PHYSICAL REVIEW A VOLUME 7, NUMBER 3 MARCH 1973

Glauber Theory of Atomic-Hydrogen Ionization by Electron Impact*†

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(Received 16 October 1972)

The high-energy Glauber, or eikonal, approximation is used to derive formulas for the scattering amplitude and cross section for the ionization of atomic hydrogen by electron impact. The scattering amplitude is expressed in terms of a double infinite sum of hypergeometric functions which may be evaluated on a computer. Total cross sections may be obtained by squaring the scattering amplitude and integrating over five final-state variables. Three integrals are trival and two must be done numerically. At sufficiently high energies, the Glauber result reduces to the expressions found in the simpler, but more restrictive, Coulomb–Born approximation.

I. INTRODUCTION

In recent years there has been success in applying the Glauber approximation[1] to atomic physics. In 1968 Franco computed[2] cross sections for the elastic scattering of electrons from hydrogen. Inelastic electron-hydrogen scattering was done[3] in 1970 by Tai, Bassel, Gerjuoy, and Franco. Following the mathematical technique[4] of Thomas and Gerjuoy, Franco developed[5] a procedure for doing elastic and inelastic electron-atom cross sections, which has been worked out for different cases by various authors.[6] A method similar to Glauber's is now being used[7] by Kohl *et al.* to work out elastic electron-molecule scattering. Somewhat earlier, Cheshire had used a similar method to calculate[8] charge exchange in proton-hydrogen scattering. Exchange contributions have been computed numerically by Byron,[9] and Reading[10] has derived some intermediate-energy corrections. In most instances, of course, the calculations may be readily modified to handle beam particles other than electrons, e.g., protons of fully stripped ions.

Ionization cross sections are now generally worked out in either the classical binary-encounter model[11] or a Born approximation, usually a Coulomb–Born approximation,[12–14] where the three-body asymptotic final state of the system includes a Coulomb wave function. Exact calculations for ionization, even in the case of electron-hydrogen scattering, have yet to be done. Consequently, there is strong motivation to consider a Glauber calculation of electron-hydrogen ionization with the hope that the techniques developed may be applied to other atomic systems.

Generally speaking, the Glauber approximation[15] includes some multiple scattering and is unitary in the high-energy limit. Since Born calculations include neither of these effects, the Glauber cross sections are often accurate over a larger energy range. For example, at 30 eV the experimental total cross section for excitation of 1s hydrogen to the $n=2$ level by electron impact is within ~5% of the Glauber prediction[3] but is about half as large as the Born prediction. At very high energies, the Glauber amplitude should reduce to the Born amplitude. One of the main strengths of the Glauber approximation in atomic physics is the ease with which it may be computed. In the scattering of electrons from hydrogen, elastic and inelastic scattering amplitudes may be found in terms of a few hypergeometric functions multiplied by simple factors. The corresponding Born calculation gives an only slightly simpler algebraic expression.

There is yet another motivation for this type of computation: namely, that it may provide an accurate source of high-partial-wave contributions to complement more exact computations of lower-partial-wave scattering amplitudes. While one of the strengths of the Glauber approximation is that a partial-wave decomposition is unnecessary, such a partial-wave decomposition in the Glauber approximation may nonetheless be useful.

II. DERIVATION

In this section we derive a Glauber amplitude for electron-hydrogen ionization. The Schrödinger

equation for this three-body atomic system may be written (in units of $\hbar = m = e = 1$) as

$$\left(-\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right)\psi = E\psi \quad , \qquad (1)$$

where the mass of the proton is much greater than the electron mass m. We rewrite Eq. (1) as

$$\left(-\tfrac{1}{2}\nabla_1^2 + h(r_2) - \frac{1}{r_1} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right)\psi = E\psi \quad , \qquad (2)$$

where

$$h(r) = -\tfrac{1}{2}\nabla^2 - 1/r - W \quad . \qquad (3)$$

In this case, $h(r)$ is the two-body Coulomb Hamiltonian with two-body energy W. The eigenstates of $h(r)$ are well-known Coulomb wave functions, $\psi_c(r)$, for $W > 0$, and the bound states of the hydrogen atom, $u_i(r)$, for $W < 0$.

