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Magnus approximation for K-shell ionization by heavy-ion impact*

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The Magnus approximation (or sudden approximation) is applied to derive the transition amplitude and the cross section for K-shell ionization of atoms by heavy-ion impact. The target electron is described by a hydrogenic wave function and the projectile as a point charge moving along a straight-line trajectory. The transition amplitude for each partial wave of the ejected electron is expressed as an infinite (but rapidly converging) sum over hypergeometric functions. To obtain the total cross section, only integrals over impact parameter and the final electron momentum have to be evaluated numerically. The approach, because it is nonperturbative, should be particularly useful for treating collisions of light atoms with much heavier projectile ions. It also allows the study of the impact-parameter dependence of the ionization process. The connection with the Glauber approximation is pointed out.

I. INTRODUCTION

K-shell ionization of atoms by collisions with energetic ions is an important process in heavy-ion physics and of considerable interest both in terms of basic theory and in various practical applications. In the theoretical investigation of these reactions, usually three approximate methods have been applied: the plane-wave Born approximation[1] (PWBA), the semiclassical approximation[2] (SCA), and the binary-encounter approximation[3] (BEA). All three approximations are valid for sufficiently high energy of the projectile. By using relativistic electron wave functions,[4] the treatment may be extended to heavy target atoms. However, it is always assumed in these calculations that the projectile is a relatively light ion such as a proton or an α particle.

Very few studies, either experimental or theoretical, have been made of the ionization of light target atoms by much heavier projectile ions. Yet such ionization processes are of considerable interest in connection with problems associated with fusion reactors and with the energy deposition of heavy ions in organic matter. It has been the purpose of the present work to develop an approach which should be particularly suitable for dealing with collisions of light atoms with heavier projectile ions.

To develop this approach one has to abandon the perturbation approach which is the basis of the Born[1] and semiclassical approximation.[2,4] If the charge of the projectile nucleus is large, its time-integrated interaction with the K electron will also be large, and a perturbation expansion will not be appropriate. The basis of this present approach is the Magnus expansion,[5,6] which is nonperturbative but rather uses the ratio of the characteristic collision time τ_{coll} to the characteristic time τ_{orb} of the unperturbed system as an expansion parameter.

The first term in this expansion leading to the (first-order) "Magnus approximation" or "sudden approximation" was originally introduced by Alder and Winther[7] and independently by Takayanagi[8] and subsequently was used by a number of others.[9-12] The approach has some relationship to the Glauber approximation,[13-17] which has also been applied to K-shell ionization[18,19] but so far only for light projectile ions.[20] The projectile charge dependence has been systematically treated from a different point of view.[21]

In this paper, we assume the projectile moves along a classical straight-line trajectory, and we study the collisional ionization process in the (first) Magnus approximation. In Sec. II, we discuss the Magnus approximation and specify our assumptions. In Sec. III, we derive expressions for the transition amplitude, the ionization probability as a function of the classical impact parameter, and the total ionization cross section. A summary discussion and some concluding remarks are presented in Sec. IV.

II. THEORETICAL BACKGROUND

Consider a beam of projectile ions (with charge number Z_p, velocity v_p) impinging on a target atom (with charge number Z_t) along a classical orbit characterized by the impact parameter b. The cross section for excitation to a specific final state f from the initial state i is given by

$$\sigma_{i\to f} = 2\pi \int_0^\infty b\, db |a_{i\to f}(b)|^2, \tag{1}$$

where $a_{i\to f}(b)$ is the excitation amplitude associated with a specific trajectory. Let T denote the time-ordering operator.[22] The excitation amplitude can then be written[22] in the usual perturbation expansion

$$a_{i\to f}=\langle f|\,T\exp\left(-\frac{i}{\hbar}\int_{-\infty}^{\infty}\tilde{H}(t)\,dt\right)|\,i\rangle \tag{2a}$$

or

$$a_{i\to f}=\delta_{if}-\frac{i}{\hbar}\langle f|\int_{-\infty}^{\infty}\tilde{H}(t)\,dt|\,i\rangle + \left(\frac{-i}{\hbar}\right)^2\langle f|\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'\tilde{H}(t)\tilde{H}(t')|\,i\rangle+\cdots . \tag{2b}$$

