Coulomb deflection in ion-atom collisions

Grzegorz Lapicki and William Losonsky*
Department of Physics, New York University, New York, New York 10003
(Received 12 January 1979)

The Coulomb-deflection factor, defined as the ratio of the Coulomb to plane-wave Born cross sections, is derived for slow but classically moving ions, and found to be in agreement with the data for K-shell ionization. When the half distance of closest approach in a head-on collision, d, is comparable to the important impact parameters ($\sim 1/q_0$, where q_0 is the minimum momentum transfer), this factor simplifies to $\exp(-\pi d q_0)$ as it has been employed in the inner-shell-ionization theory. When the impact parameters are small on the scale of the projectile de Broglie wavelength, as they are in nuclear phenomena, the Coulomb-deflection factor tends to $\exp(-2\pi d q_0)$. An extension of our results to screened Coulomb repulsion gives good agreement with the semiclassical calculations and the data for K-shell excitation in Ne^+-Ne collisions.

I. INTRODUCTION

In quantum-mechanical and semiclassical versions of the standard Born approximation, the projectile is described, respectively, as a plane wave or as a classical particle moving along a straight-line trajectory. This approximation becomes inadequate when the projectile moves so slowly that the plane wave is appreciably distorted by the Coulomb field of the target nucleus or the classical particle is significantly deflected into a Kepler orbit. In consequence, with decreasing ion velocity experimental cross sections for inner-shell vacancy production in ion-atom collisions become significantly smaller than the predictions of the plane-wave or straight-line Born approximation.

This discrepancy has been confirmed for K-shell vacancy production by semiclassical calculations. For K-shell ionization, Bang and Hansteen[1] showed that the calculations with a hyperbolic trajectory can indeed yield order of magnitude smaller cross sections than the approximation which assumes a straight-line path for the projectile. Similarly, Briggs and his collaborators[2-8] found that the cross sections for K-shell excitation in slow ion-atom collisions are markedly different when evaluated with various forms of the internuclear potential between the projectile ion and the target atom; the calculations with the Coulomb and screened Coulomb potentials resulted in significantly smaller cross sections than the approach in which the internuclear potential was neglected (straight-line approximation).

From the formulas of Bang and Hansteen,[1] Brandt and his co-workers[9,10] have extracted the Coulomb-deflection factor which was questioned on the basis of numerical[11-13] and analytical[14,15] reexamination of the Bang and Hansteen calculations. The approach of Briggs and co-workers[2-8] relies on numerical solutions of coupled-state equations. Although an elegant scaling[5,7] from one collision system to another was shown to be possible when the internuclear potential was neglected or Coulombic, no Coulomb-deflection factor has been extracted from the calculations. Moreover, the scaling[5,7] between different collision systems is not reliable[7] for screened Coulomb potentials which have to be employed to obtain agreement with experimental cross sections.

We derive a Coulomb-deflection factor C in an essentially quantum-mechanical treatment of the first Born approximation. The factor $C \equiv \sigma^{\mathrm{CWBA}}/\sigma^{\mathrm{PWBA}}$ has a universal character in that it scales the plane-wave Born approximation (PWBA) cross section σ^{PWBA} to the Coulomb-wave Born approximation (CWBA) cross section σ^{CWBA} for any inelastic collision in which the low-velocity projectile suffers relatively small loss of its energy. Because of the equivalence of the quantum-mechanical and semiclassical treatments in the Born approximation for such collisions,[16] the factor C allows one to scale the cross sections calculated for straight-line trajectories to the cross sections which are based on hyperbolic-trajectory calculations. This factor greatly simplifies analysis in that it avoids difficult numerical calculations with a hyperbolic trajectory. Moreover, in the slow collision limit of interest, the straight-line cross sections are often given analytically.

The derivation of the Coulomb-deflection factor is presented in Sec. II. In Sec. III, this factor is compared with data and calculations[1-15] for K-shell vacancy production in a target atom of atomic number Z_2 which is much larger than the atomic number Z_1 of the projectile ion ($Z_1 \ll Z_2$) and, also, in a homonuclear system ($Z_1 = Z_2$). In the Appendix, we show how to extend our approach to inelastic scattering in screened Coulomb potentials.

II. COULOMB-DEFLECTION FACTOR

Consider a nonrelativistic ion-atom collision in which the projectile ion with initial energy E_i (velocity $\vec{v}_i$ and momentum $\vec{K}_i = M\vec{v}_i$) loses the energy ΔE:

$$\Delta E = E_i - E_f = \tfrac{1}{2}M(v_i^2 - v_f^2) = (1/2M)(K_i^2 - K_f^2) \quad (1)$$

in terms of its final energy E_f (velocity $\vec{v}_f$ and momentum $\vec{K}_f = M\vec{v}_f$) and the reduced mass of the ion-atom system, M. In the independent-electron approximation, one electron is excited while all other electrons remain in their initial states and screen the nuclei. Here we consider pure Coulomb deflection, i.e., the internuclear interaction is given by the unscreened Coulomb potential. The internuclear screening is discussed in the Appendix as an extension of the results obtained in this section.

In the first Born approximation the transition amplitude T_{if} is given by

$$T_{if} = \int\int \psi_f^*(\vec{R})\phi_f^*(\vec{r})\vartheta(\vec{R},\vec{r})\psi_i(\vec{R})\phi_i(\vec{r})d^3R\,d^3r\,, \quad (2)$$

where $\vartheta(\vec{R},\vec{r})$ is the perturbing potential, $\psi_{i,f}(\vec{R})$ are the solutions of the nuclear part of the unperturbed Hamiltonian

$$\left(-\frac{1}{2M}\nabla_R^2 + \frac{Z_1Z_2}{R}\right)\psi_{i,f}(\vec{R}) = E_{i,f}\psi_{i,f}(\vec{R})\,, \quad (3)$$

with $\vec{R}$ being the position of the projectile with respect to the target,[17] and $\phi_{i,f}(\vec{r})$ are the unperturbed wave functions of the active electron at the position $\vec{r}$. In the PWBA, Z_1Z_2/R is removed from Eq. (3) and added to $\vartheta(\vec{R},\vec{r})$ in Eq. (2) where, due to the orthogonality of ϕ_i and ϕ_f, it gives no contribution to T_{if}.

We restrict ourselves to slow collisions for which a classical description of the projectile is possible so that one can use the quantum-mechanical Coulomb-deflection factor in the scaling of straight-line semiclassical calculations. The de Broglie wavelength of the projectile, $1/K_i$, is then much smaller than the half-distance of closest approach in a head-on collision, $d \equiv Z_1Z_2/Mv_i^2$, and yet the projectile orbit is not significantly modified because of the finite energy loss. With the notation $\eta_{i,f} \equiv Z_1Z_2M/K_{i,f}$, these restrictions, $\eta_i = K_i d \gg 1$ and $\Delta E/E_i \ll 1$, lead to

$$\Delta\eta \equiv \eta_f - \eta_i \cong dq_0 \text{ and } \Delta\eta/\eta_i \simeq \tfrac{1}{2}\Delta E/E_i \ll 1 \quad (4)$$

(Ref. 18). The minimum momentum transfer $q_0 \equiv K_i - K_f$ can be approximated, respectively, by $\Delta E/v_i$ for direct and by $\Delta E/v_i + \frac{1}{2}v_i$ for rearrangement collisions. The adiabaticity parameter $\Delta\eta$ determines the ratio of the characteristic time in Coulomb scattering, d/v_i, to the time of transition, $1/\Delta E$.

