

Binding effects in high-energy scattering applied to K -shell ionization*

J. Binstock and J. F. Reading

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

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The equation describing scattering of a fast ion by a K -shell electron, $i\hbar v \partial S_I / \partial Z = \exp(i\tilde{H}_e Z / \hbar v) V(\vec{r}, \vec{R}) \exp(-i\tilde{H}_e Z / \hbar v) S_I$, where $\tilde{H}_e(r) = -(\hbar^2/2m_e)\nabla_r^2 - (\hbar^2/m_e)[\partial \ln \chi_0(r)/\partial r]\partial/\partial r \equiv FT + BT$, is solved in the Glauber approximation by setting \tilde{H}_e to zero and in the Cheshire approximation by setting the binding term (BT) to zero. In this paper we solve for S_I including both the freely recoiling term (FT) and BT but neglecting their commutator. A divergence found with this method in a previous investigation of hydrogenlike atoms is removed as long as $Z_s e^2 / \hbar v < 1$. This limit represents a natural "threshold" in the method since for lower velocities the target electron is moving faster than the projectile. We apply the method in its lowest-order approximation to K -shell ionization by differently charged projectiles. A substantial improvement in the fit to the ratio r_{12} given by $r_{12} = \sigma(Z_1)Z_2^2 / \sigma(Z_2)Z_1^2$, $Z_1 > Z_2$, is found in comparison with the Glauber and Cheshire results. More experiments are needed with $Z_s \lesssim 20$ and at energies such that $Z_s e^2 / \hbar v < 1$ to test this new theory. The method has immediate applicability to any scattering problem in which the projectile has a classical trajectory.

I. INTRODUCTION

In this paper we extend a method proposed by one of us¹ to complete the sequence of improved approximations, i.e., Born, Glauber,² and Cheshire.³ The method is applied to K -shell ionization and gives an improved fit to the data⁴ when applied in lowest order to the energy region where $Z_s e^2 / \hbar v < 1$. We are at present engaged in calculating higher-order corrections, the results of which will be presented in later work.

A fundamental problem in scattering theory is that of scattering from bound systems. Recent experimental work on K -shell ionization by fast ions provides a beautiful testing ground for approximation schemes⁵ since by varying the projectile charge one can effectively explore the Born series. Furthermore, unlike the case for electron projectiles the constant-velocity approximation for the heavy projectile is accurate. This allows the unambiguous removal of the nucleus-projectile Coulomb repulsion leading to analytically integrable expressions for the scattering cross sections without the extensive use of computers.⁶ It is disturbing then to find that a sequence of widely used approximations, namely, Born, Glauber, and Cheshire, fail to fit⁶ the ratio r_{12} of cross sections $\sigma(Z_p)$ for K -shell ionization with projectiles of different charge Z_p . Here

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

The Glauber and Cheshire methods focus on the idea that for very fast projectiles the electron in the atom can be considered to be almost stationary. The mathematics of this physical idea is that we

can accurately treat the excitation energies of the electron as negligibly small or at least treat them approximately. In the Glauber approximation they are set to zero. In the Cheshire approximation the energies are calculated as if the electron had zero binding in the atom. Both these ideas are reasonable if the projectile is moving much faster than the electron in the atom but must be corrected if one wishes to extend the validity of the approximations to lower energies. In this paper we show how this may be done by not only allowing finite electron excitation energies as Cheshire does but also treating the binding of the electron in the atom. The method used is one already discussed by one of us but here we show how to remove a divergence difficulty encountered in that investigation.¹ We find, however, that we cannot extend the basic idea below a critical velocity such that $Z_s e^2 / \hbar v < 1$. This seems to us a natural "threshold" in the method since at this energy the projectile and the electron are moving at the same speed.⁷ Presumably below this projectile energy an appropriate starting point is to consider the *projectile* to be "at rest" and make corrections to that.

We apply the method in lowest order to K -shell ionization. The improved fit to the experimental data is extremely encouraging and we are now working on the higher-order corrections. A nice feature of our approach is that only three-dimensional integrals need be done numerically to obtain excitation cross sections and only four-dimensional integrals need be done to evaluate total ionization cross sections. This is two more dimensions than need be done in Born calculations

of the same processes.

Another interesting point is that the Cheshire amplitude exhibited a discontinuity^{6,8} when $Q = W$. (Here we use the notation of Merzbacher and Lewis.⁹) With this new correction this discontinuity is removed allowing the application of the method to differential cross sections.

Finally we note that though we are first applying this new theory to K -shell ionization by fast ions because we believe this is the most severe test that present experimental data provide, it is by no means limited to K -shell ionization. Elastic and excitation processes by both ions and electrons can essentially be treated in the same manner and of course we are not restricted to atomic physics. Indeed any physical process such as heavy-ion scattering, or nucleon-nucleon scattering in the quark model, or deuteron-nucleus scattering, may be treated in the same way if the path of the projectile can be accurately described with a classical trajectory.