Here, the time-dependent interaction is given in the interaction representation by

$$\tilde{H}(t)=e^{(i/\hbar)H_0t}\,V(t)\,e^{-(i/\hbar)H_0t}, \tag{3}$$

with H_0 denoting the Hamiltonian of the free-target atom and $V(t)$ is the time-dependent perturbation caused by the projectile. The first two terms of Eq. (2b) correspond to the SCA.[2]

An expansion alternative to Eq. (2) has been derived by Magnus and analyzed in detail by Pechukas and Light.[6] It leads to

$$a_{i\to f}=\langle f|\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty}\tilde{H}(t)\,dt+\frac{1}{2}\left(\frac{-i}{\hbar}\right)^2\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'[\tilde{H}(t),\tilde{H}(t')]+\cdots\right]|\,i\rangle . \tag{4}$$

In contrast to the perturbation series (2), the Magnus expansion (4) has the virtue that the transition operator is unitary at each level of approximation.

In the same way, as for Eq. (2), expansion (4) may serve as a starting point for various approximations. In the (first-order) Magnus approximation, only the first term in the exponential of (4) is retained. It can be observed that, in this approximation, only the total interaction enters or, equivalently, the operator T in Eq. (2a) is replaced by unity. The approximation will thus account only for instantaneous effects; it ignores any correlations between the values of the Hamiltonian at different times. (The time structure of the excitation process is described to the lowest order by the second term in the Magnus expansion.)

The physical interpretation above suggests that the first-order Magnus approximation will be justified if the time structure may be disregarded, that is, if the collision time τ_{coll} is small compared to the orbiting time τ_{orb} of the relevant electron, or if $\xi=\tau_{\text{coll}}/\tau_{\text{orb}}\ll 1$. In this case, it is consistent to replace $\tilde{H}(t)$ by $V(t)$ so that the transition amplitude becomes

$$a_{i\to f}=\langle f|\exp\left(-\frac{i}{\hbar}\int_{-\infty}^{\infty}V(t)\,dt\right)|\,i\rangle . \tag{5}$$

The approximation of Eq. (5) was first introduced by Alder and Winther[7] to describe multiple Coulomb excitation of deformed nuclei by energetic heavy ions and, independently, in an atomic collision problem by Takayanagi.[8] Subsequently, Eq. (5) rederived in various ways, was used by several authors.[9-12] Also, corrections resulting from the second Magnus term were investigated.[7,11]

To evaluate the right-hand side of Eq. (5), a unitary transformation is usually introduced,[7-11] which diagonalizes the interaction integral $\int V(t)\,dt$. In practice, the diagonalization is carried out in a truncated set of basis states. Unfortunately, it is difficult to estimate the error introduced by the truncation procedure. In the present work, we avoid this additional approximation. We believe that this is important, because otherwise one combines the shortcomings of the Magnus approach (no time structure) with those of the close-coupling approach (limited basis set).

Turning now to the specific problem of K-shell ionization by ion impact, we make the following assumptions: (a) the ionization process is described as a single-electron problem involving nonrelativistic hydrogenic wave functions for the initial bound and final continuum state; (b) the projectile is approximated by a point charge moving along a classical straight-line trajectory[23]; (c) the projectile velocity v_p is large enough, so that $\tau_{\text{coll}}\approx 2a_K/v_p$ is small compared to $\tau_{\text{orb}}\approx -2\pi\hbar/E_K=4\pi\hbar^3/Z_t^2me^4$ or $\xi=(2\pi)^{-1}\alpha Z_t c/v_p\ll 1$. Conditions (b) and (c) are satisfied even for heavy projectiles, provided that $Z_t/\sqrt{\epsilon_p}\ll 1$ where ϵ_p is the projectile energy measured in keV per nucleon.