Our derivation of the Coulomb-deflection factor is based on the assumption that one can extract multiplicative constants $N_{i,f}$ which relate the Coulomb wave functions $\psi_{i,f}^C$ to plane waves $\psi_{i,f}^P$, as

$$\psi_{i,f}^C = N_{i,f}\psi_{i,f}^P\,; \quad (5)$$

these constants will be determined as $\psi_{i,f}^C/\psi_{i,f}^P$ evaluated at $\vec{R}$ for which the excitation probability attains its maximum. Since for plane waves the cross section is proportional to the ratio of the final to the initial current densities of the scattered particles j_f/j_i, where $j_{i,f}^C = v_{i,f}|N_{i,f}|^2$ for $\psi_{i,f}^C$ of Eq. (5) and $j_{i,f}^P = v_{i,f}$ for $\psi_{i,f}^P$, we obtain immediately that the ratio of the Coulomb cross section σ^{CWBA} to the plane-wave cross section σ^{PWBA} is

$$C = |N_f|^2/|N_i|^2\,. \quad (6)$$

Alternatively, one derives this equation through the renormalization of amplitude T_{if}, Eq. (2), to yield the Rutherford cross section when $i=f$. The necessity for the renormalization of the Coulomb scattering amplitude is well established,[19,20] although "a clean derivation within the general framework of renormalization theory has so far not been accomplished."[20]

When the Coulomb and plane waves are compared at their origin ($R=0$), the multiplicative constants $N_{i,f}$ can easily be determined as[21]

$$N_{i,f} = e^{-\pi\eta_{i,f}/2}\Gamma(1+i\eta_{i,f}) \quad (7)$$

so that, with

$$|\Gamma(1+i\eta_{i,f})|^2 = \pi\eta_{i,f}/\sinh(\pi\eta_{i,f})$$

and with

$$\frac{1-e^{-2\pi\eta_i}}{1-e^{-2\pi\eta_f}} \simeq 1 \text{ for } \eta_{i,f} \gg 1\,,$$

$$C \cong e^{-2\pi\Delta\eta}\,. \quad (8)$$

Not surprisingly, Landau[22] found—to within a coefficient slowly varying with energy—the same Coulomb-deflection factor in the WKB approach that was applied 50 years ago to explain nuclear disintegration.[23] Gamow[24] interpreted Landau's result as essentially the ratio of transparencies for the deflected and incident particles traveling through the Coulomb potential barrier. The WKB treatment is justified when the transparencies are small[25] as they are in the slow collision regime ($\eta_{i,f} \gg 1$), and its result is identical with Eq. (8). The same $e^{-2\pi\Delta\eta}$ factor is obtained in studies of Coulomb excitation of nuclei when $\Delta\eta \to \infty$ (Ref. 26): the monopole term ($l=0$) of a multipole expansion for the perturbing potential vanishes, the dipole term ($l=1$) has the cross section $\sigma(l=1)$ proportional to $e^{-2\pi\Delta\eta}$,[27] and the higher terms ($l>1$) are of no significance since

$$\sigma(l)/\sigma(l=1)\propto(\Delta\eta)^{-2(l-1)/3}$$

(Ref. 26).

It is not appropriate, however, to compare the Coulomb and plane waves at the origin when atomic collisions are considered. The important impact parameter p_0 in the straight-line approximation for such collisions is of the order of q_0^{-1}. Thus in the expansion of the projectile wave function into the partial waves with respect to the angular momentum L, the dominating L_0 wave is such that

$$L_0\equiv K_i p_0=K_i A_0/q_0=A_0\eta_i/\Delta\eta\gg 1\,, \tag{9}$$

where $A_0\equiv p_0 q_0$ is of the order of unity. On the other hand, $L_0\simeq 0$ for nuclear phenomena since then p_0 being the size of nuclei becomes negligible in comparison with de Broglie wavelength of the projectile, $1/K_i$. In fact, we will retrieve Eq. (8) as a particular result of our approach in the $L_0\to 0$ limit.

To within a phase factor, one has

$$N_{i,f}(\eta_{i,f},L_0;\rho_{i,f})=\frac{F_{L_0}(\eta_{i,f},\rho_{i,f})}{j_{L_0}(\rho_{i,f})\rho_{i,f}}, \tag{10}$$

where $F_L(\eta,\rho)$ is the regular Coulomb wave function.[28] In the $\eta\to 0$ limit $F_L(\eta,\rho)$ reduces to the partial wave $j_L(\rho)\rho$ of the plane-wave expansion with $j_L(\rho)$ being the spherical Bessel function and $\rho\equiv KR$ the internuclear distance R on the scale of the projectile's de Broglie wavelength. Since Coulomb deflection can be viewed as a result of penetration into the classically inaccessible region, the knowledge of $F_L(\eta,\rho)$ is required in the $0\leqslant\rho\leqslant\rho_c$ range, where $\rho_c=\eta+[\eta^2+(L+1)L]^{1/2}$ denotes the distance of closest approach in Coulomb scattering.

One can generate $F_L(\eta,\rho)$ through a single recursion formula once $F_0(\eta,\rho)$ is given.[29] The $L=0$ functions, however, are tabulated only for $\rho\leqslant 20$ (Ref. 30) or for $\rho\leqslant 40$ with values of $\eta\leqslant 12$ (Ref. 31) which are too small for typical atomic collisions. Above all, tabulations allow one to calculate $F_L(\eta,\rho)$ only at certain discrete points in the η-ρ plane whereas the knowledge of $F_L(\eta,\rho)$ for a continuous set of η and ρ values is desired in evaluation of C of Eq. (6) with $N_{i,f}$ from Eq. (10). Although the F_0 function can be computed for all η and ρ by a number of well-known methods in various regions of the η-ρ plane,[32] such a calculation would involve somewhat cumbersome numerical procedures. Therefore, in our calculations of C we have used the WKB form for $F_L(\eta,\rho)$ which, with the substitution of $L(L+1)$ by $(L+\frac{1}{2})^2$, was shown to be accurate to within 5% even for $\eta=L=1$ as long as $\rho\leqslant L+\frac{1}{2}$.[33] We found that the tabulated values[34] of $F_L(\eta,\rho)$ are reproduced to within 1% when $L>10$, $\eta>5$, and ρ is not larger than $L+\frac{1}{2}$. Thus the WKB formula for $F_L(\eta,\rho)$ is sufficient when one considers slow collisions ($\eta\gg 1$) in which the $L\simeq L_0\gg 1$ waves dominate [Eq. (9)].

The important ρ, at which Eq. (10) should be evaluated is determined in the straight-line approximation as $Kp_0=L_0=A_0\eta_i/\Delta\eta$ so that

$$C_{L_0}(\Delta\eta;\rho=L_0)=\frac{|F_{L_0}(\eta_f,L_0)|^2}{|F_{L_0}(\eta_i,L_0)|^2}. \tag{11}$$

The form $e^{-\pi\Delta\eta}$ used by Brandt and his co-workers[9,10,15] as the Coulomb-deflection factor obtains when $\rho=\eta$. The WKB Coulomb wave function[33] reduces at this distance to

$$F_L(\eta,\rho=\eta)=2^{-1/2}\sin^{L+1}(\tfrac{1}{2}u_0)\cos^{-L}(\tfrac{1}{2}u_0)\times\exp[-\tfrac{1}{2}\pi\eta+(L+\tfrac{1}{2})/\cos u_0]\,, \tag{12}$$

where

$$\sin u_0\equiv\eta/[\eta^2+(L+\tfrac{1}{2})^2]^{1/2}.$$

Once Carlini's formula[35] is rewritten as

$$j_L(\eta)\eta=2^{-1/2}\sin^{1/2}(\tfrac{1}{2}u_0)\tan^{L+1/2}(\tfrac{1}{2}u_0)\times\exp[(L+\tfrac{1}{2})/\cos u_0]\,, \tag{13}$$

we find immediately from Eq. (10) that

$$N_{i,f}(\eta_{i,f},L;\rho=\eta_{i,f})=(\cos\tfrac{1}{2}u_0^{i,f})^{1/2}\exp(-\tfrac{1}{2}\pi\eta_{i,f})\,, \tag{14}$$

which by Eq. (6) leads to

$$C_L(\Delta\eta;\rho=\eta)\cong e^{-\pi\Delta\eta}. \tag{15}$$

The approximate equality sign in Eq. (15) applies in the sense that

$$\cos(\tfrac{1}{2}u_0^{i,f})\equiv[\tfrac{1}{2}(1+1/\{1+[\eta_{i,f}/(L+\tfrac{1}{2})]^2\}^{1/2})]^{1/2}$$

is a very slowly varying function of $\eta/(L+\frac{1}{2})$ and, in fact,

$$\cos(\tfrac{1}{2}u_0^f)/\cos(\tfrac{1}{2}u_0^i)\approx 1\,.$$

For $L=L_0$, Eq. (15) is identical with our Coulomb-deflection factor [Eq. (11)] when $\Delta\eta=A_0$. To discuss the deviations of this factor from $e^{-\pi\Delta\eta}$ which is used in the literature,[9,10,15] we will consider $C/e^{-\pi\Delta\eta}$.

