

THE PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 142, No. 1

4 FEBRUARY 1966

Low-Energy Electron Scattering From Atoms and Molecules: A Model

CARL J. LENANDER

Aerospace Corporation, El Segundo, California

(Received 1 October 1964; revised manuscript received 4 October 1965)

A simple model is proposed for the calculation of free-electron wave functions for low-energy electrons incident upon neutral atoms. The region of interaction of the electron with the atom may be separated into three important regions of potential: Coulomb plus exchange, Coulomb, and far-field induced polarization. The division of regions is based on mathematical and physical reasons for the characteristic behavior of wave functions in the scattering problem. Examples are given for the elastic scattering of electrons from nitrogen, oxygen, and argon. The agreement with experiment and effective-range theory is good. The application of the method to the prediction of low-energy electron scattering from homonuclear diatomic molecules is discussed.

I. ATOMS

FOR low-energy electron scattering from atoms or molecules, the important interactions are well known to be Coulomb, exchange, and induced polarization. The relative emphasis of these interactions as applied to the scattering problem appears to be the basic difference between the approximate methods of calculation that have been reported.¹⁻¹¹ However, there are certain fundamental properties of solutions to the self-consistent field and the scattering problem that must be considered in the formulation of any model. The treatment of exchange is one of the most important considerations because of its consequence of producing orthogonality between solutions of like angular symmetry.¹² The orthogonality property and its relationship to the free-electron phase shift has been discussed in

the electron-hydrogen problem by Temkin.¹³ Related to this, Helliwell¹⁴ has also observed the near radial coincidence of zeros of solutions of the same angular symmetry in a given atomic system. This appears to be true of inflection points and zeros generally.¹⁵ As an example, the second zero outward from the origin of a low-energy free-electron *s* function will nearly coincide with the nonzero inflection point of the *2s* function. However, this characteristic is not produced if only Coulomb interactions (Hartree) are considered, but is produced when exchange is added (Hartree-Fock) to the interactions, as seen in the work of Breene and Nardone.^{7,8} Also demonstrated in that paper is the stability of the second zero from the origin of the low-energy *s* wave,¹⁶ which shows the principal variation in the wave functions to occur on the exterior portion of the atom where the polarization interaction is important. This is a simplifying property of low-energy scattering solutions which would allow calculation of free-wave functions for complex scattering centers such as molecules, when the ground-state wave functions are known, by placing the appropriate zero and calculating the solution in the far field only, thus avoiding the multiple interactions inside the core. This may be seen by integrating the nonlinear differential equation

¹ D. R. Bates and H. S. W. Massey, *Phil. Trans. Roy. Soc. London* **A239**, 269 (1943).

² M. J. Seaton, *Phil. Trans. Roy. Soc. London* **A901**, 469 (1953).

³ L. B. Robinson, *Phys. Rev.* **105**, 922 (1957).

⁴ A. Temkin, *Phys. Rev.* **107**, 1004 (1957).

⁵ P. Hammerling, W. W. Shine, and B. Kivel, *J. Appl. Phys.* **25**, 760 (1957).

⁶ M. M. Klein and K. A. Brueckner, *Phys. Rev.* **111**, 1115 (1958).

⁷ R. G. Breene, Jr., and M. C. Nardone, *Phys. Rev.* **115**, 93 (1959).

⁸ R. G. Breene, Jr., and M. C. Nardone, *Phys. Rev.* **123**, 1718 (1961).

⁹ W. R. Garrett and R. A. Mann, *Phys. Rev.* **130**, 658 (1963).

¹⁰ P. M. Stone and J. R. Reitz, *Phys. Rev.* **131**, 2101 (1963).

¹¹ W. R. Garrett and R. A. Mann, *Phys. Rev.* **135**, A580 (1964).

¹² J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill Book Company, Inc., New York, 1960), Vol. II, Chap. 17.

¹³ A. Temkin, *J. Math. Phys.* **2**, 336 (1961).

¹⁴ T. M. Helliwell, *Phys. Rev.* **135**, A325 (1964).

¹⁵ The reader may satisfy himself on this by examination of any multielectron-atom Hartree-Fock solution.