We now try a solution of the form $\psi = e^{ik_0 z}\phi$, where $\frac{1}{2}k_0^2 = E$, which leads to

$$\left(-\tfrac{1}{2}\nabla_1^2 - ik_0\frac{d}{dz} + h(r_2) + V\right)\phi = 0 \quad , \qquad (4)$$

where

$$V = -1/r_1 + 1/|\vec{r}_1 - \vec{r}_2| \quad . \qquad (5)$$

We apply the eikonal approximation, i.e., assume that ϕ varies slowly over a distance of one wavelength, and drop the ∇_1^2 term, giving

$$ik_0\frac{d\phi}{dz} = (h + V)\phi \quad . \qquad (6)$$

In order to find ϕ, we have chosen to ignore the recoil energy of struck particles represented by h. This approximation is standard[8] in elastic and inelastic Glauber calculations. In the case of ionization, however, it requires some justification since it limits the energy which the ejected electron may carry off. Fortunately, at the high energies where the Glauber approximation may be applied, experiments[16] on a number of atomic systems indicated that the energy distributions are strongly peaked at low ejected-electron energies. In the case of hydrogen ionization no such data exist, but the Born–Coulomb calculations of Omidivar[17] show that the energy distributions are strongly peaked about an energy equal to $\frac{1}{4}$ the binding energy of the ejected electron. Ignoring the recoil energy corresponding to h in Eq. (6), the Glauber wave function may be expressed as

$$\psi_G(\vec{r}_1, \vec{r}_2) = u_i(\vec{r}_2)\, e^{ik_0 z_1} \times \exp\left(-\frac{i}{k_0}\int_{-\infty}^{z_1} V(\vec{r}_2,\ \vec{b} + \hat{k}_0 z')\, dz'\right) , \qquad (7)$$

where $u_i(\vec{r}_2)$ is the wave function for the initial state of the hydrogen atom itself.

In an exact formalism,[18,19] we could calculate the scattering amplitude for ionization according to

$$f = -\frac{1}{2\pi}\int (E - H)\,\phi_f^*(\vec{r}_1,\ \vec{r}_2)\,\psi_i(\vec{r}_1,\ \vec{r}_2)\, d^3r_1\, d^3r_2 \quad , \qquad (8)$$

where the exact wave function $\psi_i(\vec{r}_1,\ \vec{r}_2)$ satisfies $(E - H)\psi_i = 0$ with the usual boundary conditions as $\vec{r}_1 \to \infty$. The asymptotic wave function $\phi_f(\vec{r}_1,\ \vec{r}_2)$ may be represented by a product of Coulomb wave functions, $\psi_c^{z_1}(\vec{r}_1)\,\psi_c^{z_2}(\vec{r}_2)$, with partially screened charges z_1 and z_2 as prescribed[19] by Rudge and Seaton based, in part, on the work[20] of Peterkop. In this case,

$$(E - H)\phi_f = V\phi_f \quad , \qquad (9)$$

where

$$\hat{V}(\vec{r}_1,\ \vec{r}_2) = \frac{1 - z_1}{r_1} + \frac{1 - z_2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|} \cdot \qquad (10)$$

The expression for the scattering amplitude thus prescribed is nonsingular.

Now we shall apply the full-screening approximation already implicit in our derivation. The idea is that the ejected electron goes off with a velocity that is small compared to that of the incident electron. This corresponds to our dropping the $h(r_2)$ term in Eq. (6). The projectile electron in the final state thus is screened from the nucleus by the ejected electron, corresponding to $z_1 = 1$ and $z_2 = 0$. Our Glauber scattering amplitude may now be expressed as

$$f_G = -\frac{1}{2\pi}\int \phi_f^*(\vec{r}_1,\ \vec{r}_2)\, V(\vec{r}_1,\ \vec{r}_2)\,\psi_G(\vec{r}_1,\ \vec{r}_2)\, d^3r_1\, d^3r_2 \quad , \qquad (11)$$

where ϕ_f is a product of a Coulomb wave, representing the projectile electron. $V(\vec{r}_1,\ \vec{r}_2)$ is given by Eq. (5). Our approximate expression for the scattering amplitude f is also nonsingular. Furthermore, the screening approximation itself is exactly that used to determine ϕ_f in the standard Coulomb–Born approximation.