For the assumptions just specified, the transition amplitude (5) is written

$$a_{i\to f}(b)=\langle f|\,e^{i\chi}|\,i\rangle , \tag{6}$$

with

$$\chi(\vec{r},b)=-\frac{Z_pe^2}{\hbar}\int_{-\infty}^{\infty}\left(\frac{1}{R(t)}-\frac{1}{|\vec{r}-\vec{R}(t)|}\right)dt , \tag{7}$$

where $\vec{r}$ and $\vec{R}$ are the electron and projectile coordinates (measured from the target nucleus), respectively. The term $1/R(t)$, while ensuring convergence of the integral contributes only a constant phase to the amplitude (6).

Before proceeding to the evaluation of Eq. (6), it is instructive to establish the relation of our approach to the Glauber theory which is another nonperturbative high-energy approximation. The correspondence between wave and impact parameter treatments has been discussed by McCarroll and Salin.[24] Starting from the quantum mechanical eikonal ansatz the conventional (small-angle) Glauber scattering amplitude is derived as[13-15]

$$A_{i\to f}(\vec{q}) = \frac{ik_i}{2\pi}\int d^2b\, e^{i\vec{q}\cdot\vec{b}}\langle f|1-e^{i\chi}|i\rangle. \tag{8}$$

Here $\vec{k}_i$ is the initial projectile wave vector and $\hbar\vec{q}=\hbar(\vec{k}_f-\vec{k}_i)$ is the momentum transfer which is *assumed* to be perpendicular to $\hat{k}_i \approx \hat{k}_f$, i.e., to the beam axis. The path integral χ defined in Eq. (7) is evaluated along a rectilinear trajectory. The total cross section for exciting a specific final state is then written[14]

$$\sigma_{i\to f} = \frac{1}{k_i^2}\int_{k_i-k_f}^{k_i+k_f} q\,dq \int_0^{2\pi} d\varphi_q\,|A_{i\to f}(\vec{q})|^2. \tag{9}$$

One may obtain a result similar in form by starting from the impact parameter picture of Eq. (1). For $i\neq f$ the transition amplitude $a_{i\to f}(\vec{b})$ can be introduced (aside from an overall factor) as the two-dimensional Fourier transform of $A_{i\to f}(\vec{q})$ in the plane perpendicular to the beam axis (i.e., $\vec{q}\cdot\vec{v}_p=0$). Using the familiar representation of the delta function which reduces the double integration over the q plane to a single integration, one obtains an expression which is formally identical to Eq. (9) except for the limits of integration. In the wave picture, the limits of integration in Eq. (9) arise from the conservation of linear momentum. In the impact parameter picture, momentum conservation does not hold and $\vec{q}$ enters originally through the Fourier transform but may be interpreted[24] as transfer of transverse momentum with the limits of integration extending from zero to infinity. The upper bound is in accordance with the classical assumption of an infinitely heavy projectile. The discrepancy in the lower bound of Eq. (9) arises from the interpretation of $\vec{q}$ as *transverse* momentum transfer $\vec{q}_{tr}$ in the impact parameter picture but as *total* momentum transfer in the Glauber approximation [cf. Eq. (8)]. The latter interpretation, however, is inconsistent with the fact, that in the derivation of the conventional ("restricted"[17]) Glauber approximation the longitudinal momentum transfer $q_l \approx \Delta E/v_p$ is discarded for mathematical convenience.[13-17] Certainly, this approximation does not apply to zero-degree inelastic scattering. These difficulties have been removed, at the expense of mathematical complexity, in the "unrestricted" Glauber approximation formulated by Byron[16] and by Gau and Macek.[17]

Clearly, the present approach is related to the conventional (often quite successful[13-15,18-20]) Glauber approximation, but avoids the inconsistencies mentioned above. While it is not immediately clear which approach should be better, the semiclassical picture employed here has the appeal of greater conceptual clarity. The close correspondence between the two approaches is, of course, not surprising, because in the derivation[13] of the Glauber theory, it is assumed that the values of the interaction operator taken at different points along the trajectory commute, as in the (first) Magnus approximation.