II. BINDING TERM

The equation we need to solve to describe a fast projectile of momentum \vec{k}_0 , located at \vec{R} , scattering from a target particle located at \vec{r} , bound to the origin of our coordinate system with a single-particle wave function $\chi_0(r)$ is¹

$$i\hbar v \frac{\partial S(\vec{r}, \vec{R})}{\partial Z} = [\tilde{H}_e(r) + V(\vec{r}, \vec{R})] S(\vec{r}, \vec{R}), \quad (1)$$

$$\tilde{H}_e(r) = -\frac{\hbar^2}{2m_e} \nabla_r^2 - \frac{\hbar^2}{m_e} \frac{\partial \ln \chi_0(r)}{\partial r} \frac{\partial}{\partial r} \quad (2)$$

$$\equiv \text{FT} + \text{BT}. \quad (3)$$

Here the single-particle wave function ψ describing the system is given by

$$\psi = e^{i\vec{k}_0 \cdot \vec{R}} \chi_0(r) S(\vec{r}, \vec{R}) \quad (4)$$

and we have made this factorization with the idea in mind that if the projectile is much faster than the bound electron that $S(\vec{r}, \vec{R})$ is a slowly varying function.

The Glauber approximation to Eq. (1) is to set \tilde{H}_e to zero. If $V(\vec{r}, \vec{R})$ is a Coulomb force for a neutral system this leads to

$$S \approx S_g = \left(\frac{|\vec{R} - \vec{r}| - Z + z}{R - Z} \right)^{in}, \quad (5)$$

where here

$$n = -Z_p e^2 / \hbar v \quad (6)$$

and

$$V(\vec{r}, \vec{R}) = Z_p e^2 \left(\frac{1}{R} - \frac{1}{|\vec{R} - \vec{r}|} \right). \quad (7)$$

Cheshire³ solved Eq. (1) by setting the binding term (BT) to zero, but kept the freely recoiling term (FT).

For the Coulomb problem this approximation gives

$$S \approx S_C = e^{-\pi/2} \Gamma(1 + in) \times F(-in, 1, ik_e |\vec{R} - \vec{r}| - ik_e Z + ik_e z). \quad (8)$$

Here,

$$\vec{k}_e = m_e \vec{v} / \hbar. \quad (9)$$

We may solve Eq. (1) if we neglect FT by working in the interaction picture.¹ Defining

$$S_I = e^{i\tilde{H}_e Z / \hbar v} S \quad (10)$$

we obtain

$$i\hbar v \frac{\partial S_I}{\partial Z} = e^{i\tilde{H}_e Z / \hbar v} V e^{-i\tilde{H}_e Z / \hbar v} S_I \equiv V_I S_I. \quad (11)$$

If we now write

$$\text{BT} \equiv -\frac{\hbar^2}{m_e} \frac{\partial \ln \chi_0(r)}{\partial r} \frac{\partial}{\partial r} = \frac{\partial}{\partial p}, \quad (12)$$

we can solve for p to give

$$p = -\frac{m_e}{\hbar^2} \int^r dr \left(\frac{\partial \ln \chi_0(r)}{\partial r} \right)^{-1}. \quad (13)$$

Inverting this function gives

$$r = F(p). \quad (14)$$

If in Eq. (11) we now set FT to zero in \tilde{H}_e , we are just left with an exponentiated shift operator in the variable p . This leads to

$$i\hbar v \frac{\partial S_I}{\partial Z} = V(\hat{r} F(p + iZ/\hbar v), \vec{R}) S_I. \quad (15)$$

Equation (15) may be solved giving

$$S_I = \exp \left[\frac{-i}{\hbar v} \int_{-\infty}^Z V(\hat{r} F(p + iZ'/\hbar v), \vec{R}) dZ' \right]. \quad (16)$$

Here we use the notation $\vec{R}' \equiv (\vec{B}, Z')$.

Perhaps a concrete example will make this procedure clearer to the reader. Consider $\chi_0(r) = e^{-r^2/a_s^2}$; then

$$p = \frac{m_e}{\hbar^2} \int^r dr \frac{a_s^2}{2r} = \frac{m_e a_s^2 \ln r}{2\hbar^2} \quad (17)$$

and

$$r = e^{2\hbar^2 p / m_e a_s^2}. \quad (18)$$

Hence

$$V_I \approx V(\vec{r} e^{i2Z/k_e a_s^2}, \vec{R}). \quad (19)$$

If the potential V were a Coulomb force, this particular $\chi_0(r)$ would not present any problem in particular for large Z :

$$V(\vec{r} e^{2iZ/k_e a_s^2}, \vec{R}) \sim Z_p e^2 [|\vec{Z}|^{-1} - |\vec{Z} - \vec{r} e^{2iZ/k_e a_s^2}|^{-1}] \sim O(|Z|^{-2}), \quad (20)$$

and the integral in Eq. (16) would exist.