Using Eq. (7) for ψ_G in Eq. (11), we may integrate Eq. (11) in the standard way to obtain an expression for the Glauber scattering amplitude for ionization, namely,

$$f(\vec{q},\ \vec{k}) = \frac{ik_0}{2\pi}\int \psi_c^{*-}(\vec{r}_2)\,(1 - e^{iX(\vec{s},\vec{b})}) \times u_i(\vec{r}_2)\, e^{i\vec{q}\cdot\vec{b}}\, d^2b\, d^3r_2 \quad , \qquad (12)$$

where

$$X = -\frac{1}{k_0}\int_{-\infty}^{\infty} V(\vec{r}_1\vec{r}_2)\, dz_1 = \frac{2}{k_0}\ln\left(\frac{|\vec{b} - \vec{s}|}{b}\right) \quad . \qquad (13)$$

The configuration, shown in Fig. 1, defines the two impact parameters $\vec{b}$ and $\vec{s}$; $\psi_c^-(\vec{r}_2)$ is the two-body Coulomb wave function, and $u_i(\vec{r}_2)$ is the wave function of the initial state of the hydrogen atom.

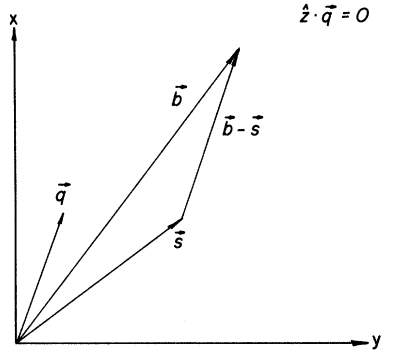

FIG. 1. Projection of the collision onto the x, y plane. The heavy nuclear mass is at the origin, $\vec{b}$ is the projection of the projectile onto the x, y plane, and $\vec{s}$ is the projection of the atomic electron. The momentum transfer $\vec{q}$ is perpendicular to the $\hat{z}$ axis.

III. CALCULATION OF SCATTERING AMPLITUDE

A. Formulation

In this section we compute the scattering amplitude for the ionization of hydrogen in the ground state by electron impact. We write the scattering amplitude as

$$f(\vec{q},\ \vec{k}) = +\frac{ik_0}{2\pi}\int \psi_c^{-*}(\vec{r})\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2ik_0}\right] \times u_0(r)\, e^{i\vec{q}\cdot\vec{b}}\, d^2b\, d^3r \ . \quad (14)$$

Here k_0 is the momentum of the incident electron, $\vec{q}=\vec{k}_0-\vec{k}_f$ is the momentum transfer, and $\vec{k}$ is the momentum of the ejected electron. The ground-state wave function of hydrogen is given by

$$u_0(r) = 2e^{-r}\, Y_{00}(\hat{r}) = e^{-r}/\sqrt{\pi} \ . \quad (15)$$

We expand the Coulomb wave function $\psi_c^-(\vec{r})$ in two-body partial waves in order to use the methods[4] of Thomas and Gerjuoy to evaluate the integrals. Specifically we expand $\psi_c^-(\vec{r})$ using[21]

$$\psi_c^-(\vec{r}) = \frac{1}{4\pi k}\sum_{l=0} i^l\,(2l+1)\, e^{-i\delta_l}\, R_{kl}(r)\, P_l(\hat{k}\cdot\hat{r}) \ . \quad (16)$$

Here

$$R_{kl}(r) = \frac{c_{kl}}{(2l+1)!}\,(2kr)^l\, e^{-ikr} \times {}_1F_1\left(\frac{i}{k}+l+1,\ 2l+2,\ 2ikr\right) \ , \quad (17)$$

$$\delta_l = \arg\Gamma\,(l+1-i/k) \ , \quad (18)$$

$$c_{kl} = \frac{2\sqrt{k}}{(1-e^{-2\pi/k})^{1/2}}\ \prod_{s=1}^{l}(s^2+1/k^2)^{1/2}\ \left(l=0\rightarrow\prod_{s=1}^{l}=1\right) \ . \quad (19)$$

The confluent hypergeometric function may be evaluated[21] according to

$$e^{-ikr}\,{}_1F_1\left(\frac{i}{k}+l+1,\ 2l+2,\ 2ikr\right) = \sum_{K=l+1}^{\infty} A_K^l(k)\,(kr)^{K-l-1} \ , \quad (20)$$

where

$$A_{l+1}^l(k)=1, \qquad A_{l+2}^l(k) = -1/k(l+1)$$

and

$$(K+l)\,(K-l-1)\,A_K^l(k) = -(2/k)\,A_{K-1}^l(k) - A_{K-2}^l(k) \ . \quad (21)$$

