Independent electron approximation for atomic scattering by heavy particles*

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Scattering from a multielectron target by a heavy particle is approximated in terms of amplitudes for scattering from individual target electrons. By treating the motion of the projectile classically and ignoring correlations, the wave function for the system is expressed as a product of single-electron wave functions. The probability amplitude for scattering into specific states is then a product of single-electron scattering amplitudes. In this approximation, cross sections for excitation and ionization involving many electrons are expressed in terms of a binomial distribution of single-electron probabilities. The standard connection of this amplitude for multiple excitation and ionization, $A^{if}(B)$, to the corresponding scattering amplitude, $f(\theta)$, is given, and the validity of this approximation is discussed.

I. INTRODUCTION

It is convenient to use an independent electron approximation in calculations of collision cross sections in multielectron atoms by heavy charged particles. In this approximation the atom is treated as a collection of electrons which independently interact with the projectile. During the time of the collision the interaction between the projectile and a given electron neither affects nor depends on the other target electrons. Thus, for example, in the calculation of single ionization, the nonparticipating electrons are ignored; i.e., their wave functions are not used in the calculation.

While most atomic collision calculations[1] have concentrated on the transition of a single electron, there have been some attempts to describe multiple transitions within a single collision. One approach is to calculate the probability for a multielectron transition by multiplying transition probabilities computed independently for each electron. As is later demonstrated, this multielectron transition probability for excitation and ionization gives a binomial distribution of the single-electron probabilities.

The idea of combining single-electron probabilities for multielectron transitions has been used by a number of authors, including applications that extend beyond the scope of this paper. Gryzinski[2] has estimated cross sections for the double ionization of helium by electron impact in this manner. Åberg[3] has used the idea for ionization by photons and electrons, while Sachenko and Demekhin[4] have considered electron rearrangement after inner-shell vacancy production. Veje[5] has recently applied the method to vacancy production in solids.

For inner-shell ionization in atoms by heavy particle impact (the problem to which this paper is addressed), the binomial distribution has been suggested[6] and used[7-11] for the analysis of high-resolution x-ray spectra,[12] which include satellite and hypersatellite lines. With a few exceptions,[13] the binomial distributions generally give a good fit to observed data when folded appropriately with Auger rates.[14]

In this paper we present a semiclassical derivation of the independent electron approximation for atomic scattering by heavy particles and the consequent binomial distribution of single-electron probabilities. Similar work has been reported[15] by Wu and Merzbacher. Our results are obtained by considering the projectile as a classical particle and ignoring correlations. Then a standard connection is given between the probability amplitude for multiple excitation and ionization, $A^{if}(B)$, and the corresponding scattering amplitude $f(\theta)$. Finally, the validity of this independent electron approximation and its relationship to various calculations is discussed.

II. REDUCTION TO INDEPENDENT ELECTRON SCATTERING TERMS

In this section we formulate the scattering amplitude for excitation and ionization in a multielectron target by heavy-particle impact as a product of single-particle wave functions, ignoring the identity of the target electrons. As we shall later remark, extension corresponding to an antisymmetrized product wave function is straightforward and is bypassed for now for simplicity.

Consider a charged particle incident on a multielectron target. We seek the wave function for the full system, $\Psi(\vec{R}, \vec{r}_1 \cdots \vec{r}_{Z_2})$, which is a solution of the Schrödinger equation,

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t},$$

where $\vec{R}$ represents the projectile coordinate, and $\vec{r}_1 \cdots \vec{r}_{Z_2}$ the set of coordinates of target electrons

measured from the target nucleus.