III. TRANSITION AMPLITUDE AND CROSS SECTIONS

In this section we calculate the transition amplitude (6) for the ionization of a K electron into a continuum state with momentum $\vec{k}$. Atomic units are used in the following presentation. Using a straight-line trajectory, one may rewrite the path integral (7) as[14]

$$\chi(\vec{r}, b) = 2\eta \ln(|\vec{b}-\vec{s}|/b), \tag{10}$$

where $\vec{s}$ is the projection of the electron coordinate $\vec{r}$ on the impact parameter plane (normal to the beam axis) and $\eta=-Z_p/v_p$. If $\lambda = Z_t^*$ and $\gamma=-Z_t^*/k$ with Z_t^* denoting the effective charge of the target nucleus, we may write the initial and final electron states in the form[25,18]

$$\Psi_{1s}(\vec{r}) = \pi^{-1/2}\lambda^{3/2}e^{-\lambda r} \tag{11}$$

and

$$\Psi_{\vec{k}}^*(\vec{r}) = \left(\frac{2k}{\pi}\right)^{1/2} e^{-\gamma\pi/2} \times\sum_{l=0}^{\infty}(-2ikr)^l\,\frac{\Gamma(l+1+i\gamma)}{(2l+1)!} \times e^{ikr}\,{}_1F_1(l+1+i\gamma, 2l+2; -2ikr) \times\sum_{m=-l}^{l} Y_{lm}(\hat{k})Y_{lm}^*(\hat{r}). \tag{12}$$

Here we have introduced a partial-wave expansion for the ejected electron and a normalization on the energy scale. Inserting Eqs. (10) to (12) into Eq. (6), we obtain a partial-wave expansion of the transition amplitude

$$a_{i\to k}(b) = (2k)^{1/2}\pi^{-1}\lambda^{3/2}e^{-\gamma\pi/2} \times\sum_{lm}(-2ik)^l\,\frac{\Gamma(l+1+i\gamma)}{(2l+1)!}\,I_{lm}(k)Y_{lm}(\hat{k}), \tag{13}$$

with

$$I_{lm}(k)=\int r^l e^{-\lambda r} e^{ikr}\left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta} Y^*_{lm}(\hat{r})\times{}_1F_1(l+1+i\gamma,2l+2;-2ikr)\,d^3r. \tag{14}$$

Owing to the symmetry of the integrand with respect to reflections on the impact parameter plane,[26] only integrals with $l+m$ an even number are different from zero. Restricting ourselves for the moment to $m\geq 0$, the spherical harmonics in Eq. (14) are expanded as

$$Y^*_{lm}(\hat{r})=e^{-im\varphi}\sin^m\theta\sum_{j=0}^{(l-m)/2}C^{(j)}_{lm}\cos^{2j}\theta, \tag{15a}$$

with

$$C^{(j)}_{lm}=(-1)^{(l+m)/2-j}\,2^{-l}\left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right)^{1/2}\times\frac{(l+m+2j)!}{[\frac{1}{2}(l+m)+j]![\frac{1}{2}(l-m)-j]!(2j)!}. \tag{15b}$$

Up to this point, our development is practically the same as the reduction by Golden and McGuire[18] for the Glauber amplitude. We can now write

$$|\vec{b}-\vec{s}|/b=(1+z^2-2z\cos\varphi)^{1/2}, \tag{16}$$

where $z=s/b=(r\sin\theta)/b$ and φ denotes the angle between $\vec{s}$ and $\vec{b}$. At this point we introduce the integral representation

$$\int_0^{2\pi}e^{im\varphi}(1+z^2-2z\cos\varphi)^{i\eta}\,d\varphi=-2\pi\cdot 2^{2i\eta}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\times\int_0^\infty t^{-2i\eta}\frac{d}{dt}[J_{|m|}(zt)J_{|m|}(t)]\,dt, \tag{17}$$

given by Thomas and Gerjuoy.[26] From this relation and the property of the spherical harmonics under complex conjugation, it is readily seen that in Eq. (13) the quantity