Collecting terms, we may write

$$\psi_c^-(\vec{r}) = \frac{1}{k}\sum_{l=0}^{\infty} i^l\, e^{-i\delta_l}\,\frac{c_{kl}}{(2l+1)!}\,(2)^l\sum_{m=-l}^{l} Y_{lm}^*(\hat{r})\, Y_{lm}(\hat{k}) \times \sum_{K=l+1}^{\infty} A_K^l(k)\, k^{K-1}\, r^{K-1} \ . \quad (22)$$

As we shall see, we will be able to set up a simple recursion scheme for computing the sum over K. The sum over l (and m) cannot be handled quite so easily. In the case of electron-hydrogen ionization, Peach[22] has shown that a few two-body partial waves are sufficient for the Coulomb–Born approximation at energies in the vicinity of a few hundred electron volts or less. Since our Glauber calculation is, in a sense, a correction to the Coulomb–Born approximation, we might expect (and indeed have found[23]) that several partial waves suffice for convergence.

B. Technique

Since the technique for each l is the same, we shall work out the dominant $l=1$ case and simply quote the results for $l=0$, 2, and 3.

In the $l=1$ case we have

$$\psi_c^-(\vec{r})\,|_{\,l=1} = \frac{i}{k}\, e^{-i\delta_1}\,\frac{c_{k1}}{3!}\,2\sum_{m=-1}^{1} Y_{1m}^*(\hat{r}^2)\, Y_{1m}(\hat{k}) \times\sum_{K=2}^{\infty} A_K^1(k)\, k^{K-1}\, r^{K-1} \ . \quad (23)$$

Substituting into Eq. (14), the $l=1$ contribution to the scattering amplitude is given by

$$f_1(\vec{q},\ \vec{k}) = -\frac{k_0}{k}\, c_{k1}\,\frac{e^{-i\delta_1}}{6\pi^{3/2}}\sum_{K=2}^{\infty} A_K^1(k)\, k^{K-1}\sum_{m=-1}^{1} Y_{1m}(\hat{k}) \times\int r^K\, Y_{1m}^*(\hat{r})\,\frac{e^{-r}}{r}\, d^3r\int e^{i\vec{q}\cdot\vec{b}}\left[1-\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2ik_0}\right] d^2b \ . \quad (24)$$

Defining

$$I_1(\lambda,\, q) = \frac{1}{(2\pi)^2}\int_0^{\infty} b\, db\int_0^{\infty} s^2\, ds\int_0^{\infty} dz\,\frac{e^{-\lambda(s^2+z^2)^{1/2}}}{(s^2+z^2)^{1/2}}$$

$$\times\int_0^{2\pi} d\phi_b\, e^{i(qb\cos\phi_b - m\phi_b)} \int_0^{2\pi} d\phi_s\, e^{-im\phi_s} \times\left[1-\left(\frac{b^2+s^2-2bs\cos\phi_s}{b^2}\right)^{i/k_0}\right], \quad (25)$$

we have

$$f_1(\vec{q},\vec{k}) = -i\,\frac{3}{8\pi}\,\frac{k_0}{k}\,2(2\pi)^2\,\frac{c_{kl}\,e^{-i\delta_1}}{6\pi^{3/2}} \times\sum_{K=2}^{\infty} A_K^l(k)\,k^{K-1}(-1)^{K-1}\,\frac{d^{K-1}}{d\lambda^{K-1}}\,I_1(\lambda,q) \times[Y_{1-1}(\hat{k})\,e^{-i\phi_q} - Y_{11}(\hat{k})\,e^{i\phi_q}]\Big|_{\lambda=1} . \quad (26)$$

The integral $I_1(\lambda, q)$ is given[4] by Thomas and Gerjuoy, who found that

$$I_1(\lambda,q) = -(4/k_0)(1-i/k_0)\left|\Gamma(1-i/k_0)\right|^2 \lambda^{-2i/k_0} q^{2i/k_0-3} \times[(1+i/k_0)\,{}_2F_1(2-i/k_0,\ 1-i/k_0;\ 2;\ -\lambda^2/q^2) \times {}_2F_1(2-i/k_0,\ 1-i/k_0;\ 1;\ -\lambda^2/q^2)] . \quad (27)$$