The full Hamiltonian of our atomic system is given by

$$H=\frac{P^2}{2M}-\frac{Z_1Z_2e^2}{R}+\sum_{j=1}^{Z_2}\frac{Z_1e^2}{|\vec{R}-\vec{r}_j|}+\sum_{j=1}^{Z_2}\left(\frac{p_j^2}{2m}+\frac{Z_2e^2}{r_j}-\sum_{k>j}^{Z_2}\frac{e^2}{|\vec{r}_k-\vec{r}_j|}\right)$$

$$=\frac{P^2}{2M}+\sum_{j=1}^{Z_2}\left(\frac{Z_1e^2}{|\vec{R}-\vec{r}_j|}-\frac{Z_1e^2}{R}\right)+\sum_{j=1}^{Z_2}\left(\frac{p_j^2}{2m}+\frac{Z_2e^2}{r_j}-\sum_{k>j}^{Z_2}\frac{e^2}{|\vec{r}_k-\vec{r}_j|}\right)$$

$$=\frac{P^2}{2M}+\sum_{j=1}^{Z_2}V(\vec{R},\vec{r}_1\cdots\vec{r}_{Z_2})+H_T$$

$$=\frac{P^2}{2M}+\sum_{j}^{Z_2}H_j(\vec{R},\vec{r}_1\cdots\vec{r}_{Z_2}). \qquad (1)$$

Here the sum over j includes the projectile-nucleus interaction, and H_T represents the Hamiltonian of the unperturbed multielectron target. We note that the $H_j(\vec{R},\vec{r}_1\cdots\vec{r}_{Z_2})$ terms contain only c numbers (i.e., commuting numbers) in the variable R, but are not sums of single-particle Hamiltonians due to the presence of the interelectron interactions, $e^2/|\vec{r}_k-\vec{r}_j|$, which produce correlations in the target electrons. It is common to approximate the $\sum_k e^2/|\vec{r}_j-\vec{r}_k|$ term by an effective potential $V(\vec{r}_j)$, so that the eigenfunctions of H_T are product wave functions.

In order to reduce $\Psi(\vec{R},\vec{r}_1\cdots\vec{r}_{Z_2})$ to a product wave function, we introduce two assumptions: (i) Assume that initially the total asymptotic wave function Ψ^i is a product wave function, and (ii) assume that $P^2/2M$ commutes with each term in H. Each of these assumptions is an approximation. In the case of the first assumption, correlations in the target wave function are ignored corresponding to the replacement of $\sum_k e^2/|\vec{r}_j-\vec{r}_k|$ by an effective $V(\vec{r}_j)$, so that H_T and H_j are sums of single-electron terms. The second assumption corresponds to treating the projectile motion classically. These are the weakest assumptions that we have found that lead to the independent electron approximation.

The first assumption may be expressed in mathematical form by writing the initial asymptotic wave function Ψ_i as

$$\Psi^i(\vec{R},\vec{r}_1\cdots\vec{r}_{Z_2})=\phi^i(\vec{R})\prod_{j=1}^{Z_2}\phi_j^i(\vec{R},\vec{r}_j). \qquad (2)$$

It is common to choose, for example, $\phi^i(\vec{R})$ as a packet of plane waves sharply peaked about the classical position $\vec{R}_c=\vec{B}+\vec{v}t$, and $\phi_j(\vec{R},\vec{r}_j)=\phi_j(\vec{r}_j)$, an effective one-electron bound-state wave function.

The second assumption now guarantees that Ψ evolves as a product wave function because the evolution[16] operator $\Omega(t_1,t_2)$ factors into a product of single-particle terms, i.e., in the Heisenberg picture,

$$\Omega(t_1,t_2)=T\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2}H(t)\,dt\right]$$

$$=T\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2}\left(\frac{P^2}{2M}+\sum_{j=1}^{Z_2}H_j(\vec{R}(t),\vec{r}_j(t))\right)dt\right]$$

$$=T\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2}\frac{P^2}{2M}\,dt\right]\times\prod_{j=1}^{Z_2}T\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2}H_j(t)\,dt\right]$$

$$=\Omega_P(t_1,t_2)\prod_{j=1}^{Z_2}\Omega_j(t_1,t_2), \qquad (3)$$

since each term in H now commutes. Here T is the time-ordering operator. This factorization of the evolution operator into a product of single-electron terms is the crux of our development. Then, at any point in time,

$$\Omega(-\infty,t)\Phi^i=\Omega_P(-\infty,t)\phi^i(\vec{R})\prod_{j=1}^{Z_2}\Omega_j(-\infty,t)\phi_j^i(\vec{R},\vec{r}_j)$$

is a product of single-particle[17] terms.