Here we use a convenient notation

$$|\vec{A}| = (\vec{A} \cdot \vec{A})^{1/2}, \quad (21)$$

implying that by $|\vec{A}|$ we mean the square root of the scalar product of \vec{A} with itself, *not* the square root of the scalar product of \vec{A} and \vec{A}^* . This we will denote by

$$\|\vec{A}\| = (\vec{A} \cdot \vec{A}^*)^{1/2}. \quad (22)$$

However, it turns out that for any binding potential which allows continuum scattering states the procedure outlined above gives trouble for Coulomb forces. This can be illustrated with a hydrogen-like wave function, $\chi_0(r) = e^{-r/a_s}$. For this case

$$\begin{aligned} e^{i\vec{H}_e Z/\hbar v} V(\vec{r}, \vec{R}) &\approx e^{iZ(\text{FT})/\hbar v} e^{iZ(\text{BT})/\hbar v} V(\vec{r}, \vec{R}) \\ &\approx e^{-iZ\nabla_r^2/2k_e} Z_p e^2 [|\vec{R}|^{-1} - |\vec{R} - \vec{r} - i\vec{c}Z|^{-1}]. \end{aligned} \quad (26)$$

Now for large Z in this approximation,

$$\begin{aligned} e^{i\vec{H}_e Z/\hbar v} V(\vec{r}, \vec{R}) &\approx Z_p e^2 e^{-iZ\nabla_r^2/2k_e} [\|Z\|^{-1} - \|Z\|^{-1} |\hat{k} - i\vec{c}|^{-1}] \\ &\approx Z_p e^2 \left\{ \|Z\|^{-1} - \sum_{l=0}^{\infty} \|Z\|^{-1} \exp\left[-\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right] \frac{iZ}{2k_e} P_l(\hat{k} \cdot \hat{c})(ic)^l \right\} \\ &\approx Z_p e^2 \sum_{l=1}^{\infty} P_l(\hat{k} \cdot \hat{c})(ic)^l \frac{\Gamma(l/2 + \frac{3}{2})}{\Gamma(l + \frac{3}{2})} \left(\frac{ik_e r^2}{2Z} \right)^{1/2} \|Z\|^{-1}. \end{aligned} \quad (27)$$

This result is derived in detail in Appendix A. Because of the $Z^{-1/2}$ factor introduced in Eq. (27) the potential now has perfectly satisfactory properties for large Z . Of course, the Legendre expansion employed is only good if

$$c \leq 1.$$

If this inequality is not satisfied we run once again into divergence problems.

These divergences arise because in an attempt to expand the exponential in powers of v^{-1} we are also expanding in a power series in Z .¹ Thus at large Z , no matter how large v , eventually the argument of the exponential will become large. This is just the mathematical consequence of the fact that the target electron will of course complete many orbits as the projectile approaches from infinity and the approximation that it is "at rest" is invalid. Nevertheless the physics of the situation is that the important interaction region is probably restricted to some region of the dimensions of the atom⁶ and during the time taken

$$V_I \approx Z_p e^2 [|\vec{R}|^{-1} - |\vec{R} - \vec{r} - i\vec{c}Z|^{-1}], \quad (23)$$

and for large Z ,

$$V_I \sim Z_p e^2 [|\vec{Z}|^{-1} - |\vec{Z} - i\vec{c}Z|^{-1}] \sim O(|\vec{Z}|^{-1}). \quad (24)$$

Here

$$c = (k_e a_s)^{-1} = (Z_s e^2/\hbar v) = (-Z_s n/Z_p), \quad (25)$$

and

$$\vec{c} = c\hat{r}.$$

Such a potential does not fall off sufficiently rapidly for large Z to make the integral in Eq. (16) convergent. This result has been discussed at some length in Ref. 1.

We now show how this divergence can be removed if c is less than unity. The idea is to keep both FT and BT in the exponential but neglect their commutator. A quantity we will need is $e^{i\vec{H}_e Z/\hbar v} \times V(\vec{r}, \vec{R})$. We can approximately evaluate it thus:

for the projectile to cross this interaction region the electron might be considered to be at rest in the first approximation. Thus the divergences might be viewed as more of a nuisance than a major difficulty. An alternative procedure would be to use our technique to produce a wave function for small Z and match it on to another wave function for large Z . We could not discover a convenient way of doing this. However, the philosophy of Glauber² is that such worries are unnecessary if one only intends to use the wave function to substitute into a t -matrix-type expression. What is essential, Glauber argues, is to have a wave function good in the interaction region in that case. And in that regard we remark that while our solution is probably not good for large Z its range of validity in this respect is much larger than for the Glauber or Cheshire approximations.

Of course we have neglected a commutator in deriving Eq. (27) and presumably if we kept all higher-order commutators we would always produce correctly convergent potentials. However,

as the reader will have no doubt grasped, this procedure is not trivial to carry out in practice.

That BT and FT do not commute can be illustrated by operating with the exponentiated FT before BT. This leads once again to divergence difficulties.

