calculations without setting  $\vec{q} \cdot \vec{Z} = 0$ .

Of course, in a real atom, the forces are long range. However, this presents no real problem as we will illustrate with the hydrogen atom. The extension to the multielectron atom or ion is straightforward and will not be presented here.<sup>12</sup>

The scattering amplitude for an excited transition is

$$f_{m,0}(\vec{q}) = -\frac{2m_p}{4\pi\hbar^2} \int e^{-i\vec{q}\cdot\vec{R}} \chi_m^*(r) \times \left( \frac{Z_p e^2}{R} - \frac{Z_p e^2}{|\vec{R}-\vec{r}|} \right) S(\vec{r}, \vec{R}) d^3r d^3R. \quad (16)$$

First of all, we assume that the integral is convergent and exists; and, in particular, that we may therefore replace the upper limit of  $Z$  by  $Z_0$  a distance that is large compared to  $a_s$ . The lower limit is treated as follows. A heavy projectile is unaffected by the light electron. Its wave function  $\phi$  given by scattering from the nucleus alone would be  $\Gamma(1-in)e^{n\pi/2} F(in, 1, ik(R-Z))$ . Here  $n = -Z_p e^2/\hbar v$ . We assumed, in deriving Eq. (3), that the argument of the hypergeometric function was large, and hence arrive at

$$\lim_{Z \rightarrow -\infty} \phi = \exp[-in \ln(R-Z)] = \exp\left(in \int^Z \frac{dZ}{R}\right) \quad (17)$$

This is just another way of deriving the phase factor already discussed, but it brings out the correct boundary condition that we need. We now write

$$S_I = e^{-in \ln(R-Z)} S_{IM}(\vec{r}; \vec{B}, Z), \quad (18)$$

and note that we must have

$$\lim_{Z \rightarrow -\infty} S_{IM}(\vec{r}; \vec{B}, Z) = e^{in \ln(R-Z)} \chi_0(r), \quad (19)$$

and similarly

$$\lim_{Z \rightarrow -\infty} S_M(\vec{r}; \vec{B}, Z) = e^{in \ln(R-Z)} \chi_0(r). \quad (20)$$

We can now write as before

$$\begin{aligned} \sigma_{m,0} &= \int d^2B \left| \int \chi_m^*(r) S_{IM}(\vec{r}; \vec{B}, Z_0) \right. \\ &\quad \times \left. [(B^2 + Z_0^2)^{1/2} - Z_0]^{-in} d^3r \right|^2 \\ &= \int d^2B \left| \int \chi_m^*(r) S_{IM}(\vec{r}; \vec{B}, Z_0) d^3r \right|^2. \quad (21) \end{aligned}$$

We may therefore calculate the total cross section from a pseudoamplitude

$$f'_{m,0}(\vec{q}) = \frac{2m_p}{4\pi\hbar^2} \int d^2B d^3r \times \int_{-\infty}^{Z_0} dZ e^{-i\vec{q}\cdot\vec{R}} \chi_m^*(r) \frac{Z_p e^2}{|\vec{R}-\vec{r}|} S_M(\vec{r}, \vec{R}). \quad (22)$$

### III. THE CHESHIRE AND GLAUBER APPROXIMATIONS

In the Sec. II we have shown that we need to calculate  $S_M$  as accurately as possible from Eq. (14) with the boundary condition of Eq. (20). The generalization of this for a neutral atom of nuclear charge  $Z_N$  is that for large negative  $Z$  we need

$$S_M(\vec{r}_1, \dots, \vec{r}_N; B, Z) \sim A \chi_0(r_1, \dots, r_N) (R-Z)^{iZ_N}.$$

$A$  is the antisymmetrization operator.<sup>12</sup> We may split the phase factor involved into  $Z_N$  equal parts, which we associate with a single-particle wave function in an independent particle model; i.e., we write

$$\begin{aligned} S_M(\vec{r}_1, \dots, \vec{r}_N; \vec{B}, Z) &= A \prod_i S_i(\vec{r}_i; \vec{B}, Z) \\ &\sim A \prod_i \chi_i(r_i) (R-Z)^{in}. \end{aligned}$$

It then turns out that to calculate the total inelastic cross section for producing a  $K$ -shell hole, we can use Eqs. (14), (20), and (22); the only difference between the general atom and the hydrogen case is that  $\chi_0(r)$  is now given by  $e^{-r/a_s}$ . The essential character of the problem as a single-particle problem, though, is unchanged.