III. PROBABILITY AMPLITUDES AND MULTIPLE IONIZATION CROSS SECTIONS

The probability amplitude $A^{i\alpha}(t)$ that the evolution operator carries Ψ^i into a particular state Ψ^α is given by the overlap of $\Omega(t,-\infty)\Psi^i$ with Ψ^α, i.e.,

$$A^{i\alpha}(t)=\langle\Psi^\alpha\,|\,\Omega(t,-\infty)\,|\,\Psi^i\rangle\,.$$

If we choose the Ψ^α to be orthonormal[18] eigenfunctions of the asymptotic Hamiltonian, then the Ψ^α may be represented as before by a product of single-electron wave functions, and, at any time,

$$A^{i\alpha}(t)=\left\langle\phi^\alpha(\vec{R})\prod_{j=1}^{Z_2}\phi_j^\alpha(\vec{r}_j)\,|\,\Omega(t,-\infty)\,|\times\phi^i(\vec{R})\prod_{j=1}^{Z_2}\phi_j^i(\vec{r}_j)\right\rangle.$$

Since the wave packet is sharply peaked about $\vec{R}_c=\vec{B}+\vec{v}t$, $A^{i\alpha}$ is a function of both impact parameter $\vec{B}$ and time t. Using the product nature of the evolution operator, we have

$$A^{i\alpha} = \langle \phi^{\alpha}(\vec{R}) \,|\Omega_P(t,-\infty)\,| \phi^{i}(\vec{R})\rangle \times \prod_{j=1}^{Z_2} \langle \phi_j^{\alpha}(\vec{r}_j) \,|\Omega_j(t,-\infty)\,| \phi_j^{i}(\vec{r}_j)\rangle = \prod_{j=0}^{Z_2} a_j^{i\alpha}(t) . \quad (4)$$

That is, the probability amplitude for the transition $i \to \alpha$ for a system with Z_2 electrons is a product of single-electron probability amplitudes [including the $j=0$ term, which is $\langle \phi^{\alpha}(\vec{R})\,|\Omega_P(t,-\infty)\,|\phi^{i}(\vec{R})\rangle$, here simply corresponding to straightline internuclear motion].

The square of this scattering amplitude, $|A^{if}(+\infty)|^2$, is the probability for scattering from an initial state Ψ^i characterized by a particular impact parameter $\vec{B}$ to a final state Ψ^f (replacing α by f). The total cross section for a beam of particles, uniformly distributed over impact parameter, is found by integrating the asymptotic transition probability over the impact parameter of the projectile, namely, with $A^{if}(+\infty) \equiv A^{if}(B)$,

$$\sigma^{if} = \int d^2B \,|A^{if}(B)\,|^2 = \int d^2B \prod_{j=0}^{Z_2} |a_j^{if}(B)\,|^2 . \quad (5)$$

The integral over $\vec{B}$ corresponds to an incoherent sum of probabilities for processes that are distinguishable; i.e., the transition from $\vec{B}_1$ is distinguishable from the transition from $\vec{B}_2$. This incoherence corresponds to our classical notion of a particle.

We note that the cross section for excitation of a single electron s in this approximation[19] is given by

$$\sigma_s^{if} = \int d^2B \,|a_s^{if}(B)\,|^2 \prod_{j\neq s}^{Z_2} \sum_f |a_j^{if}(B)|^2 = \int d^2B \,|a_s^{if}(B)\,|^2$$

since $\sum_f |a_j^{if}\,|^2 = 1$ for all j. Correspondence of this probability amplitude to a scattering amplitude is discussed in Sec. IV. Conceptually, in our classical treatment of the projectile, we assume that there is a one-to-one correspondence between the impact parameter and scattering angle of the projectile. Thus summing differential cross sections over impact parameters is equivalent to a sum over scattering angles.