III. SECOND BORN TERM

In this section we illustrate the procedures outlined above in a calculation including the second Born term for S. We have

$$S_2 = 1 - in \int_{-Z_0}^Z e^{i\tilde{H}_e(Z' - Z) / \hbar v} \times (|\vec{R}' - \vec{r}|^{-1} - |\vec{R}'|^{-1}) dZ'. \quad (28)$$

It is convenient to treat the nuclear repulsion and the electron-projectile potential separately so we introduce an infinite cutoff $-Z_0$ as a lower bound on the integral. If everything is correct our answer should not depend on Z_0 , and it does not.

$$a_l(q, cZ'') = \int d^3\rho (-i)^l (2l+1) j_l(q\rho) P_l(\hat{c} \cdot \hat{\rho}) |\vec{\rho} + i\vec{c}Z''|^{-1} \quad (32)$$

$$= 2\pi \int_0^\infty \rho^2 d\rho \int_{-1}^{+1} dx (-i)^l (2l+1) j_l(q\rho) P_l(x) (\rho^2 + 2icZ''\rho x - c^2Z''^2)^{-1/2}. \quad (33)$$

We must now proceed with a little care. If

$$cZ'' < \rho, \quad (34)$$

we may correctly write

$$(\rho^2 + 2icZ''\rho x - c^2Z''^2)^{-1/2} = \rho^{-1} \sum_{l=0}^\infty P_l(x) \times \left(\frac{-icZ''}{\rho} \right)^l. \quad (35)$$

On the other hand, if

$$cZ'' > \rho, \quad (36)$$

then

$$a_0(q, cZ'') = 4\pi \int_0^{lcZ''} d\rho \rho j_0(q, \rho) [1 - (1 - \rho^2/c^2Z''^2)^{1/2}] + 4\pi \int_{lcZ''}^\infty d\rho \rho j_0(q, \rho) = \frac{4\pi}{q^2} \int_0^1 dx \cos[qcZ''(1-x^2)^{1/2}]. \quad (38)$$

For the purposes of this present calculation a_0 is all we will need as we shall ignore all the higher-order terms in our Legendre expansion. We are presently engaged in calculating the effect of these and will report on this in later work. Here we are

We therefore write

$$S_2 = S_e + S_N,$$

where

$$S_N = -in \ln(|R - Z| / 2Z_0) \quad (29)$$

and

$$S_e \approx \left[1 - \frac{in}{(2\pi)^3} \int_0^{Z_0} dZ'' \int d^3q d^3\rho e^{iZ'' \nabla_r^2 / 2k_e} \times e^{i\hat{q} \cdot (\vec{R} - \vec{r} - \vec{Z}'')} e^{-i\hat{q} \cdot \vec{\rho}} |\vec{\rho} + i\vec{c}Z''|^{-1} \right]. \quad (30)$$

We expand the integral on $\vec{\rho}$ in terms of a Legendre expansion in the function $P_l(\hat{q} \cdot \hat{c})$, i.e.,

$$\int d^3\rho e^{-i\hat{q} \cdot \vec{\rho}} |\vec{\rho} + i\vec{c}Z''|^{-1} = \sum_{l=0}^\infty a_l(q, cZ'') P_l(\hat{q} \cdot \hat{c}). \quad (31)$$

Here

$$(\rho^2 + 2icZ''\rho x - c^2Z''^2)^{-1/2} = \frac{1}{(-c^2Z''^2)^{1/2}} \sum_{l=0}^\infty P_l(x) \left(\frac{\rho}{-icZ''} \right)^l. \quad (37)$$

The reason is that the $|\vec{\rho} + i\vec{c}Z''|$ is a two-branched function. Which sheet we arrive at from analytically continuing from the inequality of Eq. (34) to Eq. (36) depends on the sign of x . That we must analytically continue the square root of course goes back to our use of the shift operator when we assumed our function $|\vec{R} - \vec{r}|$ was infinitely differentiable.

However, once having realized this, it is straightforward to proceed, and in particular we derive

mainly concerned with presenting the method and demonstrating its practicability. We do note though that a_0 is the leading-order term, since if we set c to zero we would obtain the Cheshire approximation to S in Eq. (30), and all the other a_l 's

are zero in this limit. It might be argued that since we are trying to calculate a correction term of order c and since Eq. (38) is "obviously" second order in c we should first of all be concerned with a calculation of a_1 , setting c to zero in a_0 . We do not have a perturbation theory in c in mind though. To begin with, since the Cheshire amplitude has a discontinuity⁸ in it there is not a simple analytic behavior of the corrected amplitude at c equal to zero. In fact it contains terms proportional to

$$S_e = \left[1 - \frac{in}{2\pi^2} \int_0^{Z_0} dZ'' \int d^3q \int_0^1 dx \exp\left(\frac{-iq^2 Z''}{2k_e} + i\vec{q} \cdot (\vec{R} - \vec{r} - \vec{Z}'')\right) \cos[(qZ''(1-x^2)^{1/2})q^{-2}] \right]. \quad (39)$$

We can now make use of all the work that has been done on the Cheshire approximation.⁸ We write, introducing a "dummy" angular \vec{c} dependence,

$$\int_0^1 dx \cos[qcZ''(1-x^2)^{1/2}] = \frac{1}{4\pi} \frac{\partial}{\partial c} \left[c \int d\Omega_c \int_0^1 dx e^{i\vec{q} \cdot \vec{c}(1-x^2)^{1/2} Z''} \right].$$

With this substitution we see that the only modification that we have over the Cheshire result as far as the \vec{q} and Z'' integrations are concerned is that we have an extra factor in the $e^{-i\vec{q} \cdot \vec{Z}''}$ term, i.e.,

$$e^{-i\vec{q} \cdot \vec{Z}''} \rightarrow e^{-i\vec{q} \cdot \vec{Z}'' \cdot [\hat{k} - \vec{c}(1-x^2)^{1/2}]} \quad (40)$$

This leads to a "rule": replace \hat{k} by $\hat{k} - \vec{c}(1-x^2)^{1/2}$ and the answer is the same as for the Cheshire approximation. Of course, since we can work out all the integrals involving \vec{q} and Z'' in the Cheshire

$(c^2)^{1/2}$ because of this.