Writing

$$S_M(\vec{r}; \vec{R}) = \chi_0(r) \phi(\vec{r}; \vec{R})$$

we obtain

$$i\hbar v \frac{\partial \phi}{\partial Z} = \left( -\frac{\hbar^2}{2m_e} \nabla_r^2 + \frac{\hbar^2}{m_e a_s} \frac{\partial}{\partial r} - \frac{Z_p e^2}{|\vec{R}-\vec{r}|} \right) \phi(\vec{r}, \vec{R}).$$

The first two terms on the right-hand side of this equation are called the freely recoiling term (FT) and the binding term (BT),<sup>9</sup> respectively. The Glauber approximation sets FT and BT equal to zero and gives a solution

$$\phi_0 = (|\vec{R}-\vec{r}| - Z + z)^{in}.$$

The Cheshire approximation sets BT equal to zero and gives a solution

$$\phi_C = \Gamma(1+in) e^{-n\pi/2} F(-in, 1, ik_e (|\vec{R}-\vec{r}| - Z + z)).$$

We note that, if we are at such high energies that

the argument of  $F$  is large, then  $\phi_C = \phi_G$ . The reason that we can use this limit as an accurate approximation to derive Eq. (17) is the fact that  $k \gg k_e$ . It might be noted as an aside that if we are using electrons as projectiles, the only consistent approximation is to neglect FT as we have already neglected a term of this order in obtaining Eq. (3).

If we use  $\phi_C$  or  $\phi_G$  in Eq. (22), we note that we can take the limit  $Z_0$  to infinity without difficulty, because as long as  $q_z$  is nonzero, the integral converges. In an inelastic process,  $q_z$ , of course, is never zero. Changing variables ( $\vec{R} - \vec{r}$ ) to  $\vec{R}'$  in an exactly equivalent manner to the Born approximation as described by Merzbacher and Lewis, gives, in the Glauber approximation

$$f'_C(\vec{q}) = F(\vec{q}, m) t_C(\vec{q} + \vec{k}_e, \vec{k}_e), \quad (23)$$

where

$$F(\vec{q}, m) = \int \chi_m^*(r) \chi_0(r) e^{-i\vec{q} \cdot \vec{r}} d^3r, \quad (24)$$

and

$$t_C(\vec{q} + \vec{k}_e, \vec{k}_e) = (Z_p e^2 2m_p / \hbar^2) e^{n\pi/2} \times \Gamma(1 + in) |2q_z|^{in} (q^{-2})^{1+in}. \quad (25)$$

We thus deduce that the Glauber approximation for an inelastic cross section gives  $\sigma_G$ , where

$$\sigma_G = |\Gamma(1 + in)|^2 e^{n\pi} \sigma_B \quad (26)$$

and  $\sigma_B$  is the Born result. Applying this result to ionization gives  $r_{12} < 1$ .

To obtain the result of Eq. (25), it is necessary to perform the integral  $I$ , where

$$I = \int e^{-i\vec{q} \cdot \vec{r}} (r - z)^{in} r^{-1} d^3r. \quad (27)$$

This integral is straightforward to evaluate if we use the fact that

$$(r - z)^{in} = [\Gamma(-in)]^{-1} \int_0^\infty e^{t(z-r)} t^{-in-1} dt \quad (28)$$

In Eq. (28) we allow  $n$  a small positive imaginary part to be taken to zero at the end of the calculation. Thus

$$I = \frac{4\pi}{\Gamma(-in)} \int_0^\infty \frac{t^{-in-1} dt}{(\vec{q} + i\hat{k}t)^2 + t^2} \\ = \frac{4\pi}{\Gamma(-in)} \int_0^\infty dx \int_0^\infty e^{-(q^2 + 2iq_z t)x} t^{-in-1} dt. \quad (29)$$

In Eq. (29),  $\hat{k}$  is a unit vector in the  $z$  direction. Performing the  $t$  integration gives

$$I = 4\pi(2iq_z)^{in} \int_0^\infty dx e^{-q^2 x} x^{in} \\ = 4\pi(2iq_z)^{in} \Gamma(1 + in) (q^{-2})^{in+1}. \quad (30)$$

In our problem  $q_z$  is negative. Hence

$$I = 4\pi |2q_z|^{in} \Gamma(1 + in) (q^{-2})^{in+1} e^{n\pi/2}. \quad (31)$$

The Cheshire approximation gives

$$t_C(\vec{q} + \vec{k}_e, \vec{k}_e) = (Z_p e^2 2m_p e^{-n\pi/2} / \hbar^2) \Gamma(1 + in) (q^{-2})^{in+1} \\ \times (q^2 + 2\vec{k}_e \cdot \vec{q})^{in}, \quad (32)$$

a result which may be derived in an exactly analogous manner to that above, if we use

$$\frac{\Gamma(b-a)\Gamma(a)}{\Gamma(b)} F(a; b; x) = \int_0^1 e^{xt} (1-t)^{b-a-1} t^{a-1} dt.$$

We first note that if  $k_e$  is large, then  $t_C$  and  $t_G$  agree, apart from a factor  $(k_e)^{in}$ . This comes from the fact that we have written the Glauber wave function as  $(r - z)^{in}$ , as opposed to the asymptotic form for the Cheshire approximation  $[k_e(r - z)]^{in}$ .

