Electron-Impact Ionization of Ne and Ar in the Eikonal and Born Approximations*

S. J. Wallace,† R. A. Berg, and A. E. S. Green
Department of Physics and Astronomy, University of Florida, Gainesville, Florida 32601
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Utilizing the first Born approximation and an eikonal/closure approximation plus Bethe's generalized-oscillator-strength (GOS) formalism, we evaluate s- and p-shell ionization of Ne and Ar. Partial-wave contributions to the GOS are calculated using an analytic independent-particle model (IPM) whose parameters have been established in previous work on excitation GOS's. For single ionization of Ne and Ar shells (K shell excepted), total cross sections and cross sections differential in the energy of the secondary electron are calculated for electron-impact energies near threshold to 10 keV. The eikonal/closure approximation which is developed in detail for large atoms differs from the Glauber theory by not assuming sudden passage of the projectile in which the time dependence of the bound electron and the energy transfer to the projectile may be neglected. In the single-scattering limit, the theory produces a simple factor multiplying the usual Born approximation amplitude, which leads to improved agreement with experiment at low energy.

I. INTRODUCTION

Electron-impact ionization of heavy atoms is an important process in many applications, e.g., studies of energy deposition in the upper atmosphere and in biological systems. However, the analysis of heavy atoms is complicated by their many-electron nature, particularly when one considers scattering theories of higher sophistication than the often used Born approximation.

The many-body nature of the atom is approximated in the present work by an independent-particle model, a technique which is often used in the study of large nuclei.[1] A series of studies has established a simple independent-particle model for atoms in which a two-parameter analytic potential[2] approximates the common attraction binding all electrons to the parent ion. One-electron (occupied) energy levels are accurately computed in this model[2] based on suitable values of the two parameters and reasonable elastic differential scattering cross sections[3–5] have been obtained for collisions of electrons with rare-gas atoms. The model has also been used previously with the generalized-oscillator-strength (GOS) formalism[6] to calculate electron-impact excitation of Ne, Ar, Kr, and Xe.

The electron-impact ionization process is considered in the present work using the eikonal approximation as well as the standard Born treatment.[7,8] Recent studies applying the Glauber high-energy approximation[9] to electron-hydrogen collisions[10–13] have obtained substantial improvement over the Born approximation for elastic and inelastic scattering. The Glauber theory is based on the eikonal approximation and on the assumption of sudden passage of the projectile in which the target particles may be regarded as immobile. The sudden passage assumption is in the spirit of the impulse approximation[14] but also entails neglect of the energy transfer in a reaction. However, as pointed out by Franco,[10] the neglect of the energy transfer in the Glauber theory is a weak assumption at large impact parameters (corresponding to small scattering angles), where the eikonal approximation is best established. In the present work, an eikonal/closure approximation is developed which incorporates nonzero energy transfer into the Glauber eikonal theory in a consistent way. The effect of large energy transfer is to reduce the ionization probability for large-impact-parameter collisions.

The eikonal theory is developed in several stages in Sec. II, where the eikonal approximation (without the sudden passage assumption) is discussed. The independent-particle model is used to simplify the many-electron scattering matrix element to a determinantal form involving one-electron matrix elements. From this result, approximations of increasing tractability are obtained by using the independent-particle potential to represent the distorting potential due to $Z-1$ inert core electrons on a one-electron transition. The one-electron transition matrix element is approximated by use of closure to sum over intermediate virtual transitions. Finally, the scattering amplitude is separated into a single-scattering term plus a distortion term. The resulting single-scattering term, which will be referred to as the eikonal/closure approximation (without distortion), consists of a universal factor multiplying the Born amplitude.

In Sec. III we discuss the calculations which employ the partial-wave GOS formalism for electron-impact ionization of closed subshells. Comparisons of our GOS calculations (based on the Green–Sellin–Zachor potential[2]) with the work of McGuire[15,16] and Manson[17] (who used a Hermann–Skillman[18] potential) have been briefly reviewed elsewhere.[19] Results for the outer-shell ionization GOS of Ne

are presented. The Bethe surfaces[20-23] of Ne are developed as a series of cuts at constant ejected electron energy and constant momentum transfer. Section IV presents cross-section results for single ionization of Ne and Ar shells (K shell excepted) based on the eikonal/closure approximation (without distortion) and on the Born approximation. Comparisons are made with the experimental data.[24-28] Concluding remarks are made in Sec. V.

II. EIKONAL FORMALISM

A. Eikonal Approximation for Inelastic Scattering

The eikonal approximation is based on approximating the exact scattering wave by a set of straight-line rays which propagate through the interaction with fixed impact vector $\vec{b}$ parallel to what is generally defined to be the z axis. Although other choices have recently been proposed,[29] we follow Glauber[9] in choosing the z axis parallel to the average momentum $\vec{k} = \frac{1}{2}(\vec{k}_i + \vec{k}_f)$ for inelastic as well as elastic collisions. This choice is also motivated by studies of the corrections to the Glauber approximation for potential scattering.[30]

For elastic scattering, the fact that the momentum transfer $\vec{K} = \vec{k}_i - \vec{k}_f$ is perpendicular to Glauber's z direction occasions a simplification in the theory and calculations. For inelastic scattering the component $K_z = (k_i^2 - k_f^2)/2|\vec{k}|$ is nonzero but, to retain the simplifications, it is generally ignored. The object of the present development is to incorporate nonzero K_z into the Glauber-type eikonal theory.

In the following statement of the eikonal approximation, we use atomic units in which energies are expressed in units of the Rydberg ($R = e^2/2a_0 = 13.6$ eV), lengths are expressed in units of the Bohr radius ($a_0 = 0.529$ Å), and masses are expressed in units of the electron mass.

The eikonal T matrix can be cast in the form of an impact-parameter representation in which the impact vector $\vec{b}$ lies in a plane perpendicular to the average momentum $\frac{1}{2}(\vec{k}_i + \vec{k}_f)$ which serves to define a z direction. The momentum transfer $\vec{K} = \vec{k}_i - \vec{k}_f$ can be decomposed into parts K_z and $\vec{K}_\perp$ which are parallel and perpendicular to the z axis. These are expressed as follows:

$$K_z = \tfrac{1}{2}\beta W/v\,, \quad \beta = [\tfrac{1}{2} + \tfrac{1}{2}(1-\nu^2)^{1/2}\cos\theta]^{-1/2}\,,$$
$$\nu = W/2Pv\,, \tag{1}$$
$$K_\perp = |\vec{K}_\perp| = P\beta(1-\nu^2)^{1/2}\sin\theta\,. \tag{2}$$

Here the scattering angle of the projectile is θ (in the center-of-mass system) and the wave number P is given by

$$P = [\tfrac{1}{2}(k_i^2 + k_f^2)]^{1/2} = [M(E - \tfrac{1}{2}W)]^{1/2}\,. \tag{3}$$

W is the energy loss of the incident particle. The velocity v is defined by $v = P/M$ in terms of the reduced mass M ($M = 1$ for electron impact). The inelasticity parameter ν appearing in Eq. (1) is the ratio of energy loss W to twice the average projectile kinetic energy. The c.m. energy is E. Note that here and in what follows, the energy variables often carry a factor $\frac{1}{2}$ which is not present in the a.u. system ($e = \hbar = m_e = 1$). Also when W is set to zero, the usual variables are obtained [$K_z = 0$, $K_\perp = 2P\sin\frac{1}{2}\theta$, $P = (ME)^{1/2}$].

In terms of the above parameters the leading order eikonal scattering amplitude takes the form of a two-dimensional Fourier transform

$$T_{fi} = \frac{P}{2\pi i}\int d^2b\, e^{i\vec{K}_\perp\cdot\vec{b}}\langle\epsilon_f|\,U_0(\vec{b},\vec{b}_T)\,|\epsilon_i\rangle\,, \tag{4}$$

from which the differential cross section is obtained as follows:

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\,|T_{fi}|^2\,. \tag{5}$$

The unitary operator governing the target atom transition between energy eigenstates $|\epsilon_i\rangle$ and $|\epsilon_f\rangle$ is

$$U_0(\vec{b};\vec{b}_T) = T\left\{\exp\left[\frac{i}{-2v}\int_{-\infty}^{\infty} dz\, V\left(\vec{r};\vec{r}_T\left(\beta\frac{z}{v}\right)\right)\right]\right\}\,. \tag{6}$$

The operator U_0 governs the "time dependence" of the target in response to passage of the projectile along a straight-line path $\vec{r} = \vec{b} + vt\hat{k}$ in which the projectile z coordinate plays the role of "time," i.e., $t = z/v$. The symbol T in (6) is the time-ordering operator applied to trajectory time z/v. Corrections due to curvature of the projectile's path have been developed,[31,32] but they are complicated and will be ignored for the present.

The above formalism deviates from Glauber's original development by presence of $\beta = P/|\vec{k}|$ in (6). Note from (1) that $\beta \approx 1/\cos\frac{1}{2}\theta \approx 1$ for high-energy small-angle scattering, and thus β represents a minor change arising from choosing the eikonal propagation along the average momentum $\vec{k}$. As it stands, the leading approximation (6) of the eikonal formalism contains important improvements over the Born approximation which is obtained by expanding (6) to leading order in the interaction. The second- and higher-order powers of the interaction present in Eq. (6) are corrections to the Born term, and they must be retained to obtain approximate unitarity.

The transition operator U_0 is "time" ordered in the parameter z/v because the Heisenberg "time"-dependent interaction

$$V(\vec{r},\vec{r}_T(\beta z/v)) = e^{i\beta H_T z/2v}V(\vec{r},\vec{r}_T)\,e^{-i\beta H_T z/2v} \tag{7a}$$

involves the "time"-dependent coordinate operators

$$\vec{r}_T(\beta z/v) = e^{i\beta H_T z/2v}\vec{r}_T e^{-i\beta H_T z/2v}, \tag{7b}$$

which do not commute at different values of the "time." The interaction $V(\vec{r}, \vec{r}_T)$ of course depends on the collection of coordinates $\vec{r}_T = \{\vec{r}_1, \ldots, \vec{r}_{N+1}\}$ which specify the locations of the target particles [the $(N+1)^{\text{th}}$ one is the nucleus]. For electron impact we have in Rydberg units

$$V(\vec{r}; \vec{r}_T) = \sum_{i=1}^{N} \frac{2}{|\vec{r} - \vec{r}_i|} - \frac{2Z}{|\vec{r}|}, \tag{8}$$

where the coordinate $\vec{r}_{N+1}$ of the atomic nucleus relative to the atom's center of mass has been ignored.

B. Independent-Particle Assumption

For simplicity, the target atom is described by an independent-particle Hamiltonian H_T^0 which consists of a sum of commuting one particle Hamiltonians h_i as follows:

$$H_T = H_T^0 + \delta V, \quad H_T^0 = \sum_i h_i, \quad h_i = P_i^2 + V_c(\vec{r}_i). \tag{9}$$

In the approximation $H_T = H_T^0$ each electron feels the same central potential due to the nucleus and $N-1$ other electrons. Green, Sellin, and Zachor have successfully parameterized the atomic independent-particle potential by the analytic form[2]

$$\begin{aligned} V_c(r) &= -(2/r)[(N-1)\Omega(r) + Z - N + 1], \\ \Omega(r) &= [H(e^{r/d} - 1) + 1]^{-1}, \end{aligned} \tag{10}$$

where parameter values H and d have been defined by previous studies. For a neutral atom one of course has $N = Z$. Correlation effects due to the interactions in δV are ignored in the model but they are in a sense minimized by choice of an optimized independent-particle potential.

Amus'ya *et al.*[33] have recently shown that correlation effects can be quite important in GOS calculations at small momentum transfer for electron impact ionization of Ar. Our bound-state and final continuum-state electron wave functions, which are obtained by numerically integrating the radial Schrödinger equation using the effective potential above, may not be as accurate as those of Amus'ya *et al.*

The eikonal framework of Eq. (4) is much simpler in the independent-particle model because the single-particle operators h_i and r_i commute with the corresponding operators of the other electrons. Substituting the approximation $H_T = H_T^0$ in (7) and (6) simplifies the unitary operator U_0 of Eq. (6) to a direct product of commuting unitary operators which act in the subspace of each target particle:

$$U_0(\vec{b}; \vec{b}_T) = e^{i\chi_N(\vec{b})} \prod_{i=1}^{N} U_0^{(1)}(|\vec{b} - \vec{b}_i|), \tag{11}$$

$$\begin{aligned} U_0^{(1)} &= T\left[\exp\left(\frac{-i}{v}\int_{-\infty}^{\infty} dz \, \frac{1}{|\vec{r} - \vec{r}_i(\beta z/v)|}\right)\right], \\ \vec{r}_i\left(\frac{\beta z}{v}\right) &= e^{ih_i\beta z/2v}\vec{r}_i e^{-ih_i\beta z/2v}. \end{aligned} \tag{12}$$

The phase $\chi_N(b)$ arises from the nuclear term in the interaction, Eq. (8). In this approximation the "time" dependence of the ith-electron coordinate is governed by the independent-particle Hamiltonian h_i. A simpler form of the factorization property, Eq. (12), is very well known[9] at high energy when the "time" dependence can be ignored altogether. Then one obtains the Glauber theory by approximating $K_z = \beta\Delta\epsilon/2v = 0$. This limit is, however, inappropriate to a class of inelastic-scattering problems in which the Coulomb potential governs large-impact-parameter collisions because setting K_z to zero produces an infinite forward-scattering amplitude just as in the elastic channel.[10] To avoid singular results at small angles, one must retain the "time" dependence in Eq. (12).

The determinantal wave functions appropriate to an atom in the independent-particle model take their simplest form for closed-shell atoms such as the rare gases. Then a single determinant of the space states ϕ_i and spin states χ_i suffices to describe the atom's ground state,

$$|\epsilon\rangle = A_N|\phi_1(1)\chi_1(1)\rangle|\phi_2(2)\chi_2(2)\rangle\cdots|\phi_N(N)\chi_N(N)\rangle, \tag{13}$$

where A_N is the antisymmetrizing operator for N particles. The fine structure of the atomic levels is ignored so that each level contains $N_{nl} = 2(2l+1)$ electrons differing only in magnetic and spin quantum numbers.

Before discussing the inelastic scattering, there are several points which should be understood about the elastic channel in the present formalism. Elastic scattering is of course described by the matrix element $\langle\epsilon_i|U_0|\epsilon_i\rangle$ and since in Eq. (11) U_0 is a symmetric product, the result may be expressed as the determinant of an $N\times N$ matrix of one-particle transition matrix elements:

$$\begin{aligned} S_A(\vec{b}) &= \langle\epsilon_i|U_0|\epsilon_i\rangle \\ &= e^{i\chi_N(\vec{b})}\,\mathrm{Det}\langle\phi_m\chi_m|U_0^{(1)}(\vec{b} - \vec{b}')|\phi_n\chi_n\rangle \\ &= e^{i\chi_N(\vec{b})}\,[\mathrm{Det}\langle\phi_m|U_0^{(1)}(\vec{b} - \vec{b}')|\phi_n\rangle]^2. \end{aligned} \tag{14}$$

In the third line we have used the orthogonality of spin states and assumed spin degeneracy to simplify the original determinant to the square of the determinant of an $\frac{1}{2}N\times\frac{1}{2}N$ matrix[34] involving only the space states. In principle this elastic-scattering amplitude could be calculated; however, that is unnecessary in the present case. It is well known that the elastic scattering can be equivalently described by a potential (which is in general complex). A recent treatment of this problem has been

made by Joachain and Mittleman,[35] who derive an optical potential for elastic scattering.

An analysis by Berg, Purcell, and Green[5] has, however, shown that the elastic scattering of electrons by rare gases is adequately described using exactly the same potential $V_c(\vec{r})$ as above. One simply adjusts the parameter N to the value $Z+1$ to describe the interaction of the impact electron with the neutral atom, exclusive of any polarization effects. In the eikonal formalism, this means that the electron-atom elastic-channel scattering can be described by an impact-parameter amplitude[30] $S_A(b)$ based on the potential $V_c(\vec{r})$ plus, in general, a polarization potential $V_p(\vec{r})$. If needed, the imaginary part of the potential could, of course, be included.

Inelastic scattering differs by excitation of one (or more) electrons to excited states. The single-particle excited states are calculated using the model potential, Eq. (10), and are therefore orthogonal to each occupied level of the ground-state atom. The simplest situation occurs when a single electron (from say any state ϕ_j of the nl shell) is excited to an unoccupied level ϕ_α with quantum numbers designated by α. The excitation energy is $\Delta\epsilon = \epsilon_\alpha - \epsilon_{nl}$ and the corresponding final-state wave function for the atom is

$$|\epsilon_f\rangle = A_N |\phi_1(1)\chi_1(1)\rangle \cdots |\phi_\alpha(j)\chi_\alpha(j)\rangle \cdots |\phi_N(N)\chi_N(N)\rangle . \quad (15)$$

The resulting inelastic amplitude $\langle\epsilon_f|U_0|\epsilon_i\rangle$ is a determinant which differs from the elastic amplitude, Eq. (14), since the jth row involves single-particle transition matrix elements between each initial state and the state $\phi_\alpha\chi_\alpha$. The full ionization amplitude is obtained by expanding said determinant about the jth row; and the result is that one obtains a direct-ionization term equal to the jj matrix element multiplied by its minor plus exchange terms involving the other matrix elements of the row multiplied by their respective minors.

The amplitude for direct ionization of an electron from a specific initial state is approximated by using, as above, a potential scattering amplitude to describe the $Z-1$ electrons which remain in their original states. The resulting expression for a direct transition is thus written as

$$\langle\epsilon_f|U_0|\epsilon_i\rangle \approx \langle\phi_\alpha\chi_\alpha|U_0^{(1)}(\vec{b}-\vec{b}_j')|\phi_{nlm_l}\chi_{m_s}\rangle S_{A^+}(\vec{b}) + \text{exchange terms}, \quad (16)$$

where $S_{A^+}(\vec{b})$ is the elastic scattering amplitude corresponding to the $Z-1$ inert electrons and the nucleus.[36] The subscript A^+ designates a singly ionized atom and the potential $V_c(\vec{r})$ of Eq. (10) can be used for this elastic scattering factor. Since we must in the end average over the magnetic and spin quantum numbers, the use of the same spherically symmetric distorting potential for all nl shell transitions is reasonable.

C. Eikonal/Closure Approximation

As already emphasized, the energy transfer should not be ignored. To deal with it we must calculate the "time" dependence of the operator $U_0^{(1)}$ occurring in the transition matrix-element, Eq. (16). This is done exactly in first order and approximately in the higher orders by employing a form of the closure approximation as follows. We expand Eq. (12) for $U_0^{(1)}$ in powers of the time-dependent two-electron interaction

$$e^{i\beta hz/2v}\frac{1}{|\vec{r}-\vec{r}'|}e^{-i\beta hz/2v}$$

to obtain the following form for the single-particle transition matrix element:

$$\langle\phi_\alpha|U_0^{(1)}|\phi_{nl}\rangle = \frac{-i}{v}\langle\phi_\alpha|\int_{-\infty}^{\infty}dz_1\, e^{i\beta hz_1/2v}\frac{1}{|\vec{r}_1-\vec{r}'|} \times e^{-i\beta hz_1/2v}|\phi_{nl}\rangle + \left(\frac{-i}{v}\right)^2\langle\phi_\alpha|\int_{-\infty}^{\infty}dz_1 \times e^{i\beta hz_1/2v}\frac{1}{|\vec{r}_1-\vec{r}'|}e^{-i\beta hz_1/2v}\int_{-\infty}^{z_1}dz_2 \times e^{i\beta hz_2/2v}\frac{1}{|\vec{r}_2-\vec{r}'|}e^{-i\beta hz_2/2v}|\phi_{nl}\rangle + \cdots . \quad (17)$$

Here the projectile coordinates $\vec{r}_1 = z_1\hat{k}+\vec{b}$, $\vec{r}_2 = z_2\hat{k}+\vec{b}$, and so on, all have the same impact vector $\vec{b}$ but differing z coordinates, and the target coordinates are designated by $\vec{r}' = z'\hat{k}+\vec{b}'$. A little manipulation casts the leading term here (which is the Born amplitude) into the form

$$-(2i/v)\langle\phi_\alpha|e^{iK_z z'}K_0(K_z|\vec{b}-\vec{b}'|)|\phi_{nl}\rangle , \quad K_z = \tfrac{1}{2}\beta W/v , \quad W = \epsilon_\alpha - \epsilon_{nl} . \quad (18)$$

The modified Bessel function K_0 appears by virtue of the integral over $z_1 - z'$, which takes the form

$$\int_{-\infty}^{\infty}d\zeta\frac{e^{iK_z\zeta}}{(\zeta^2+|\vec{b}-\vec{b}'|^2)^{1/2}} = 2K_0(K_z|\vec{b}-\vec{b}'|), \quad (19)$$

and the Hamiltonian operators on the left- and right-hand side of the terms in Eq. (17) have taken the values ϵ_α and ϵ_{nl} appropriate to the eigenstates on which they act. Note that K_z plays the role of a screening parameter. If the Coulomb interaction $|\vec{r}-\vec{r}'|^{-1}$ were exponentially screened by a factor $e^{-\mu|\vec{r}-\vec{r}'|}$, one would obtain $(\mu^2+K_z^2)^{1/2}$ in place of K_z in the right-hand side of (19). Thus nonzero K_z has the same effect as $K_z = 0$ with nonzero μ, i.e., screening.

Ignoring higher-order terms in Eq. (17) and using the above Born term in Eq. (16) corresponds to a distorted-wave Born approximation.[37] How-

ever, to obtain an approximately unitary amplitude we must consider the higher-order terms. In the Glauber theory this calculation is simple because each h of (17) is set to zero. We approximate h in a somewhat more realistic way by allowing it to take on values in the range $\epsilon_\alpha \le h \le \epsilon_{nl}$ in such a way that Eq. (17) can still be calculated. For example, the second-order term of Eq. (17) is calculated by inserting a complete set of single particle eigenstates $|\phi_\gamma\rangle$ to obtain

$$\sum_\gamma \left(\frac{-i}{v}\right)^2 \langle\phi_\alpha| \int_{-\infty}^{\infty} dz_1\, e^{i\beta\epsilon_\alpha z_1/2v} \frac{1}{|\vec{r}_1 - \vec{r}\,'|} e^{-i\beta\epsilon_\gamma z_1/2v} |\phi_\gamma\rangle \times \langle\phi_\gamma| \int_{-\infty}^{z_1} dz_2\, e^{i\beta\epsilon_\gamma z_2/2v} \frac{1}{|\vec{r}_2 - \vec{r}\,'|} e^{-i\beta\epsilon_{nl} z_2/2v} |\phi_{nl}\rangle . \tag{20}$$

We approximate this term by fixing ϵ_γ at the average energy $\frac{1}{2}(\epsilon_\alpha + \epsilon_{nl})$ and then invoke closure $\sum_\gamma |\phi_\gamma\rangle\langle\phi_\gamma| = 1$ to render the $z_1 - z'$ integrals to a tractable form. The result is

$$(1/2!)\langle\phi_\alpha| e^{iK_z z'}[-(2i/v)K_0(\tfrac{1}{2}K_z|\vec{b} - \vec{b}\,'|)]^2 |\phi_{nl}\rangle , \tag{21}$$

where we have used the special case $n = 2$ of the formula

$$I_n = \int_{-\infty}^{\infty} dz_1\, f(z_1) \int_{-\infty}^{z_1} dZ_2\, f(z_2) \cdots \int_{-\infty}^{z_{n-1}} dz_n\, f(z_n) = \frac{1}{n!}\left(\int_{-\infty}^{\infty} dz_1\, f(z_1)\right)^n . \tag{22}$$

The above procedure can be extended to evaluate all the terms in the expansion of $U_0^{(1)}$. For example, in the nth-order term, one fixes all the intermediate-state energies at $(1/n)(\epsilon_\alpha - \epsilon_{nl})$ and then uses closure to render the $z_i - z'$ integrals into the form Eq. (22). In this way, the eikonal transition operator $U_0^{(1)}$ in (16) is replaced by an approximate transition operator which, apart from a factor $e^{iK_z z'}$, is

$$T_e(K_z|\vec{b} - \vec{b}\,'|) = \sum_{n=1}^{\infty} \left[\frac{-2i}{v} K_0\left(\frac{1}{n} K_z|\vec{b} - \vec{b}\,'|\right)\right]^n \frac{1}{n!} . \tag{23}$$

In this expression the screening effect of K_z is the only difference from the Glauber result. For the exponentially screened Coulomb potential mentioned above, the Glauber result is obtained by replacing K_z/n in (23) with $(\mu^2 + K_z^2/n^2)^{1/2}$ and taking the limit $K_z = 0$. For a Coulomb interaction, the screening parameter μ is allowed to become very small and this leads to the usual constant phase times $e^{2i|\vec{b}-\vec{b}'|/v}$ in place of (23). Since the modified Bessel function $K_0(x)$ falls off as $x^{-1/2}e^{-x}$, one can see that for large relative impact parameter $S \equiv |\vec{b} - \vec{b}\,'|$, each term of (23) is proportional to a screening factor $e^{-K_z S}$.

Equation (23) is simply one method of incorporating nonzero K_z into a consistent eikonal theory and its derivation involves the rather arbitrary device of splitting K_z into n equal portions $K_{z1}, K_{z2}, \ldots, K_{zn}$ for an nth-order scattering. Since the screening constant at large S is simply K_z, i.e., the sum of the magnitudes of the pieces, it is, however, likely that other divisions of K_z would produce at least as much screening at large S.

The direct inelastic scattering amplitude can now be expressed by collecting the above results:

$$T_{fi} = \frac{P}{2\pi i} \int d^2b\, e^{i\vec{K}_\perp \cdot \vec{b}} S_{A^+}(\vec{b}) \times \langle\phi_\alpha\chi_\alpha| e^{iK_z z'} T_e(K_z|\vec{b} - \vec{b}\,'|)|\phi_{nlm}\chi_\mu\rangle . \tag{24}$$

This is our basic approximation based on the eikonal formalism. An alternative statement of the result can be made by introducing the scattering amplitudes $T_{A^+}(\vec{q})$ corresponding to e-A^+ elastic scattering and $T_e(K_\perp; K_z)$ corresponding to e-e inelastic scattering, respectively,

$$T_{A^+}(\vec{q}) = \frac{P}{2\pi i} \int d^2b\, e^{i\vec{q}\cdot\vec{b}}[S_{A^+}(\vec{b}) - 1], \tag{25}$$

$$T_e(K_\perp, K_z) = \frac{P}{2\pi i} \int d^2b\, e^{i\vec{K}_\perp \cdot \vec{b}} T_e(K_z|\vec{b}|) . \tag{26}$$

Then Eq. (24) can be cast into a more convenient form as follows:

$$T_{fi} = T_e(K_\perp; K_z)\langle\phi_\alpha\chi_\alpha| e^{i\vec{K}\cdot\vec{r}\,'} |\phi_{nlm}\chi_\mu\rangle + (i/2\pi P) \int d^2\vec{q}\, T_{A^+}(|\vec{K}_\perp - \vec{q}|) T_e(q; K_z) \times \langle\phi_\alpha\chi_\alpha| e^{i(\vec{q}\cdot\vec{b}\,' + K_z z')} |\phi_{nlm}\chi_\mu\rangle . \tag{27}$$

Here the leading term is our eikonal/closure approximation for the single scattering (without distortion) in which the eikonal amplitude $T_e(K_\perp; K_z)$ replaces the usual Born amplitude $T_B(K^2) = -2M/K^2$. The second term corresponds to the leading-order effect of the distorting potential.

Figure 1 illustrates this decomposition of the reaction amplitude into a single-scattering e-e term plus a double-scattering term in which the

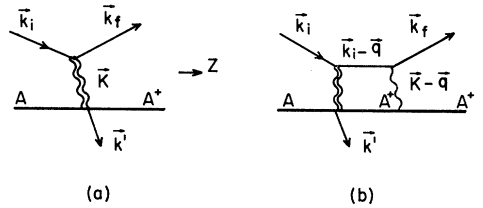

FIG. 1. Diagrams illustrating (a) the single-scattering and (b) the double-scattering (distortion) contributions to single-ionization. The ejected electron momentum is $\vec{K}'$ and the heavy line represents the atom (A) or ionized atom (A^+). The double-scattering term is approximated by a single-electron ionization in conjunction with an elastic in a potential model of the ion.

inert core of the atom A is approximated by a potential. The atom (which is taken to have infinite mass compared to an electron) is indicated by the lower heavy line and the impact electron by the upper lines. The momentum $\vec{k}'$ indicates the secondary electron. The double wavy lines here for momentum transfer are used to indicate our approximation to the inelastic e-e scattering. They actually correspond to summing all ladder diagrams for photon exchange as in Fig. 2 using the eikonal approximation. By this we mean that both electrons are constrained to move on straight-line paths and each virtual photon exchanged in an nth-order diagram carries $1/n$ times the z component of over-all momentum transfer K_z.

D. Relationship to the Born Approximation

For the present, we do not calculate the effects of the distorting potential but concentrate on the rather simpler single-scattering term in Eq. (27). The large impact-parameter collisions which contribute strongly to forward scattering are expected to be more affected by the improved treatment of K_z (inelasticity) than by distortion effects. Thus the approximation we use is calculationally similar to the usual Born treatment. To expressly isolate this difference as a simple factor we calculate the ratio of T_e to the Born amplitude as follows:

$$F=\frac{-K^2}{2M}\frac{P}{i}\int_0^\infty db\, bJ_0(K_\perp b)T_e(K_z b)$$

$$=\tfrac{1}{2}iv(1+Q^2)\int_0^\infty db'\,b'J_0(Qb')T_e(b'). \qquad (28)$$

In the first line the integration over directions of $\vec{b}$ in Eq. (26) has been carried out and the result divided by $-2M/K^2$. The second line is obtained by integrating over the scaled impact parameter $b'=K_z b$ and introducing the ratio of momentum transfer perpendicular and parallel to z,

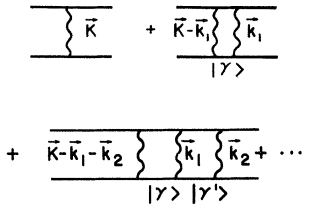

FIG. 2. Ladder-series diagrams for nonrelativistic photon exchange, calculated in the eikonal approximation to obtain a unitarized two-body amplitude. In the lower line the bound electron makes a transition from the initial $|n1\rangle$ state through various intermediate states $|\gamma\rangle$ to the final state $|\alpha\rangle$. In summing over the intermediate states using the closure approximation, the Pauli exclusion principle is ignored, i.e., already occupied levels are included in the sum to obtain a simple result.

$$Q\equiv K_\perp/K_z=(1-\nu^2)^{1/2}(\sin\theta)/\nu. \qquad (29)$$

Numerical calculations have been made of this factor which is applicable to any e-e single scattering with energy transfer to a virtual photon. Because of its presumably wide range of applicability, we have developed analytic curve fits to $|F(Q,v)|^2$. The direct numerical results along with the analytic curve fits to the function are plotted in Figs. 3 and 4. The curve fit we use is given by the formula

$$|F(Q,v)|^2=\frac{v^4}{v^4+3.77v^2+1}\times\left(1+\frac{Q^2}{(0.54+0.441v^2+0.0119v^4)^2}\right)^{-1}. \qquad (30)$$

For the present, the factor $|F(Q,v)|^2$ has been evaluated at kinematical conditions appropriate to electron-impact ionization. The results are equally applicable to proton ionization at the same velocity and Q values.

The parameter Q used here is a function of the impact energy E, energy loss W, and momentum transfer K of the impact particle as follows:

$$Q^2=4(vK/W)^2(1-K^2/4P^2)-1,\quad P^2=M(E-\tfrac{1}{2}W), \qquad (31)$$

and for electron impact, $M=1$. Note from (31) that the optical limit ($K^2\to 0$) for fixed energy loss W requires $Q^2\to -1$, whereas the physical range of Q^2 is positive as seen from (29). Lassettre, Skerbele, and Dillon[38] have given arguments which show that in the limit $K^2\to 0$, the cross section for electron-impact ionization should approach the photoionization cross section in which $F(Q,v)$ is replaced by unity. This requirement is not incompatible with (28) because the integral (which is convergent for $Q^2>-1$) tends to infinity as $Q^2\to -1$ but the factor $1+Q^2$ tends to zero. It is conjectured that the limit is $F(Q,v)\to 1$ as $K^2\to 0$; however, the analytic function (30) is seen to be deficient in this respect and probably should not be used outside the range given in Fig. 3.

Owing to neglect of the distortion effects which are present in the second term of (27), the correction factor $|F(Q,v)|^2$ to the Born approximation is always less than unity and is a decreasing function of Q, i.e., of the sine of the scattering angle. This behavior is not expected to be universally realistic when distortion effects are included. Hence the reliability of the single-scattering term of (27) [in which $T_e(K_\perp, K_z)$ is equal to $-2MF(Q,v)/K^2$] is presumably limited to small scattering angles. Integrated cross sections are dominated by small-angle scattering events, however, and this limitation is not serious unless one is specifically interested in the large-angle differential scattering.

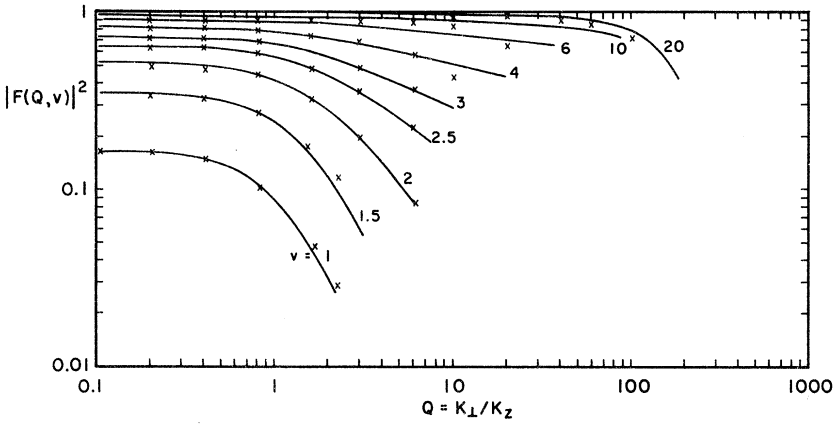

FIG. 3. Absolute magnitude squared $|F(Q, v)|^2$ of the ratio of the unitarized e-e scattering amplitude to the Born approximation is plotted as a function of the scaled momentum transfer $Q = K_\perp/K_z$ for various velocities v which are in units of αc. The curve fit function of Eq. (30) produces the points indicated by x.

E. Effect of the Exclusion Principle on Closure

In reality, the situation is not as simple as depicted above because the closure approximation must be handled with more care. The difficulty arises because we have neglected the exchange terms in (16), which, in addition to providing exchange mechanisms, also enforce the exclusion principle on the direct one-electron transition.

Because of the Pauli exclusion principle, a single-particle state $|\phi_\gamma\rangle$ which is already occupied by one of the atomic electrons is not an admissible intermediate state for the direct single-particle transition of another electron. The determinantal wave function of the complete atom vanishes if two electrons occupy the same single-particle state. Thus the sum over intermediate states must properly be limited to just the unoccupied single-particle states.

The projection operator onto the unoccupied states is written as

$$\hat{\rho} \equiv \sum_{\gamma > \gamma_0} |\phi_\gamma\rangle\langle\phi_\gamma| , \tag{32}$$

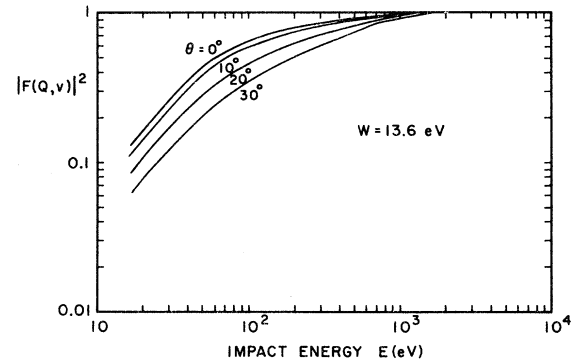

FIG. 4. Same information as in Fig. 3 is shown as a function of electron-impact energy E in eV at fixed values of the scattering angle θ for an energy loss W of 1 Ry.

and we note that it does not commute with the position operator $\vec{r}\,'$ of the bound electron. For hydrogen, $\hat{\rho}$ is unity, since no states are excluded by the Pauli principle. The deviation of $\hat{\rho}$ from unity obviously increases as the target atomic number increases. Although the effect is expected to be nonnegligible for heavy atoms, a detailed treatment is beyond the scope of this paper.

However, we note that it is possible to parametrize the effect of the incompleteness ($\hat{\rho} \neq 1$) by proceeding in the spirit of the optical model. The matrix element in (17) is simply a complex number for each value of the impact parameter b. Thus a function $\rho(b)$ can be found such that correct matrix element, incorporating the projection operator $\hat{\rho}$ of (32), is equal to

$$T_e(\rho; K_z|\vec{b} - \vec{b}\,'|) \equiv \rho^{-1} \sum_{n=1}^{\infty} \left[\frac{-2i\rho}{v} K_0\left(\frac{1}{n} K_z|\vec{b} - \vec{b}\,'|\right)\right]^n \frac{1}{n!} . \tag{33}$$

The parameter ρ is here inserted in the same way that the operator $\hat{\rho}$ enters and this permits the Born approximation ($\rho = 0$) and eikonal/closure approximation ($\rho = 1$) limits to be readily obtained.

A constant value ρ has the effect of shifting the velocity v in (23) to v/ρ. Thus a factor $|F(Q, v/\rho)|^2$ can be obtained from (28) or (30) and as $\rho \to 0$ the high-velocity behavior $|F|^2 \to 1$ is obtained indicating a smooth connection with the Born approximation.

F. Relationship to Other Theories

The fact that the eikonal/closure approximation yields a kinematical factor times the Born amplitude suggests a similarity with the impulse approximation (IA)[14] and with the approximation of Vainshtein, Presnyakov, and Sobelman (VPS).[39] Coleman[40] has recently reviewed the IA and VPS methods and has shown the relationship of the VPS theory to an extended impulse approximation.

The idea behind the IA and VPS methods is to

treat the scattering of the projectile electron (e) and an *immobile* bound electron (e') as a Coulomb scattering process. Due to the energy transfer, an off-energy-shell scattering amplitude is needed. The VPS approximation and extended impulse approximation includes, in addition, what we have called distortion effects; i.e., effects due to the Coulomb potential of the nucleus are included (approximately) in the e-e' scattering amplitude. However, both approximations ignore the *time dependence* of the bound electron which provides the principal new effect in the eikonal/closure approximation of Eq. (27).

In the IA and VPS methods, the target atom initial and final states provide distributions of initial and final momentum values for e' over which the e-e' potential scattering amplitude must be averaged. With few exceptions, a peaking approximation is used to evaluate this average. A sharp peak is presumed in the forward e-e' scattering amplitude allowing evaluation of the momentum distribution only at the corresponding values of e' momentum. As a result, both the IA and VPS methods obtain results similar to the first term of (27) but with different factors in place of the e-e' scattering amplitude $T_e(K_\perp, K_z)$. However, Coleman[40] cautions that the peaking approximation is likely to be valid only at extremely high energies.

It is worth noting that a peaking approximation could be applied to the second term of Eq. (27) to approximate the distortion effect. The resulting formula would then bear a strong analogy to the VPS approximation. However, a much more reliable (but also more difficult) calculation would proceed directly from (27).

Since the principal new effect of the present development is included in the eikonal/closure approximation (without distortion) and the peaking approximation is dubious, our present calculations are made neglecting the distortion term of (27).

III. IONIZATION FORM FACTOR: GOS CALCULATIONS

The ionization-cross-section differential in energy loss W, and the element $d\Omega$ of solid angle is, in our single-scattering approximation,

$$\frac{d^2\sigma}{dW\,d\Omega} = \frac{4k_f}{k_i}\frac{|F(Q,v)|^2}{K^4}\frac{1}{2(2l_0+1)} \times N_{nl}\sum_{m\mu\nu}\int d\hat{k}'\,|\,I(\vec{k}',\vec{K})\chi_\mu^\dagger\chi_\nu|^2\,, \quad (34)$$

with the factor $F(Q, v)$ as given in Sec. II representing the only difference from the Born approximation. An average is performed over the $N_{nl} = 2(2l_0+1)$ equivalent spin and magnetic substates of the nl shell. Also we sum over final spin orientations and integrate over the directions $\hat{k}'$ of the ejected electron's momentum $\vec{k}'$. The form factor of the ionizing reaction which promotes an electron of nl shell to a single-particle continuum state with asymptotic momentum $\vec{k}'$ is

$$I(\vec{k}',\vec{K}) = \langle\phi_{\vec{k}'}\,|\,e^{i\vec{K}\cdot\vec{r}}\,|\,\phi_{nlm}\rangle\,. \quad (35)$$

The final state $\phi_{\vec{k}'}$ is normalized per unit energy $T = k'^2$ and solid angle according to

$$\langle\phi_{\vec{k}'}\,|\,\phi_{\vec{k}''}\rangle = \delta(k'^2 - k''^2)\delta^{(2)}(\Omega' - \Omega'')\,, \quad (36)$$

and thus asymptotically approaches $[k'/2(2\pi)^3]^{1/2}$ times a phase-shifted Coulomb wave.

The generalized oscillator strength (GOS) for the ionization process is (after performing the spin sums)

$$\frac{df}{dW} = \frac{WN_{nl}}{K^2(2l_0+1)}\sum_m\int |I(\vec{k}',\vec{K})|^2\,d\hat{k}'\,, \quad (37)$$

so that the double-differential cross section takes the form

$$\frac{d^2\sigma}{dW\,d\Omega} = 4\frac{k_f}{k_i}\frac{|F(Q,v)|^2}{K^2}\frac{1}{W}\frac{df}{dW}\,. \quad (38)$$

With the exception of the factor $|F(Q, v)|^2$, this is the standard expression as derived originally by Bethe[20] and more recently by Mott and Massey,[22] Massey and Burhop,[23] and by Rudge.[7]

Performing a series of mathematical manipulations of the matrix element (35) (McGuire[16] and Berg[41] give details) we have

$$\frac{df}{dW} = \frac{2N_{nl}W}{\pi k'K^2}\sum_{l'=0}^{\infty}(2l'+1)\sum_{l=|l'-l_0|}^{l'+l_0}(2l+1) \times\begin{pmatrix} l' & l & l_0\\ 0 & 0 & 0\end{pmatrix}^2 |I_{l'll_0}|^2\,, \quad (39)$$

where $\begin{pmatrix} l_1 & l_2 & l_3\\ m_1 & m_2 & m_3\end{pmatrix}$ is a Wigner 3-j symbol[42] and the reduced matrix elements are

$$I_{l'll_0} = \int P_{l'}^*(k'r)\,j_l(Kr)\,P_{n_0l_0}(r)\,dr\,. \quad (40)$$

In this expression $P_{n_0l_0}(r)$ is the radial bound-state wave function, $P_{l'}(k'r)$ is the radial continuum wave function, and $j_l(Kr)$ is a spherical Bessel function.

In the present calculations of df/dW, the potential V_c of (10) is used. Accurate numerical integrations of the radial Schrödinger equations for both $P_{n_0l_0}(r)$ (using the Hermann–Skillman code) and $P_{l'}(k'r)$ (using the Noumerov method) are performed. Table I lists the potential parameters H and d which have been determined[6] to give accurate

TABLE I. Potential parameter values used in the model.

	Ne	Ar	Kr	Xe
H	2.2188	3.4687	5.5066	6.8051
d	0.7145	0.9971	1.0550	1.1752

excited-state energy levels for rare-gas atoms. In this respect, the potential (10) is superior to the Hermann–Skillman potential[18] used by Manson[17] and McGuire.[15,16]

Our calculations of the GOS are performed with l and l' values in (39) limited to a maximum value of 13. McGuire, who has used a similar limit (12) for his calculations,[15,16] has discussed the likely errors introduced by this truncation. Also the direct computation[41] of (40) is presumably superior to the method used by McGuire, which employs a series of straight-line segments to approximate $rV(r)$, where $V(r)$ is the Hermann–Skillman potential. Reference 19 contains comparisons of our GOS values with those of Manson and McGuire.

Calculations have been performed for outer and inner shells of neon and argon. The outer-shell GOS results for Argon have been discussed in Ref. 19. For neon, we present typical outer-shell GOS results which provide the dominant contribution to over-all ionization.

Neon Ionization GOS

The most hydrogenlike atom in the present study is Ne, for which Figs. 5 and 6 illustrate our calculational results. These plots depict "cuts" at constant T and K^2 of the Bethe surface df/dW for Ne ionization. Inokuti[8] has cited the importance

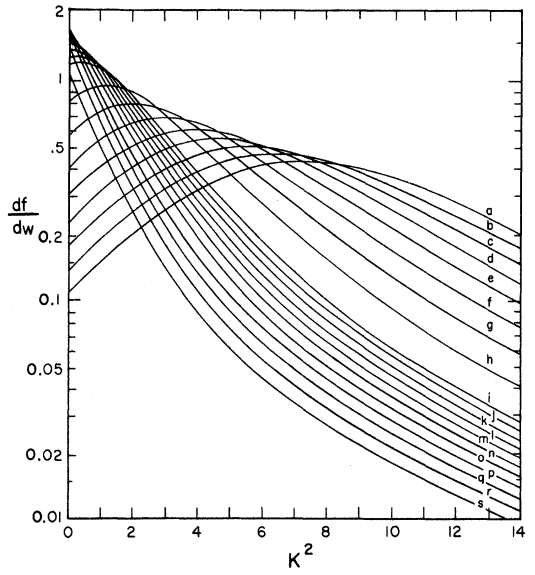

FIG. 5. Model calculations of the total GOS in units of Ry^{-1} vs K^2 at constant T for Ne. The energy (T) values for the curves are as follows (Ry):

a-10	f-5	k-1.6	p-0.6
b-9	g-4	l-1.4	q-0.4
c-8	h-3	m-1.2	r-0.2
d-7	i-2	n-1.0	$s-10^{-6}$.
e-6	j-1.8	o-0.8	

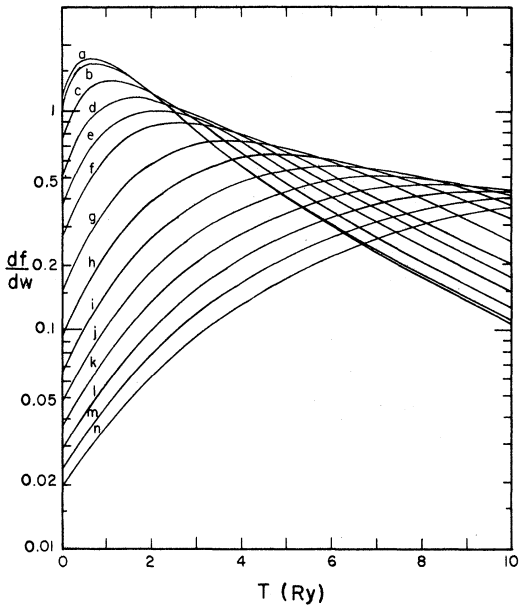

FIG. 6. Model calculations of the total GOS in units of $(Ry)^{-1}$ vs T at constant K^2 for Ne. The K^2 values for the curves are as follows (a_0^{-2}):

$a-10^{-4}$	f-2	k-7
b-0.1	g-3	l-8
c-0.5	h-4	m-9
d-1.0	i-5	n-10.
e-1.5	j-6	

of the Bethe surface as being its comprehensive representation of the inelastic scattering phenomenon.

We note that at large values of K^2 and T, our surface is similar to the hydrogenic case with the Bethe ridge extending out into the $K^2 = T$ plane and being approximately centered over the $K^2 = T$ line as expected from energy conservation in the quasi-elastic scattering limit. Figure 6 displays the only qualitative change between our Ne calculation and hydrogenic results. As one starts at $T = 0.0$ Ry and goes to higher energy for the $K^2 = 10^{-4}$ curve, the GOS builds up to a maximum at $T \approx 0.6$ Ry before falling off whereas in the hydrogenic case, the maximum would be at $T = 0.0$ Ry. Thus the most probable secondary electron energies are nonzero, which, of course, is not the case in hydrogen.

IV. CROSS SECTIONS

The cross sections for ionization are calculated in two steps. The first integration of (38) is over angles of scattering of the primary electron to obtain the cross section $d\sigma/dT \equiv S(E, T)$ differential in energy of the secondary electron. Employing $x \equiv K^2 = k_i^2 + k_f^2 - 2k_i k_f \cos\theta$ to convert the integration over $d\Omega = 2\pi d(\cos\theta)$ to one over the momentum transfer squared x, the result is

$$S(E, T)=\frac{4\pi}{EW}\int_{x-}^{x+}\frac{dx}{x}\frac{df}{dW}(x)\left|F\left(Q, \frac{v}{\rho}\right)\right|^2, \quad (41)$$

where

$$x\pm=2ME\left[1-\frac{W}{2E}\pm\left(1-\frac{W}{E}\right)^{1/2}\right]. \quad (42)$$

The eikonal/closure factor is calculated as in (30) using the connection between x and Q^2 as given in (31).

The parameter ρ indicated in (41) is zero if one wishes to obtain the Born approximation or unity to obtain the full eikonal/closure result.

Single-ionization cross sections are calculated by integrating over the secondary electron energy T:

$$\sigma(E)=\int_0^{(E-I)/2}dT\,S(E, T). \quad (43)$$

The upper limit of integration corresponds to the midpoint of the total distribution due to primary plus secondary electrons. Thus we follow the convention of counting electrons with kinetic energies $T<\frac{1}{2}(E-I)$ as secondaries and the balance as primaries. This rule is not rigorous and would presumably be improved upon at low energy by a treatment of exchange effects in computing the total electron distribution.[7]

The comparison of theory with experiment is most readily accomplished by first considering the ionization cross sections. Figures 7 and 8 present shell by shell partial contributions to Ne and Ar ionization cross sections in both the Born and eikonal/closure approximations. The outer-shell results in the Born approximation are in reasonable agreement with McGuire's Born-approximation calculations,[15] which are shown for comparison. Our results for Ne are consistently higher than those of McGuire. Clearly, the outer-shell electrons dominate the process at all energies; however, the inner-shell contributions are not negligible at high energy. The innermost K shell has been omitted in both cases. At high energy the two theoretical curves are in good agreement; however, the eikonal/closure approximation provides a marked reduction in the cross sections at low energies relative to the Born approximation.

Figures 9 and 10 show our single-ionization cross sections (summed over subshells) for Ne and Ar. The experimental data, obtained from the review by Kieffer and Dunn,[24] are from various experiments as indicated (see Ref. 24 for original sources). We show maximum and minimum experimental cross-section values at representative energies, and these are based on measurements of total ion current. Thus the experimental points include multiple-ionization effects which are not in the theoretical curves. Kieffer and Dunn[24] present data which show that the single-ionization cross sections for Ne and Ar tend to be about 10 to

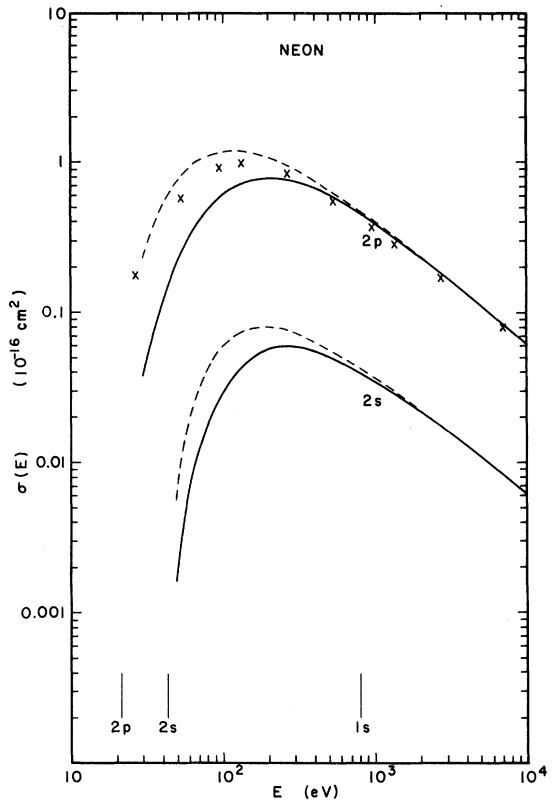

FIG. 7. Partial cross sections for ionization of Ne shells. Vertical bars represent ionization threshold energies for shell indicated. Dashed lines are Born approximation results; solid lines are eikonal/closure approximation results; ×'s are results of McGuire, Ref. 15.

15% lower than the total (or gross) ionization data points given in Figs. 9 and 10 at energies above 200 eV.

For this reason the theoretical single-ionization curves should be compared to the lower experimental points in each plot. Also we note that the average of experimental data compiled by Green and McNeal[26] for E up to 1000 eV tends to pass between the extremes shown in Figs. 9 and 10.

For Ne, the eikonal/closure approximation produces more accurate results than the Born approximation near the peak cross-section values; however, we note at high energy a disturbingly large difference between our calculations and the experiments. The discrepancy of about 30% at high energy in Fig. 9 arises partially from inaccuracies in the GOS near threshold. Our outer-shell calculations tend to agree with those of McGuire to about 10% at high energy (Fig. 7); thus both calculations appear to yield higher than expected total ionization cross sections when inner-shell effects and multiple-ionization effects are included. The agreement with experiment is not

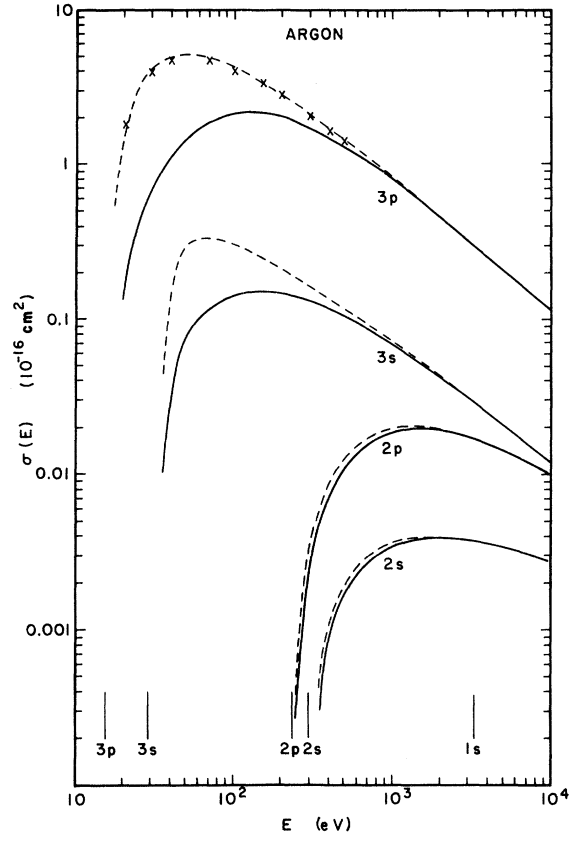

FIG. 8. Partial cross sections for ionization of Ar shells. Vertical bars represent ionization threshold energies for shell indicated. Dashed lines are Born approximation results; solid lines are eikonal/closure approximation results; ×'s are results of McGuire, Ref. 15.

unreasonable, however, in Fig. 9. It is possible that polarization effects, which can be important near the ionization threshold, are limiting the accuracy which can be attained with the present independent-particle model wave functions.

For Ar the agreement between theory and experiment at high energy is much better. However, below 100 eV, the Born approximation gives about double the experimental cross section, and the eikonal/closure result about one-half the experimental result. In Fig. 10 we also show an intermediate theoretical curve based on $\rho = 0.6$ (corresponding crudely to partial closure) which does fit the experimental data rather well. Thus for Ar the results are about equally poor for the Born and eikonal/closure approximations and only by parametrizing the effect of the Pauli principle via $\rho = 0.6$ is decent agreement with experiment obtained. Of course, using a nonunity value of ρ is at the present time a heuristic device. Still the procedure permits improved estimates of the secondary electron distributions in energy. Figures 11 and 12 show the secondary electron distributions for Ne with $\rho = 1$ and Ar with $\rho = 0.6$. These distributions are thus compatible with the cross sections shown in the corresponding curves in Figs. 9 and 10. The data points are from the experiment by Opal, Beaty, and Peterson[25] at 500 eV. In general, the agreement of theory and experiment is good, with some notable exceptions in the vicinity of 10-eV secondary electron energy. These discrepancies at low secondary electron energy are possibly due to core polarization effects and also multiple-ionization processes which we have ig-

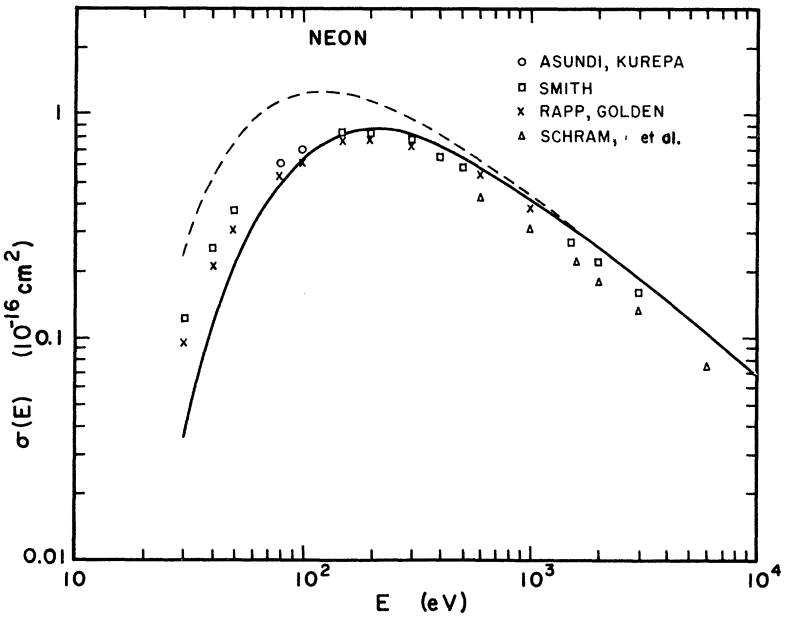

FIG. 9. Comparison of theoretical single-ionization and experimental gross-ionization cross sections for Ne. Dashed line is Born approximation. Solid line is eikonal/closure approximation. Data points are from Ref. 24.

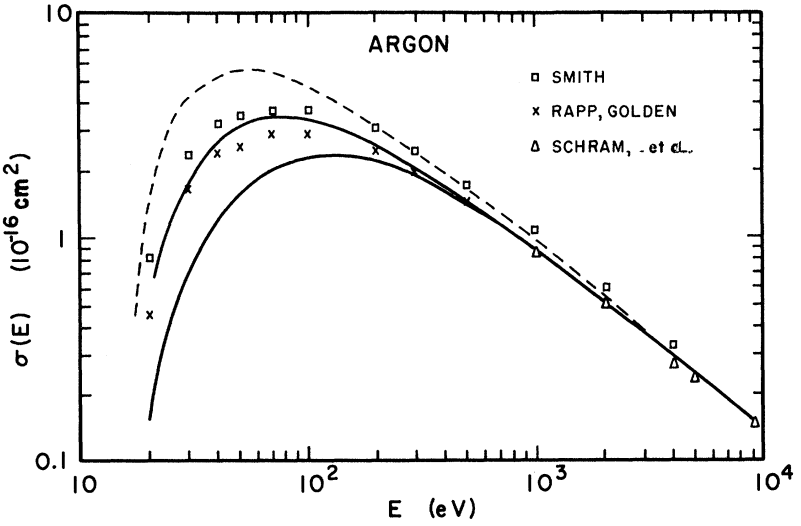

FIG. 10. Comparison of theoretical single-ionization and experimental gross-ionization cross sections for argon. Dashed line is Born approximation. Lowest solid line is eikonal/closure approximation with $\rho = 1$, intermediate solid line is same with $\rho = 0.6$. Data points are from Ref. 24.

nored. The distortion and exchange effects which also have been ignored are not expected to cause a large effect at this impact energy (500 eV).

V. CONCLUDING REMARKS

The calculational procedures to obtain the Bethe surfaces and cross sections for many-shell atoms are, at this time, rather long and costly but not prohibitive. Thus we conclude that the independent-particle model of Green, Sellin, and Zachor[2] provides a quite reasonable method of calculating ionization GOS's for a number of atoms over a wide range or energy losses and momentum transfers. The use of an analytic potential lends the calculation an adaptability which is not now present in the self-consistent field method.

Our results on the Bethe surface indicate that there is much more structure for low K^2 and T values than might have been expected from the use of hydrogenic wave functions for the ejected electron. This fact indicates that there is a need to use realistic wave functions in GOS calculations. To obtain good agreement with photoionization experiments in the optical limit ($K^2 \to 0$), it may also be necessary to account for polarization effects or simply to use more accurate wave functions such as computed by Amus'ya *et al.*[33] Note that the independent-particle model used in this work does give quite good total cross sections at $E = 4$ KeV in Fig. 10. The effect of correlations on the GOS demonstrated by Amus'ya *et al.* at this energy does not seem to affect the total cross section. On the experimental side, measurements of angular differential cross sections for heavier atoms are quite rare. If the incident energy is high enough, measurements of this kind can be converted into GOS's[43] for comparison with theory and will indicate how well or poorly the analytic potential model is doing. At the present time, there is need for more angular distribution data.

The success of the eikonal/closure approximation for heavy atoms is partial and thus does not

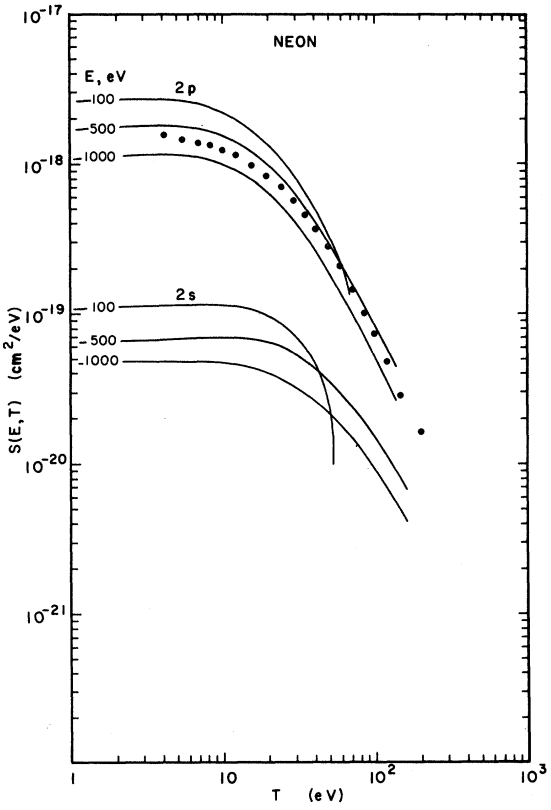

FIG. 11. Distribution in energy T of the secondary electrons in electron-impact ionization of Ne. Results are based on eikonal/closure approximation ($\rho = 1$). Data points are from Ref. 25 for 500 eV.

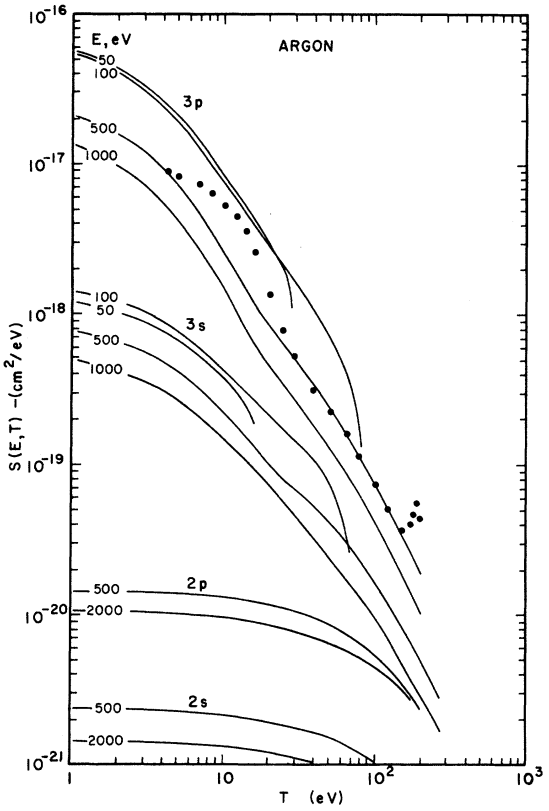

FIG. 12. Distribution in energy T of the secondary electrons in electron-impact ionization of Ar. Results are based on eikonal/closure approximation ($\rho = 0.6$). Data points are from Ref. 25 for 500 eV.

permit broad conclusions to be drawn. However, the method does incorporate nonzero energy transfer $\Delta\epsilon$ into a consistent eikonal theory and remains tractable. Clearly $\Delta\epsilon$ can have a substantial screening effect of the long-range forces.

The distortion effects which we have not calculated can be included in a straightforward way, as discussed in Sec. II, to make the calculation of cross sections reliable at low energy. Since a reliable means of incorporating the effect of the Pauli principle on single-particle transitions is not presently available (either in the Glauber or eikonal/closure approximations), the theory is probably limited to light atoms. A clean test of the eikonal closure theory would be obtained for hydrogen, where other theoretical results are available.

For applications which demand reliable cross-section values at low energies and/or heavy atoms, it appears necessary at present to use more detailed but more empirical modifications of the Born approximation such as that of Green and Dutta[44] or else resort to an extension of the distorted-wave Born approximation along the lines of the work of Sawada *et al.*[45]

Inner-shell ionization has been shown to be a small (10%) part of the single-ionization Ne and Ar cross sections. However, a much more substantial contribution can be anticipated to the average energy loss per ionization due to the more tightly bound inner shells. Also the subsequent production of multiple ionization due to Auger mechanisms once an inner-shell vacancy is produced tends to increase importance of inner-shell calculations.

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†Present address: Lyman Laboratory of Physics, Harvard University, Cambridge, Mass. 02138

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