Furthermore the angular dependence of the higher-order terms in the expansion leads to certain orthogonality properties which will probably reduce their effect in K -shell ionization, though only a detailed calculation will confirm whether this is really true.

Working in this lowest-order approximation then we substitute Eqs. (31) and (38) into Eq. (30). We replace ∇_r^2 by $-q^2$ and arrive at

result to obtain the second Born term [e.g., by an expansion in n of Eq. (8)], similarly we can work out all the integrals in Eq. (39). Furthermore, since we could in the Cheshire approximation substitute S_c into an expression for the scattering amplitude $\langle \chi_f | V | \psi \rangle$ and work out all the integrals on \vec{R} and \vec{r} so we can here. And of course we end up with an expression to first order in n for the cross section σ_K for producing a K -shell hole, as simple as the Cheshire result, viz.,

$$\sigma_K = \int dW dQ \frac{d^2\sigma_B(Q, W)}{dW dQ} \left[1 - \frac{1}{4\pi} \frac{\partial}{\partial c} \left(c \int d\Omega_c \int_0^1 dx n\pi [1 - 2\vec{c} \cdot \hat{k}(1-x^2)^{1/2} + c^2(1-x^2)]^{-1/2} \right. \right. \\ \left. \left. \times \text{sgn}[q^2 + 2\vec{k}_e \cdot \vec{q} - 2k_e \vec{c} \cdot \vec{q}(1-x^2)^{1/2}] \right) \right]. \quad (41)$$

Here Q and W are defined as in Merzbacher and Lewis⁹ in terms of the momentum transfer \vec{q} given to the projectile, and the kinetic energy of the ejected electron. That the factor $[1 - 2\vec{c} \cdot \hat{k}(1-x^2)^{1/2} + c^2(1-x^2)]^{-1/2}$ should be present in Eq. (41) is not obvious from the rule but is correct as can be shown by carrying out all the integrations necessary to arrive at the result. This is done in Appendix B.

The most important point to notice about Eq. (41) is that the discontinuity or "sign function" present in the Cheshire approximation as $(1 + 2\vec{k}_e \cdot \vec{q}/q^2)$ changes sign is still here, but it no longer produces a discontinuity in the differential cross section as the Cheshire approximation did. The approximate treatment described is good enough to remove this unfortunate aspect of the Cheshire approach which by neglecting binding effects in the dynamics but not in the kinematics gave this unphysical discontinuity.

It turns out that we can do one more integration in Eq. (41) simply and one more after that if we are prepared to introduce derivatives of elliptic integrals. We found that in the absence of simple polynomial formulas for the elliptic integrals it was simpler to leave the problem as the four-dimensional integral given in Appendix B. The results of applying this method to the calculation of ν_{12} are presented in Sec. IV.

IV. K -SHELL IONIZATION AND ν_{12}

The ratio ν_{12} defined in Sec. I provides an extremely severe test for any theory of scattering from bound systems.⁵ Furthermore by varying the charges of the projectiles involved we can effectively explore the Born series as a power series in the coupling constant n . Such freedom is a nuclear physicist's dream but an atomic physicist's reality. In Figs. 1-5 we plot the results for Glauber, Cheshire, and this approximation and

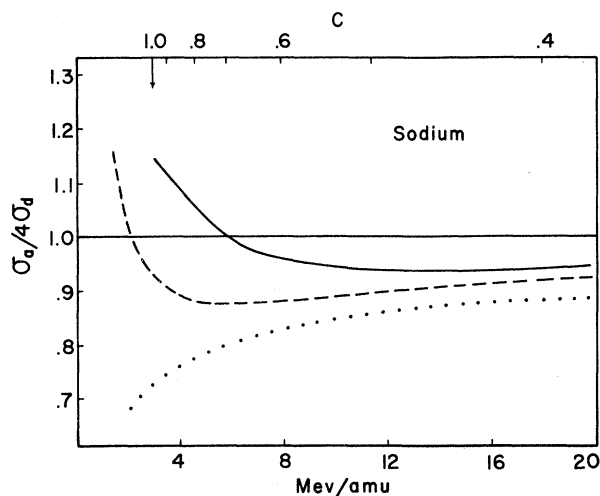


FIG. 1. Theoretical results for α -particle and deuteron scattering in sodium. Dotted line, obtained from the Glauber approximation; broken line, from the Cheshire approximation. Solid curve, work of this paper. The figure illustrates that r_{12} is predicted to be below 1 at high energies.

compare them with the available experimental results for alpha and deuteron scattering from sodium, chlorine, calcium, titanium, and copper.