C. Results

Following the techniques described above, the scattering amplitude for ionization of hydrogen by electron impact may be expressed in the Glauber approximation as

$$f(\vec{q},\vec{k}) = \frac{-ik_0}{\sqrt{k}}\,\frac{1}{\pi^{3/2}}\,\frac{1}{1-e^{-2\pi/k}} \times\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(-2ik)^l}{(2l+1)!}\,e^{i\delta_l}p(l,k)\,Y_{lm}^*(\hat{k}) \times\sum_{K=0}^{\infty} A_{l+K+1}^l(k)\,(-k)^K\,\frac{d^{K+1}}{d\lambda^{K+1}}\,I_{lm}\Big|_{\lambda=1} . \quad (28)$$

In this expression k_0 is the momentum of the incident electron, k the momentum of the ejected electron, and $\vec{q}$ is the momentum transfered to the hydrogen atom.

The coefficients $p(l, k)$ and $A_{l+K+1}^l(k)$ are given by

$$p(l,k) = \begin{cases} 1, & l=0 \\ \prod_{s=1}^{l}(s^2+1/k^2)^{1/2}, & l\neq 0 \end{cases} \quad (29)$$

and

$$A_{l+1}^l(k) = 1, \quad A_{l+2}^l(k) = -1/k(l+1), \quad (K+l)(K-l-1)\,A_K^l(k) = -(2/k)\,A_{K-1}^l(k) - A_{K-2}^l(k). \quad (30)$$

The terms I_{lm} are defined by

$$I_{lm} = \iint r^l\,\frac{e^{-\lambda r}}{r}\,Y_{lm}(\hat{r})\,e^{i\vec{q}\cdot\vec{b}}\,\Gamma(\vec{b},\vec{s})\,d^3r\,d^2b , \quad (31)$$

where

$$\Gamma(\vec{b},\vec{s}) = 1-(|\vec{b}-\vec{s}|/b)^{2i/k_0} . \quad (32)$$

The I_{lm} integrals are given by

$$\begin{aligned} I_{00} &= [(2\pi)^2/\sqrt{4\pi}]\,I_0 , \\ I_{11} &= -(3/8\pi)^{1/2}\,e^{i\phi_q}2(2\pi)^2\,I_1 , \\ I_{1-1} &= (3/8\pi)^{1/2}e^{-i\phi_q}2(2\pi)^2\,I_1 = -e^{-2i\phi_q}I_{11} , \\ I_{22} &= \tfrac{1}{4}(15/2\pi)^{1/2}e^{2i\phi_q}2(2\pi)^2\,I_2 , \\ I_{20} &= \tfrac{1}{2}(5/4\pi)^{1/2}2(2\pi)^2(2I_2'-I_2) , \\ I_{2-2} &= e^{-4i\phi_q}I_{22} , \\ I_{33} &= -\tfrac{1}{4}(35/4\pi)^{1/2}e^{3i\phi_q}2(2\pi)^2\,I_3 , \\ I_{31} &= -\tfrac{1}{4}(21/4\pi)^{1/2}e^{i\phi_q}2(2\pi)^2(4I_3'-I_3) , \\ I_{3-1} &= -e^{-2i\phi_q}I_{31} , \\ I_{3-3} &= -e^{-6i\phi_q}I_{33} . \end{aligned} \quad (33)$$

The I_n and I_n' are given in terms of hypergeometric functions, namely,

$$I_0 = -(4i/k_0)\left|\Gamma(1-i/k_0)\right|^2\lambda^{-(2+2i/k_0)}q^{-2+2i/k_0}\,{}_2F_1(1-i/k_0,\ 1-i/k_0;\ 1;\ -\lambda^2/q^2) ,$$

$$I_1 = -(4/k_0)(1-i/k_0)\left|\Gamma(1-i/k_0)\right|^2\lambda^{-(2+2i/k_0)}q^{-3+2i/k_0} \times[(1+i/k_0)\,{}_2F_1(2-i/k_0,\ 1-i/k_0;\ 2;\ -\lambda^2/q^2) - {}_2F_1(2-i/k_0,\ 1-i/k_0;\ 1;\ -\lambda^2/q^2)] ,$$

