72, 3933 (1967).

[13] R. A. Bonham, J. Chem. Phys. 36, 3260 (1962).

[14] U. Fano and J. W. Cooper, Phys. Rev. 137, A1364 (1965).

[15] W. Gautschi and W. F. Cahill, in *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (U. S. GPO, Washington, D. C., 1964), Appl. Math. Series 55, Chap. 5.

[16] A. T. Jusick, C. E. Watson, L. R. Peterson, and A.E.S. Green, J. Geophys. Res. 72, 3943 (1967).

[17] R. S. Stolarski, V. A. Dulock, C. E. Watson, and A.E.S. Green, J. Geophys. Res. 72, 3953 (1967).

[18] C. E. Watson, V. A. Dulock, R. S. Stolarski, and A. E. S. Green, J. Geophys. Res. 72, 3961 (1967).

[19] D. J. Strickland and A. E. S. Green, J. Geophys. Res. 74, No. 26 (1969).

[20] J. D. Dow and R. S. Knox, Phys. Rev. 152, 50 (1966).

[21] A. Gold and R. S. Knox, Phys. Rev. 113, 834 (1959).

[22] J. W. Cooper, Phys. Rev. 128, 681 (1962).

[23] J. Geiger, Z. Physik 177, 138 (1964).

[24] G. M. Lawrence and H. S. Liszt, Phys. Rev. 178, 122 (1969).

[25] E. L. Lewis, Proc. Phys. Soc. (London) 92, 817 (1967).

[26] G. M. Lawrence, Phys. Rev. 175, 40 (1968).

[27] P. G. Wilkinson, J. Quant. Spectry. Radiative Transfer 5, 503 (1965).

[28] J. Koch, Kgl. Fysiograf. Sallskap. Lund Forh. 19, 173 (1949).

[29] J. M. Vaughan, Phys. Rev. 166, 13 (1968).

[30] D. K. Anderson, Phys. Rev. 137, A21 (1965).

[31] Y. K. Kim, M. Inokuti, G. E. Chamberlain, and S. R. Mielczarek, Phys. Rev. Letters 21, 1146 (1968).

[32] C. E. Kuyatt (private communication).

[33] L. A. Vainshtein and I. I. Sobel'man, J. Quant. Spectry. Radiative Transfer 8, 1491 (1968).

[34] V. Ya. Veldre, A. V. Lyash, and L. L. Rabik, Opt. Spectry. (USSR) 19, 182 (1965).

[35] B. L. Moiseiwitsch and S. J. Smith, Rev. Mod. Phys. 40, 238 (1968).

[36] T. Sawada, J. E. Purcell, and A. E. S. Green, following paper, Phys. Rev. A 4, 192 (1971).

[37] R. S. Stolarksi and A. E. S. Green, J. Geophys. Res. 72, 3967 (1967).

[38] A. E. S. Green and C. A. Barth, J. Geophys. Res. 72, 3974 (1967).

[39] L. R. Peterson and A. E. S. Green, J. Phys. B 1, 1131 (1968).

[40] R. A. Berg and A. E. S. Green (unpublished).

[41] L. R. Peterson and J. E. Allen, Jr. (unpublished).

PHYSICAL REVIEW A VOLUME 4, NUMBER 1 JULY 1971

Distorted-Wave Calculation of Electron Impact Excitation of the Rare Gases*

T. Sawada, J. E. Purcell,† and A. E. S. Green
University of Florida, Gainesville, Florida 32601

(Received 11 January 1971)

A distorted-wave (DW) formulation with exchange is given for the electron impact excitation of the rare gases from $(n_0p)^6$ to $(n_0p)^5nl$ configurations. A practical form employing the pure LS-coupling scheme is used in conjunction with the phenomenologically determined independent-particle model (IPM) and the DW potentials of real central forms to compute cross sections averaged over fine structures. Numerical work is carried out for Ne $2p\rightarrow 3s$ and Ar $3p\rightarrow 4s$ electron impact excitations. The distorted generalized oscillator strengths (DGOS), which converge to the generalized oscillator strengths (GOS) in the limit of the Born approximation, as well as integrated cross sections, are obtained over a wide range of energies, so that the systematic variation of the cross sections in relation to the results of the Born approximation can be studied. The results of the angular distributions at lower energies are in reasonable agreement with the data by Nicoll and Mohr.

I. INTRODUCTION

The electron impact excitation of the rare gases has been studied in the Born approximation by Ganas and Green, based upon the analytic atomic IPM of Green, Sellin, and Zachor.[1,2] In order to extend their work to lower-energy regions, it is necessary to investigate the effects of distortion as well as exchange contributions. We study these effects using the DW approximation based upon the same IPM[2] and the same DW potential that has been applied to the elastic scattering analysis.[3]

Very few DW calculations have been reported for atoms heavier than hydrogen and helium, with the exception of the work by Massey and Mohr on the low-energy data of Ne and Ar obtained by Nicoll and Mohr.[4,5] If the excitation cross sections of individual levels in a fine structure were required, one would have to first obtain Hartree-Fock (HF) atomic wave functions and HF potentials of the initial and final states. A detailed DW formulation appropriate for such a computation has been proposed recently by Shelton and Leherissey[6] with particular emphasis on a transition from the LS-coupled ground state to a J_Cl-coupled excited state.

In this work, however, we are interested primarily in obtaining cross sections averaged over an energy interval whose width is of the order of the level splitting of the fine structure. Such cross sections would be obtained experimentally either by taking the corresponding average of fine resolution measurements or by using an incident electron beam of "poor" energy resolution. The concept of cross sections averaged over many fine resonances is familiar in the nuclear optical model and constitutes the basis of that model.[7] Although the states involved here are not resonances but states below the ionization threshold, we employ a similar averaging process. Accordingly, we compute averaged cross sections directly based upon the IPM and the optical model using model potentials determined phenomenologically.[2,3] Such an approach is not only a useful one but is, in fact, the only practical course if one wants to obtain reliable estimates of hundreds of cross sections for use in electron-energy deposition studies.

In Sec. II, the DW formulation appropriate to our approach is briefly discussed, and the choice of the distorting potentials for the direct and exchange amplitudes is made. DGOS is defined such that it approaches the GOS in the limit of the Born approximation. In Sec. III, the detailed formulas of reaction amplitudes and cross sections of the excitation from $(n_0p)^6$ to $(n_0p)^5nl_n$ configurations for both singlet and triplet final states are presented assuming the pure LS-coupling scheme of the atomic wave functions. The results of numerical calculations for the Ne $2p \rightarrow 3s$ and Ar $3p \rightarrow 4s$ excitations are provided in Sec. IV in terms of the DGOS and integrated cross sections. Comparisons are made with the results of the Born approximation with appropriate discussions. We chose these reactions partly because of the choice of the LS-coupling scheme made for the atomic wave functions. The formulation, however, should be applicable for other excitations as well as for heavier rare-gas atoms, whenever we intend to calculate average cross sections. The main reson for choosing these reactions is that there are experimental data available for comparison with the theory.[4] Furthermore, the comparison is more meaningful since these reactions produce simple but pronounced diffraction patterns which are necessary to test the DW angular distributions, unlike the results for helium or higher excitations in Ne and Ar.

II. METHOD OF ANALYSIS

The ground- and excited-state atomic wave functions ψ_0 and ψ_n are constructed from single-electron wave functions bound in the IPM potential of the form[1] (in a.u.)

$$V_B(r) = -\frac{2}{r}\left\{\frac{Z-1}{H(e^{r/d}-1)+1}+1\right\} . \qquad (2.1)$$

In the study of generalized oscillator strengths of the rare gases, Ganas and Green[2] found sets of values of parameters H and d in (2.1) that reproduce quite well the positions of levels of $(n_0p)^5nl_n$ configurations averaged over fine splittings. In this work we use the parameter values obtained by them. The ground-state wave function ψ_0 is the Slater determinant of the $(n_0p)^6$ electron wave functions, and the excited-state wave function ψ_n is constructed as a properly antisymmetrized combination of the $(n_0p)^5nl_n$ product wave functions LS coupled to produce a state with the total angular momentum J and its z component M. The actual forms of ψ_0 and ψ_n, and the values of H and d used, are given in Sec. III.

We denote the plane-wave function for the jth electron by $\phi_0(j)$,

$$\phi_0(j) = e^{i\vec{k}_0\cdot\vec{r}_j}\sigma^{m_s}(j) , \qquad (2.2)$$

where $\vec{k}_0$ is the initial momentum and σ^{m_s} is the spin eigenfunction. We also denote the ground-state atomic wave function by $\psi_0(\bar{j})$, indicating that the jth electron is the projectile and hence is not present in ψ_0, and the total wave function by $\Psi_0^{(+)}(j)$, in which only the jth electron has an incoming plane wave in the incident channel but all electrons have outgoing spherical waves in all open channels, and similarly for ϕ_n, ψ_n, and $\Psi_n^{(-)}$ for the final state, where $\Psi_n^{(-)}$ now has the incoming boundary condition. Then the exact amplitude for the direct process in which electron 0 comes in and is scattered out inelastically by exciting the atom from the $(n_0p)^6$ to the $(n_0p)^5nl_n$ configuration is proportional to M^D, where

$$M^D = \langle\psi_n(\bar{0})\phi_n(0)|\sum_{j\neq0} v_{0j} + U(0)|\Psi_0^{(+)}(0)\rangle \qquad (2.3a)$$

$$= \langle\Psi_n^{(-)}(0)|\sum_{j\neq0} v_{0j} + U(0)|\psi_0(\bar{0})\phi_0(0)\rangle \qquad (2.3b)$$

in the post- and prior-interaction forms, respectively. In (2.3), $U(j)$ is the nuclear Coulomb interaction acting upon the jth electron, and v_{ij} is the Coulomb interaction between the ith and the jth electrons, and we have ignored magnetic interactions that might exist. The sum $\sum v_{0j}$ is over all the $(n_0p)^6$ electrons in the ground-state atom, which will be denoted by 1, 2, ..., 6.

The amplitude for the exchange process in which the incident electron 0 drops into the nl_n orbit while electron 1 is knocked out from the n_0p orbit is proportional to M^E, where

$$M^E = \langle\psi_n(\bar{1})\phi_n(1)|\sum_{j\neq1} v_{1j} + U(1)|\Psi_0^{(+)}(0)\rangle \qquad (2.4a)$$

$$= \langle\Psi_n^{(-)}(1)|\sum_{j\neq0} v_{0j} + U(0)|\psi_0(\bar{0})\phi_0(0)\rangle \qquad (2.4b)$$

in the post- and prior-interaction forms, respectively.

We define a distorting potential $V_0(j)$ and its eigenfunction $\chi_0^{(\pm)}(j)$ for an electron in the incident channel,

$$[(E-E_0)-K_j-V_0(j)]\,\chi_0^{(\pm)}(j)=0\ , \tag{2.5}$$

where K_j is the kinetic energy operator, E is the total energy, and E_0 is the eigenenergy of ψ_0. We define $V_n(j)$ and $\chi_n^{(\pm)}(j)$ similarly for the outgoing channel. Using the Gell-Mann–Goldberger relation for problems with two potentials,[8,9] we obtain from (2.3) and (2.4)

$$M^D=\langle\psi_n(\bar{0})\chi_n^{(-)}(0)|\sum_{j\neq0}v_{0j}+U(0)-V_n(0)|\Psi_0^{(+)}(0)\rangle \tag{2.6a}$$

$$=\langle\Psi_n^{(-)}(0)|\sum_{j\neq0}v_{0j}+U(0)-V_0(0)|\psi_0(\bar{0})\chi_0^{(+)}(0)\rangle \tag{2.6b}$$

and

$$M^E=\langle\psi_n(\bar{1})\chi_n^{(-)}(1)|\sum_{j\neq1}v_{1j}+U(1)-V_n(1)|\Psi_0^{(+)}(0)\rangle \tag{2.7a}$$

$$=\langle\Psi_n^{(-)}(1)|\sum_{j\neq0}v_{0j}+U(0)-V_0(0)|\psi_0(\bar{0})\chi_0^{(+)}(0)\rangle\ . \tag{2.7b}$$

The DW approximation corresponds to approximating the exact total wave functions $\Psi_0^{(+)}$ and $\Psi_n^{(-)}$ by their elastic channel components $\psi_0\chi_0^{(+)}$ and $\psi_n\chi_n^{(-)}$, respectively, observing that usually elastic scattering is the dominant process and hence other components in $\Psi_0^{(+)}$ and $\Psi_n^{(-)}$ can be ignored. In other words, the coupling between pairs of states is assumed to be small. Thus the method will fail if there are pairs of states that are coupled strongly, such as vibrational states in collisions with molecules.

Under this approximation, the direct amplitude becomes

$$M^{D,\mathrm{DW}}=6\langle\psi_n(\bar{0})\chi_n^{(-)}(0)|\,v_{01}\,|\psi_0(\bar{0})\chi_0^{(+)}(0)\rangle\ , \tag{2.8}$$

where the orthogonality of ψ_0 and ψ_n has been used to eliminate the contributions of $U(0)-V_n(0)$ and $U(0)-V_0(0)$ in (2.6), thereby eliminating the post-prior asymmetry. The factor 6 comes from the fact that, owing to the antisymmetry of ψ_0 and ψ_n, each n_0p^6 electron contributes the same. For the exchange amplitude, the post-prior asymmetry still remains and we have

$$M^{E,\mathrm{DW}}(\text{post})=\langle\psi_n(\bar{1})\chi_n^{(-)}(1)|\sum_{j\neq1}v_{1j}+U(1)-V_n(1)|\psi_0(\bar{0})\chi_0(0)\rangle\ , \tag{2.9a}$$

$$M^{E,\mathrm{DW}}(\text{prior})=\langle\psi_n(\bar{1})\chi_n^{(-)}(1)|\sum_{j\neq0}v_{0j}+U(0)-V_0(0)|\psi_0(\bar{0})\chi_0(0)\rangle\ . \tag{2.9b}$$

The choice of the distorting potentials V_0 and V_n is discussed next. For the direct amplitude, the form of the potential used is

$$V(r)=-\frac{2}{r}\,\frac{Z}{H(e^{r/d}-1)+1}\ , \tag{2.10}$$

with the same parameter values used for $V_B(r)$ of (2.1). This potential has been used by Berg, Purcell, and Green[3] in their study of elastic scattering from the rare gases, and found to reproduce experimental angular distributions quite well. The effect of a polarization potential was found to be restricted to extremely forward angles, and hence we neglect the polarization potential in this work. They also reported that the effect of an imaginary surface absorptive potential added to $V(r)$ was very small, and hence we also ignore the imaginary potential. The effects of the polarization potential and the imaginary potential should, however, be investigated further. Since we intend to produce average cross sections, any spin-orbit interactions present in the electron-atom interactions are omitted in $V_B(r)$ and $V(r)$.

Although, strictly speaking, the initial and the final states should have different distorting potentials, we simply use the same potential $V(r)$ of (2.10) assuming that the influence of a single electron excited in the final state upon the outgoing electron is small compared with the rest of the interactions.

Since $V(r)$ vanishes exponentially at large distance, the direct amplitude can be computed as

$$M^D=(M^D-M^B)+M^B\ , \tag{2.11}$$

where M^B is the Born amplitude. For the last term, i.e., M^B, we use the well-known expression due to Bethe,

$$M^B=\left\langle\psi_n(\bar{0})\left|\frac{4\pi e^2}{K^2}\sum_{j=1}^{6}e^{i\vec{K}\cdot\vec{r}_j}\right|\psi_0(\bar{0})\right\rangle\ , \tag{2.12}$$

where $\vec{K}$ is the momentum transfer,

$$\vec{K}=\vec{k}_0-\vec{k}_n\ . \tag{2.13}$$

For the first term of (2.11), i.e., M^D-M^B, the partial-wave expansion is used with detailed expressions given in Sec. III. The advantage of computing in this manner is that, since the effect of distortion vanishes rapidly from a certain partial wave l and higher owing to the exponential damping of $V(r)$, the difference M^D-M^B as a function of l vanishes rapidly beyond that value of l. This is unlike M^D itself, where we must include an extremely large number of partial waves in order to attain a sufficient numerical accuracy owing to the long-range nature of the Coulomb interaction.

For the exchange amplitude, if we use the same distorting potential $V(r)$ as used for the direct amplitude, then, for example, the term $U(0) - V_0(0)$ of (2.9b) gives a nonzero contribution, since then the bound states and the scattering states are not orthogonal to each other. In fact, the contribution happens to be quite large even at high energies where one expects exchange effects to be negligible. Also, there occur small but non-negligible contributions from the terms v_{0j} with $j \neq 1$ of (2.9b) which correspond to "knockout" processes if the scattered electron 1 comes out at forward angles, and "pick-up" processes if it is backward. In view of the mass difference between an electron and an atom, the contributions from these processes should be extremely small. In order to avoid these difficulties, we use the potential $V_B(r)$ given by (2.1) that is employed to obtain bound-state wave functions for the distorting potential of the exchange amplitude, thus making the bound states and scattering states orthogonal to each other. Then the post-prior asymmetry of $M^{E,\mathrm{DW}}$ also disappears, and we find from (2.9)

$$M^{E,\mathrm{DW}} = \langle \psi_n(\bar{1}) \chi_n^{(-)}(1) | v_{10} | \psi_0(\bar{0}) \chi_0^{(+)}(0) \rangle \; ; \qquad (2.14)$$

the same expression has been obtained by others[6,10] with HF potentials rather than phenomenological ones.

Thus, the distorted waves χ appearing in the direct amplitude (2.8) are different from the distorted waves χ in the exchange amplitude (2.14). One may be tempted to use $V_B(r)$ also for the direct amplitude. However, this is not desirable, since then the relation to the analyses of elastic scattering[3] and GOS[2] is lost, and even the Born amplitude has to contain the Coulomb distortion, which is unreasonable for the inelastic scattering of electrons against a neutral atom. The use of different distorting potentials for direct and exchange processes may seem odd at first sight, but the derivation of (2.6) and (2.7) from (2.3) and (2.4) is valid. The question is whether or not the choice made here provides a better basis for the DW approximation.

The total scattering amplitude for the transition $(n_0 p)^6 \rightarrow (n_0 p)^5 n l_n$ is, apart from the factor $- m_e / 2\pi\hbar^2$,

$$M^{\mathrm{DW}} = M^{D,\mathrm{DW}} - 6 M^{E,\mathrm{DW}} \; , \qquad (2.15)$$

and the differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{k_n}{k_0} \left(\frac{m_e}{2\pi\hbar^2} \right)^2 \frac{1}{2} \sum | M^{\mathrm{DW}} |^2 \; , \qquad (2.16)$$

where the sum is over initial and final magnetic substates. In presenting the results of angular distributions, we define the DGOS $f_d(x, E)$ by

$$f_d(x, E) = \frac{k_0}{4 k_n} \frac{x}{a_0^2} x_t \frac{d\sigma}{d\Omega} \; , \qquad (2.17)$$

where $x = K^2 a_0^2$, a_0 being the Bohr radius and x_t the excitation energy (in rydbergs). The main reason for introducing $f_d(x, E)$ is, of course, that this goes over to the GOS in the limit of the Born approximation, where f_d becomes a function of x only. Another reason is that $f_d(x, E)$ provides a better test of the theory, since, owing to the strong weighting factor x in $f_d(x, E)$, even a slight structure in $d\sigma/d\Omega$ becomes pronounced in $f_d(x, E)$.

In terms of $f_d(x, E)$, the integrated cross section $\sigma = \int (d\sigma/d\Omega)\, d\Omega$ becomes

$$\sigma = \frac{4\pi}{k_0^2 x_t} \int_{x_l}^{x_u} \frac{f_d(x, E)}{x} \, dx \; , \qquad (2.18)$$

where x_l and x_u are $(k_0 - k_n)^2 a_0^2$ and $(k_0 + k_n)^2 a_0^2$, respectively, corresponding to the 0° and 180° scatterings.

III. MATHEMATICAL AND COMPUTATIONAL DESCRIPTIONS

The initial-state atomic wave function $\psi_0(\bar{0})$ is given by

$$\psi_0(\bar{0}) = \sum_{m_s, m_l} (\tfrac{1}{2}, -m_s, \tfrac{1}{2}, m_s | 0, 0)(1, -m_l, 1, m_l | 0, 0) \times \Psi(n_0 p^5; \tfrac{1}{2}, -m_s, 1, -m_l) \psi(n_0 p; m_s m_l) \; , \qquad (3.1)$$

where the usual notation $(j_1, m_1, j_2, m_2 | j_{12}, m_{12})$ is used for the Clebsch-Gordan coefficients,[9] $\Psi(n_0 p^5)$ is the properly antisymmetrized wave function of $(n_0 p)^5$ electrons, and $\psi(nl)$ is the bound (nl) electron wave function. The final-state wave function $\psi_n(\bar{0})$ of the $(n_0 p)^5 (n l_n)$ configuration is given by

$$\psi_n(\bar{0}) = \sum_{M_S M_L} (S M_S L M_L | J M) \sum_{m_s' m_l' M_S' M_L'} (\tfrac{1}{2} M_s' \tfrac{1}{2} m_s' | S M_s) \times (1 M_L' l_n m_l' | L M_L) \frac{1}{\sqrt{6}} \left(1 - \sum_{j=2}^{6} P_{1j} \right) \times \Psi(n_0 p^5; \tfrac{1}{2} M_s' 1 M_L'; 23456) \psi(n l_n; m_s' m_l'; 1) \; , \qquad (3.2)$$

where P_{1j} is the permutation operator for electron 1 and electron j. A similar expression applies for $\psi_n(\bar{1})$ with 1 in (3.2) replaced by 0. The bound-state single-electron wave function ψ is obtained by solving the Schrödinger equation with the potential $V_B(r)$ of (2.1), using the Herman-Skillman code. The potential parameters used throughout this work are taken from the work of Ganas and Green,[2]

$$H = 2.22, \quad d = 0.715 a_0 \quad \text{for Ne} \, ,$$
$$H = 3.47, \quad d = 0.997 a_0 \quad \text{for Ar} \; . \qquad (3.3)$$

We introduce the multipole expansion of v_{01},

$$v_{01}=\frac{e^2}{|\vec{r}_0-\vec{r}_1|}=\sum_{b\beta}\frac{4\pi e^2}{2b+1}\,\frac{r_<^b}{r_>^{b+1}}\,Y_{b\beta}^*(\hat{r}_0)Y_{b\beta}(\hat{r}_1)\ , \tag{3.4}$$

where $Y_{b\beta}(\hat{r})$ are the spherical harmonics and $r_<$ and $r_>$ are the smaller and the larger of r_1 and r_2. The partial-wave expansions of the distorted waves are also introduced:

$$\chi_0^{(+)}(0)=(4\pi)^{1/2}\sum_l i^l(2l+1)^{1/2}Y_{l0}(\hat{r}_0)f_l(k_0,r_0)\sigma^{m_i}(0)\ , \tag{3.5a}$$

$$\chi_n^{(-)}(0)=(4\pi)^{1/2}\sum_{l'm_l'} i^{l'}Y_{l'm_l'}^*(\hat{k}_n)Y_{l'm_l'}(\hat{r}_0)f_{l'}^*(k_n,r_0)\sigma^{m_f}(0), \tag{3.5b}$$

and similarly for $\chi_n^{(-)}(1)$, where σ is the spin eigenfunction and where the z axis has been chosen along $\vec{k}_0$. The radial parts of the distorted waves f_l are obtained by solving the radial Schrödinger equation with the potential $V(r)$ of (2.10) for the direct amplitude and with the potential $V_B(r)$ of (2.1) for the exchange amplitude, using the potential parameters given by (3.3). The asymptotic forms of these functions are

$$f_l(k,r)\underset{r\to\infty}{\longrightarrow} e^{i\delta_l}\cos\delta_l(\mathcal{F}_l(kr)-\tan\delta_l\,\mathcal{G}_l(kr))\ , \tag{3.6}$$

where δ_l is the phase shift due to the potentials V or V_B, and where $\mathcal{F}_l$ and $\mathcal{G}_l$ are the spherical Bessel functions of the first and the second kind[11] for the direct process, and $F_l(kr)/kr$ and $-G_l(kr)/kr$ for the exchange process, where F_l and G_l are the regular and irregular Coulomb functions.[11]

Substituting (3.1), (3.2), (3.4), and (3.5) into (2.8), we find

$$M^{D,\mathrm{DW}}=4\pi\sum_{ll'}i^{l-l'}Y_{l',-M}(\hat{k}_n)(l',-M,L,M|\,l,0)\times P_{Ll_n}^{ll'}\,\delta_{S,0}\delta_{m_i,m_f}\ , \tag{3.7}$$

$$P_{Ll_n}^{ll'}=\delta_{L,J}(2l'+1)^{1/2}(l'0L0|\,l0)g_{Ll_n}^{ll'}\ , \tag{3.8}$$

with

$$g_{Ll_n}^{ll'}=\frac{4\pi e^2}{2L+1}\left(\frac{6(2L+1)}{4\pi}\right)^{1/2}(10l0|\,l_n0)\times\langle f_{l'}^*(k_n,r_0)R_{nl_n}(r_1)|\,r_<^L/r_>^{L+1}|\,R_{n_0p}(r_1)\times f_l(k_0,r_0)\rangle\ , \tag{3.9}$$

where $R_{nl_n}(r_1)$ and $R_{n_0p}(r_1)$ are the radial parts of $\psi(nl_n)$ and $\psi(n_0p)$. Similarly, we find from (2.14)

$$M^{E,\mathrm{DW}}=4\pi\sum_{ll'M'}i^{l-l'}Y_{l',-M+M'}(\hat{k}_n)\times(l',-M+M',L,M-M'|\,l,0)\times(\tfrac{1}{2},-m_f,\tfrac{1}{2},m_f|\,0,0)(\tfrac{1}{2},-m_f,\tfrac{1}{2},m_i|\,S,M')\times(S,M',L,M-M'|\,J,M)\sum_\alpha Q_{Ll_n\alpha}^{ll'}\ , \tag{3.10}$$

where

$$Q_{Ll_n\alpha}^{ll'}=(-)^{\alpha+l_n+l}\,\tfrac{1}{6}[(2\alpha+1)(2l_n+1)(2L+1)]^{1/2}\times(l_n0\alpha0|\,l0)\begin{Bmatrix} l & l' & L\\ 1 & l_n & \alpha\end{Bmatrix}h_{\alpha l_n}^{ll'}\ , \tag{3.11}$$

where the quantity in the curly bracket is the $6j$ symbol,[9] and

$$h_{\alpha l_n}^{ll'}=\frac{4\pi e^2}{2\alpha+1}\left(\frac{6(2\alpha+1)}{4\pi}\right)^{1/2}(10\alpha0|\,l'0)\times\langle f_{l'}^*(k_n,r_1)R_{nl_n}(r_0)|\,r_<^\alpha/r_>^{\alpha+1}|\,R_{n_0p}(r_1)f_l(k_0,r_0)\rangle\ . \tag{3.12}$$

In the following subsections, we treat the excitation of singlet states and triplet states separately.

A. Excitation of Singlet States

Substituting $M^{D,\mathrm{DW}}$ of (3.7) and $M^{E,\mathrm{DW}}$ of (3.10) with $S=0$ into (2.15), we find

$$M^{\mathrm{DW}}=4\pi\sum_{ll'}i^{l-l'}Y_{l',-M}(\hat{k}_n)(l',-M,L,M|\,l,0)\times\delta_{m_i,m_f}W_{Ll_n}^{ll'}\ , \tag{3.13}$$

where

$$W_{Ll_n}^{ll'}=P_{Ll_n}^{ll'}-3\sum_\alpha Q_{Ll_n\alpha}^{ll'}\ . \tag{3.14}$$

As explained in Sec. II, we compute M^{DW} according to (2.11). For the term $M^{\mathrm{DW}}-M^B$, the partial-wave expansion of M^B is given the same way as for $M^{D,\mathrm{DW}}$ of (3.7) except that $f_l(k,r)$ is now replaced by the spherical Bessel function $j_l(kr)$. Denoting the radial matrix element g of (3.9) thus redefined for the Born approximation by $g_{Ll_n}^{B,ll'}$, we write, similar to (3.8),

$$\overline{P}_{Ll_n}^{ll'}=\delta_{L,J}(2l'+1)^{1/2}(l0L0|\,l0)\times\{g_{Ll_n}^{ll'}-g_{Ll_n}^{B,ll'}\} \tag{3.15}$$

and, similar to (3.14),

$$\overline{W}_{Ll_n}^{ll'}=\overline{P}_{Ll_n}^{ll'}-3\sum_\alpha Q_{Ll_n\alpha}^{ll'}\ . \tag{3.16}$$

Thus the difference term $M^{\mathrm{DW}}-M^B$ becomes

$$M^{\mathrm{DW}}-M^B=4\pi\sum_{ll'}i^{l-l'}Y_{l',-M}(\hat{k}_f)(l',-M,L,M|\,l,0)\times\delta_{m_i,m_f}\overline{W}_{Ll_n}^{ll'}\ . \tag{3.17}$$

On the other hand, from (2.12) we obtain

$$M^B = \delta_{m_i,m_f}\delta_{L,J}\frac{4\pi}{(2L+1)^{1/2}}\, i^L Y^*_{LM}(\hat{K})h^B_L(K) , \quad (3.18)$$

where

$$h^B_L(K) = \frac{4\pi e^2}{K^2}\left(\frac{6(2L+1)}{4\pi}\right)^{1/2}(10L0|\, l_n 0)$$
$$\times \langle R_{nl_n}(r)|\, j_L(Kr)|\, R_{n_0 p}(r)\rangle . \quad (3.19)$$

The cross section for the excitation of singlet states is composed of three terms,

$$\frac{d\sigma}{d\Omega}(S=0) = \left(\frac{d\sigma}{d\Omega}\right)^B + \left(\frac{d\sigma}{d\Omega}\right)^D + \left(\frac{d\sigma}{d\Omega}\right)^I . \quad (3.20)$$

The first term is the usual Born cross section, the second term is of purely distortion origin and is due to $|M^{\mathrm{DW}} - M^B|^2$, and the last term is the interference between M^B and $M^{\mathrm{DW}} - M^B$. Choosing the Z axis along $\vec{\mathrm{K}}$ for the first term, and along $\vec{\mathrm{k}}_0$ for the second and third terms, we find

$$\left(\frac{d\sigma}{d\Omega}\right)^B = \gamma |\, h^B_L(K)|^2 , \quad (3.21)$$

$$\left(\frac{d\sigma}{d\Omega}\right)^D = \gamma \sum_\lambda \sum_{ll'\bar{l}\bar{l}'} C_{\lambda L}(ll';\bar{l}\bar{l}')\overline{W}^{\bar{l}\bar{l}'*}_{Ll_n}\overline{W}^{ll'}_{Ll_n}P_\lambda(\cos\theta) , \quad (3.22)$$

and

$$\left(\frac{d\sigma}{d\Omega}\right)^I = \gamma\frac{2}{(2L+1)^{1/2}}\sum_{ll'} i^{l-l'-L}\,\mathcal{Y}^{ll'}_L(\theta)(R_e\overline{W}^{ll'}_{Ll_n})h^B_L(K) , \quad (3.23)$$

where

$$C_{\lambda L}(ll'\bar{l}\bar{l}')$$
$$= i^{l-l'-\bar{l}+\bar{l}'}(-)^L[(2l+1)(2l'+1)(2\bar{l}+1)(2\bar{l}'+1)]^{1/2}$$
$$\times(l0\bar{l}0|\,\lambda 0)(l'0\bar{l}'0|\lambda 0)\begin{Bmatrix} l & L & l' \\ \bar{l}' & \lambda & \bar{l} \end{Bmatrix} . \quad (3.24)$$

$$\mathcal{Y}^{ll'}_L(\theta) = \sum_M (l', -M, L, M|\, l, 0)Y_{l',-M}(\hat{k}_f)Y_{LM}(\hat{K}) , \quad (3.25)$$

$$\gamma = 4\pi(k_n/k_0)(m_e/2\pi\hbar^2)^2 , \quad (3.26)$$

and $P_\lambda(\cos\theta)$ is the Legendre polynomial, θ being the scattering angle. The coefficient $C_{\lambda L}$ has the following symmetry property:

$$C_{\lambda L}(ll';\bar{l}\bar{l}') = C_{\lambda L}(l'l;\bar{l}'\bar{l}) = C_{\lambda L}(\bar{l}\bar{l}';ll')$$
$$= C_{\lambda L}(\bar{l}'\bar{l};l'l) . \quad (3.27)$$

This relation is used to greatly economize the multiple summation in (3.22), and also to check the computation of the $C_{\lambda L}$ coefficients. The function $\mathcal{Y}(\theta)$ is a real function of θ only, since $\vec{\mathrm{K}}$ lies on the scattering plane.

The form factor $\langle R_{nl_n}(r_1)|r^L_</r^{L+1}_>|R_{n_0 p}(r_1)\rangle$ appearing in the radial matrix element of g given by (3.9) has an extremely long-range contribution, far beyond the point where the radial functions f_l attain their asymptotic forms (3.6). In order to economize the numerical work while maintaining sufficient accuracy, the contribution to the matrix element from the asymptotic region is calculated accurately using (3.6). Thus, we convert the integral to an almost analytic expression of a quickly converging series of integrals, each integral ranging over a period of sine or cosine functions from peak to peak. This method is especially suited for use with (3.15), since then the outer contributions to g and g^B cancel each other for large partial waves.

B. Excitation of Triplet States

No direct process contributes to the excitation of triplet states within our formalism, and hence from (2.15) the amplitude is proportional to $M^{\mathrm{DW}} = -6M^{E,\mathrm{DW}}$ with $S=1$. As is evident from (3.12), the partial-wave expansion of $M^{E,\mathrm{DW}}$ involves the overlap integral $h^{ll'}_{\alpha l_n}$ which vanishes quickly as a function of l and l' beyond certain values of l and l'. Thus the amplitude $M^{E,\mathrm{DW}}$ converges quickly as a function of l and l', unlike $M^{D,\mathrm{DW}}$. After summing over magnetic substates, we find

$$\frac{d\sigma}{d\Omega} = 9\gamma\frac{2J+1}{2L+1}\sum_\lambda\sum_{ll'\bar{l}\bar{l}'} C_{\lambda L}(ll';\bar{l}\bar{l}')\sum_\alpha Q^{ll'}_{Ll_n\alpha}$$
$$\times\sum_{\bar{\alpha}} Q^{\bar{l}\bar{l}'*}_{Ll_n\bar{\alpha}}P_\lambda(\cos\theta) , \quad (3.28)$$

with the same definitions of $C_{\lambda L}$, Q, and γ given previously. Without spin-orbit interactions, all three states $J=L+1$, L, and $L-1$ are degenerate, and hence summing over three corresponding cross sections, we find

$$\frac{d\sigma}{d\Omega} = 27\gamma\sum_\lambda\sum_{ll'\bar{l}\bar{l}'} C_{\lambda L}(ll';\bar{l}\bar{l}')$$
$$\times\sum_\alpha Q^{ll'}_{Ll_n\alpha}\sum_{\bar{\alpha}} Q^{\bar{l}\bar{l}'*}_{Ll_n\bar{\alpha}}P_\lambda(\cos\theta) . \quad (3.29)$$

Here again the symmetry property of the coefficient $C_{\lambda L}$, Eq. (3.27), serves to greatly simplify the multiple summation.

IV. RESULTS AND DISCUSSIONS

The theoretical predictions of DGOS as a function of $\xi = x/x_t$ are shown in Figs. 1 and 2 for Ne $(2p)^6 \to (2p)^5 3s$ and Ar $(3p)^6 \to (3p)^5 4s$ excitations at various incident energies. The solid curves rep-

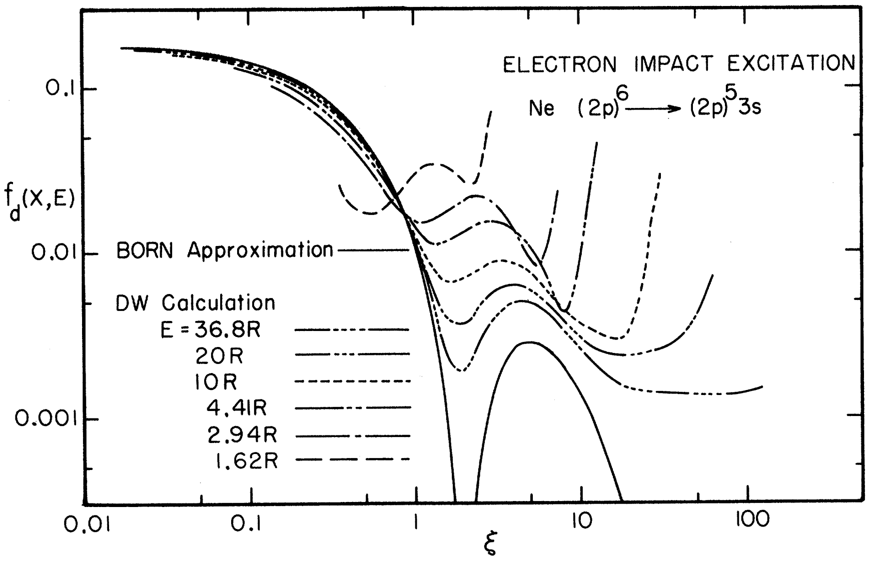

FIG. 1. DGOS for the electron impact excitation of Ne from $(2p)^6$ to $(2p)^5 3s$ configurations as a function of $\xi = x/x_t = K^2 a_0^2/x_t$ at various incident energies.

resent the results of the Born approximation, that is, the GOS which, when extrapolated to zero momentum transfer, yields the optical oscillator strengths ~0.184 for Ne and ~0.327 for Ar. In reality, these strengths are split among components of the fine structure. Therefore, they should be compared with the sums of experimentally determined ^1P and ^3P strengths. The fact that our extrapolated values come fairly close to the experimental optical oscillator strengths[12] indicates that the use of the *LS*-coupling scheme for the atomic wave functions with averaging is reasonable, at least for the reactions presented.

As can be seen from Figs. 1 and 2, the effect of distortion remains small, and hence the Born approximation remains good, for small momentum transfer even at energies as low as 10 Ry. The effect of distortion sets in for larger momentum transfer, and in fact even at 36.8 Ry the Born limit is not quite reached beyond the first diffraction minimum. The results at low energies, where the exchange effects are appreciable, are presented as the sum of singlet and triplet excitations. Not many data are available to compare with our results, but the low-energy data by Nicoll and Mohr[4] suit our purpose quite well since the energy resolution in their work is large enough to allow us to compare their data with our averaged cross sections directly. In Figs. 3 and 4, we show the comparison with their data. For Ar, the cross-section data are taken from the table given by Nicoll and Mohr, but for Ne the data have to be read from

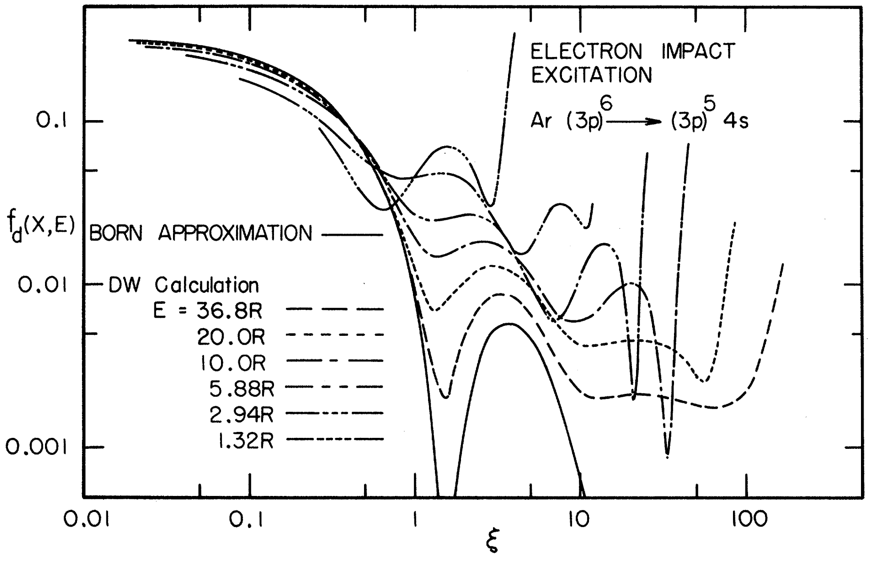

FIG. 2. DGOS for the electron impact excitation of Ar from $(3p)^6$ to $(3p)^5 4s$ configurations as a function of ϵ at various incident energies.

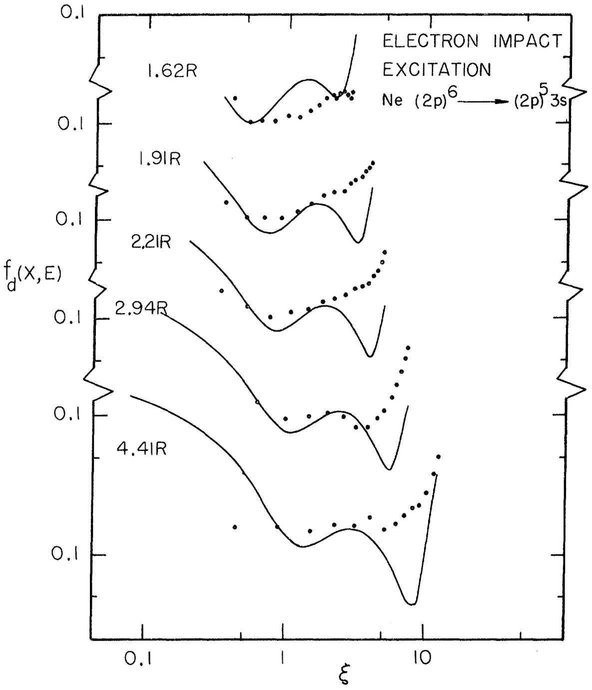

FIG. 3. Electron impact excitation of Ne $2p \rightarrow 3s$ at low energies. The dots are the experimental DGOS transformed from the cross-section data read off from the figure given by Nicoll and Mohr (Ref. 4). The solid curves are the sums of predictions for the singlet and triplet final states.

their figure.[4] Then these data are transformed to the DGOS using (2.17), by normalizing them arbitrarily to the theoretical values at $\theta = 30°$ for Ne and at $\theta = 10°$ for Ar, to bring about the seemingly best agreement between theory and experiment. Any fluctuation of the data seen in Fig. 3 for Ne may be due to our error in reading from the figure as mentioned above.

At energies larger than 2.21 Ry the theoretical values of the DGOS, $f_d(x, E)$, for Ar have two peaks, whereas Ne has only one peak, and all go up sharply at the extreme backward angles. These expectations appear to be borne out by the experimental data. As mentioned near the end of Sec. II, $f_d(x, E)$ provides a better test of the theory than the differential cross section. This can be seen, for example, in Fig. 4 for Ar beyond 2.21 Ry. The data exhibit a slight structure in the region around $\xi \sim 1$ which, as can be seen from Fig. 2, corresponds to the first peak in the Born approximation. This structure is not pronounced in the experimental differential cross section.

At all energies shown in Fig. 3 for Ne, and at lower energies in Fig. 4 for Ar, the theory predicts a dip at backward angles which is not seen in the data. Furthermore, although the characteristic change in the shape of $f_d(x, E)$ for Ar in going from 2.21 to 1.47 Ry is reproduced, the theory fails to give the characteristic change in going from 1.32

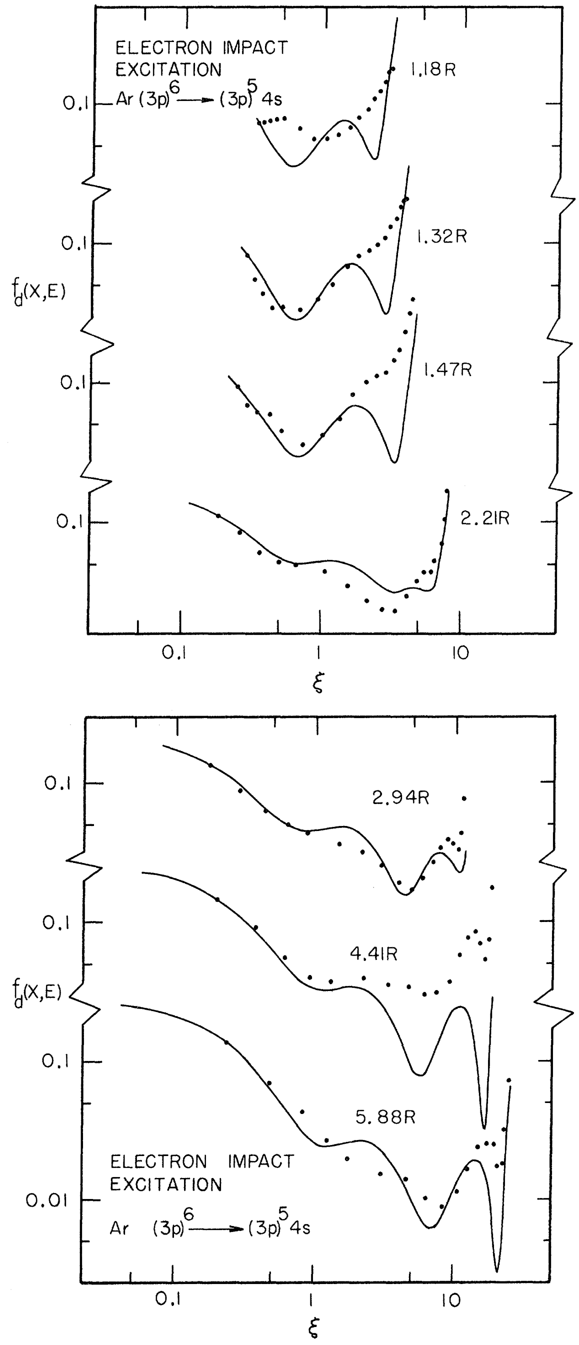

FIG. 4. Low-energy electron impact excitation of Ar $3p \rightarrow 4s$. The dots are the experimental DGOS transformed from the cross-section data given by Nicoll and Mohr (Ref. 4) and the solid curves are the sums of predictions for the singlet and triplet final states.

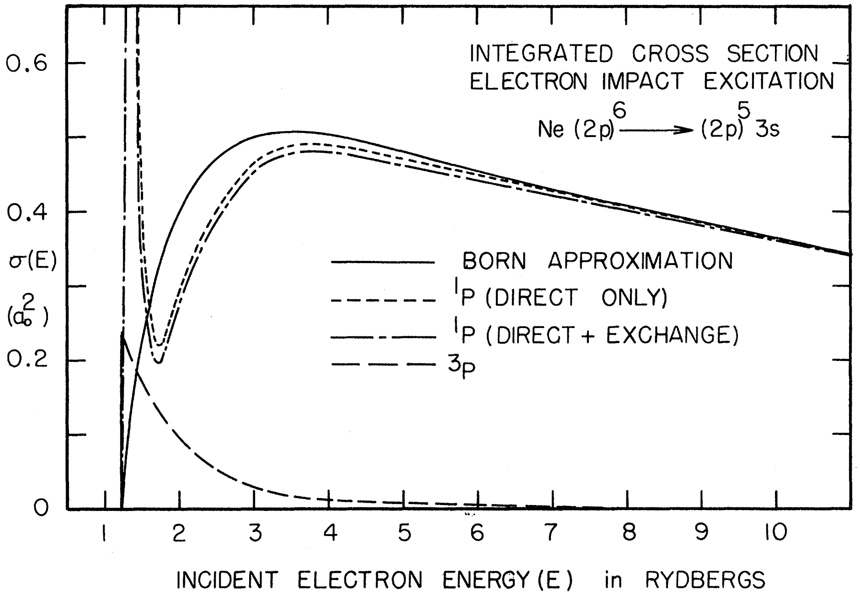

FIG. 5. Integrated cross section σ (in a_0^2) for Ne $2p \rightarrow 3s$ electron impact excitation. The solid curve is for the Born approximation, the short-dashed curve is for the singlet cross section with direct process only, the dot-dashed curve is for the singlet cross section including exchange, and the long-dashed curve is for the triplet cross section.

to 1.18 Ry as seen in the data. These difficulties of the theory may be corrected in part by carrying out potential parameter searches for better fits to the data. However, the reasonable fits to the data shown in Figs. 3 and 4 obtained by the same potential parameters that reproduce elastic scattering and bound-state data[2,3] encourage us to believe that the results shown in Figs. 1 and 2 are not far from reality, except perhaps at very low energies.

The integrated cross sections are presented in Figs. 5 and 6. Although the effect of distortion on the DGOS is important as we have just seen, its effect on the integrated cross section σ is much less important, so that the Born approximation seemingly holds quite well down to fairly low energies. As pointed out previously, for $f_d(x, E)$ at forward angles where the main contribution to σ arises, the Born approximation is good down to relatively low energies. For even lower energies where the Born approximation fails at forward angles, there occurs a certain amount of compensation between the contributions from forward angles and those from backward angles, as can be seen from Figs. 1 and 2. It should be noticed that the effect of distortion on $f_d(x, E)$ at large x is reduced in computing σ by the factor $1/x$ that appears in (2.18).

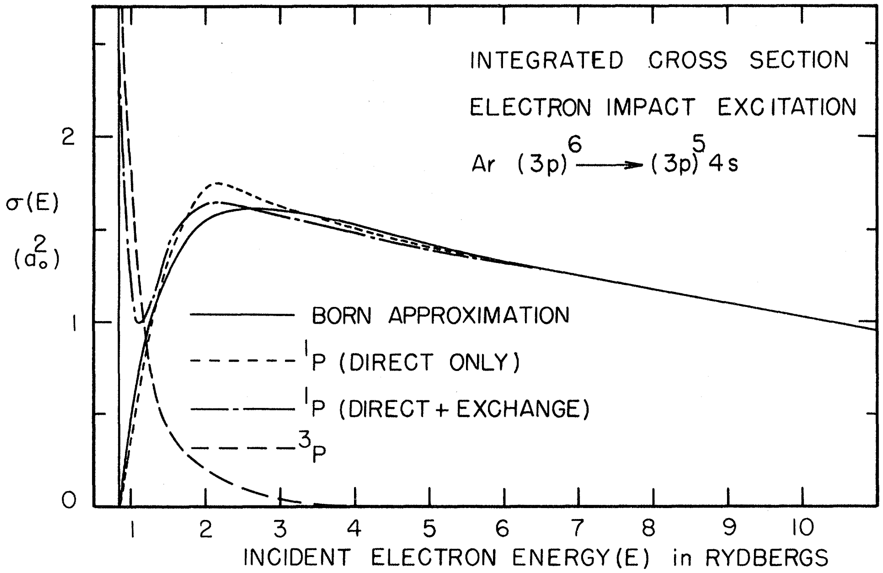

FIG. 6. Integrated cross section σ (in a_0^2) for Ar $3p \rightarrow 4s$ (see caption to Fig. 5).

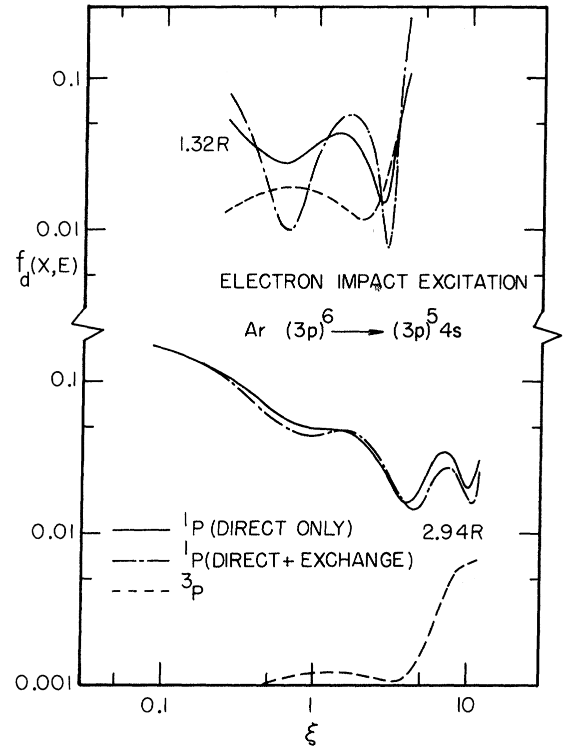

FIG. 7. Direct and exchange contributions to DGOS for Ar $3p \rightarrow 4s$ at the incident energies 1.32 and 2.94 Ry. The solid curve is for the singlet cross section with direct process only, the dot-dashed curve is for the singlet cross section with exchange, and the dashed curve is for the triplet cross section.

There appears a resonance peak in σ near threshold for Ne as shown in Fig. 5, occasioned by the presence of a sharp rise of the p-wave phase shift through 90° in the inelastic channel just above the threshold in the direct amplitude. A similar but nonresonant peak appears in σ for Ar at threshold as shown in Fig. 6. There is no sharp resonance in phase shifts for Ar, although the d-wave phase shifts rise through 90° at around 2.8 Ry in the incident channel and at the corresponding energy in the outgoing channel, which may be responsible for bringing σ closer to the Born approximation. The peak at threshold is due, however, to the finite contribution of the exchange amplitude at threshold caused by the use of the distorting potential with an attractive Coulomb tail.[13] A similar but smaller effect is present in Ne also but it is overwhelmed by the resonance effect. The energy dependence of the exchange contributions can be seen from the plot of the triplet cross sections shown in Figs. 5 and 6. These peaks may or may not be realistic. If there is such a peak in the data, the theory is capable of reproducing it. If no peak exists in the data, the choice of the distorting potential may have to be altered if one desires a good representation down to very low energies. Recent measurement by Sharpton *et al.*[14] of the optical excitation functions of Ne show no resonance in $3s_2(J=1)$ and $3s_4(J=1)$ levels. However, their $3s_3(J=0)$ and $3s_5(J=2)$ excitation functions show narrow peaking at threshold similar to the triplet cross section shown in Fig. 5.

For the sake of completeness, we present in Fig. 7 the separate contributions to $f_d(x, E)$ from the direct and exchange processes at two representative energies for Ar. The figures show entirely different dependences of $f_d(x, E)$ on the momentum transfer leading to the excitation of ^1P and ^3P states.

To summarize, the DW method presented here gives a reasonably reliable estimate of averaged DGOS and integrated cross sections over a wide range of energies except perhaps at very low energies. It is hoped that the results are useful in the application to atmospheric physics. Electrons arising as secondary particles (e.g., photoelectrons, secondary electrons from electron or proton primaries) with energies below 5 Ry play a major role in such studies.[15,16] Thus it is imperative to allow for departures from the Born-Bethe approximation in dealing microscopically with energy deposition. Semiempirical efforts to incorporate distortion and exchange effects have already been made in this connection.[17] The present study, while still involving phenomenological consideration, is a more fundamental approach towards incorporating such effects. As can be seen from the figures, the effects which we consider play a major role even for energies as high as $E \sim 5$ Ry. Unfortunately the lack of experimental data in the domain where distortion and exchange effects play an important role is a serious problem and it is hoped that this study might stimulate such measurements. Meanwhile, our theoretical calculations should serve as a firmer basis for incorporating DW modification into realistic calculations of electron-energy deposition.

ACKNOWLEDGMENTS

The authors would like to thank R. A. Berg and Dr. P. S. Ganas for their assistance with these calculations.

---

*Work supported by the Air Force Office of Scientific Research.

†Present address: Georgia State University, Atlanta, Ga.

[1] A. E. S. Green, D. L. Sellin, and A. S. Zachor, Phys. Rev. 184, 1 (1969).

[2] P. S. Ganas and A. E. S. Green, preceding paper, Phys. Rev. A 4, 192 (1971).

[3] R. Berg, J. Purcell, and A. E. S. Green, Phys. Rev. A 3, 508 (1971).

[4] F. H. Nicoll and C. B. O. Mohr, Proc. Roy. Soc. (London) A142, 320 (1933); A142, 647 (1933).

[5] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) A146, 880 (1934).

[6] W. N. Shelton and E. S. Leherissey (unpublished).

[7] A. E. S. Green, T. Sawada, and D. S. Saxon, *The Nuclear Independent Particle Model* (Academic, New York, 1968).

[8] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964); T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Englewood Cliffs, N. J., 1962).

[9] A. Messiah, *Quantum Mechanics* (Wiley, New York, 1965).

[10] D. C. Cartwright, Ph. D. thesis, California Institute of Technology, Report No. CALT-532-12, 1967 (unpublished).

[11] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965).

[12] G. M. Lawrence, Phys. Rev. 175, 40 (1968); E. L. Lewis, Proc. Phys. Soc. (London) 92, 817 (1967); D. N. Stacey and J. M. Vaughan, Phys. Letters 11, 105 (1964).

[13] N. F. Mott and H. S. Massey, *Theory of Atomic Collisions* (Clarendon, Oxford, England, 1965); H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Clarendon, Oxford, England, 1969); G. F. Drukarev, *The Theory of Electron-Atom Collisions* (Academic, New York, 1965).

[14] F. A. Sharpton, R. M. St. John, C. C. Lin, and F. E. Fajen, Phys. Rev. A 2, 1305 (1970).

[15] R. S. Stolarski and A. E. S. Green, J. Geophys. Res. 72, 3967 (1967).

[16] A. E. S. Green and C. A. Barth, J. Geophys. Res. 70, 1083 (1965).

[17] A. E. S. Green and S. K. Dutta, J. Geophys. Res. 72, 3933 (1967).

PHYSICAL REVIEW A VOLUME 4, NUMBER 1 JULY 1971

Cross Sections for Collisions of the Second Kind in a Helium-Neon Discharge

R. Arrathoon
Bell Telephone Laboratories, Murray Hill, New Jersey 07974

(Received 30 November 1970)

The collisional transfer of energy between two excited states in a gas discharge may be described by a two-body inelastic cross section. The energy dependence of the two-body cross section for collisions of the second kind between the He 2^1S metastable and Ne $3s_2$ states has been investigated. This process is primarily responsible for populating the upper level of the 6328-Å laser transition. Pulsed afterglow measurements were performed as a function of gas temperature and pressure. The experiments were conducted at low gas temperatures so that the effect of energy transfer from the helium metastable level to other nearby neon levels could be minimized. The measured decay rates departed substantially from that predicted by using an energy-independent cross section. A unit-step cross section for the He 2^1S – Ne $3s_2$ resonant transfer process with a value of $(1.0 \pm 0.15) \times 10^{-15}$ cm^2 and with a threshold energy corresponding to the energy difference between the two levels was determined.

I. INTRODUCTION

The discrete character of energy levels in a gas discharge requires that an inelastic collision between an excited atom and a normal atom, resulting in a transition to a higher excited state, be accompanied by the exchange of a certain minimum threshold energy. For collisions of the second kind, involving energy transfer from excited states of one species to those of another species by collisions with ground-state atoms, this minimum threshold energy corresponds to the energy difference between the two excited levels. The energy for the process is supplied by a change in the kinetic energy of the atoms. When collisions are the primary mechanism for kinetic-energy exchange among the atoms, their motion may be described by a Maxwellian energy distribution at a specific gas temperature.

The usual way of characterizing two-body gas collisions is to define a velocity-averaged cross section at a particular temperature, which is energy independent. This cross section is normally used to describe energy transfer between energy levels which are within a few kT of each other. Since the actual cross section must have a minimum threshold energy, any attempt to use such a cross section over a wide range of gas temperatures can result in serious errors. The interaction is often further complicated at higher temperatures by the presence of inelastic transfer to other nearby ener-