The first thing to note is that in the region $c < 1$ there is quite a paucity of experimental data. This is in part due to the comparative difficulty of accurately measuring the x-ray yield provided by K -shell ionization for atoms with Z_s less than 20. The chlorine and calcium data for example are "relative." However, probably the most overwhelming reason for not performing experiments at higher energies is the "misconception" that the

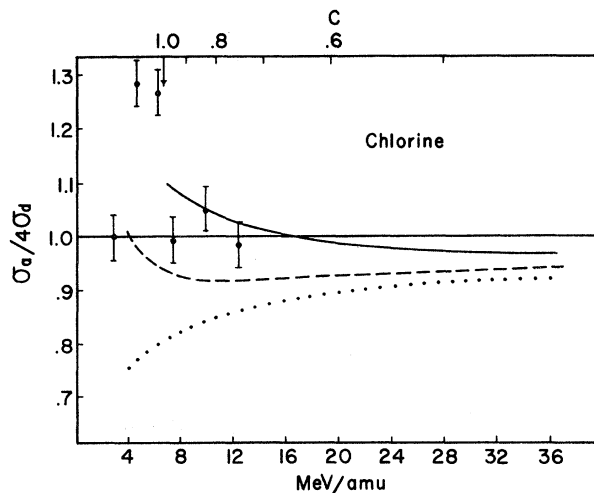


FIG. 2. Same as for Fig. 1, but for chlorine. The experimental points are taken from Ref. 4.

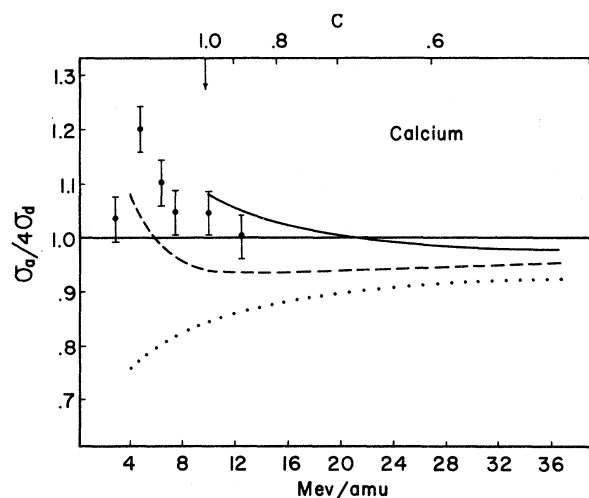


FIG. 3. Same as for Fig. 1, but for calcium. The experimental points are taken from Ref. 4.

Born approximation is supposed to be valid at these energies. Whether the second Born term is indeed negligibly small in this region only the experiments will finally show but certainly none of the three approximations described here would lead one to believe that it is supposed to be. On the contrary, for sodium, Fig. 1, at 10–20 MeV, it is predicted that r_{12} should be less than unity by 5% and experiments with more highly charged ions would certainly increase this.

The theoretical prediction⁶ that r_{12} should be less than unity at high energies as the Glauber theory says is still maintained by this new approximation but the high-energy crossover point is moved up somewhat over the Cheshire result.

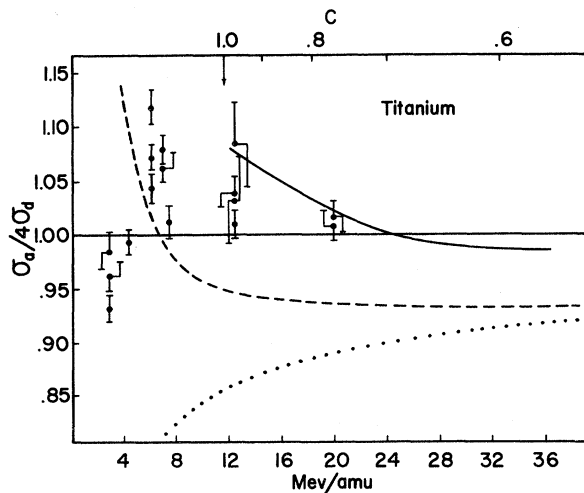


FIG. 4. Same as for Fig. 1, but for titanium. The experimental results are taken from Ref. 4.

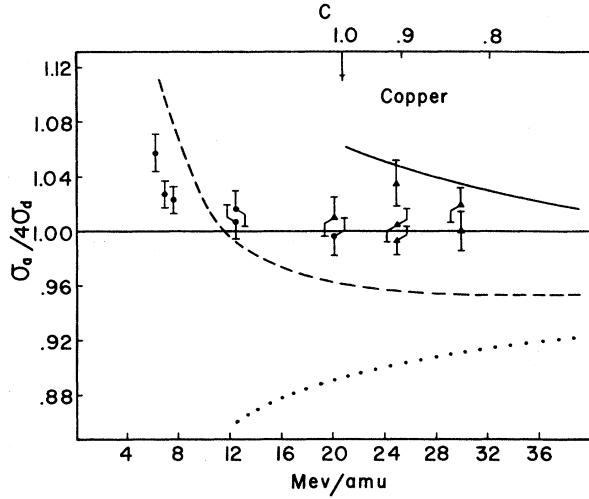


FIG. 5. Same as for Fig. 1, but for copper. The black dots are the experimental points taken from Ref. 4. The triangles are new unpublished data very kindly given to us by R. L. Watson and T. Hardt.

This seems to be in agreement with the experiments. *Over all of course this new approximation is seen to give a substantial improvement in the agreement with the experiments, though there is still plenty of room for further theoretical work.*

This result is certainly encouraging enough for us to try to keep higher-order terms and extend the method beyond the second Born approximation.

When this is done we will try the approach on excitation processes and then on systems other than the Coulomb type.

V. CONCLUSION

We have presented a method which allows extension of the Glauber method to lower velocities but not lower than the velocity of the bound particle. For scattering from hydrogenlike atoms the discontinuity found in the differential cross section for the Chesire method is removed. An application to *K*-shell ionization in the theory's lowest order shows that only a four-dimensional integral need be evaluated numerically to obtain the total cross section for producing a *K*-shell hole. The fit to the experimental data leaves room for improvement but is substantially better than with the Glauber or Chesire approximation. The theoretical prediction that r_{12} will approach unity at high energies from below 1 is still maintained.

APPENDIX A

We show here that for large Z

$$I \equiv e^{-iZ\nabla_r^2/2k_e} P_l(\hat{q} \cdot \hat{r}) = P_l(\hat{q} \cdot \hat{r}) \frac{\Gamma(l/2 + \frac{3}{2})}{\Gamma(l + \frac{3}{2})} \left(\frac{ik_e r^2}{2Z} \right)^{1/2}.$$

We first note that

$$\begin{aligned} & e^{-iZ\nabla_r^2/2k_e} P_l(\hat{q} \cdot \hat{r}) \\ &= P_l(\hat{q} \cdot \hat{r}) \exp \left[\left(-\frac{1}{r^2} \frac{\partial r^2}{\partial r} \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) \frac{iZ}{2k_e} \right] \\ &= P_l(\hat{q} \cdot \hat{r}) \exp \left[\left(-\frac{1}{r^2} \frac{\partial r^2}{\partial r} \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) \frac{iZ}{2k_e} \right] \int_0^\infty dr' \delta(r-r') \\ &= P_l(\hat{q} \cdot \hat{r}) \exp \left[\left(-\frac{1}{r^2} \frac{\partial r^2}{\partial r} \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) \frac{iZ}{2k_e} \right] \frac{2}{\pi} \int_0^\infty dr' r'^2 \int_0^\infty dp p^2 j_l(pr) j_l(pr') e^{-\epsilon p^2} \\ &= P_l(\hat{q} \cdot \hat{r}) \frac{2}{\pi} \int_0^\infty dr' r'^2 \int_0^\infty dp^2 e^{-p^2(\epsilon - iZ/2k_e)} j_l(pr) j_l(pr'). \end{aligned}$$

It should be understood that ϵ can only be set to zero after the integration. The p integration can be performed¹⁰ to give

$$I = P_l(\hat{q} \cdot \hat{r}) \int_0^\infty \frac{dr' r'^2 e^{-(r^2+r'^2)/4(\epsilon - iZ/2k_e)}}{(rr')^{1/2} 2(\epsilon - iZ/2k_e)} I_{l+1/2} \left(\frac{rr'}{2(\epsilon - iZ/2k_e)} \right).$$

The r' integration can now be performed.¹⁰ It is convergent as r' goes to infinity because the Gaussian cutoff overwhelms the exponential blow up of the Bessel function. It gives

$$I = P_1(\hat{q} \cdot \hat{r}) \frac{\Gamma(l/2 + \frac{3}{2})}{\Gamma(l + \frac{3}{2})} \left(\frac{ik_e \gamma^2}{2Z} \right)^{1/2} \left[1 + O\left(\frac{1}{Z}\right) \right],$$

which is the desired result for large Z .

APPENDIX B

Here we fill in some of the steps in the derivation of Eq. (41) and then show how Eq. (41) may be reduced to a four-dimensional quadrature.

The Cheshire-type integral we have to consider from Eqs. (39) and (40) is of the form

$$I = \frac{-in}{2\pi^2} \int_0^{Z_0} dZ'' \int d^3q q^{-2} \times e^{-i\alpha^2 Z'' / 2k_e + i\mathbf{q} \cdot (\vec{R} - \vec{r} - Z'' \vec{K})},$$

where

$$\vec{K} = \hat{k} - \hat{c}(1 - x^2)^{1/2}.$$

We perform the integration over \vec{q} by first of all integrating on the angles and then using the fact that

$$\frac{\sin(\alpha q y)}{q \alpha} = \int_0^y \cos(y \alpha q) dy,$$

where

$$\alpha = |\vec{R} - \vec{r} - Z'' \vec{K}|,$$

to allow us to perform the q integration. We obtain

$$\begin{aligned} S_2 &= -i \int_0^1 dx \int \frac{d\Omega_c}{4\pi} \frac{\partial}{\partial c} \left[\frac{nc}{K} \left(\ln |R - Z| + \ln k_e K - i\pi/2 - \Gamma'(1) + E_1(\rho k_e K) \right) \right] \\ &= \int_0^1 dx \int \frac{d\Omega_c}{4\pi} \frac{\partial}{\partial c} \left[cn \frac{\partial}{\partial n} \left[\Gamma(1 + in/K) e^{-n\pi/2K} F(-in/K, 1, ik_e K_\rho) (K k_e (R - Z))^{-in/K} \right] \Big|_{n=0} \right]. \end{aligned} \quad (42)$$