$$I_2 = -(4i/k_0)(1-i/k_0)^2(2-i/k_0)\left|\Gamma(1-i/k_0)\right|^2\lambda^{-(2+2i/k_0)}q^{-4+2i/k_0} \times[(2+i/k_0)\,{}_2F_1(3-i/k_0,\ 2-i/k_0;\ 3;\ -\lambda^2/q^2) - 2\,{}_2F_1(3-i/k_0,\ 2-i/k_0;\ 2;\ -\lambda^2/q^2)] ,$$

$$I_2' = (4i/k_0)\left|\Gamma(1-i/k_0)\right|^2\lambda^{-(4+2i/k_0)}q^{-2+2i/k_0}[2\,{}_2F_1(1-i/k_0,\ 1-i/k_0;\ 1;\ -\lambda^2/q^2)$$

$$-(1-i/k_0)\,{}_2F_1(2-i/k_0,\ 1-i/k_0;\ 1;\ -\lambda^2/q^2)]\ ,$$

$$I_3=(8/3k_0)(1-i/k_0)^2(2-i/k_0)^2(3-i/k_0)|\Gamma(1-i/k_0)|^2\lambda^{-(2+2i/k_0)}q^{-5+2i/k_0}$$

$$\times[(3+i/k_0)\,{}_2F_1(4-i/k_0,\ 3-i/k_0;\ 4;\ -\lambda^2/q^2)-3\,{}_2F_1(4-i/k_0,\ 3-i/k_0;\ 3;\ -\lambda^2/q^2)]\ ,$$

$$I_3'=-(8/k_0)(1-i/k_0)|\Gamma(1-i/k_0)|^2\lambda^{-(4+2i/k_0)}q^{-3+2i/k_0}[2\,{}_2F_1(2-i/k_0,\ 1-i/k_0;\ 2;\ -\lambda^2/q^2)$$

$$+(2-i/k_0)(1-i/k_0)\,{}_2F_1(3-i/k_0,\ 2-i/k_0;2;\ -\lambda^2/q^2)-4(1-i/k_0)\,{}_2F_1(2-i/k_0;\ 2;\ -\lambda^2/q^2)]\ . \quad (34)$$

In order to evaluate the derivatives of the I_{lm}'s in Eq. (28), a recurrence relation for the derivatives of the ${}_2F_1$'s is helpful. Noting that[24]

$$\frac{d}{dz}\,{}_2F_1(a,b;c;z)=\frac{ab}{c}\,{}_2F_1(a+1,b+1;c+1:z)\ , \quad (35)$$

and defining

$$f_0\equiv{}_2F_1(a,b;c;z)\ ,\quad g_0\equiv{}_2F_1(a,b;c+1;z)\ , \quad (36)$$

it may be quickly established from the Gauss relations that[25]

$$f_{n+1}=[(1-z)(a+n)(b+n)]^{-1}[(a+b-c+n)f_n$$

$$+(c-a)(c-b)g_n]\ ,$$

$$g_{n+1}=\frac{(c+n+1)(c+n)}{(a+n)(b+n)z}(f_n-g_n)\ . \quad (37)$$

The two ${}_2F_1$'s needed initially may be computed numerically from convergent-series expansions.[26]

IV. CROSS SECTIONS

The ionization cross section may be evaluated by considering inelastic scattering of an electron of incident momentum $\vec{k}_0$ to a final momentum $\vec{k}_f$. In the inelastic case the differential cross section is given (in units of a_0^2, where $a_0=0.529\times10^{-8}$ cm) by

$$\frac{d\sigma}{d\hat{k}_f}=\frac{k_f}{k_0}|f(\vec{q})|^2\ , \quad (38)$$

where $\vec{q}=\vec{k}_0-\vec{k}_f$. In ionization there is an extra vector variable in the final state, namely, the momentum $\vec{k}$ of the ejected electron. Consequently, the differential cross section may be expressed[27] as

$$\frac{d^5\sigma}{d^3k\,d\hat{k}_f}=\frac{k_f}{k_0}|f(\vec{k},\vec{q})|^2\ . \quad (39)$$

In measurements with azimuthal symmetry (where the final-state magnetic quantum numbers are summed over), $d^5\sigma$ is independent of ϕ_{k_f} and reduces to $2\pi d^4\sigma$.