Figure 1 shows that C_{L_0} of Eq. (11) is practically independent of η_i and somewhat sensitive to the choice of $A_0\equiv p_0q_0$. The values of A_0 depend on the method of deciding what is the most important impact parameter p_0 in the $P(p)p$ distribution, where $P(p)$ is the excitation probability for a given collision process as calculated in the straight-line approximation at the impact parameter p. One can define p_0 as the impact parameter at which

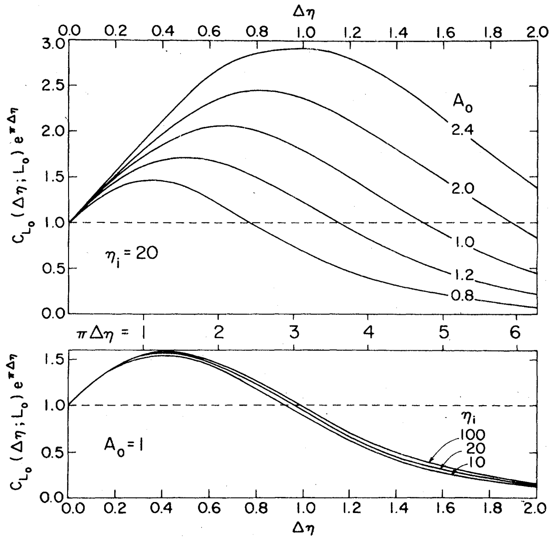

FIG. 1. Coulomb-deflection factor $C_{L_0}(\Delta\eta;L_0)$, derived from Eq. (11) and divided by $e^{-\pi\Delta\eta}$, as a function of $\Delta\eta \simeq dq_0$ for various choices of $\eta_i \equiv Z_1Z_2/v_i$ with $A_0=1$ (lower figure) and of $A_0 \equiv p_0q_0$ with $\eta_i=20$ (upper figure). Note that C_{L_0} is virtually independent of η_i for all $\Delta\eta$ and closely equal to $e^{-\pi\Delta\eta}$ when $\Delta\eta = A_0$. By Eq. (7), $L_0=A_0\eta_i/\Delta\eta \gg 1$.

$P(p)p$ attains a maximum or take

$$p_0 \equiv \int_0^\infty pP(p)p\,dp \Big/ \int_0^\infty P(p)p\,dp\,.$$

Correspondingly, we obtain[36] $A_0=1.2$ or 1.8 for ionization of an s state, $A_0=1.7$ or 2.3 for ionization of a p state, and $A_0=0.8$ or 0.9 for K-shell exciation in the homonuclear collisions considered by Briggs.[7] In Sec. III, we will assume that $A_0=0.85$ for K-shell excitation in Ne^{+}-Ne collision, and $A_0=1.5$ and 2 for s- and p-state ionization.

Figures 2 and 3 illustrate, respectively, how critically the Coulomb-deflection factor depends on the choice of the partial wave at $L=L_0$ and at $\rho=L_0$. We have evaluated $C_L(\Delta\eta;L_0)$ for the $0.3 \leq L/L_0 \leq 3.0$ range which covers about 90% of the area under the normalized $P(p)p$ curve. As shown in Fig. 2, F_L gives the same result as F_{L_0} to within a factor of 2 even when $\Delta\eta$ is not close to unity. Actually the uncertainty of the Coulomb-deflection factor is somewhat smaller because already $\frac{2}{3}$ of the normalized $P(p)p$ distribution is covered when $0.5 \leq L/L_0 \leq 2.0$ and the underestimate of the C_{L_0} factor for $L<L_0$ appears to nearly offset the overestimate for $L>L_0$. Figure 3 shows a similar compensation when $C_{L_0}(\Delta\eta;\rho)$ is considered around $\rho=L_0$ (filled circles). The open circles represent the calculation at $\rho=\eta$ which results essentially in the $e^{-\pi\Delta\eta}$ dependence given by Eq. (15).

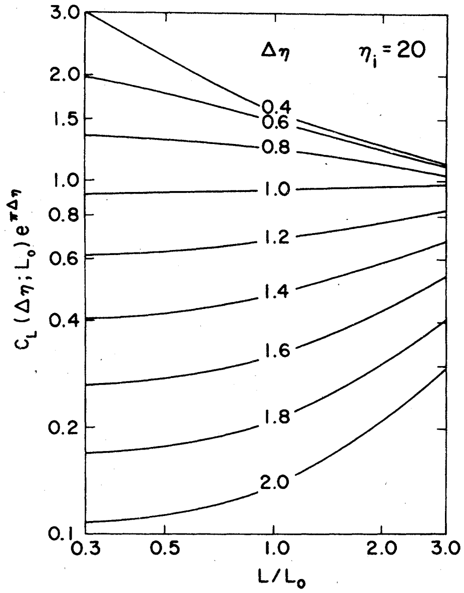

FIG. 2. Coulomb-deflection factor $C_L(\Delta\eta;L_0)$ divided by $e^{-\pi\Delta\eta}$ as a function of L/L_0 for $\eta_i=20$ and various $\Delta\eta$.

The Coulomb-deflection factor reduces practically to unity at the distance of closest approach in the Coulomb scattering

$$\rho_c = \eta + [\eta^2 + (L+\tfrac{1}{2})^2]^{1/2}$$

since for $\eta \gg 1$ (Ref. 37) the function

$$F_L(\eta, \rho=\rho_c) = \frac{\Gamma(1/3)}{2\sqrt{\pi}}\left(\frac{\rho_c}{3}\right)^{1/6}\left[1+\left(\frac{L+\frac{1}{2}}{\rho_c}\right)^2\right]^{-1/6} \tag{16}$$

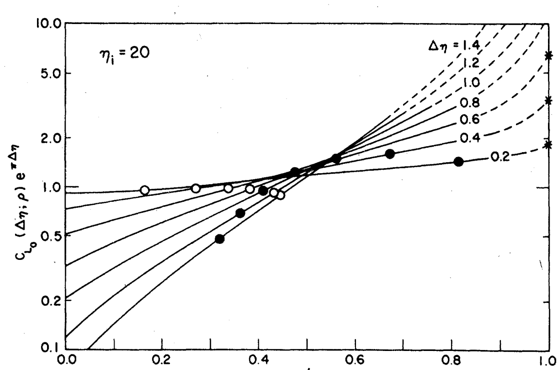

FIG. 3. Coulomb-deflection factor $C_{L_0}(\Delta\eta;\rho)$ divided by $e^{-\pi\Delta\eta}$ as a function of ρ/ρ_c for various $\Delta\eta$ with

$$\rho_c \equiv \eta_i + [\eta_i^2 + (L_0+\tfrac{1}{2})^2]^{1/2}$$

and $\eta_i=20$. The open circles at $\rho=\eta$ are according to Eq. (15) and the filled circles at $\rho=L_0$ are calculated from Eq. (11). The dashed curves are drawn where the WKB evalaution of $F_{L_0}(\eta,\rho)$ begins to lose its validity, and the stars at $\rho=\rho_c$ mark the points where $C_{L_0}(\Delta\eta;\rho_c)=1$ as expected on the basis of Eq. (16).

has an extremely weak dependence on η. The $\rho/\rho_c > 1$ region is expected to become insignificant since for such ρ values $F_L(\eta, \rho)$ exhibits an oscillatory behavior, and, therefore, tends to cancel out with contributions of other F_L functions in the transition amplitude T_{if} of Eq. (2). On the other hand, the $\rho/\rho_c \ll 1$ values become accessible in nuclear collisions. At $\rho = 0$ Eq. (10) reads[28]

$$N_{i,f}(\eta_{i,f}, L; 0) = \left\{ \frac{2\pi\eta_{i,f}}{e^{2\pi\eta_{i,f}} - 1} \prod_{s=1}^{L} \left[1 + \left(\frac{\eta_{i,f}}{s} \right)^2 \right] \right\}^{1/2}. \tag{17}$$

With $\eta_{i,f} \gg 1$ and ρ being identified with L_0 (the $L_0 \to 0$ limit), Eq. (17) leads to

$$C_0(\Delta\eta; 0) \simeq e^{-2\pi\Delta\eta}, \tag{18}$$

which, as anticipated, is identical with Eq. (8).