By writing Eq. (42) as a derivative with respect to n we illustrate the simplicity of the rule of Eq. (40); i.e., the second Born term for the wave function is, apart from the integrations over Ω_c and x still to be performed, the same as Cheshire's with the proviso that n is replaced by n/K and \vec{k}_e is replaced by $k_e \vec{K}$. Using this fact together with the knowledge that keeping only terms up to third order in n in Cheshire gives⁶

$$\sigma_K = \int dW dQ \frac{d^2 \sigma_B(Q, W)}{dQ dW} [1 - n\pi \text{sgn}(q^2 + 2\vec{k}_e \cdot \vec{q})],$$

$$\sigma_K = \int dW dQ \frac{d^2 \sigma_B(Q, W)}{dW dQ} \left[1 + \int_0^1 dx' F(c(1 - x'^2)^{1/2}) \right],$$

$$I = -in \left(\frac{2k_e}{\pi} \right)^{1/2} e^{-i\pi/4} \int_0^1 dy \int_0^{Z_0} dZ'' Z''^{-1/2} \times e^{i\alpha^2 y^2 k_e / 2Z''}.$$

We would like to take the limit as $Z_0 \rightarrow \infty$ but may not yet because the integral over y would diverge at $y=0$. Instead we rewrite the integral on y in two parts: an integral I_1 from zero to infinity and an integral I_2 from one to infinity to be subtracted off. We can now perform the y integration in I_1 and the Z'' integration in I_2 as in the latter case we may correctly take Z_0 to be infinite. We obtain

$$I = I_1 - I_2 = -in \left[\int_0^{Z_0} \frac{dZ''}{\alpha} - \frac{2}{K} \int_1^\infty e^{i\rho k_e y^2} \frac{dy}{y} \right],$$

where

$$\rho = |\vec{R} - \vec{r}| - \hat{K} \cdot [\vec{R} - \vec{r}].$$

Performing the Z'' integration and using the fact that

$$\Gamma'(1) = \int_1^\infty \frac{e^{-t}}{t} dt - \int_0^1 \frac{1 - e^{-t}}{t} dt,$$

we obtain

$$\begin{aligned} I &= \frac{-in}{K} \left[\ln \left(\frac{2Z_0}{\rho} \right) - \Gamma'(1) - \ln \left(\frac{i}{k_e K_\rho} \right) \right. \\ &\quad \left. + \int_0^1 \frac{e^{i\rho k_e K t} - 1}{t} dt \right]. \end{aligned}$$

Thus

we derive Eq. (41).

Equation (41) can be reduced to a four-dimensional integral, by performing the $\partial/\partial c$ differentiation and then integrating one term by parts with respect to the $\hat{c} \cdot \hat{k}$ angular variable. If we write

$$\hat{c} \cdot \hat{k} = x,$$

$$\hat{c} \cdot \hat{q} = x \hat{q} \cdot \hat{k} + \cos \phi (1 - x^2)^{1/2} [1 - (\hat{q} \cdot \hat{k})^2]^{1/2}$$

so that $d\Omega_c = dx d\phi$, it happens that the ϕ integration can be easily done. The result is

where, if $c' = c(1 - x'^2)^{1/2}$,

$$F(c') = -n\pi \operatorname{sgn}(\gamma(c')) \theta(|\gamma(c')| - |\lambda|) + n \int_{x_1(c')}^{x_2(c')} \frac{dx[\gamma(c')(1 - c'x) + \lambda(c' - x)]\theta(1 - |\gamma(c')|)}{(1 + c'^2 - 2c'x)^{1/2} \{ [x - x_1(c')][x_2(c') - x] \}^{1/2} (1 - x^2)},$$

$$\left. \begin{array}{l} x_2(c') \\ x_1(c') \end{array} \right\} = \gamma(c')\lambda \pm [1 - \gamma^2(c')]^{1/2}(1 - \lambda^2)^{1/2},$$

$$\gamma(c') = \frac{q^2 + 2\vec{k}_e \cdot \vec{q}}{2q k_e c'} = \frac{(Q - W)}{2Q^{1/2}} \frac{Z_S e^2}{\hbar v} \frac{1}{c'},$$

$$\lambda = \hat{q} \cdot \hat{k} = \frac{-W}{2Q^{1/2}} \frac{Z_S e^2}{\hbar v},$$

and Q and W are as defined in Merzbacher and Lewis.⁹ Here θ is the usual step function.

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