In order to evaluate total cross sections one must integrate over the remaining final-state variables, namely,

$$\sigma=\int_0^{k_{\max}}k^2\,dk\int d\hat{k}\int d\hat{k}_f\ \frac{k_f}{k_0}|f(\vec{k},\vec{q})|^2\ , \quad (40)$$

where

$$k_0^2-I=k_f^2+k^2$$

and

$$k_{\max}=k_0^2-I,\quad I=27.2\ \text{eV}\ . \quad (41)$$

Note that the integrals over $d\hat{k}$ are trivial: The only dependence of $f(\vec{q},\vec{k})$ on $\hat{k}$ in Eq. (28) is through $Y_{lm}(\hat{k})$, and the Y_{lm}'s, of course, are orthonormal. Hence, there are two integrations to be done numerically in order to evaluate total ionization cross sections.

It must be noted, at this point, that the power-series expansion in k of $f(\vec{k},\vec{q})$ will not converge numerically to a well-defined result for $k\gtrsim0.71k_{\text{orb}}$, where k_{orb} is the momentum of the orbiting electron. This divergence is not so serious as it might at first appear, since the cross sections peak near $k=\frac{1}{2}k_{\text{orb}}$ and rapidly fall off with increasing k. Furthermore, the series appears to be the sort which may be summed with Padé approximants [i.e., it behaves something like $\sum_{n=0}^{\infty}(-k/\sqrt{2})^n$]. A Padé approximant of the series would also be likely to improve the convergence rate in k for $k<0.71k_{\text{orb}}$. A less elegant procedure for finding total cross sections would be to fit $d\sigma/dk$ to the shape of the Born cross section for $k>0.71k_{\text{orb}}$, since the shapes of both approximations are remarkably similar for $k<0.71k_{\text{orb}}$. In any event, we expect our scattering amplitude to be accurate only in the region where $k<k_{\text{orb}}$ owing to approximations in the derivation.

V. DISCUSSION

While the choice of the direction of the z axis is not specified in our derivation, we have found that it must be taken perpendicular to the direction of the momentum transfer $\vec{q}$ in order to give agreement with the results of the Coulomb–Born approxi-

mation. As Gerjuoy has emphasized[28] the Coulomb–Born approximation may be recovered from Eq. (10) by keeping the first nonzero term of an expansion of $(1 - e^{i\chi})$ in powers of χ only if $\hat{z}$ is perpendicular to $\vec{q}$. If another choice is made (such as taking $\hat{z}$ parallel to $\vec{k}_0$) the angular distributions for the ejected electrons differ substantially with the predictions of the Coulomb–Born approximations at beam energies as large as 500 eV or more. Choosing $\hat{z}$ perpendicular to $\hat{q}$ is easy. Defining

$$\vec{z} = \vec{k}_0 + \alpha \vec{k}_f \quad \text{and} \quad \vec{q} = \vec{k}_0 - \vec{k}_f \tag{42}$$

we require that

$$\vec{z} \cdot \vec{q} = (\vec{k}_0 + \alpha \vec{k}_f) - (\vec{k}_0 - \vec{k}_f) = 0 \ , \tag{43}$$

which leads immediately to

$$\alpha = (\vec{k}_0 \cdot \vec{k}_f - k_0^2)/(\vec{k}_0 \cdot \vec{k}_f - k_f^2) . \tag{44}$$

In integrating over $\hat{k}$ the dependence of the cross sections on α disappears [cf. Eq. (28)]. Hence the choice of the direction of the z axis is irrelevant in computing $d^2\sigma/dkdq$, for example.

Exchange contributions to the cross section are ignored in our calculation. A straightforward calculation of the exchange amplitude in Glauber approximation could be time consuming. Rudge and Seaton have shown[19] that the exact exchange scattering amplitude $g(\vec{k}_f, \vec{k})$ is simply related to the exact direct amplitude $f(\vec{k}_f, \vec{k})$ by $g(\vec{k}_f, \vec{k}) = f(\vec{k}, \vec{k})$. Here $\vec{k}_f$ is the final velocity of the incident electron and $\vec{k}$ the final velocity of the atomic electron. Our direct scattering amplitude was derived under conditions corresponding to $k_f \ll k$, so that it is not useful to employ the relation of Rudge and Seaton where $g(\vec{k}_f, \vec{k})$ is large. An easy approximation[19] which may be used to include exchange contributions approximately is to replace k_{max} in Eq. (40) by $k_{max}/\sqrt{2}$. In the case of the ionization of hydrogen by electrons, exchange contributions are expected to be a small fraction of the total cross section, however.