$$I_{l,-|m|}=(-)^l I_{l,|m|}\,. \tag{18}$$

Owing to this symmetry, we may immediately obtain the partial transition amplitudes I_{lm} for $m<0$ from our explicit treatment of the cases $m\geq 0$. At first we confine ourselves to $m\geq 1$. In this case, integration by parts may be carried out[26] on the right-hand side of Eq. (17). Introducing Eqs. (15) and (17) into Eq. (14) and collecting θ-dependent terms, we arrive at the integral[27]

$$\int_0^\pi \sin^{m+1}\theta\cos^{2j}\theta J_m\left(\frac{rt}{b}\sin\theta\right)d\theta=2^{j+1/2}\Gamma(j+\tfrac{1}{2})\left(\frac{rt}{b}\right)^{-j-1/2}J_{m+j+1/2}\left(\frac{rt}{b}\right). \tag{19}$$

It would be possible to do the t integration[28] as the next step; however, this is not practical[28] for the further reduction. Nevertheless, it can be verified that after t integration a distinction between the cases $m=0$ and $m\geq 1$ is not necessary; for $m=0$ the differentiation in Eq. (17) has to be carried out explicitly. When integrated over θ and t, the two resulting hypergeometric functions are combined through an appropriate Gauss relation.[29] This, however, leads precisely to the result obtained by partial integration in Eq. (17) (applicable for $m\geq 1$ only) and specialization to $m=0$ *after* t integration.

To perform the r integration as the next step, we introduce the standard integral representation[30] of the confluent hypergeometric function into Eq. (14) and insert the expressions (15), (17), and (19) to obtain the partial transition amplitude

$$I_{lm}=2\pi\cdot 2^{2i\eta}(-2i\eta)\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\frac{\Gamma(2l+2)}{\Gamma(l+1+i\gamma)\Gamma(l+1-i\gamma)}\times\sum_{j=0}^{(l-m)/2}C^{(j)}_{lm}2^{j+1/2}\Gamma(j+\tfrac{1}{2})b^{j+1/2}J^{(j)}_{lm}, \tag{20a}$$

with

$$J^{(j)}_{lm}=\int_0^1 dx\,x^{l+i\gamma}(1-x)^{l-i\gamma}\int_0^\infty dr\,r^{l-j+3/2}e^{-\alpha r}\times\int_0^\infty dt\,t^{-(j+3/2+2i\eta)}J_m(t)J_{m+j+1/2}\left(\frac{r}{b}t\right), \tag{20b}$$

where $\alpha=\lambda-ik(1-2x)$. The r integration[31] leads to a hypergeometric function with a terminating power expansion in the variable $-t^2/\alpha^2b^2$. If the finite series is written explicitly, we get

$$J^{(j)}_{lm}=2^{-(m+j+1/2)}\frac{(l+m+2)![\frac{1}{2}(l-m)-j]!}{\Gamma[-\frac{1}{2}(l-m)+j-\frac{1}{2}]}\sum_{\nu=0}^{(l-m)/2-j}\frac{\Gamma(-\nu-\frac{1}{2})b^{l-j+7/2+2\nu}}{\nu![\frac{1}{2}(l-m)-j-\nu]!\Gamma[\frac{1}{2}(l+m)+\frac{3}{2}-\nu]}\times\int_0^1 dx\,x^{l+i\gamma}(1-x)^{l-i\gamma}\alpha^{2\nu+1}\int_0^\infty dt\,t^{l-2j-1-2\nu-2i\eta}(\alpha^2b^2+t^2)^{-(l-j+2)}J_m(t). \tag{21}$$

The t integration[32] now yields a sum of two generalized hypergeometric functions ${}_1F_2(a; b, c; z)$, which can be written as a convergent series in the whole z plane ($z = -\alpha^2 b^2/4$) and may be expected to converge rapidly. For each term in the series, the remaining integral over x can be identified with the fundamental integral representation[33] of the hypergeometric function.