In order to compute explicit cross sections for multiple ionization, it is useful to differentiate between the probability that an electron is excited to a particular state, and the probability that it is not excited. Since each electronic wave function evolves independently, we may apply unitarity to each single-electron wave function. Thus $|a_j^{i\vec{k}}(B)\,|^2$ is the probability that the jth electron is scattered into a final state, denoted by $\vec{k}$, and $1-|a_j^{i\vec{k}}(B)\,|^2$ is the probability of scattering into a final state other than $\vec{k}$. Here $\vec{k}$ denotes either a bound or a continuum excited state.

The probability for producing a vacancy in the single-electron picture via excitation or ionization is given by

$$P_S = \sum \int d\vec{k} \,|a^{i\vec{k}}(B)\,|^2 , \quad (6)$$

where the label S designates the state originally occupied by the electron. The probability for not producing a vacancy is $1-P_S$.

Obtaining the expression for multiple-ionization cross section is now a simple matter of specifying and counting the final states with and without a vacancy. In a particular atomic shell S with a total of N electrons, if the single-electron vacancy production probabilities P_S are identical, then there are $\binom{N}{n}$ possible ways to produce n vacancies with a probability

$$\binom{N}{n} P_S(1-P_S)^{N-n} ,$$

where $\binom{N}{n}$ is the binomial coefficient.

Thus if we consider a target with atomic shells $S=K,L,M,\ldots$, the cross section for removing $n_1=k$ of the $N_1=K$ electrons, $n_2=l$ of the $N_2=L$ electrons, $n_3=m$ of the $N_3=M$ electrons, etc., is given by

$$\sigma_{klm} = \int d^2B \left[\binom{K}{k}(P_K)^k(1-P_K)^{K-k} \times \binom{L}{l}(P_L)^l(1-P_L)^{L-l} \times \binom{M}{m}(P_M)^m(1-P_M)^{M-m}\ldots\right] . \quad (7)$$

The cross section summed over all final states, except those in the K and L shell, is represented by

$$\sigma_{kl} = \int d^2B \left[\binom{K}{k}(P_K)^k(1-P_K)^{K-k}\binom{L}{l} \times (P_L)^l(1-P_L)^{L-l}\right].$$

If one wishes to allow the single-electron probabilities within a shell to vary, it is straightforward to modify[7] the counting procedure.

IV. CONNECTION OF THE PROBABILITY AMPLITUDE A^{if} TO THE SCATTERING AMPLITUDE $f(\theta)$

In Sec. III, total cross sections for multiple excitation and ionization are expressed as an integral over impact parameters of the square of

the probability amplitude $A^{if}(B)$. Alternatively, a total cross section may be computed as an integral over scattering angles of the square of the scattering amplitude $f(\theta)$. Since we have had difficulty in expressing multiple excitation and ionization cross sections in terms of $f(\theta)$ directly, we discuss in this section in a standard fashion the relationship between $f(\theta)$ and $A^{if}(B)$.

The connection between $f(\theta)$ and $A^{if}(B)$ is most simply made classically, namely,

$$|f(\theta)|^2 = |A^{if}(B)|^2 \frac{B}{\sin\theta}\left(\frac{d\theta}{dB}\right)^{-1}, \tag{8}$$

where θ is the classical scattering angle for a projectile with incident impact parameter B interacting via an interparticle potential $V_c(R)$. In order to identify $V_c(R)$ and to justify the use of classical relationships, we expand the quantum-mechanical scattering amplitude in partial waves (ignoring the unscattered contribution) according to[20]

$$f(\theta) = \frac{-i}{2k}\sum_l^\infty (2l+1)e^{i2\delta_l} A_l^{if} P_l(\cos\theta), \tag{9}$$

where[21]

$$A_l^{if} = \langle \Psi_l^{ef} | \Omega^e(+\infty, -\infty) | \Psi^{ei} \rangle$$

is the amplitude of the electronic state $\langle \Psi_l^{ef}|$ in the outgoing wave as $R \to \infty$. The internuclear distortion of the scattering wave may be represented by the phase shift δ_l, which may be determined from an effective internuclear potential $V_c(R)$. Although this potential determines the deflection angle of the projectile, for heavy particles, where the deflection is slight, it may be ignored (as we have done). For heavy particles the effect of $V_c(R)$ is to contribute an overall phase δ_l to the probability amplitude, $A^{if}(B) = e^{2i\delta_l} A_l^{if}$, with $l = kB$, so that the two amplitudes[22] give the same total cross sections, corresponding to

$$\begin{aligned}\sigma &= 2\pi\int_{-1}^{1} |f(\theta)|^2 d(\cos\theta) \\ &= \frac{2\pi}{k^2}\sum_l (l+\tfrac{1}{2})|A_l^{if}|^2 \\ &\simeq 2\pi\int_0^\infty B|A^{if}(B)|^2 dB,\end{aligned}$$

assuming that the greatest contributions come from large l. Then $P_l(\cos\theta) \cong J_0((l+\frac{1}{2})\theta)$ with $\sin\theta \cong \theta$ and

$$f(\theta) \cong -ik\int_0^\infty dB\, B \exp[2i\delta(l=kB)]\, A_{l=kB}^{if} J_0(kB\theta). \tag{10}$$

This expression corresponds to summing[23] all diffraction contributions of $f(\theta)$ from various impact parameters. In Fig. 1, the wave amplitude at

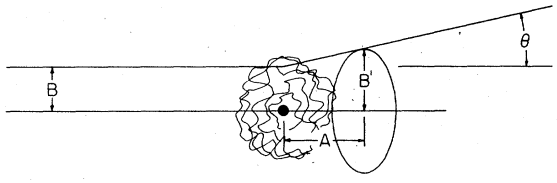

FIG. 1. Scattering illustration.

B' is $A^{if}(B')e^{i2\Delta(B')}$, where Δ is the phase difference between an unshifted wave and the true phase at B'. Beyond the plane at $Z = A$, defining the boundary of the scattering region we have

$$f(\theta) = ik\int_0^\infty B'\,dB'\, e^{2i\Delta(B')} A_{l=kB'}^{if} \times\left\{\frac{1}{2\pi}\int_0^{2\pi} d\phi' \exp(iqB'\cos\phi')\right\},$$

where the momentum transfer is $q \simeq k\theta$. The integral over ϕ' corresponds to a sum of wave amplitudes from contributions about the annulus at fixed B'. The term in the brackets is $J_0(qB')$. For heavy projectiles, $B \cong B'$, and

$$f(\theta) \cong -ik\int_0^\infty B A_{l=kB}^{if} e^{2i\Delta(B)} J_0(kB\theta)\, dB,$$

where $\Delta(B)$ corresponds to $\delta_{l=kB}$.

The classical relationship between $f(\theta)$ and $A^{if}(B)$ follows upon using the asymptotic expression for $P_l(\cos\theta)$ [or $J_0(kB\theta)$] and evaluating the above integral by the method of stationary phase. A_l^{if} is assumed to vary slowly in l (or B). The point of stationary phase corresponds[24] to

$$2\frac{d\delta_l}{dl} = \pm\theta,$$

which, with $l = kB$, is the classical scattering condition for a particle with impact parameter B to scatter via[25] $V_c(R)$ into θ. Thus $\theta = \theta(B)$, which we assume for the present to give a one-to-one relationship between θ and B. After a little algebra, the classical relationship given above between $|f(\theta)|^2$ and $|A^{if}(B)|^2$ then follows.

In this development the scattering amplitude $f(\theta)$, corresponding to the transition of more than one electron, is expressed in terms of the multielectron probability amplitude $A^{if}(B)$. We have not found a practical technique[26,27] for computing $f(\theta)$ directly for multielectron transitions.

The validity of this picture rests on replacing the sum over l by an integral, and assuming that the quantum-mechanical diffraction,[28] $\phi \sim l^{-1}$, is small compared with the scattering angle θ. For heavy particles, impact-parameter studies[29] suggest that most contributions to total cross sections correspond to $l = MvB \sim M$ (typically 2000 in atomic

units). The diffraction requirement depends on the choice of the internuclear potential $V_c(R)$, which determines $\theta(B)$. For inner-shell processes, it is conventional to regard[30] $V_c(R)$ as a screened Coulomb potential, whence $\theta \cong d_0/B$, where $d_0 = Z_1 Z_2/E$ is the distance of closest approach in a head-on collision (Z_1, E are the charge and energy of the projectile, and Z_2 the screened nuclear charge of the target at the collision site). Thus for screened Coulomb scattering it is required that $\theta > \phi = (MvB)^{-1} = \theta v/2Z_1Z_2$. Such a simple estimate[31-33] suggests that the classical approximation is valid at low velocities, $v \leq 2Z_1Z_2$.

V. DISCUSSION

The region of validity of our independent electron approximation corresponds to the limitations of the approximations used, namely, classical treatment of the projectile, discussed in Sec. IV, and neglect of correlations. Although we do not understand all possible effects due to correlations, some restriction is apparent. The effect of ignoring correlations in the initial unperturbed wave function is tied to the validity[34] of the uncorrelated Hartree-Fock approximation.[35] Correlations in the final-state wave functions, discussed below, may be important[36] in some circumstances. For applications cited[12] we distinguish between inner and outer atomic shells. During the interaction, target correlations in inner shells are neglected. Outer-shell activity is treated using sum rules[19] (illustrated at the end of Sec. III) so that it is effectively ignored. In our picture we also separate inner-shell excitation processes from deexcitation processes, i.e., the effects of final-state rearrangement are considered apart from the excitation process. This corresponds to the sudden approximation where the target wave function is frozen, except for those electrons directly affected during the interaction.

Electron correlation effects in the final state, following the passage of the projectile through the target, must be small in order for our method to be valid. Shakeoff and shakeup at high energies are examples[3,37-39] of final-state correlation contributions corresponding to rearrangement of the target wave function occurring after the projectile has interacted with the target. In photoabsorption[40] this effect appears to be the crucial determinant of multiple excitation and ionization. However, the probabilities for multiple excitation and ionization due to this final-state rearrangment are often small,[37-39] i.e., much less than 1, particularly for electrons in inner atomic shells. In contrast, when the projectile charge Z_1 is not small compared to the target charge Z_2, direct Coulomb multiple-ionization probabilities[12,41] are relatively large. In applying our methods one should ensure that direct Coulomb ionization probabilities are large compared to correlation probabilities. For example, in atoms between $Z_2 = 20$ and $Z_2 = 40$ the probability of L-shell ionization due to shakeoff following K-shell vacancy production has been estimated[39] at less than a few percent, that is, an order of magnitude less than the probability obtained[12,41] via direct Coulomb ionization by 30-MeV oxygen ions.

The scattering interaction itself may also produce correlations which we have ignored in the independent electron approximation. Calculations which go beyond the independent electron approximation now exist: for example, Glauber calculations[42] and close-coupling calculations with (or without) pseudostates.[43] These include eikonal calculations which employ a phase integral over an interparticle potential, mixing the wave functions of the projectile and target so that the resulting wave function is no longer a product of single-electron wave functions. In some cases (for single-electron excitation[44] and ionization[45]), the mixing terms contributing to the scattering amplitude $f(\theta)$ can be separated from the single-particle terms and studied separately. The effects of these coupling terms seem to be more evident in differential cross sections than in total cross sections.

In our independent electron approximation, the total wave function was presented using a simple product wave function ignoring the identity of the target electrons, e.g.,

$$\Psi^i = \phi^i(\vec{R}) \prod_{j=1}^{Z_2} \phi_j^i(\vec{R}, \vec{r}_j) .$$

This corresponds to a Hartree wave function for the multielectron target. Our development is unchanged, however, if an antisymmetrized product wave function is used, namely,

$$\Psi^i = \phi^i(\vec{R}) A \prod_{j=1}^{Z_2} \phi_j^i(\vec{R}, \vec{r}_j) ,$$

where A is the antisymmetrization operator. Now Ψ^i corresponds to an antisymmetrized sum of single-particle wave functions. As before, each term evolves independently so that the resulting probability amplitude is an antisymmetrized product of single-electron probability amplitudes. In this case, Ψ corresponds to an uncorrelated Hartree-Fock wave function.

The expression for multiple-excitation and ionization cross sections in Sec. III is defined in terms of the probability $P(B)$ for the transition of a single electron. A variety of classical[46,47] and semiclassical methods[33,48] for computing $P(B)$ are available. For example, the probability for ionization

of inner-shell electrons has been expressed[49] and tabulated[41] in the semiclassical Coulomb approximation using first-order perturbation theory. The multiple-ionization cross section computed[7] using these first-order probabilities correspond to some form of higher-order perturbation theory since the first-order contribution to multiple ionization is zero when the initial and final states are orthogonal. Also, the single-electron probability $P(B)$ does not correspond to the excitation of a single electron with no change permitted in the wave functions of the other electrons, but rather $P(B)$ corresponds to the probability of exciting a particular electron with an implicit sum[19] over all possible final states of the other electrons, as demonstrated in Sec. III.

This independent electron approximation reduces a many-body scattering calculation to a simple statistical distribution of single-electron probabilities. Since the binomial distribution itself is specified, the remaining problem is to determine the single-electron probabilities. Under some conditions, one may use first-order perturbation theory.[41] In other circumstances, where approximate calculations of $P(B)$ are not applicable, it may be useful to fit[12,50] observed distributions with an empirical probability $P(B)$. In some instances, it is reasonable to approximate $P(B)$ by $P(\overline{B})$, where $\overline{B}$ is a value of B contributing strongly to the total cross section. For example, if $P_K \ll 1$, and if $P_K(B)$ falls to zero within the interval where $P_L(B) \cong P_L(0)$, corresponding to $\overline{B}=0$, then

$$\sigma_{kl} = \int 2\pi B\, dB \binom{K}{k} [P_K(B)]^k [1-P_K(B)]^{K-k} \times \binom{L}{l} [P_L(B)]^l [1-P_L(B)]^{L-l}$$

$$\cong \binom{L}{l} [P_L(0)]^l [1-P_L(0)]^{L-l} \int 2\pi B\, dB \binom{K}{k} [P_K]^k = \binom{l}{L} [P_L(0)]^l [1-P_L(0)]^{L-l} \sigma_k .$$

The empirical vlaue of $P(\overline{B})$ may then be compared to direct observations of the impact-parameter dependence of vacancy production cross sections, providing experimental tests of the independent electron approximation.

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[17]Note that $[H_i(t_1), H_k(t_2)]$ is nonzero if $i=k$ and $t_1 \neq t_2$, i.e., $H_j(t_1)$ and $H_j(t_2)$ commute only if $t_1=t_2$.

[18]Nonorthogonality enters into the problem of atomic charge transfer. This problem is not addressed here. This orthogonality follows if H tends to the same asymptotic Hamiltonian initially and finally.

[19]J. H. McGuire and J. R. Macdonald, Phys. Rev. A 11, 146 (1975); J. S. Briggs and A. G. Roberts, J. Phys. B 7, 1370 (1974); J. F. Reading, Phys. Rev. A 8, 3262 (1973).

[20]N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University, London, 1965), p. 797.

[21]The integral over the projectile wave packet is conventionally omitted. When included, as in $A^{if}(B)$, the wave packet is localized with an impact parameter B and each wave packet has a relative phase of $e^{2i\delta(B)}$, corresponding to an internuclear interaction $V_c(R)$.

[22]It is conventional to regard $A^{if}(B)$ as the coefficients of the expansion of the full scattering wave function in time-dependent perturbation theory. Thus $A^{if}(B)$ is a function of a continuous variable B near $B=0$, unlike $e^{i2\delta l}A_l^{if}$ for small l, where l is discrete. We assume that small l contributes little to our amplitudes so that this difference may be ignored. Then for straight-line trajectories, it may be easily shown that $e^{i2\delta l}A_{l=kB}^{if}$ and $A^{if}(B)$ are equal.

[23]C. L. Cocke (private communication) pointed out this well-known fact to us. See, e.g., J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962), pp. 292–294.

[24]M. R. C. McDowell and J. P. Coleman, *Introduction to the Theory of Ion-Atom Collisions* (North-Holland, Amsterdam, 1970), p. 54.

[25]We note that a plausible choice for $V_c(R)$ is the distorting potential in a distorted-wave Born approximation (DWBA) approach.

[26]Y. Hahn and K. M. Watson [Phys. Rev. A 7, 491 (1973)] use a semiclassical projection operator for ionization by electron impact at high energies.

[27]A. Russek, Phys. Rev. 132, 246 (1963) and related papers describe an alternate statistical procedure for predicting ionization probabilities by heavy-particle impact.

[28]Reference 24, p. 9.

[29]For example, E. Laegsgaard, J. V. Anderson, and L. C. Feldman, Phys. Rev. Lett. 29, 1206 (1972); C. L. Cocke and R. Randall, Phys. Rev. Lett. 30, 1016 (1973).

[30]E. Everhart, G. Stone, and R. J. Carbone, Phys. Rev. 99, 1218 (1955).

[31]Reference 20, p. 110.

[32]On the other hand, total cross sections in the semiclassical approximation are often valid at high velocities as well (Ref. 24, Chap. 4, Appendix 4.1), even though the classical interpretation breaks down for Coulomb potentials. Also, the equivalence of the Rutherford differential cross section classically and quantum mechanically suggests a broader range of validity.

[33]J. Eichler has considered a related development using the Magnus expansion, as described by P. Pechukas and J. C. Light, J. Chem. Phys. 44, 2897 (1966); W. Magnus, Commun. Pure Appl. Math. 7, 649 (1954). The Magnus expansion gives an exponential series containing integrals over the commutator $[H_I(t_1), H_I(t_2)]$, where $H_I(t)$ is the Hamiltonian in the interaction representation. For the projectile we ignore such commutator terms, which for Coulomb interactions are proportional to delta functions.

[34]H. P. Kelly, in Ref. 12, Chap. 8.

[35]J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York, 1960), Vols. I and II.

[36]T. Åberg (private communication).

[37]F. Wuilleumier and M. O. Krause, Phys. Rev. A 10, 242 (1974); C. S. Fadley, Chem. Phys. Lett. 25, 225 (1974); M. Ya Amusia, V. K. Ivanov, N. A. Cherepkov, and L. V. Chernysheva, Phys. Lett. A 40, 361 (1972); H. P. Kelly, Phys. Rev. A 6, 1048 (1972); T. N. Chang, T. Ishihara, and R. T. Poe, Phys. Rev. Lett. 27, 838 (1971); T. A. Carlson, Phys. Rev. 156, 142 (1967).

[38]T. Åberg, in Ref. 12, Chap. 9. Also Ref. 3.

[39]T. Åberg, Phys. Rev. 156, 35 (1967).

[40]J. W. Cooper, in Ref. 12, Chap. 3.

[41]J. M. Hansteen, O. M. Johnson, and L. Kobach, At. Data Nucl. Data Tables 15, 305 (1975).

[42]E. Gerjuoy and B. K. Thomas, Rep. Prog. Phys. 37, 1345 (1974).

[43]M. R. Flannery and K. J. McCann, J. Phys. B 7, 2518 (1974). In this paper there are no applications to multielectron targets. Nevertheless, it represents an extension past the Glauber approximation, which includes mixing terms in multielectron systems. Hence in application to multielectron targets, we expect mixing terms to arise in this approach.

[44]B. K. Thomas and F. T. Chan, Phys. Rev. A 8, 252 (1973); F. T. Chan and S. T. Chen, Phys. Rev. A 9, 2393 (1974).

[45]J. E. Golden and J. H. McGuire, Phys. Rev. A 15, 499 (1977). The mixing terms, explicitly ignored by Golden and McGuire, have been evaluated by B. K. Thomas and A. M. Halpern, Bull. Am. Phys. Soc. 21, 1251 (1976).

[46]R. Abrines and I. C. Percival, Proc. Phys. Soc. Lond. 88, 873 (1966).

[47]R. Olson and A. Salop (private communication).

[48]Reference 24, Chap. 4, and references contained therein.

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[50]C. P. Bhalla, in *Beam Foil Spectroscopy*, Vol. 2, edited by I. A. Sellin and D. J. Pegg (Plenum, New York, 1976), p. 629.