In the derivation of the Coulomb-deflection factor, Eq. (11), we have tacitly assumed that $L_i = L_f \simeq L_0$ since $(L_f - L_i)/L_0 \simeq \Delta\eta/\eta_i \ll 1$ [see Eq. (4)] so that the classical projectile trajectory is well defined.[38] It may be argued that such an approach is strictly valid only as long as the angular momentum of the electron is conserved. This assumption is made in the semiclassical calculations for K-shell ionization[11-15] which, in the monopole approximation to the perturbing potential, consider only the transition to the $1s$ state in the continuum of the target atom.[1] However, these calculations deviate from C_{L_0} of Eq. (11) and from $e^{-\pi\Delta\eta}$, Eq. (15), as $\Delta\eta/\eta_i$ increases. One can view such deviations as an inherent breakdown in the equivalence between a semiclassical approach and our essentially quantum-mechanical treatment when $\Delta\eta/\eta_i$ is not negligible.

We conclude that the form $e^{-\pi\Delta\eta}$, Eq. (15), ought to give estimates of the Coulomb-deflection factor, Eq. (11) or Fig. 1, good to an accuracy of a factor of ~2. Given the straight-line impact-parameter-dependent probability $P(p)$ for a specific collision process, we can determine A_0 and the PWBA cross section which is easily scaled to the CWBA results by multiplication with $e^{-\pi\Delta\eta}$ or $C_{L_0}(\Delta\eta; L_0)$, where L_0 is $A_0\eta_i/\Delta\eta$.

III. INNER-SHELL-VACANCY PRODUCTION: A TEST OF THE COULOMB-DEFLECTION FACTOR

A. K-shell excitation in symmetric collisions ($Z_1 = Z_2$)

Briggs and co-workers[2-8] have reported calculations for K-shell excitation in Ne^+-Ne collisions. These semiclassical calculations were performed numerically with the neglect of the internuclear potential as well as with the Coulomb potential, Z_1Z_2/R, and Bohr's screened Coulomb potential, Eq. (A1). The resulting cross sections varied by orders of magnitude depending on the choice of the potential; very close agreement with experiment[39] was obtained when the screened potential was used.

If the internuclear potential is neglected, *ab initio* $2p\pi$-$2p\sigma$ coupled-state calculations[7] yield a straight-line impact-parameter-dependent function P. This probability of producing a hole (or a K-shell vacancy in the separated-atom nomenclature) in the collision is solely dependent on $(k/v_i)^{1/3}p$ if one sets $\Delta E = kR^2$, with $k \equiv \frac{1}{40} Z_1^* Z_2^* (Z_1^* + Z_2^*)^2$ in a small-R expansion.[40] By integration over all impact parameters the straight-line semiclassical, or equivalently, the PWBA cross section is obtained as

$$\sigma^{\text{PWBA}} = 2\pi \int_0^\infty P(p)p\,dp = N_0 \left(\frac{v_i}{k} \right)^{2/3}. \tag{19}$$

We have read the P function from Fig. 3 of Ref. 7 and found that N_0 is 2.4 for N^+-N collisions. Because of the universality of P, especially for symmetric collisions, one may use this constant in Eq. (19) for the analysis of Ne^+-Ne collisions. With the identification $\Delta\eta = dq_0$ [Eq. (4)] and with the Coulomb-deflection factor $e^{-\pi\Delta\eta}$ or, more refined, Eq. (11) at $A_0 = 0.85$, we can scale σ^{PWBA} to σ^{CWBA}.

We determine q_0 as $q_0 = \langle\Delta E\rangle/v_i$, with

$$\langle\Delta E\rangle \equiv \int_0^\infty \Delta E(R_0)P(p)p\,dp \bigg/ \int_0^\infty P(p)p\,dp. \tag{20}$$

For R_0 we take the distance of closest approach, i.e., the solution of

$$E_i(1 - p^2/R_0^2) = V(R_0), \tag{21}$$

which is $R_0 = d + (d^2 + p^2)^{1/2}$ for the pure Coulomb potential $V = Z_1Z_2/R$. As discussed in the Appendix, for screened Coulomb potentials $R_0 \to R_0'$, $d \to d'$, $q \to q_0'$, and $\Delta\eta \to \Delta\eta' = d'q_0'$. For $\Delta E(R_0)$ in Eq. (20), we take

$$\Delta E(R_0) = kR_0^2/[1 + 0.122(bR_0)^2 + 0.0729(bR_0)^4]^{1/2}. \tag{22}$$

With Briggs' reduced unit of length

$$b \equiv \{Z_1^{*2} Z_2^{*2} [\tfrac{1}{2}(Z_1^* + Z_2^*)]^4 M/(Z_1Z_2)\}^{1/7},$$

Eq. (22) reproduces to within 8% the Hartree-Fock results for ΔE that were used in calculations of Briggs and co-workers (see Fig. 4 of Ref. 7). Such a fit, valid for all internuclear separations R, is necessary because the deflected projectiles do not probe the small-R-expansion region. If one were to evaluate in Eq. (20) $\Delta E(R_0)$ at $R_0 = p$, corresponding to undeflected projectiles, the data plot as the open circles in Fig. 4 in gross disagreement with the $e^{-\pi\Delta\eta}$ factor.

Figure 4 displays the ratio of K-shell excitation cross sections for Ne^{+}-Ne collisions calculated[2,8] with a hyperbolically deflected trajectory to the cross sections evaluated with the straight-line path or equivalently $C = \sigma^{CWBA}/\sigma^{PWBA}$. The dash-dotted and dashed curves versus $\pi\Delta\eta$ and $\pi\Delta\eta'$, respectively, are the C's for pure[2] and screened[8] Coulomb potentials. The closeness of these curves indicates that our procedure developed to incorporate the screening effect (see the Appendix) is adequate; the difference between them reflects on the inherent difficulty in the determination of $\langle\Delta E\rangle$. The solid line represents the $C = e^{-x}$, with $x = \pi\Delta\eta$ or $\pi\Delta\eta'$. Good agreement with the data[39] is obtained when the experimental ratios are plotted as a function of $\pi\Delta\eta'$, the screened argument of the Coulomb-deflection factor. As an example of the difference between the Coulomb and the screened