Thus, the final result (valid for $m \geqslant 0$) is expressed as an infinite but presumably rapidly converging sum over hypergeometric functions

$$
\begin{aligned}
I_{lm} = {} & (-1)^{(l-m)/2} 4\pi\eta^2 2^{2i\eta - m} [\Gamma(i\eta)]^2 (l+m+2)! \\
& \times \sum_{j=0}^{(l-m)/2} C_{lm}^{(j)} \frac{\Gamma(j+\frac{1}{2})[\frac{1}{2}(l-m)-j]!}{\Gamma[-\frac{1}{2}(l-m)+j-\frac{1}{2}](l-j+1)!} \sum_{\nu=0}^{(l-m)/2-j} \frac{(-1)^\nu \Gamma(-\nu-\frac{1}{2}) b^{l+4+2\nu}}{\nu ! [\frac{1}{2}(l-m)-j-\nu]! \Gamma[\frac{1}{2}(l+m)+\frac{3}{2}-\nu]} \\
& \times \sum_{n=0}^{\infty} \left[A_n (\lambda - ik)^{-l+m-3+2n-2i\eta} {}_2F_1\left(l-m+3-2n+2i\eta,\, l+1+i\gamma;\, 2l+2;\, \frac{-2ik}{\lambda - ik}\right) \right. \\
& \qquad \left. + B_n (\lambda - ik)^{2\nu+2n+1} {}_2F_1\left(-2\nu-2n-1,\, l+1+i\gamma;\, 2l+2;\, \frac{-2ik}{\lambda-ik}\right) \right],
\end{aligned}
\tag{22}
$$

with the coefficients

$$
A_n(b) = b^{-(l-m+2\nu+4-2n+2i\eta)} \frac{2^{-(m+1+2n)} \Gamma[\frac{1}{2}(l+m)-j-\nu+n-i\eta]}{\Gamma[-\frac{1}{2}(l-m)-\nu-1+n-i\eta](m+n)!n!}
\tag{23a}
$$

and

$$
B_n(b) = -b^{2n} \frac{2^{-(l+2\nu+5+2n+2i\eta)}(l-j+1+n)!}{\Gamma[\frac{1}{2}(l+m)+3+\nu+n+i\eta]\Gamma[\frac{1}{2}(l-m)+3+\nu+n+i\eta]n!} .
\tag{23b}
$$

The expression (22) has to be inserted into Eq. (13) to get the transition amplitude. It is noteworthy that the transition amplitude is well-behaved as $b \to 0$. For $b \to \infty$, the orthogonality of the wave function in Eq. (14) leads to a vanishing amplitude.

From the transition amplitude (13), one immediately obtains the cross section for ionizing a given electron from the K shell of the target atom into a final state characterized by the electron energy E and the solid angle $d\Omega$ (in units of a_0^2, a_0 Bohr radius), namely,

$$
\frac{d^2\sigma}{dE\, d\Omega} = 2\pi \int_0^\infty b\, db |a_{i \to \vec{k}}|^2 .
\tag{24}
$$

If the ejected electron is not detected, one has to integrate over the energy and angle variable to get the total cross section for a given center-of-mass energy E_p of the projectile. The cross section is expressed in terms of the excitation probability $P(E_p, b)$ integrated over all impact parameters as

$$
\sigma(E_p) = 2\pi \int_0^\infty b\, db P(E_p, b),
\tag{25}
$$

with

$$
P(E_p, b) = \frac{2\lambda^3}{\pi^2} \int_0^{k_{\max}} k^2\, dk\, e^{-\gamma\pi} \times \sum_{lm} (2k)^{2l} \frac{|\Gamma(l+1+i\gamma)|^2}{[(2l+1)!]^2} |I_{lm}(k)|^2 .
\tag{26}
$$

Here, the wave number $k_{\max}$ is determined by the energy loss of the projectile. In practice, however, the cross section is expected to become negligible[34] at electron energies far below the projectile energy, consistent with the adopted approximations. The cross sections (24) and (25) have to be multiplied with a factor of 2 if initially there are two electrons in the K shell.