¹⁶ Reference 8, Fig. 2.

for the phase shift¹⁷

$$\frac{d\eta}{dr} = -kV(r) \left[\frac{\sin(kr + \eta(r))}{k} \right]^2 \quad (1)$$

for the s wave, where η is the phase shift, k is the square root of the energy in rydbergs and $V(r)$ is the scattering potential. The phase shift at a zero R of the wave function would be $-kR$. The integration for the phase shift would then range from R to ∞ . And the important contributions to the phase shift would then come from the potential on the outside of that zero.

However, if a good approximate potential could be used that would accurately produce Hartree-Fock (HF) solutions out to the point of the appropriate node, then that potential could be used as the scattering potential for the inner core region.

It is much more important in any approximation scheme that good solutions be obtained rather than making approximations that produce good ionization potentials for the bound states, because it is the functional character of the solutions which is useful in partial wave analysis and effective range theory. Thus, a method is needed which will produce good approximations to the Hartree-Fock solutions in the region of interest. Such a method is the parameterized-Slater-modified Hartree-Fock method (PSHF)¹⁸ which is especially attractive because it eliminates the coupled terms in the Hartree-Fock equations and thus automatically ensures orthogonality for solutions of like

TABLE I. Comparison of Hartree-Fock (HF) and parameterized-Slater-modified Hartree-Fock (PSHF) $2s$ wave functions. The inflection-point zeros occur at $r=0.274$ a.u. (HF) and $r=0.276$ a.u. (PSHF).

r (atomic units)	HF $2P^a$	PSHF
0.01	0.090	0.094
0.04	0.282	0.293
0.10	0.410	0.426
0.14	0.379	0.392
0.20	0.241	0.248
0.25	+0.086	+0.087
0.30	-0.079	-0.083
0.40	-0.388	-0.398
0.50	-0.632	-0.643
0.60	-0.800	-0.812
0.70	-0.902	-0.911
0.80	-0.951	-0.956
0.90	-0.960	-0.961
1.00	-0.941	-0.937
1.20	-0.851	-0.845
1.60	-0.610	-0.605
2.00	-0.401	-0.397
2.40	-0.252	-0.249
3.00	-0.120	-0.121
4.00	-0.0325	-0.0343
5.00	-0.0085	-0.0093
6.00	-0.0025	-0.0025

^a Reference 19.

¹⁷ B. R. Levy and J. B. Keller, J. Math. Phys. 4, 54 (1963).

¹⁸ C. J. Lenander, Phys. Rev. 130, 1033 (1963).

angular symmetry. The accuracy of this method may be judged from the comparison with the oxygen $2s$ HF solution in Table I.¹⁹ The region where the PSHF method breaks down is values of r considerably outside the important nodal point, which does not affect the bound solutions because they are exponentially decaying in that region, but would affect the low-energy free solutions because they are increasing to large values in that region. The region where the PSHF method begins to break down is about where the Hartree (H) potential form is becoming dominant so the scattering potential must make a transition from the former to the latter in the region outside the node. Next, it will be shown that the induced polarization potential rises in importance as the H potential diminishes and is negligible on the interior of the atom so that an appropriate approximate polarization potential may be added for the entire radial region.

The treatment of polarization by some authors has been parametric and has been adjusted in such a way as to serve as both exchange and polarization. Because the sign of the interaction is the same, an overemphasis of polarization in the absence of exchange will tend to compensate for the absence. In these cases of parametric treatment of polarization,^{6,9,11} the region of interaction is extended to the interior of the core charge distribution when polarization, as will be shown, is principally a surface effect and a perturbation on the atomic field, not the same size or larger than the atomic field in the region of the maxima of the outer electrons. Because of this, that method does not give the proper behavior of the cross section below 0.5 eV.

One writes the induced polarization potential from first-order perturbation theory as

$$V_I(r) = 2 \sum_n \sum_{l=0}^{\infty} \frac{|\langle g | V_l | n \rangle|^2}{E_n - E_g}, \quad (2)$$

where g is the ground state, n are excited configurations, and the V_l are the terms in the expansion of r_{12}^{-1} in spherical harmonics of order l . Then for values of r greater than R_s , an indicator of the atom's radial size, defined by

$$\epsilon = 1 - \frac{1}{N} \int_0^{R_s} \sum_{i=1}^N P_i^2(r) dr, \quad (3)$$

where $P_i(r)$ is a one-electron ground-state radial wave function, ϵ is a small number such as 0.01 and the sum is over the ground-state electrons which number N , the induced potential, in lowest order, comes from the terms for $l=1$. This gives rise to the asymptotic interaction potential

$$V_I = \alpha/r^4 = \sum_n \alpha_{gn}/r^4, \quad (4)$$

where the α_{gn} are the partial polarizabilities from Eq.