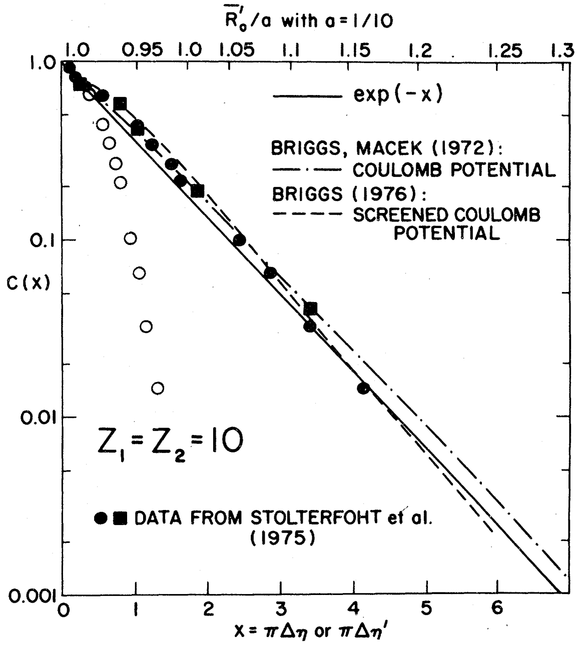

FIG. 4. Coulomb and screened Coulomb-deflection factors, $C(x)$, for K-shell excitation in Ne^{+}-Ne collisions. The dash-dotted and dashed curves plotted, respectively, vs $x = \pi\Delta\eta$ and $x = \pi\Delta\eta'$, are the results of the semiclassical calculations with Coulomb (Ref. 2) and screened Coulomb (Ref. 8) potentials. They follow closely the solid line e^{-x}. Experimental cross sections (Ref. 39) divided by the PWBA cross sections, Eq. (19), based on Ref. 7, are in agreement with this line only when plotted vs $x = \pi\Delta\eta'$ (solid symbols). The open symbols result if $\Delta\eta'$ is determined from $\langle\Delta E\rangle$ being evaluated with $\Delta E(p)$ instead of $\Delta E(R_0')$. As discussed in the Appendix, it is necessary to employ a screened Coulomb potential when $\bar{R}_0'/a > 1$.

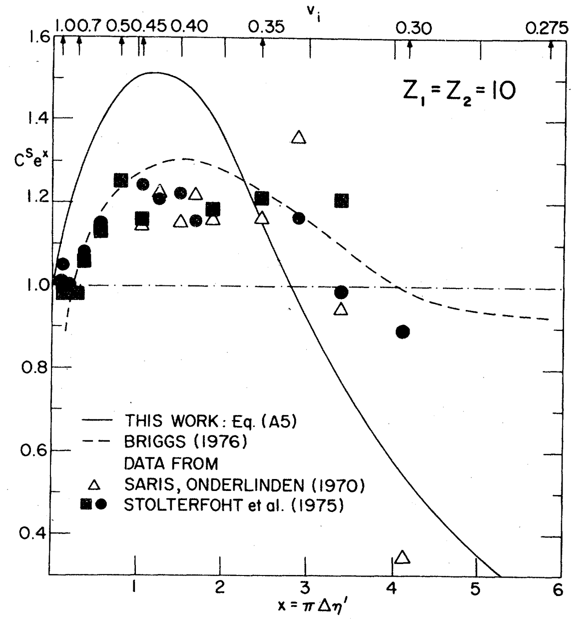

FIG. 5. Screened Coulomb-deflection factor divided by $e^{-\pi\Delta\eta'}$ for K-shell excitation in Ne^{+}-Ne collisions. The semiclassical calculations (dashed curve) of Ref. 8 and the data of Refs. 39 and 41 are in good agreement with the screened Coulomb-deflection factor $C^S = C_{L_0'}(\Delta\eta'; L_0')$ of Eqs. (A5), (A6), and (11) (solid curve).

Coulomb potentials, one has for a Ne^{+}-Ne collision at $v_i = 0.3$ the values $\pi\Delta\eta = 9.26$ and $\pi\Delta\eta' = 4.16$. Then $e^{9.3-4.2} = 164$, i.e., the measured cross section at $v_i = 0.3$ is two orders of magnitude larger than the prediction of the theory which assumes that the internuclear potential is purely Coulombic. The curve drawn on the basis of Eq. (A5) would be indiscernibly close to Briggs' screened Coulomb curve (dashed curve).

The Coulomb-deflection factors for screened Coulomb repulsion are examined in a magnified way in Fig. 5. In addition to the data[39] shown in Fig. 4, we plot the data from Ref. 41 which agree with those of Ref. 39 except of the lowest velocity $v_i = 0.3$; other data[42] for Ne^{+}-Ne collisions are within the ~20% experimental uncertainty but they do not extend down to $v_i = 0.3$.[43] The Coulomb factor, although it changes by almost three orders of magnitude, is predicted by $e^{-\pi\Delta\eta'}$ nearly to within the uncertainties of the data and agrees to within ~30% with Briggs' calculations.[8] The divergence between the solid and dashed curves at the lowest velocities may be due to inherent difficulties in our determination of $\langle\Delta E\rangle$ which is needed to obtain $\Delta\eta'$. Good agreement is also found between the exponential factor, the data, and calculations that were reported by Peterson *et al.*[44] for the isotope dependence of the K-shell-

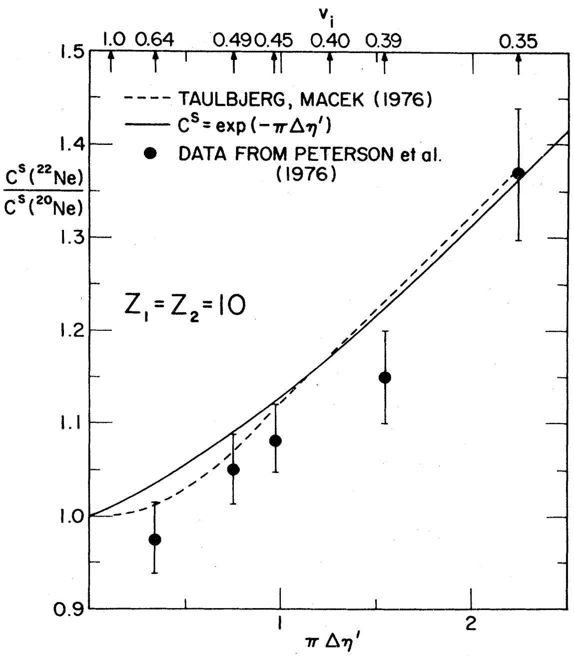

FIG. 6. Isotope effect for K-shell excitation in Ne^+-Ne collisions: the larger cross sections for ^{22}Ne than ^{20}Ne are explained in terms of the smaller Coulomb-deflection effect for the heavier isotope. The data and the results of the semiclassical calculations (dashed curve) are shown as reported in Ref. 44. The solid curve is based on the simple approximation to the screened-Coulomb-deflection factor derived in this work. As can be seen from Fig. 5, Eq. (A5) would be in excellent agreement with the dashed curve and the data.

vacancy production in slow Ne^+-Ne collisions (see Fig. 6).

B. Inner-shell ionization in nonsymmetric collisions ($Z_1 < Z_2$)

Based on the perturbed stationary-state (PSS) approach,[45] Brandt and coworkers[10,15] have developed a direct ionization theory for $Z_1 \ll Z_2$. Since electron capture contributes negligibly to inner-shell ionization in such collisions, the ratios of experimental cross sections to predictions of the PSSR theory—which accounts also for the relativistic (R) effect in the description of an inner shell[15]—determine semiempirically the Coulomb-deflection factor. Figure 7 demonstrates that the locus of these ratios based on the data[46] for K x-ray production by protons follows $C = e^{-\pi\Delta\eta_0}$.[47]

They do not confirm the result of semiclassical calculations in the monopole approximation.[11-13,15] Their scatter does not allow one to decide whether the refinement of the Coulomb deflection as calculated from Eq. (11) is warranted.

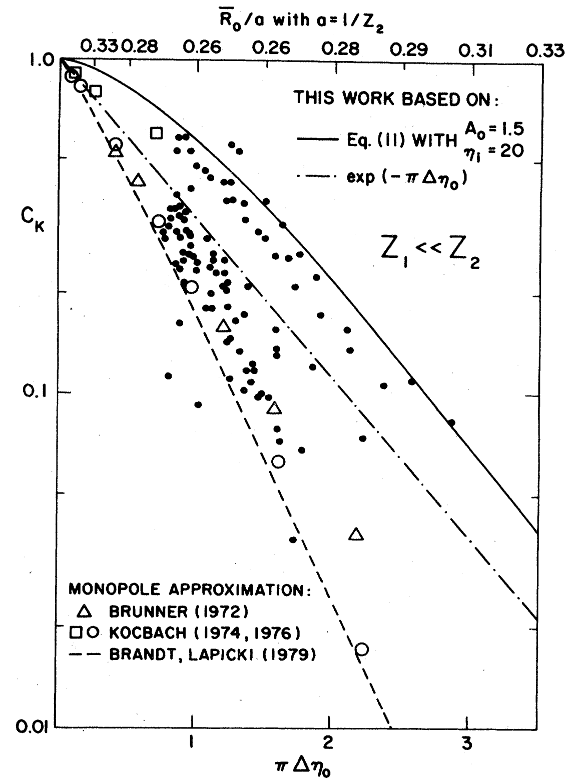

FIG. 7. Coulomb-deflection effect for K-shell ionization by protons in the $Z_1 \ll Z_2$ collisions. The closed circles represent a semiempirical determination of this effect once the ratios of the x-ray production data (Ref. 46) to the predictions of the PSSR theory for direct ionization (Refs. 10 and 15) are plotted vs $\pi\,\Delta\eta_0$ as explained in Ref. 47. The open symbols and dashed curve are the numerical (Refs. 11–13) and analytical (Ref. 15) results of the semiclassical approach (Ref. 1). The dash dotted and solid curves are based on, respectively, $e^{-\pi\Delta\eta_0}$, and Eq. (11) with $A_0 = 1.5$ and $\eta_i = 20$ as derived in this work. As discussed in the Appendix, it is sufficient to use a pure Coulomb potential when $\bar{R}_0/a < 1$.

C. Summary

We conclude from Figs. 4–7 that the form $e^{-\pi\Delta\eta}$ introduced as Coulomb-deflection factor in inner-shell ionization theory[9] is reliable within the scatter of data. Just as $e^{-2\pi\Delta\eta}$ is appropriate for nuclear processes so is $e^{-\pi\Delta\eta}$ for slow ion-atom collisions which occur at impact parameters comparable to the half-distance of closest approach, d [see Eq. (15)]. When collisions take place at other impact parameters, one should use the more general Eq. (11) or Fig. 1 to determine the Coulomb-deflection factor. Even then its values may differ by a factor of 2 because of the uncertainties in the choice of parameters which enter in Eq. (11). Equation (15) was found to be in good agreement with the Coulomb-deflection factor derived in semiclassical calculations for K-shell excitations in homonuclear collisions. It is expected to apply in any slow atomic collision for which a classical description of the projectile is possible.

Our derivation is basically quantum mechanical in that it considers the properties of the wave function of the projectile. One might be surprised that, by comparison with semiclassical calculations, its results are more accurate for quasimolecular excitation than for inner-shell ionization with $Z_1 \ll Z_2$ in which the Coulomb deflection is of lesser significance. This apparent paradox may be resolved if viewed as the lack of equivalence between the quantum-mechanical and semiclassical treatments when the energy loss ΔE cannot be neglected in comparison with the projectile energy E_i. We note that in Ne^+-Ne collision $\Delta E/E_i$ barely exceeds 1% whereas in inner-shell ionization $\Delta E/E_i$ can be as large as 10%. Although the Coulomb-deflection factor derived in this work gives overall a better agreement with experiment than the factors found in semiclassical approximation, the results of both approaches should be treated with caution unless $\Delta E/E_i \ll 1$. Otherwise, calculations based on a fully quantum-mechanical theory with projectiles described by Coulomb waves or a semiclassical approximation with the consideration[48] of projectile energy loss are needed.

ACKNOWLEDGMENTS

We would like to thank Werner Brandt and Kenneth F. Stanton for helpful discussions and criticism of the manuscript, and John S. Briggs for sending numerical results of his calculations that we have used in Figs. 4 and 5. This work was supported in part by the U. S. Department of Energy.

APPENDIX: SCREENED COULOMB-DEFLECTION FACTOR

It is necessary to account for screening of the nuclei when the projectile does not penetrate deeply into the K shell, i.e., when $\overline{R}_0' \gtrsim a$. Here $\overline{R}_0'$ is the distance of the closest approach evaluated for a screened potential at

$$\overline{p} \equiv \int_0^\infty pP(p)p\,dp \Big/ \int_0^\infty P(p)p\,dp\,,$$

and a is the K-shell radius. On the other hand, the screening is of no importance when $\overline{R}_0' \ll a$. In particular, the screening plays no role in the $Z_1 \ll Z_2$ inner-shell ionization processes unless one considers the high velocities at which the Coulomb-deflection effect ceases to be significant (see Fig. 7).

We extend the validity of Eqs. (11) and (15) to screened Coulomb potentials. Commonly used screened potentials are the Bohr potential[49]

$$V^B(R) = Z_1Z_2e^{-\mu_B R}/R\,, \tag{A1}$$

with

$$\mu_B \equiv (Z_1^{2/3} + Z_2^{2/3})^{1/2}\,,$$

and the Firsov potential[50]

$$V^F(R) = Z_1Z_2\Phi(\mu_F R/0.8853)/R\,, \tag{A2}$$

with $\mu_F \equiv (Z_1^{1/2} + Z_2^{1/2})^{2/3}$, where Φ is the Thomas-Fermi screening function. For small R, these potentials can be approximated by

$$V^S(R) = Z_1Z_2(1 - A\mu R)/R\,, \tag{A3}$$

the Coulomb potential minus the constant $Z_1Z_2A\mu$ which is independent of the internuclear distance R. The major contribution to inelastic collisions comes from the distances for which $\mu R < 1$. We find that Eq. (A3), with $A = 0.60$ and μ standing for μ_B or μ_F depending on the choice of potential, fits Eqs. (A1) and (A2) to within 20% over the $0 \leqslant \mu R \leqslant 1.2$ range. The Lindhard form for the screened Coulomb potential[51] is approximated by Eq. (A3) with even greater accuracy. A 20% uncertainty is usually associated with the statistical model for the internuclear potential[50] and is comparable with the uncertainties encountered in the quantum-mechanical calculation of the neon-neon interaction.[52] The solutions of

$$\left(-\frac{1}{2M}\nabla_{\vec{R}}^2 + V^S\right)\psi_{i,f}(\vec{R}) = E_{i,f}\psi_{i,f}(\vec{R}) \tag{A4}$$

are still given by Coulomb wave functions, Eq. (3), but with the eigenenergies $E'_{i,f} = E_{i,f} + A\mu Z_1Z_2$.[53] Thus we obtain the screened Coulomb-deflection factor C^S through the replacement of $\Delta\eta = dq_0$ in the argument of the Coulomb-deflection factor, Eq. (11) and $e^{-\pi\Delta\eta}$, by $\Delta\eta' = d'q_0'$, i.e., with $L_0' = A_0\eta_i/\Delta\eta'$

$$C^S = C_{L_0'}(\Delta\eta' = d'q_0'; L_0')\,. \tag{A5}$$

Here

$$d' \equiv d/(1 + A\mu Z_1Z_2/E_i) = d/(1 + 2A\mu d)$$

and

$$q_0' \equiv \langle\Delta E\rangle/[v_i(1 + 2A\mu d)^{1/2}]\,, \tag{A6}$$

where

$$\langle\Delta E\rangle = \int_0^\infty \Delta E(R_0')P(p)p\,dp \Big/ \int_0^\infty P(p)p\,dp$$

is with R_0' found by numerical solution of Eq. (21) in which $V(R_0')$ is given by Eq. (A1) or (A2).[54] Equation (A5) is rigorous as long as $2A\mu d \ll 1$. Note that in the $0 < \mu R < 1.2$ range of validity for Eq. (A3), $\mu d < 0.6$ or, with $A = 0.60$, $2A\mu d < 0.72$ since R is the distance of closest approach.

*Also Maritime College, SUNY, Bronx, N. Y. 10465

[1]J. Bang and J. M. Hansteen, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 31, No. 13 (1959).
[2]J. S. Briggs and J. Macek, J. Phys. B 5, 579 (1972).
[3]J. S. Briggs, in *Proceedings of the International Conference on Inner-Shell Ionization Phenomena and Future Applications, Atlanta, 1972*, edited by R. W. Fink, S. T. Manson, M. Palms, and P. V. Rao (U.S. AEC, Oak Ridge, TN, 1973), p. 1209.
[4]J. H. Macek and J. S. Briggs, J. Phys. B 6, 841 (1973); Comments At. Mol. Phys. 14, 97 (1973).
[5]J. S. Briggs and J. H. Macek, J. Phys. B 6, 982 (1973).
[6]K. Taulbjerg and J. S. Briggs, J. Phys. B 8, 1895 (1975); 8, 1909 (1975).
[7]K. Taulbjerg, J. S. Briggs, and J. Vaaben, J. Phys. B 9, 1351 (1976).
[8]J. S. Briggs, in *The Physics of Electronic and Atom Collisions: Invited Lectures, Review Papers and Progress Reports of the IX International Conference on the Physics of Electronics and Atomic Collisions, Seattle, 1975*, edited by J. S. Risley and R. Geballe (University of Washington, Seattle, 1976), p. 384; Rep. Prog. Phys. 39, 217 (1976).
[9]W. Brandt, R. Laubert, and I. Sellin, Phys. Lett. 21, 518 (1966); Phys. Rev. 151, 56 (1966).
[10]G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973); 17, 1655 (1978); W. Brandt and G. Lapicki, *ibid.* 10, 474 (1974); G. Lapicki, Ph.D. thesis (New York University, 1975) (unpublished); G. Lapicki and W. Losonsky, Phys. Rev. A 15, 896 (1977).
[11]K. Brunner, Ph.D. thesis (Würzburg University, 1972) (unpublished); K. Brunner and W. Hink, Z. Phys. 262, 181 (1973).
[12]L. Kocbach, Phys. Fenn. Suppl. S1 9, 46 (1974).
[13]L. Kocbach, Phys. Norv. 8, 187 (1976).
[14]P. A. Amundsen, J. Phys. B 10, 2177 (1977).
[15]W. Brandt and G. Lapicki, Phys. Rev. A 20, 465 (1979).
[16]J. W. Frame, Proc. Camb. Philos. Soc. 27, 511 (1931); N. F. Mott, *ibid.* 27, 553 (1931); A. M. Arthurs, *ibid.* 57, 901 (1961) (s-s transitions in the first Born approximation); R. McCarroll and A. Salin, C. R. Acad. Sci. (Paris) 263, 329 (1966) (all transitions in the first Born approximation); B. L. Moiseiwitsch, Proc. Phys. Soc. 87, 885 (1966) (all orders of the Born approximation); D. S. F. Crothers and A. R. Holt, Proc. Phys. Soc. 88, 75 (1966); A. V. Vinogradov, in *Proceedings (Trudy) of the P. N. Lebedev Physics Institute*, edited by D. V. Skobel'tsyn (Nauka, Moscow, 1970), Vol. 51, p. 45, translation available from Consultants Bureau, New York, 1971 (even for slow collisions as long as the reduced mass $M\rightarrow\infty$). This equivalence has been also proved for rearrangement collisions: R. Shakeshaft and L. Spruch, Phys. Rev. A 8, 206 (1973); and R. Shakeshaft, J. Phys. B 6, 1357 (1973).
[17]J. S. Briggs, J. Phys. B 8, L485 (1975). We restrict ourselves to the homonuclear ($Z_1=Z_2$, $M_1=M_2$) and highly nonsymetric ($Z_1 \ll Z_2$, $M_1 \ll M_2$) collisions for which the center of charge coincides with the center of mass.
[18]With $q_0=\Delta E/v_i$,

$$\Delta\eta=\frac{dq_0 2}{[1+(1-\Delta E/E_i)^{1/2}](1-\Delta E/E_i)^{1/2}} \simeq dq_0[1+3/4(\Delta E/E_i)+O(\Delta E/E_i)^2]$$

can be approximated by $\Delta\eta\simeq dq_0$ to about $75(\Delta E/E_i)\%$.
[19]S. Okubo and D. Feldman, Phys. Rev. 117, 292 (1960); R. A. Mapleton, J. Math. Phys. 2, 478 (1960); G. Gorshkov, Zh. Eksp. Teor. Fiz. 40, 1481 (1961) [Sov. Phys. JETP 13, 1037 (1961)]; J. D. Dollard, J. Math. Phys. 5, 729 (1964); W. F. Ford, J. Math. Phys. 7, 626 (1965); G. L. Nutt, J. Math. Phys. 9, 796 (1968); W. W. Zachary, J. Math. Phys. 12, 1379 (1971); J. C. Y. Chen and A. C. Chen, Adv. At. Mol. Phys. 8, 71 (1972); D. Zwanziger, Phys. Rev. D 7, 1082 (1973); E. Prugovečki and J. Zorbas, J. Math. Phys. 14, 1398 (1973), 15, 268(E) (1974); E. Prugovečki, Phys. Lett. 49B, 305 (1974); M. J. Roberts, J. Phys. Lett. 49B, 305 (1974); M. J. Roberts, J. Phys. B 7, L397 (1974); J. R. Taylor, Nuovo Cimento B 23, 313 (1974); S. N. Banerjee, J. Phys. B 8, L225 (1975); K. Nakano, Prog. Teor. Phys. 56, 1174 (1976); M. Kolsrud, Nuovo Cimento B 38, 61 (1977); J. Zorbas, J. Math. Phys. 18, 1112 (1977); E. O. Alt, W. Sandhas, and H. Ziegelmann, Phys. Rev. C 17, 1981 (1978); J. Zorbas, J. Math. Phys. 19, 2426 (1978); K. A. A. Hamza, Nuovo Cimento B 49, 247 (1979).
[20]J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons*, 2nd ed. (Springer, New York, 1976), see Suppl. S4, pp. 513 and 525.
[21]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics Nonrelativistic Theory* (Pergamon, London, 1958), p. 422.
[22]L. Landau, Phys. Z. Sowjet. 1, 88(1932) [English translation: Collected papers of L. D. Landau, edited by D. ter Haar (Pergamon, New York, 1965), p. 52]; see also H. A. Bethe, Rev. Mod. Phys. 9, 69 (1937) and E. Guth, Phys. Rev. 68, 280 (1945).
[23]G. Gamow, Z. Phys. 51, 204 (1928). For an account of early history of tunneling see E. Condon, Am. J. Phys. 46, 319 (1978).
[24]G. Gamow, *Structure of Atomic and Nuclear Transformations*, 2nd ed. (Clarendon, Oxford, 1937), Chap. IX, pp. 179 and 180.
[25]See Ref. 24, Chap. V, p. 94.
[26]K. A. Ter-Martirosyan, Zh. Eksp. Teor. Fiz. 22, 284 (1952) [English translation: first book below, p. 15]; K. Alder and A. Winther, *Coulomb Excitation* (Academic, New York, 1965); L. C. Biederharn and P. J. Brussaard, *Coulomb Excitation* (Clarendon, Oxford, 1965); J. M. Eisenberg and W. Greiner, *Excitation Mechanisms in the Nucleus* (North-Holland, Amsterdam, 1970), Chap. 8; K. Alder and A. Winther, *Electromagnetic Excitation Theory of Coulomb Excitation Theory of Coulomb Excitation with Heavy Ions* (North-Holland, Amsterdam, 1975).
[27]M. Pauli and D. Trautmann, J. Phys. B 11, 667 (1978). See Eq. (A14), I. Yu. Skobelev and A. V. Vinogradov, J. Phys. B 11, 2899 (1978), Eq. (8).
[28]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965), Chap. 14, p. 538, Eq. (4.1.3).
[29]See Ref. 28, p. 543, Table 14.7, Example 1.
[30]See Ref. 28, pp. 546–552, Table 14.1.
[31]A. Tubis, *Tables of Coulomb Wave Functions* (Los Alamos Scientific Laboratories, Los Alamos, New Mexico, 1958), No. LA-2150.
[32]C. E. Fröberg, Rev. Mod. Phys. 27, 399 (1955).
[33]F. L. Yost, J. A. Wheeler, and G. Breit, Phys. Rev. 49, 176 (1936), Eq. (38).

[34]A. V. Luk'yanov, I. V. Teplov, and M. K. Akimova, *Tables of Coulomb Wave Functions* (Computing Center of the Academy of Sciences of the USSR, Moscow, 1961), translation available from Macmillan, New York, 1965.

[35]G. N. Watson, *Theory of Bessel Functions* (University Press, Cambridge, 1922), pp. 7 and 227.

[36]In the slow collision limit, $P(p)$ for inner-shell ionization is identical with the W_S function that was given in Ref. 10 [W. Brandt and G. Lapicki (1974) and G. Lapicki and W. Losonsky (1977)]. As discussed in Sec. III A, we have read $P(p)$ for excitation in a N^+-N collision from Fig. 3 of Ref. 7. It is interesting to note that a semiempirical determination of mean impact parameters [P. Armbruster, H.-H. Behancke, S. Hagmann, D. Liesen, F. Folkmann, and P. H. Mokler, Z. Phys. 288, 277 (1978)] yields $A_0 = 0.8 \pm 0.1$ for $2p\sigma$ excitations of super-heavy quasimolecules with $Z_1 + Z_2 > 137$.

[37]See Ref. 28, Eq. (14.6.14).

[38]In Eq. (9) L_0 is defined in terms of η_i. It has been advocated in studies of nuclear [Ref. 26 and B. J. B. Crowley, Ann. Phys. 117, 323 (1979)] and atomic [L. A. Vainshtein and A. V. Vinogradov, J. Phys. B 3, 1090 (1970)] excitations that an average of η_i and η_f, η_{av}, be used instead. Both the arithmetic and geometric averages yield

$$\eta_{av} \simeq \eta_i [(1 + 1/4(\Delta E/E_i)].$$

Using this η_{av} instead of η_i in the determination of L_0 would result in only a 5% higher values of C_{L0} of Eq. (11) even at the largest $\Delta E/E_i$ that is attainable in the measurements discussed in Sec. III.

[39]N. Stolterfoht, D. Schneider, D. Burch, B. Aagaard, E. Boving, and B. Fastrup, Phys. Rev. A 12, 1313 (1975).

[40]Following Briggs, we use $Z^*_{1,2} = Z^*_{1,2} - 0.5$ (Ref. 2) for a Coulomb potential and $Z^*_{1,2} = Z^*_{1,2} - 1$ for a screened Coulomb potential (Ref. 7).

[41]F. W. Saris and D. Onderlinden, Physica 49, 441 (1970).

[42]P. K. Cacak, D. C. Kessel, and R. E. Rudd, Phys. Rev. A 2, 1327 (1970); H. Tawara, C. Foster, and F. J. de Heer, Phys. Lett. 43A, 266 (1973); K. H. Schartner, H. Schafer, and R. Hippler, Phys. Lett. 46A, 31 (1973); T. P. Hoogkamer, Ph.D. thesis (University of Amsterdam, 1977) (unpublished) and T. P. Hoogkamer, P. H. Woerlee, R. J. Fornter, and F. W. Saris, J. Phys. B 10, 3245 (1977).

[43]To convert x-ray and Auger-electron production excitation cross sections, we have used experimentally determined fluorescence yields ω_K (see Fig. 12 of Ref. 39) for Ne^+-Ne collisions. At $v_i = 0.3$, these yields appear to approach $\omega_K = 0.018$ which is equal to recently recommended value [see M. O. Krause, J. Phys. Chem. Ref. Data 8, 307 (1979)] for a neon atom with a single K-shell hole. The assumption of the fluorescence yield corrected for multiple excitation could only widen the discrepancy between the cross sections of Refs. 39 and 41 at $v_i = 0.3$.

[44]R. S. Peterson, S. B. Elston, I. A. Sellin, R. Laubert, F. K. Chen, and C. A. Peterson, Phys. Rev. Lett. 37, 984 (1976).

[45]G. Basbas, W. Brandt, and R.H. Ritchie, Phys. Rev. A 7, 1971 (1973).

[46]P. R. Bevington and E. M. Bernstein, Bull. Am. Phys. Soc. 1, 98 (1956); J. M. Hansteen and S. Messelt, Nucl. Phys. 2, 526 (1957); E. Merzbacher and W. Lewis, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1958), Vol. 34, p. 166; S. Messelt, Nucl. Phys. 5, 435 (1958); R. C. Jopson, H. Mark, and C. D. Swift, Phys. Rev. 127, 1612 (1962); J. M. Khan and D. L. Potter, *ibid.* 133, A890 (1964); J. M. Khan, D. L. Potter, and R. D. Worley, *ibid.* 139, A1735 (1965); W. Brandt, R. Laubert, and I. A. Sellin, in Ref. 10; W. Brandt and R. Laubert, Phys. Rev. 178, 225 (1969); K. G. Harrison, H. Tawara, and F. J. de Heer, Physica 66, 16 (1973); G. Basbas, W. Brandt, and R. Laubert, in Ref. 10; K. Brunner and W. Hink, in Ref. 11; T. L. Criswell and T. J. Gray, Phys. Rev. A 10, 1145 (1974); N. A. Khelil and T. J. Gray, *ibid.* 11, 893 (1975); S. R. Wilson, F. D. McDaniel, J. R. Rowe, and J. L. Duggan, *ibid.* 16, 903 (1977); M. Kamiya, K. Ishii, K. Sera, S. Morita, and H. Tawara, *ibid.* 16, 2295 (1977); C. Bauer, R. Mann, and W. Rudolph, Z. Phys. A 287, 27 (1978). The ratios based on the data of R. Anholt [Phys. Rev. A17, 983 (1978)], which are not shown in Fig. 7, follow very closely the results of semiclassical calculations performed in the monopole approximation (dashed curve and open symbols in Fig. 7).

[47]The ratios are plotted versus $\pi \Delta\eta_0$, where $\Delta\eta_0 \equiv \Delta\eta(\mathcal{E}_f = 0)$ is evaluated at the ionization edge. The curves were obtained by the integration of various Coulomb-deflection factors over the final energies $\mathcal{E}_f$ of the electron ejected into the continuum of the target atom (see Ref. 15).

[48]L. A. Vainshtein and A. V. Vinogradov, J. Phys. B 3, 1090 (1970); A. A. Andrianov, Teor. Mat. Fiz. 33, 337 (1977) [Theor. Math. Phys. 33, 1058 (1978)]; S. D. Augustin and H. Rabitz, J. Chem. Phys. 69, 4195 (1978).

[49]N. Bohr, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 18, No. 8 (1948).

[50]O. B. Firsov, Zh. Eksp. Teor. Fiz. 33, 696 (1957) [Sov. Phys. JETP 6, 534 (1958)].

[51]J. Lindhard (unpublished). See E. Bonderup, *Lecture notes on penetration of charged particles through matter* (University of Aarhus, Aarhus, 1978), Eq. (13.45).

[52]P. T. Wedepohl, Proc. Phys. Soc. 92, 79 (1967).

[53]It should be noted that any change in the internuclear potential requires a redefinition of the perturbing potential ϑ in Eq. (2). Such a change, however, does not alter our derivation of Coulomb-deflection factor in Sec. II because a constant with respect to the electronic variables gives no contribution to the transition amplitude in the first Born approximation.

[54]In the determination of $\Delta\eta'$ we have relied on the Bohr potential which was used in the calculations of Briggs *et al.* [K. Taulbjerg (private communication)]. The use of the Firsov potential would change the values of our screened Coulomb-deflection factor by only a few percent.