Some numerical calculations[23] have been done on the IBM 360/65 at Texas A&M University. Differential cross sections consume a few seconds while total cross sections require a few minutes on the computer. In the Coulomb–Born approximation, the differential cross section may be expressed as a relatively simple algebraic expression. About 1 sec of computer time was used in doing the two numerical integrals required to evaluate a total Coulomb–Born cross section. Macek has suggested[29] that by working in hyperbolic coordinates one may be able to avoid the expansion in l, and thus save both programming time and run time. The technique has not yet been tried.

Unitarity may in general be used to relate the ionization scattering amplitudes for elastic and inelastic scattering. While we have not explicitly demonstrated this relationship, it is interesting to note that the Glauber ionization amplitude goes to infinity as q goes to zero, as does the elastic scattering amplitude. For ionization, however, $q = 0$ violates the constraints of energy momentum conservation.

Finally, let us point out that the dependence of our Glauber cross section on projectile charge z differs from the simple z^2 dependence of the Born calculation, and the classical binary-encounter[11] calculations. In the limit as $z/k_0 \to 0$, of course, our Glauber calculation goes over to the Born result.

ACKNOWLEDGMENTS

We wish to thank E. Gerjuoy, M. Mittleman, J. Reading, R. Stagat, S. Geltman, J. Macek, M. Seaton, and V. Franco for helpful discussions and suggestions.

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*Work supported by the U. S. Air Force Office of Scientific Research, Office of Aerospace Research, under Grant No. 71-1979A.

†Much of this work was done at Texas A&M University, and some was also done at the Joint Institute for Laboratory Astrophysics, Boulder, Colo. 80302.

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PHYSICAL REVIEW A VOLUME 7, NUMBER 3 MARCH 1973

X-Ray Scattering by Atoms According to the Thomas–Fermi Model with Quantum Corrections*

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(Received 11 September 1972)

Using an accurate numerical solution of the Thomas–Fermi model with quantum-mechanical corrections, the author obtains a description of coherent and incoherent scattering of x rays by the inert gases, which is in excellent agreement with detailed Hartree–Fock calculations. The results are somewhat better than those given by the Thomas–Fermi–Dirac model, and are a substantial improvement over those given by the Thomas–Fermi model alone.

I. INTRODUCTION

Recently, a new integration technique[1] was used to obtain an accurate solution to the differential equation which determines the first-order quantum-mechanical corrections of exchange, inhomogeneity, and correlation[2,3] to the semiclassical Thomas–Fermi model of the atom,[4] and this gives a new potential field to describe the electron density about an atom. This improvement has been shown to lead to total energies of neutral atoms,[3] and diamagnetic susceptibilities and atomic polarizabilities of the inert gases,[1] among other properties, which are in substantially better agreement with experiment than are the similar values calculated by the exact Thomas–Fermi model. The purpose of this paper is to show that the improved Thomas–Fermi model also gives an excellent description of the coherent (elastic) and incoherent (inelastic) scattering of x rays by the inert gases.

According to the Thomas–Fermi model of the atom, including the quantum-mechanical corrections, the Coulomb potential about a spherically symmetric neutral atom of atomic number Z, namely, $V(r) = -Ze^2/r$, is replaced by the modified potential

$$V(r) = (-Ze^2/bx)[\psi(x) + ay(x)], \tag{1}$$

where $r = bx$, $a = \frac{1}{8}(6\pi Z)^{-2/3}$, $b = (6\pi)^{2/3} a_B / 8Z^{1/3} = 0.88534 a_B Z^{-1/3}$, and $a_B = \hbar^2/me^2$ is the Bohr radius for hydrogen. $\psi(x)$ is the well-known solution of the Thomas–Fermi equation[4] and is given approximately by[5]

$$\psi = \left(\frac{1 + 1.81061x^{1/2} + 0.60112x}{1 + 1.81061x^{1/2} + 1.39515x + 0.77112x^{3/2} + 0.21465x^2 + 0.04793x^{5/2}} \right)^2 , \tag{2}$$

with a maximum error of $\delta\psi < 1.2 \times 10^{-5}$. $y(x)$ is the solution to the equation owing to Kompaneets and Pavlovskii,[2,3] which gives the quantum-mechanical corrections. This solution has been discussed in detail previously[1] and can be represented approximately by the following power series: