Mean-electric-field approximation to multiple ionization in distant collisions

L. Végh
Institute of Nuclear Research of the Hungarian Academy of Sciences, H-4001 Debrecen, P.O. Box 51, Hungary
(Received 27 November 1984)

The description of ion-atom collisions in a mean-electric-field approximation is discussed. In this method the sum of the interactions between the projectile and the electrons of the target is expressed as the sum of the Coulomb field acting on the center of charge of the target electrons and a residual interaction. For distant (high-energy) collisions the residual interaction can be neglected. The calculation of the scattering amplitude corresponding to the mean electric field is performed within the framework of the first Born approximation. It is shown that for high-energy collisions the scattering amplitude is a product of single-electron scattering amplitudes and the cross sections of the multiple ionization follow the binomial distribution. A simple expression is derived for the cross section of n-vacancy production. The calculated ionization cross sections and mean numbers of outer-shell vacancies in the presence of an inner-shell vacancy are in satisfactory agreement with experimental values for high projectile energies.

I. INTRODUCTION

For calculations of multiple-excitation and -ionization cross sections the single-particle model[1-2] meets with a remarkable success. In this description, which has also been denoted the "independent-electron approximation," the projectile moves classically and the wave function of the target electrons is expressed as a product of single-electron wave functions. Then the probability amplitude of the scattering is the product of single-electron scattering amplitudes, and the multiple-ionization transition probabilities $P_n(b)$ for removing n electrons from a shell containing N electrons in a collision with impact parameter b are given by

$$P_n(b)=\binom{N}{n}[P_s(b)]^n[1-P_s(b)]^{N-n} . \tag{1}$$

Here $\binom{N}{n}$ are the binomial coefficients with $P_s(b)$ being the transition probability calculated in a single-electron model. The differential cross section is of the form

$$d\sigma^n=2\pi P_n(b)b\,db . \tag{2}$$

The validity of the binomial distribution in formula (1) has been discussed within the independent-Fermi-particle model,[3] which contains the electron correlations due to the antisymmetry of the atomic wave function. The results of such coupled-channel calculations[3] show that the correlations largely cancel because of a tendency of the scattering amplitudes to have random phases. This implies that the binomial distribution (1) is a good approximation to the multiple-ionization scattering amplitude.

In this paper we present a description of multielectron excitation and ionization processes which is based on the use of the Coulomb field acting on the center of charge of the target electrons. This approximation is constructed within a fully quantum-mechanical framework using the momentum transfer to characterize the collision. As is demonstrated later, the operator of the two-body Coulomb interaction acting between the projectile and the center of charge of the target electrons may induce multielectron transitions even in the first Born approximation.

II. THE SCATTERING AMPLITUDE

We discuss ion-atom collisions where the incident ion is fully ionized. In this section we use some elements of the formalism developed in a previous paper of the author.[4]

A. Coordinates and momenta

To describe the collision in the laboratory system we use the following coordinates. Let $\mathbf{R}_P$ and $\mathbf{R}_T$ be the coordinates of the projectile and target nuclei, respectively, and $\mathbf{R}_1,\ldots,\mathbf{R}_{Z_T}$ the coordinates of the Z_T target electrons, Z_T being the atomic number of the target. The corresponding momenta are $\mathbf{P}_P$, $\mathbf{P}_T$, and $\mathbf{P}_1,\ldots,\mathbf{P}_{Z_T}$.

We define a new set of coordinates as

$$\begin{aligned}\mathbf{r}_j&=\mathbf{R}_j-\mathbf{R}_T ,\\ \mathbf{R}&=\mathbf{R}_P-\mathbf{R}_A ,\\ \mathbf{R}_{\text{c.m.}}&=\frac{m\sum_{j=1}^{Z_T}\mathbf{R}_j+M_T\mathbf{R}_T+M_P\mathbf{R}_P}{M_T+Z_Tm+M_P} ,\end{aligned} \tag{3}$$

where m is the electron mass, M_P and M_T are the masses of the projectile and target nuclei, respectively, and $\mathbf{R}_A$ is the coordinate of the center of mass of the target atom:

$$\mathbf{R}_A=\frac{M_T\mathbf{R}_T+m\sum_{j=1}^{Z_T}\mathbf{R}_j}{M_T+Z_Tm} . \tag{4}$$

The conjugated momenta for coordinates (3) have the form

$$\mathbf{p}_j=\frac{M_T\mathbf{P}_j-m\mathbf{P}_T}{M_T+m} , \tag{5}$$

$$\mathbf{P}=\frac{(M_T+Z_Tm)\mathbf{P}_P-M_P\left[\mathbf{P}_T+\sum_{j=1}^{Z_T}\mathbf{P}_j\right]}{M_T+Z_Tm+M_P}\,, \tag{6}$$

$$\mathbf{P}_{\text{c.m.}}=\mathbf{P}_T+\sum_{j=1}^{Z_T}\mathbf{P}_j+\mathbf{P}_P\,. \tag{7}$$

B. The Hamiltonian

The Hamiltonian is given by

$$H=T_{\text{c.m.}}+T_{PA}+H_A+\frac{Z_PZ_Te^2}{|\mathbf{R}_P-\mathbf{R}_T|}-\sum_{j=1}^{Z_T}\frac{Z_Pe^2}{|\mathbf{R}_P-\mathbf{R}_j|}\,, \tag{8}$$

$$H_A=\sum_{j=1}^{Z_T}\left[\frac{\mathbf{p}_j^2}{2m}-\frac{Z_Te^2}{r_j}+\sum_{\substack{i=1\\ i>j}}^{Z_T}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}\right]. \tag{9}$$

Here $T_{\text{c.m.}}$ is the kinetic energy operator of the center of mass and T_{PA} is that of the atom-projectile relative motion, and Z_P is the atomic number of the projectile. The symbol H_A represents the Hamiltonian of the target atom. We split the Hamiltonian (8) into three parts in the following way:

$$H=H_0+V_{PT}+V_{PE} \tag{10}$$

with

$$H_0=T_{\text{c.m.}}+T_{PA}+H_A\,, \tag{11}$$

$$V_{PT}=\frac{Z_PZ_Te^2}{|\mathbf{R}_P-\mathbf{R}_T|}\,, \tag{12}$$

$$V_{PE}=-\sum_{j=1}^{Z_T}\frac{Z_Pe^2}{|\mathbf{R}_P-\mathbf{R}_j|}\,. \tag{13}$$

The initial and final asymptotic wave functions corresponding to the eigenfunctions of H_0 (11) have the form

$$\Psi_a(\mathbf{R},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})=(2\pi)^{-3/2}\exp(i\mathbf{P}_a\cdot\mathbf{R}/\hbar)\Phi_a(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\,, \qquad a=i,f \tag{14}$$

where $\mathbf{P}_i$ and $\mathbf{P}_f$ are the conjugated momenta (6). The quantities Φ_i and Φ_f are eigenfunctions of H_A, $\Phi_i(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})$ is the initial ground-state atomic wave function, and $\Phi_f(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})$ describes the final state of the Z_T electron-target nucleus system. The motion of the center of mass of the whole system is separated off and is not considered. For the sake of simplicity the spin indices are neglected.

C. The mean interaction

The source of the multiple ionization is the simultaneous interaction of the atomic electrons with the projectile. We describe this process by a mean Coulomb field of the target electrons. Using the center-of-charge (-mass) coordinate of the target electrons fixed to the target nucleus

$$\mathbf{R}_e=\frac{1}{Z_T}\sum_{j=1}^{Z_T}\mathbf{r}_j \tag{15}$$

we split the sum of the projectile-target electron interactions (13) into two parts as follows:

$$-Z_Pe^2\sum_{j=1}^{Z_T}\frac{1}{|\mathbf{R}_{PT}-\mathbf{r}_j|}=V_M(|\mathbf{R}_{PT}-\mathbf{R}_e|)+V_R(\mathbf{R}_{PT},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\,, \tag{16}$$

$$V_M(|\mathbf{R}_{PT}-\mathbf{R}_e|)=\frac{-Z_PZ_Te^2}{|\mathbf{R}_{PT}-\mathbf{R}_e|} \tag{17}$$

with $\mathbf{R}_{PT}=\mathbf{R}_P-\mathbf{R}_T$. The quantities $V_M(|\mathbf{R}_{PT}-\mathbf{R}_e|)$ can be regarded as the mean interaction between the projectile and the Z_T target electrons and $V_R(\mathbf{R}_{PT},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})$ as a residual interaction. Considering the multipole expansion

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=\sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}P_l\left[\frac{\mathbf{r}_1\cdot\mathbf{r}_2}{r_1r_2}\right] \tag{18}$$

we can see that in the region $R_{PT}>r_j$ $(j=1,\ldots,Z_T)$ the monopole and dipole terms of the left-hand side of Eq. (16) and that of the mean interaction (17) coincide, that is, the residual interaction starts with quadrupole terms. The collisions where the main contributions come from the region $R_{PT}>r_j$ are the "distant" collisions. For an atomic orbit with radius r_n in the case of distant collisions the relation

$$\frac{1}{q_{\min}}=\frac{v}{\Delta E}>\frac{r_n}{\hbar} \tag{19}$$

is fulfilled,[5] where v is the velocity of the projectile, ΔE is the energy transfer, and $q_{\min}$ is the minimum momentum transfer to the electron on this orbit. For distant collisions the residual interaction V_R can be neglected. In what follows we restrict ourselves to the investigation of high-energy collisions where the condition (19) of distant collisions is valid.

D. The Born approximation

We denote the contribution of the mean Coulomb field (17) to the scattering amplitude in the first Born approximation by T_M^B. Using the asymptotic initial and final wave functions given by (14) T_M^B can be written as

$$T_M^B=\left\langle\Psi_f(\mathbf{R},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\left|\frac{-Z_PZ_Te^2}{|\mathbf{R}_{PT}-\mathbf{R}_e|}\right|\Psi_i(\mathbf{R},\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\right\rangle$$
$$=-(2\pi)^{-3}Z_PZ_Te^2\int d\mathbf{R}\,d\mathbf{r}_1\cdots d\mathbf{r}_{Z_T}\Phi_f^*(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\frac{e^{-i\mathbf{q}\cdot\mathbf{R}/\hbar}}{|\mathbf{R}_{PT}-\mathbf{R}_e|}\Phi_i(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\,, \tag{20}$$

where

$$\mathbf{q}=\mathbf{P}_f-\mathbf{P}_i \tag{21}$$

is the momentum transfer to the target atom. According to the relations (3), (4), and (15) the $\mathbf{R}_{PT}-\mathbf{R}_e$ coordinate can be expressed as

$$\mathbf{R}_{PT}-\mathbf{R}_e=\mathbf{R}-\frac{k_M}{Z_T}\sum_{j=1}^{Z_T}\mathbf{r}_j \tag{22}$$

with

$$k_M=\frac{M_T}{M_T+Z_T m}\approx 1 . \tag{23}$$

Applying Bethe's integral[6]

$$\int \frac{e^{i\mathbf{K}\cdot\mathbf{R}}}{|\mathbf{R}-\mathbf{x}|}d\mathbf{R}=\frac{4\pi}{K^2}e^{i\mathbf{K}\cdot\mathbf{x}} \tag{24}$$

the $T_M^B(\mathbf{q})$ amplitude in (20) can be given as

$$T_M^B(\mathbf{q})=\frac{-Z_P Z_T e^2\hbar^2}{2\pi^2 q^2}\left\langle \Phi_f(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\left|\exp\left[-i\frac{k_M}{Z_T}\frac{\mathbf{q}}{\hbar}\sum_{j=1}^{Z_T}\mathbf{r}_j\right]\right|\Phi_i(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\right\rangle \tag{25}$$

which is the matrix element of a Z_T-body operator which contains the coordinates of the atomic electrons in a symmetrical form. Excluding the electron-electron correlations, the Born series corresponding to the sum of the projectile-electron interactions (13) can give contributions to the n-body transitions only from the nth-order terms. In distant collisions, where the mean-electric-field approximation is valid, the n-body transitions can be described even in the first of the Born terms of the mean interaction.

Using Eq. (24) the first Born term of the projectile-nucleus interaction (12) which we denote by $T_{\rm rec}^B(\mathbf{q})$ can be written as

$$T_{\rm rec}^B(\mathbf{q})=\frac{Z_p Z_T e^2\hbar^2}{2\pi^2 q^2}\left\langle \Phi_f(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\left|\exp\left[-i\frac{k_{\rm rec}}{Z_T}\frac{\mathbf{q}}{\hbar}\sum_{j=1}^{Z_T}\mathbf{r}_j\right]\right|\Phi_i(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})\right\rangle , \tag{26}$$

$$k_{\rm rec}=\frac{Z_T m}{M_T+Z_T m} . \tag{27}$$

As $k_{\rm rec}$ is small, $T_{\rm rec}^B(\mathbf{q})$ can have considerable values only at very large recoil momenta q, and in the calculation of the total ionization cross sections can be neglected.[4]

For distant collisions, which according to relation (19) correspond to high-energy projectiles, the characteristic momentum transfers are small enough to justify our further approximations. Hence, if we apply for the atomic wave functions $\Phi_a(\mathbf{r}_1,\ldots,\mathbf{r}_{Z_T})$ a Slater determinant, the part of the amplitude corresponding to the exchange terms can be neglected and we can write

$$T_M^B(\mathbf{q})=\frac{-Z_P Z_T e^2\hbar^2}{2\pi^2 q^2}\prod_{j=1}^{Z_T}A_{fi}^j\left[\frac{k_M}{Z_T}\frac{\mathbf{q}}{\hbar}\right] \tag{28}$$

with

$$A_{fi}^j(\mathbf{K})=\langle\varphi_f^j(\mathbf{r}_j)\,|\,\exp(-i\mathbf{K}\cdot\mathbf{r}_j)\,|\,\varphi_i^j(\mathbf{r}_j)\rangle , \tag{29}$$

where $\varphi_i^j(\mathbf{r}_j)$ and $\varphi_f^j(\mathbf{r}_j)$ are the single-electron wave functions of the jth electron in the initial and final state, respectively.

Formula (28) shows that for high-energy projectile the scattering amplitude is a product of single-electron scattering amplitudes. This result has been obtained without the assumptions on the product wave function of the target and on the classical motion of the projectile made by McGuire and Weaver[2] in the single-particle model.

To calculate ionization and excitation of outer shell electrons we shall apply the amplitude (28). In inner-shell processes the momentum transferred to the outer-shell electrons can be neglected. In this case we replace in Eq. (28) Z_T by Z_ν, where Z_ν is the number of atomic electrons given by the sum which runs from the K shell up to the ionized main shell. That is, at the excitation and ionization of electrons in a given shell, according to Eq. (28) each of the electrons of this shell and the electrons inside obtain the momentum $\mathbf{q}/Z_\nu$. Below we use the number Z_ν instead of Z_T.

III. THE CROSS SECTIONS

A. Inelastic cross section

The differential cross section for the transition with momentum transfer $\mathbf{q}$ leading to a final state f using the scattering amplitude (28) can be given as

$$\frac{d\sigma^f}{dq}=8\pi\left[\frac{Z_P Z_\nu e^2}{v}\right]^2\frac{1}{q^3}\prod_{j=1}^{Z_\nu}a_{fi}^j\left[\frac{k_M}{Z_\nu}\frac{\mathbf{q}}{\hbar}\right] , \tag{30}$$

where a_{fi}^j is the squared single-electron amplitude for the jth electron:

$$a_{fi}^j(\mathbf{K})=|\,A_{fi}^j(\mathbf{K})\,|^2 . \tag{31}$$

B. Inelastic cross section at a given momentum transfer

The inelastic cross section $\sigma(q)$ at a given momentum transfer q can be calculated by summing over the possible final states f. Considering the completeness relation of the single-electron amplitudes we can write

$$\sum_{f\neq i} a_{fi}^{j}(\mathbf{K}) = 1 - a_{ii}^{j}(\mathbf{K}) , \tag{32}$$

the sum runs over the possible bound and continuum atomic electron states except the ground state. If there are n vacancies in the orbit ν ($\nu = n_0 lm$) which contain N electrons in its ground state, from formulas (29)—(32) follows

$$f_\nu(q/Z_\nu) = 1 - \frac{1}{2l+1}\sum_m \left| \left\langle \varphi_\nu(\mathbf{r}) \left| \exp\left[i \frac{k_M}{Z_\nu} \frac{\mathbf{q}\cdot\mathbf{r}}{\hbar} \right] \right| \varphi_\nu(\mathbf{r}) \right\rangle \right|^2 , \tag{34}$$

where l is the quantum number of the orbital momentum and the sum is over the magnetic quantum numbers m. Expanding the exponential operator into a partial-wave series

$$\exp(i\mathbf{K}\cdot\mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(Kr) Y_{lm}^*(\hat{\mathbf{K}}) Y_{lm}(\hat{\mathbf{r}}) \tag{35}$$

we obtain after straightforward calculations the following expression for $f_\nu(K)$:

$$f_\nu(K) = 1 - \sum_{l'} (2l'+1)(l0l'0 \mid l0) F_{ll'}^2(K) \tag{36}$$

with

$$F_{ll'}(K) = \int_0^\infty dr\, r^2 j_{l'}(Kr) \varphi_{n_0}^2(r) , \tag{37}$$

where $j_{l'}(Kr)$ is a spherical Bessel function.

We notice that by introducing the new variable

$$b = \frac{2Z_P Z_\nu e^2}{vq} \tag{38}$$

the differential cross section (33) can be written in a form analogous to the semiclassical cross-section formula (2)

$$d\sigma_\nu^n = 2\pi b\, db \binom{N}{n} f_\nu \left[\frac{2Z_P e^2}{vb} \right]^n \left[1 - f_\nu \left[\frac{2Z_P e^2}{vb} \right] \right]^{N-n} . \tag{39}$$

C. Inelastic cross section integrated over the momemtum transfer

Now we consider the cross section of the process leading to the final state f which can be obtained by integrating the differential cross section (30) over the momentum transfer q:

$$\sigma^f = \int_{q_{\min}}^{q_{\max}} dq \frac{d\sigma^f}{dq} . \tag{40}$$

Introducing the new variable

$$q' = q/Z_\nu$$

and using (30) the total cross section σ^f can be expressed as

$$\sigma^f = 8\pi \left[\frac{Z_P e^2}{v} \right]^2 \int_{q_{\min}/Z_\nu}^{q_{\max}/Z_\nu} \frac{dq}{q^3} \prod_{j=1}^{Z_\nu} a_{fi}^j(k_M \mathbf{q}/\hbar) . \tag{41}$$

$$\frac{d\sigma_\nu^n}{dq} = 8\pi \left[\frac{Z_P Z_\nu e^2}{v} \right]^2 \binom{N}{n} \frac{1}{q^3} f_\nu \left[\frac{q}{Z_\nu} \right]^n \times \left[1 - f_\nu \left[\frac{q}{Z_\nu} \right] \right]^{N-n} , \tag{33}$$

where $f_\nu(q/Z_\nu)$ is given by the elastic form factor as

For the determination of $q_{\min}$ and $q_{\max}$ we use the relation between the momentum and energy transferred to the target atom. The absolute value of the momentum transfer (21) is given as

$$q^2 = P_f^2 + P_i^2 - 2P_i P_f \cos\vartheta , \tag{42}$$

where ϑ is the center-of-mass scattering angle. The energy transfer in the laboratory system to the atom with initial energy E_i and final energy E_f can be expressed as

$$E_f - E_i = \frac{P_{fL}^2}{2M_P} - \frac{P_{iL}^2}{2M_P} + \frac{(\mathbf{P}_{iL} - \mathbf{P}_{fL})^2}{2(M_T + Z_T m)} , \tag{43}$$

here the label L relates to the laboratory system. The third term is the kinetic energy transferred to the target atom which can be neglected when only projectile-electron interactions are considered. Furthermore, in this case the scattering angle ϑ and the transferred momentum compared to the projectile momentum are very small. Then we obtain from relations (42) and (43) that

$$E_f - E_i \approx \frac{P_{iL}(P_{fL} - P_{iL})}{M_P} = v(P_{fL} - P_{iL}) = vq_{||} = \mathbf{v}\cdot\mathbf{q} , \tag{44}$$

that is, the component of $\mathbf{q}$ parallel to $\mathbf{P}_i$ is fixed by the energy conservation and that its perpendicular component has the value

$$q_\perp = P_i \vartheta . \tag{45}$$

The lower integration limit $q_{\min}$ is determined by the minimum value of q from Eq. (44) as given by (19):

$$q_{\min} = q_{||} = \frac{E_f - E_i}{v} . \tag{46}$$

In the case of n-electron ionization the threshold of the momentum transfer is

$$q_{\text{th}} = \frac{E_B^n}{v} , \tag{47}$$

where E_B^n is the energy needed to remove n electrons from the atom.

The upper limit $q_{\max}$ can be calculated using the kinematics of the process. Instead of this kinematical limit which can practically be taken as infinity we use as the maximum of $q_\perp$ the characteristic value

$$q_{\perp\max}=\frac{2Z_\nu Z_P e^2}{v r_\nu} \tag{48}$$

where r_ν is the root-mean-square radius of the investigated shell. This choice of $q_{\perp\max}$ corresponds to the momentum transfer from the projectile to the Z_ν electrons concentrated in one point in a collision with impact parameter r_ν. Equation (48) is an asymptotic form of the expression valid for the Rutherford scattering:

$$q_{\perp\max}=Z_\nu 2mv\frac{Z_P e^2/mv^2}{[(Z_P e^2/mv^2)^2+r_\nu^2]^{1/2}} \tag{49}$$

for the limit $r_\nu \gg Z_P e^2/mv^2$. Using Eqs. (46) and (48) $q_{\max}$ can be written as

$$\begin{aligned} q_{\max}&=(q_{\parallel}^2+q_{\perp\max}^2)^{1/2} \\ &=\frac{1}{v}[(E_f-E_i)^2+(2Z_\nu Z_P e^2/r_\nu)^2]^{1/2} . \end{aligned} \tag{50}$$

The reduction of the kinematic upper limit to $q_{\max}$ as given in Eq. (50) makes it possible to fulfill the condition of distant collisions for velocities

$$\frac{2Z_P e^2}{\hbar v}<1 . \tag{51}$$

If this relation is valid the contributions which correspond to the spatial region where the strength of the mean-field interaction strongly exceeds that of the sum of the projectile-electron interactions are removed from integral (41). Since $Z_\nu e^2/r_\nu$ has the order of magnitude of the binding energy of the ionized electrons for low projectile charges, $q_{\max}$ is close to $q_{\min}$. The limits (46) and (50) show that the region of momentum transfer for high-energy projectiles is fairly confined.

D. The multi-ionization cross section

The total cross section σ_ν^n of the n-vacancy production can be obtained by integrating the cross section (41) over the momenta $\mathbf{p}_1,\ldots,\mathbf{p}_n$ of the ionized electrons as follows:

$$\sigma_\nu^n=8\pi\left[\frac{Z_P e^2}{v}\right]^2 \times\int d\mathbf{p}_1\cdots d\mathbf{p}_n\int_{q_{\min}/Z_\nu}^{q_{\max}/Z_\nu}\frac{dq}{q^3}\prod_{j=1}^{Z_\nu}a_{f,i}^j(k_M\mathbf{q}/\hbar) . \tag{52}$$

Unfortunately, in the limits of integration over q, given by Eqs. (46) and (50), the term E_f-E_i given as

$$E_f-E_i=E_B^n+\sum_{i=1}^{n}p_i^2/2m \tag{53}$$

also depend on the momenta p_i. We get rid of this dependence by approximating E_f-E_i by the constant I_n defined as

$$E_f-E_i\sim I_n\equiv E_B^n+n\frac{q_{\perp\max}^2}{Z_\nu^2 2m} , \tag{54}$$

where the momentum $q_{\perp\max}/Z_\nu$ given by (48) is assumed to take the characteristic value of the momenta of the directly ionized electrons.

With constant integration limits and neglecting the contributions corresponding to excitations to bound atomic states, for the integrations over $\mathbf{p}_i$ we can apply the treatment discussed in Sec. III B. Through relations (32), (34), and (52) the cross section of the n-vacancy production in the orbit ν with N electrons in the ground state can be written as

$$\sigma_\nu^n=8\pi\left[\frac{Z_P e^2}{v}\right]^2\binom{N}{n}\int_{q_{\min}/Z_\nu}^{q_{\max}/Z_\nu}\frac{dq}{q^3}f_\nu(q)^n[1-f_\nu(q)]^{N-n} . \tag{55}$$

This cross-section formula is valid for high projectile energies where the condition (19) of the distant collisions is fulfilled and the upper momentum-transfer limit is small enough to allow the omission of the exchange terms of the scattering amplitude (25). The high projectile energy allows further simplification of the formula (55) as given in Sec. III E.

E. Multiple-vacancy production in high-energy limit

If we restrict ourselves to the study of atomic orbits with orbital momentum $l=0$, then in formula (36) only the term corresponding to the spherical Bessel function of zeroth order gives contribution. Even in the case of atomic orbits with $l>0$ at small momentum transfers the essential contribution comes from the term of zeroth order. If the projectile velocity is so high that the inequality

$$\frac{Z_P e^2}{\hbar v}\ll 1 \tag{56}$$

is fulfilled, i.e., $q/\hbar Z_\nu$ is small compared to the inverse radius of the atomic orbit, see Eq. (48), the zeroth-order Bessel function is duly approximated with the first two terms of its power-series expansion

$$j_0(k_M r q/\hbar)\approx 1-\frac{1}{6}\left[k_M\frac{q}{\hbar}r\right]^2 \tag{57}$$

and from Eqs. (36) and (37)

$$f_\nu(q)\approx\tfrac{1}{3}k_M^2\frac{q^2}{\hbar^2}\langle r^2\rangle_\nu \tag{58}$$

follows. If the relation

$$\frac{2Z_P e^2}{r_\nu}\gg\frac{I_n}{Z_\nu} \tag{59}$$

holds then the assumption $I_n=0$ seems valid. With approximation (58) we can perform the integration in the cross-section formula (55) analytically. Taking k_M equal to unity and neglecting the higher-order terms according to the condition (56) and using (59) we obtain

$$\sigma_\nu^n=\pi\langle r^2\rangle_\nu\binom{N}{n}\left[\frac{2Z_P e^2}{\sqrt{3}\hbar v}\right]^{2n} \times\left[\frac{1}{n-1}-\frac{N-n}{n}\left[\frac{2Z_P e^2}{\sqrt{3}\hbar v}\right]^2\right] . \tag{60}$$

This relation shows that the n-vacancy production decreases as $v^{-2n} \sim E_P^{-n}$ with the projectile energy E_P. The properties of the electron orbit are suppressed into the mean-squared radius $r_\nu^2 = \langle r^2 \rangle_\nu$ of the shell.

F. One-electron ionization

Now we discuss the difference between the cross-section formula given by the mean-electric-field approximation (55) for ionization of one electron,

$$\sigma_\nu^1 = 8\pi \left[\frac{Z_P e^2}{v} \right]^2 N \int_{q_{\min}/Z_\nu}^{q_{\max}/Z_\nu} \frac{dq}{q^3} f_\nu(q)[1-f_\nu(q)]^{N-1} , \tag{61}$$

and that corresponding to the conventional Born approximation,

$$\sigma_\nu = 8\pi \left[\frac{Z_P e^2}{v} \right]^2 N \int_{q_{\min}}^{2mv} \frac{dq}{q^3} f_\nu(q) . \tag{62}$$

Since at high velocities the $(N-1)$th power in Eq. (61) may to a good approximation be set equal to unity, the main difference between the expressions is in the limits of the momentum-transfer integral. As the integrand behaves like $1/q$ [see Eq. (58)], in transforming the integral (61) the Z_ν number in the limits can be omitted. Since the value of the integral is determined by the lower limit, the different upper limits cannot make a drastic difference between the cross-section values calculated from Eqs. (61) and (62).

IV. VACANCY PRODUCTION IN THE PRESENCE OF AN INNER-SHELL VACANCY

As is well known,[5] the intensive inner-shell vacancy production occurs at impact parameters close to the inverse of the minimum momentum transfer defined by relation (19). This distance, also called the adiabatic radius, has values similar to those of the inner-shell radius r_n for swift collision. The radius of an inner-shell orbit is much less than that of the outer-shell orbits. Therefore, when producing an inner-shell vacancy the projectile has the opportunity to transfer the maximum amount of momentum to the outer-shell electrons. According to this argument the mean ionization probability for the outer shell ν at zero impact parameter, denoted by $P_\nu(0)$, corresponds to the factor f_ν defined in (34) at momentum transfer $q_{\max}/Z_\nu$ [see also relation (39)]. Using relation (50) for $q_{\max}$ we can write

$$P_\nu(0) \approx f_\nu \left[\frac{2Z_P e^2}{v r_\nu} \right] , \tag{63}$$

where according to inequality (59) we have neglected the parallel component of $q_{\max}$. For a high-energy projectile, in approximation (58), we obtain

$$P_\nu(0) \approx \frac{4}{3} \left[\frac{Z_P e^2}{\hbar v} \right]^2 . \tag{64}$$

The relation (63) shows that the mean ionization probability at zero impact parameter depends on the properties of the projectile only through the ratio Z_P/v. This scaling property has been recently discussed within the framework of a simplified binary-encounter model.[7]

If the projectile is not fully ionized, we determine the projectile effective charge Z_p using a screened charge based on the Gáspár potential[8] as discussed in Ref. 9. If the atomic number of the projectile is Z_N and its ionic charge is I, Z_P can be expressed as

$$Z_P = I + (Z_N - I) \frac{e^{-\nu_0 r_\nu}}{1+\kappa r_\nu} . \tag{65}$$

We parametrized ν_0 and κ as in Ref. 10:

$$\begin{aligned} \nu_0(Z_N) &= (0.1306 \times 10^{-2} Z_N + 0.2765) Z_N^{1/3} , \\ \kappa(Z_N) &= (0.3453 \times 10^{-2} Z_N + 0.9406) Z_N^{1/3} . \end{aligned} \tag{66}$$

The screening described by relation (66) corresponds to the case when the projectile moves at the center of the target atom.

V. RESULTS

When calculating the $f_\nu(q)$ factors in (36) we have used nonrelativistic screened hydrogenic wave functions. We have followed the screening procedure of Slater.[11] In this case the calculation of the integral (37) can be performed in analytical form. We have neglected the difference between the subshells of the given main shell using the wave function of the s subshell for the main shell.

A. Ionization cross sections

We present calculations for He and Ne targets at proton impact in the energy range 0.01—4 MeV and compare them with the experimental data.[12] In the investigated region for the Ne target, the multiple outer-shell ionization is far more probable than the multiple ionization occurring via K-shell ionization followed by Auger decay.[13,14] It has been demonstrated by DuBois[15] that in the energy region 0.015—0.1 MeV the simultaneous electron capture plus ionization and the direct multiple ionization of the outer shell dominate over direct single target ionization.

In the calculation of $q_{\min}$ from Eqs. (46) and (54) for the He and Ne targets we have used experimental and calculated[16] binding energies, respectively. For Ne we have averaged over the energy values corresponding to the $2s$ and $2p$ subshells. Contributions arising from the Auger decay following the K-shell ionization of Ne have been neglected.

At higher projectile energies where the mean-electric-field approximation and the Born approximation become valid there is satisfactory agreement between the calculated and experimental multi-ionization cross sections, see Fig. 1. At projectile energies $E_P > 0.5$ MeV we also give the results calculated by the approximate formula (60). The results slightly exceed the cross sections calculated without approximations. The single-ionization cross sections calculated by the mean-electric-field approximation (61) and by the conventional formula (62) agree remarkably. This agreement supports the arguments that in the

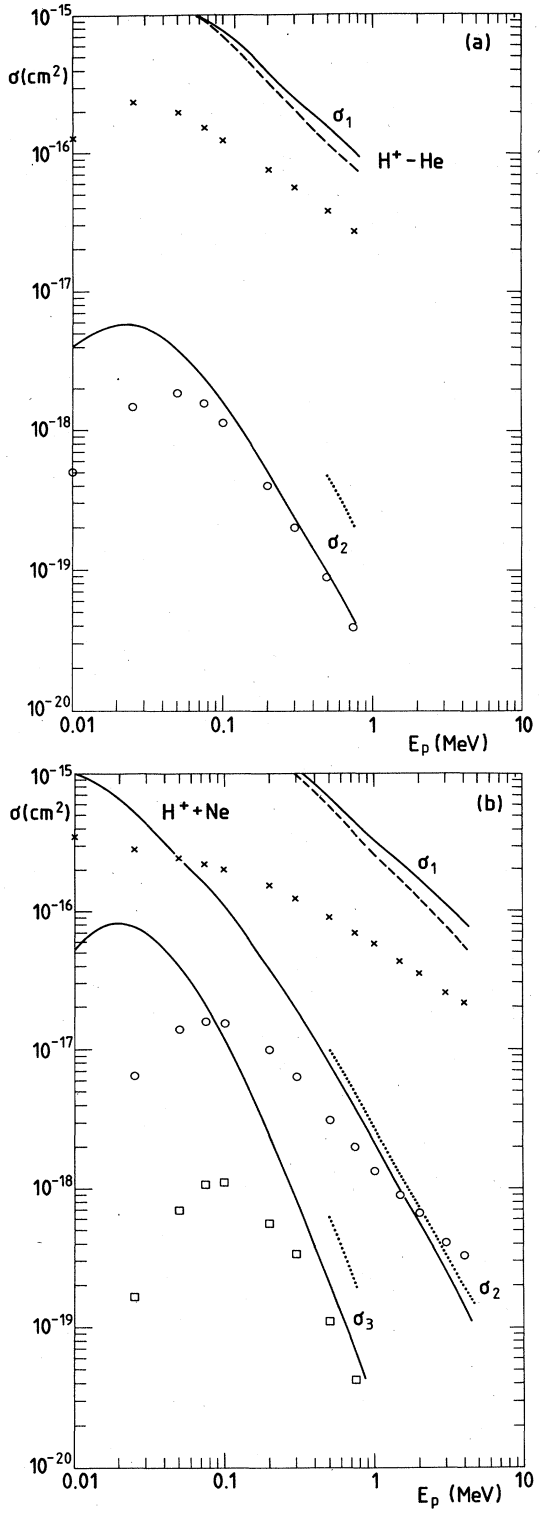

FIG. 1. Multiple-ionization cross sections for (a) H^+-He and (b) H^+-Ne collisions. The data are taken from the work of DuBois *et al.* (Ref 12): ×, single vacancy; ○, double vacancy; □, triple vacancy. Solid lines correspond to the mean-electric-field approximation, dashed lines are the single-ionization values calculated by the conventional formula (62), dotted lines correspond to the simple approximate formula (60) of the mean-electric-field model.

case of single-electron ionization the two approximations are equivalent.

B. Vacancy production in the presence of an inner-shell vacancy

There are a number of experimental data for Ne targets for the average number of L-shell vacancies produced simultaneously with a K-shell vacancy. Figure 2 shows the data of papers[17–20] compared with the theoretical curve calculated according to the relation (63) with effective charge defined by (65). The results, presented as a function of the dimensionless scaling parameter $Z_P c/v$, at high energies, which corresponds to smaller values of $Z_P c/v$, show a good agreement with the values evaluated from the measured spectra.

VI. DISCUSSION

The region of validity of the mean-electric-field approximation corresponds to the high projectile energies where the contributions due to the residual interaction and to the higher Born terms of the mean interaction seem to be negligible. In this region the approximations connected with the choice of limits of the momentum transfer integral given by formulas (48) and (54) obviously cause negligible errors.

The application of this method for lower projectile energies is hindered by a number of difficulties. If the condition for distant collision is poorly fulfilled then the cross sections are strongly overestimated. The contributions corresponding to electron-electron correlations for low energies may be important.

The choice of atomic wave function can affect seriously the results only at lower projectile energies, at high energies it has little influence on the results. At high energies the cross section depends only on the low-momentum behavior of the elastic form factors, which is determined by the asymptotic behavior of the wave function. Since the asymptote is determined by the binding energy, the atomic wave functions of correct binding energy should be

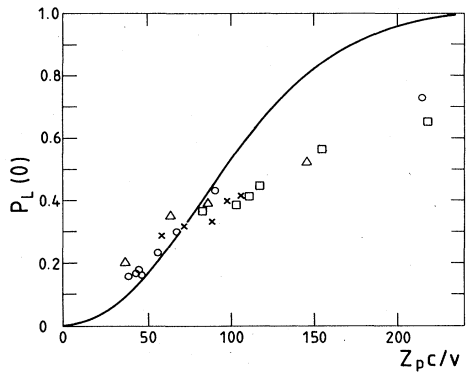

FIG. 2. Mean L-shell ionization probability at zero impact parameter for Ne as a function of the scaling parameter of the projectile $Z_p c/v$ compared with experimental data: □, Brown *et al.* (Ref. 17), ×, Kauffman *et al.* (Ref. 18); ○, Schneider *et al.* (Ref. 19); △, Kádár *et al.* (Ref. 20). Solid line has been calculated by relation (63).

appropriate for the description of multiple ionization.

The importance of the contributions of inner-shell vacancies via Auger decays as compared to the multiple ionization has to be discussed in each case separately. Within the present framework we cannot properly determine the role of the simultaneous capture and ionization mechanism as compared to the direct single target ionization.

In conclusion we can say that the mean-electric-field approximation seems to be a consequent description of the multi-electron transitions at high energies. The method is tractable, moreover, the very simple approximate formula derived for multiple-vacancy production may be a useful tool to estimate the multiple-ionization cross sections for different physical problems.

[1]J. M. Hansteen and O. P. Mosebekk, Phys. Rev. Lett. **29**, 1361 (1972).
[2]J. H. McGuire and L. Weaver, Phys. Rev. A **16**, 41 (1977).
[3]R. L. Becker, A. L. Ford, and J. F. Reading, Phys. Rev. A **29**, 3111 (1984).
[4]L. Végh, J. Phys. B **16**, 4175 (1983).
[5]J.Bang and J. M. Hansteen, K. Dan. Vidensk. Selsk. Mat-Fys. Medd. **31**, No. 13 (1959); J. M. Hansteen, in *Advances in Atomic and Molecular Physics,* edited by D. R. Bates (Academic, New York, 1975), Vol. 11, p. 299.
[6]H. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930).
[7]B. Sulik, G. Hock, and D. Berényi, J. Phys. B **17**, 3239 (1984).
[8]R. Gáspár, Acta Phys. Acad. Sci. Hung. **2**, 611 (1952).
[9]L. Végh and L. Sarkadi, J. Phys. B **16**, L727 (1983).
[10]A. Jakob, F. Rösel, D. Trautmann, and G. Baur, Z. Phys. A **309**, 13 (1982).
[11]J. C. Slater, Phys. Rev. **36**, 57 (1930).
[12]R. D. DuBois, L. H. Toburen, and M. E. Rudd, Phys. Rev. A **29**, 70 (1984).
[13]S. T. Manson, R. D. DuBois, and L. H. Toburen, Phys. Rev. Lett. **51**, 1542 (1983).
[14]M. Eckhardt and K.-H. Schratner, Z. Phys. A **312**, 321 (1983).
[15]R. D. DuBois, Phys. Rev. Lett. **52**, 2348 (1984).
[16]F. P. Larkins, J. Phys. B **4**, 14 (1971).
[17]M. D. Brown, J. R. McDonald, P. Richard, J. R. Mowat, and I. A. Sellin, Phys. Rev. A **9**, 1470 (1974).
[18]R. L. Kauffman, C. W. Woods, K. A. Jamison, and P. Richard, Phys. Rev. A **11**, 872 (1975).
[19]D. Schneider, M. Prost, R. DuBois, and N. Stolterfoht, Phys. Rev. A **25**, 3102 (1982).
[20]I. Kádár, S. Ricz, V. A. Schegolev, B. Sulik, D. Varga, J. Végh, D. Berényi, and G. Hock, J. Phys. B **18**, 275 (1985).