We also note that  $t_C$  is discontinuous at the point where  $(q^2 + 2\vec{k}_e \cdot \vec{q})$  is zero. This discontinuity has been noted by other authors<sup>7</sup> for the Cheshire approximation, and for this integral by Ford,<sup>13</sup> who calculated the off-energy-shell  $t$ -matrix elements for a cutoff Coulomb potential to which the integral exactly corresponds. This latter statement merely reflects the fact that for a Coulomb potential cutoff at some large radius, say,  $R_0$ , the wave function  $\psi^{(+)}$  inside the potential region is apart from a phase factor,  $e^{ikz} F(-in, 1, ik(r - z))$ . The correspondence between the integral and the off-energy-shell  $t$  matrix then follows from the fact that

$$t(\vec{k}_e + \vec{q}, \vec{k}_e) \equiv \langle \vec{k}_e + \vec{q} | \frac{1}{r} | \psi_{k_e}^{(+)} \rangle.$$

The discontinuity in  $t_C$  is not physical. It is a result of our approximation in neglecting BT. The fact that the electron is bound is what makes the scattering off energy shell, and produces what is normally an "unphysical" discontinuity. This discontinuity has appeared because we have treated the electron as free (i.e., we have neglected BT) as far as the dynamics are concerned, but we have treated the electron as if it were not free as far as the kinematics are concerned. Nevertheless, the discontinuity is integrable and produces perfectly reasonable smooth total cross sections. In particular, if  $I_K > T_m$ , we never reach the discontinuity, and we derive

$$\sigma_C = |\Gamma(1 + in)|^2 e^{-n\pi} \sigma_B. \quad (33)$$

Applied to the ionization problem, this gives  $r_{12} > 1$ . For  $I_K < T_m$  the discontinuity is reached, and in the notation of Merzbacher and Lewis, we obtain the result of Eq. (33) for all those final-state energies such that

$$Q > W,$$

and the result of Eq. (26) if

$$Q < W.$$

Thus  $r_{12}$  is an average of the two results, depending on the kinematic region one is scattering into. It is interesting to note from our quasi-classical description of the process that Eq. (33) merely reflects that the electron density is modified over the Born result by a factor of  $|\Gamma(1+in)|^2 e^{-n\pi}$  at the point  $\vec{R} = \vec{r}$ . As the energy increases, the projectile can expel the electron at a larger and larger separation. The density increased over the Born result at the origin falls as  $|\vec{R} - \vec{r}|$  increases. By plotting

$$|\Gamma(1+in)|^2 e^{-n\pi} |F(-in, 1, ik_e(|\vec{R} - \vec{r}| - Z + z))|^2$$

as a function of its argument, we can find that the density starts *decreasing* over the Born result at a separation  $d$  for small  $n$  such that

$$k_e d \sim 1.$$

By the uncertainty principle, this corresponds to a momentum transfer such that

$$q \sim k_e.$$

This is exactly the point at which the effect changes sign due to the discontinuity. This reasoning, of course, does not explain why the change is discontinuous; it merely helps us to understand the sign change of the effect.

#### IV. APPLICATION TO IONIZATION

We applied the two approximations discussed above to the experiments mentioned previously.<sup>2</sup> We used standard wave functions for  $F(q, m)$  with

the usual screening charges  $Z_s$ , and performed the calculation in a way exactly analogous to the method of Merzbacher and Lewis.<sup>4</sup> The results for  $r_{12}$  are plotted in Figs. 1-3. The upper curve is the envelope obtained by using Eq. (33), and the lower curve is the Glauber result of Eq. (26). The Cheshire approximation, the solid line, which averages these two results, is seen to be in much better agreement with experiment than either envelope. However, the fit to the data is by no means convincing. In particular, with the possible exception of copper, none of the experiments show  $r_{12}$  less than unity at the high-energy end. However, the energies measured so far are comparatively low, and it would be of great interest to perform further experiments to test this theoretical prediction. Another reason for the lack of agreement between theory and experiment may be the approximate form factor  $F(q, m)$ . The device of replacing the other atomic electrons by a screening charge is highly suspect for the ejected electron. No provision is made for the Perey<sup>14</sup> effect, which can alter the wave functions considerably.

The major approximation, of course, is the neglect of BT. This can be estimated<sup>9</sup> to give errors of the order of  $(Z_n/Z_p)n^2$  and becomes important as the energy is lowered. Our next task will be to try and incorporate BT into the calculation.

In summary, we have shown that with the removal of the projectile nuclear repulsion, very simple analytic formulas may be obtained for the Cheshire and Glauber approximations within a consistent small-angle high-energy framework. Both of these approximations predict that  $r_{12}$  is less than unity at high energies; the Cheshire approximation is in better agreement with the experiments at lower energies. However, in order to correctly understand  $r_{12}$ , it is clear that advances must be made in both the description of the electronic wave functions used, and in the projectile's interaction with a bound electron.

\*Work supported by a grant from the Air Force Office of Scientific Research, No. AFSOR-73-2484.

<sup>1</sup>G. Basbas, W. Brandt, R. Laubert, A. Rakowski, and A. Schwarzschild, Phys. Rev. Lett. **27**, 171 (1971); G. Basbas, W. Brandt, and R. Laubert, Phys. Lett. A **34**, 277 (1971); G. D. Doolen, J. H. McGuire, M. Mittleman, Phys. Rev. A **7**, 1800 (1973); J. S. Hansen, Phys. Rev. Rev. A **8**, 822 (1973).

<sup>2</sup>C. W. Lewis, R. L. Watson, and J. B. Natowitz, Phys. Rev. A **5**, 1773 (1971); R. L. Watson and L. H. Toburen, Phys. Rev. A **7**, 1853 (1973).

<sup>3</sup>J. R. Macdonald, L. M. Winters, M. D. Brown, L. D.

Ellsworth, T. Chiao, and E. W. Pettus, Phys. Rev. Lett. **30**, 251 (1973).

<sup>4</sup>E. Merzbacher and H. W. Lewis, in *Encyclopedia of Physics*, edited by S. Flugge (Springer, Berlin, 1957), Vol. XXXIV, p. 106.

<sup>5</sup>K. Omidvar, H. L. Kyle, and E. C. Sullivan, Phys. Rev. A **5**, 1174 (1972).

<sup>6</sup>R. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1958), Vol. II.

<sup>7</sup>I. M. Cheshire, Proc. Phys. Soc. Lond. **84**, 89 (1964); M. R. C. McDowell and J. P. Coleman, *Introduction to*

*the Theory of Ion-Atom Collisions* (Elsevier, New York, 1970), p. 367 and Chap. 7.

<sup>8</sup>A. M. Halpern and J. Law, *Phys. Rev. Lett.* 31, 4 (1973); J. H. McGuire, *Phys. Rev. A* 8, 2760 (1973).

<sup>9</sup>J. F. Reading, *Phys. Rev. A* 1, 1642 (1970).

<sup>10</sup>H. Tai, R. H. Bassel, E. Gerjuoy, and V. Franco, *Phys. Rev. A* 1, 1819 (1970); J. M. McGuire, M. B. Hidalgo, G. D. Doolen, and J. Nuttall, *Phys. Rev. A* 7, 973 (1973).

<sup>11</sup>An alternative proof of this result which is more rigorous though, perhaps, not so instructive, is to use the generalized optical theorem by B. Bransden and J. F. Reading [*Phys. Rev.* 179, 982 (1969)]. Here

$$\sigma_{m10} = \text{Im} \left( \frac{1}{\hbar v} \right) \int d^3R d^3r d^3r' \chi_m^*(r') [V(\vec{r}', \vec{R}) + W(R)] \\ \times \psi(\vec{r}', \vec{R}) \chi_m(r) \psi^*(\vec{r}, \vec{R}).$$

The phase factor produced by  $W$  cancels as does the term proportional to  $W(R)$ , as it is real.

<sup>12</sup>J. F. Reading, *Phys. Rev. A* 8, 3262 (1973).

<sup>13</sup>W. F. Ford, *J. Math. Phys.* 7, 626 (1966).

<sup>14</sup>F. G. Perey and D. S. Saxon, *Phys. Lett.* 10, 107 (1964); N. Austen, *Phys. Rev.* 137, B752 (1965); J. F. Reading, *Phys. Rev.* 153, 1377 (1967).