IV. DISCUSSION AND CONCLUDING REMARKS

The cross sections given in Eqs. (24) and (25) are expressed as integrals over the impact parameter. The impact parameter by itself is not a measurable quantity. However, for a repulsive Coulomb force acting between the target and the projectile nucleus there is a one-to-one correspondence between the impact parameter b and the deflection angle θ_p (in the center-of-mass system). The relation is established[2] via the eccentricity ϵ of the hyperbolic path, which is connected to the deflection angle by $\epsilon = (\sin\frac{1}{2}\theta_p)^{-1}$ and also to the impact parameter by $\epsilon^2 = 1 + b^2/d^2$ where $d = Z_p Z_t e^2/2E_p$ is half the distance of closest approach. Under these conditions, therefore, the impact parameter is accessible to experimental investigation. In our calculations we have assumed straight-line trajectories, but the path integral (7), and hence the ionization probability (26), will not differ very much from the case where Rutherford orbits are used instead (provided θ_p is not too large). Thus, one may use our formulas and still associate a scattering angle with each impact parameter. The differential cross section with respect to projectile deflection then is

$$\frac{d\sigma}{d\Omega_p} = P(E_p, b)\frac{d\sigma_R}{d\Omega_p}, \qquad (27)$$

where $d\sigma_R/d\Omega_p = \frac{1}{4}\epsilon^4 d^2$ is the differential Rutherford cross section. According to Bang and Hansteen[2] the differential cross section calculated in this way from a theory using straight-line trajectories has a shape very similar to the cross section derived from Rutherford orbits.

The dependence of the cross section on the projectile is entirely contained in the parameter $\eta \sim Z_p/v_p$. In our approximation, the cross sections should hence be a universal function of Z_p/v_p. As was noted in Ref. 20, this is not so in the Glauber approximation, because the minimum momentum transfer does not scale with Z_p/v_p.

As has been discussed in Sec. II, the present formulation has much in common with the Glauber approach[18-20] but we believe that the final expressions are simpler to evaluate than the corresponding results from Glauber theory. Moreover, since the Magnus approximation is the first term of an expansion, it is a straightforward, although rather involved, procedure to include the next higher term in the expansion (4). For some applications, the possibility of obtaining the impact-parameter dependence of the cross sections would be of considerable interest.

We conclude the discussion by pointing out some effects that are neglected in the present treatment. (a) We have disregarded all the complex processes which the outer target electrons may experience. (b) Electron capture into the continuum[35] may be significant, especially if the projectile charge exceeds the target charge. However, it is very difficult to include this effect. (c) If the projectile is only partially stripped, the projectile electrons will contribute to the interaction with the target K electrons. To the lowest order, in particular for $Z_p \gg Z_t$, this effect might be accounted for by introducing an effective charge also for the projectile.

We believe that the present approach makes it possible to calculate K-shell ionization cross sections for systems which in the past were not easily amenable to theoretical treatment. Detailed calculations of the ionization cross section for a number of ion-atom collision systems are in progress.

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[1]E. Merzbacher and W. H. Lewis, *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1958), Vol. 34, p. 166.

[2]J. Bang and J. M. Hansteen, Kgl. Danske Vidensk. Selsk., Mat.-Fys. Medd. 31, No. 13 (1959).

[3]J. D. Garcia, E. Gerjuoy, and J. Welker, Phys. Rev. 165, 66 (1968); J. D. Garcia, Phys. Rev. A 1, 280 (1970); 4, 955 (1971); L. Vriens, Proc. Phys. Soc. Lond. 90, 935 (1966); E. Gerjuoy, Phys. Rev. 148, 54 (1966); M. Gryzinski, *ibid.* 138, A336 (1965).

[4]P. A. Amundsen and L. Kocbach, J. Phys. B 8, L122 (1975); P. A. Amundsen, *ibid.* 9, 971 (1975).

[5]W. Magnus, Commun. Pure Appl. Math. 7, 649 (1954).

[6]P. Pechukas and J. C. Light, Chem. Phys. 44, 3897 (1966).

[7]K. Alder and A. Winther, Kgl. Danske Vidensk. Selsk., Mat.-Fys. Medd. 32, No. 8 (1960); K. Alder, *Reactions Between Complex Nuclei*, edited by A. Ghiorso, R. M. Diamond, and H. E. Conzett (University of California Press, Berkeley, 1963), p. 253.

[8]K. Takayanagi, Prog. Theor. Phys. Suppl. 25, 43 (1963); Sci. Rep. Saitama Univ. IIIA, No. 2, 65 (1959).

[9]K. H. Kramer and R. B. Bernstein, Chem. Phys. 40, 200 (1964).

[10]J. Callaway and E. Bauer, Phys. Rev. 140, A1072 (1965); J. Callaway and A. F. Dugan, Phys. Lett. 21, 295 (1966).

[11]D. Baye and P. H. Heenen, J. Phys. B 6, 105 (1973).

[12]H. Kruger and E. W. Knapp, J. Phys. B 9, 1629 (1976).

[13]R. J. Glauber, *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959), Vol. I, p. 315.
[14]E. Gerjuoy and B. K. Thomas, Rep. Prog. Phys. 37, 1345 (1974).
[15]C. Quigg and C. J. Joachain, Rev. Mod. Phys. 46, 279 (1974).
[16]F. W. Byron, Jr., Phys. Rev. A 4, 1907 (1971).
[17]J. N. Gau and J. Macek, Phys. Rev. A 10, 522 (1974).
[18]J. H. McGuire, M. B. Hidalgo, G. D. Doolen, and J. Nuttall, Phys. Rev. A 7, 973 (1973); J. E. Golden and J. H. McGuire, *ibid.* 12, 80 (1975).
[19]H. Narumi, A. Tsuji, and A. Miyamoto, Prog. Theor. Phys. 54, 740 (1975); H. Narumi, T. Sekimura, and A. Tsuji, Circ. Nucl. Fusion Jpn. Suppl. 3, 34, 5 (1975); also, B. K. Thomas, Bull. Am. Phys. Soc. 19, 1191 (1974).
[20]J. E. Golden and J. H. McGuire, J. Phys. B 9, L11 (1976).
[21]J. F. Reading, Phys. Rev. A 1, 1642 (1970); 8, 3262 (1973); J. F. Reading and E. Fitchard, *ibid.* 10, 168 (1974); J. Binstock and J. F. Reading, *ibid.* 11, 1205 (1975); J. F. Reading, A. L. Ford, and E. Fitchard, Phys. Rev. Lett. 36, 573 (1976).
[22]The "chronological" operator T orders a product of time-dependent operators such that, reading from left to right, the operators at later times come first, cf. F. J. Dyson, Phys. Rev. 75, 486 (1949).
[23]In neglecting the Coulomb deflection, we assume (cf. Ref. 1) that the distance $2d$ of closest approach is much smaller than the K-shell radius; i.e., $d/a_K = Z_p Z_t \alpha^2 \cdot mc^2/E_p \ll 1$ where $\alpha = e^2/\hbar c = 1/137$, m is the electron mass and E_p the projectile c.m. energy.
[24]R. McCarroll and A. Salin, C. R. Acad. Sci. (Paris) 263, 329 (1966); also Ref. 25, Appendix 4.1.
[25]M. R. C. McDowell and J. P. Coleman, *Introduction to the Theory of Ion-Atom Collisions* (North-Holland, Amsterdam, 1970), p. 246.
[26]B. K. Thomas and E. Gerjuoy, J. Math. Phys. 12, 1567 (1971).
[27]I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products*, 4th ed. (Academic, New York, 1965), p. 688.
[28]Reference 27, p. 692.
[29]A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. I, p. 103.
[30]Reference 29, p. 255.
[31]Reference 27, p. 711.
[32]Reference 27, p. 687.
[33]Reference 29, p. 114.
[34]K. Omidvar, Phys. Rev. 140, A26 (1965).
[35]J. Macek, Phys. Rev. A 1, 235 (1970); also A. Salin, J. Phys. B 2, 631 (1969).