¹⁹ D. R. Hartree, W. Hartree, and B. Swirles, Phil. Trans. Roy. Soc. London A238, 229 (1939).

(2) and α is the total polarizability. The contributions to the α_{gn} radial integrals are appreciable only in the region considerably outside the region where the ground-state exchange interaction is important. As an example, it may be seen that the radially dependent polarizability in oxygen has its principal contributions in the region outside of the nonzero inflection points of the $2s$ and $2p$ functions. See Table III.

Once the atomic core is penetrated ($r < R_z$), matrix elements for the interaction term which transforms as $l=0$ will be nonzero and cause the mixing of terms in the polarizability of the same symmetry as the ground state. This will lead to interactions which would be the same as those produced in a perturbation approach to the outer electron's wave function.

In the present work, the interaction inside the core is assumed to be the field of the ground state with the exchange interaction approximated by the PSHF exchange potential out to the radial value where the approximation is no longer proper, that is, the value $r=R$ where the effective charge for potential $[RV_{\text{PSHF}}(R)]$ is one. At that point the potential is continued as the H potential matched to the total potential's amplitude at that point: $V(r) = V_{\text{H}}(r)/V_{\text{H}}(R)$ this will cause the free wave function to be nearly orthogonal to the bound wave functions because the actual mismatch of the PSHF and H potentials in this region is numerically small and thus forms a good region to make the transition to the asymptotically correct H potential. The matching point will occur well outside of the nonzero inflection points of the outermost bound functions in the region where the free-functions are linear in r and nearly invariant with energy. The matching point will occur, for the case shown in Fig. 1, between the second zero of the free-function and $r=2$. It is the region out to $r \approx 4$ which determines the orthogonality to the $2s$ function, because the $2s$ function is quite small for larger r . If the PSHF potential were used all the way out to this region, the free function would automatically be orthogonal, as a property of the Sturmian set of equations. Also, the near-coincident inflection-point node of the free function will be properly placed, because it will occur inside of the matching point.

Further justification for using the atomic fields in the inner region of the atom may be seen in an examination of the HF wave functions¹⁹ for O^- and O I . The important orbitals to examine are the $2s$ and $2p$, because the s and p waves will be the most important in the low-energy scattering problem as the centrifugal term in the Hamiltonian will dominate the behavior of the higher l waves. And the s and p waves, for low energy, will have much of the character or functional behavior of the $2s$ and $2p$ core functions in the inner core region. The change in the positions of the nodes and maxima of the $2s$ and $2p$ functions with the addition of an electron to O I is little. The principal differ-

ence in the functions occurs in the outer region of the core where the potential becomes principally an H type. The effect of the longer "tail" on the O^- functions is to unshield some of the nuclear charge thus lowering the outer H potential with respect to that of the O I atom.

Thus, it is seen that there are three principal regions of interaction for the free electron wave function: interior core with Coulomb and exchange, outer core with Coulomb dominant, and the far field of the polarization potential. The radial regions are: 0 to R , $R \rightarrow R_z$ and $R_z \rightarrow \infty$, where R is the point where the effective charge for the potential equals one, and R_z is given by Eq. (3).

The polarization potentials calculated for Cs by Stone and Reitz¹⁰ and the polarization perturbation calculated by Temkin for oxygen⁴ indicate that the polarization potential rises to its maximum near the atomic radius and then decreases rapidly to some negligible value on the interior of the atom. An analytic form which describes this type of behavior and has been successfully utilized for polarization is^{9,11,20,21}

$$V_p(r) = (\alpha/2r^4)\{1 - \exp[-(r/r_0)^n]\}, \quad (5)$$

where $n \geq 4$ and r_0 is a cutoff value which will be chosen later. The most common choice is $n=8$, even though the α_{gn}/r^4 of Eq. (4) go to zero at least as r^2 . However, there is little change ($<10\%$) in the scattering results whether $n=4, 6$, or 8 as the atomic fields swamp the perturbation field on the interior of the atom. Here $n=8$ is chosen because of the rapid cutoff with decreasing r after the maximum of Eq. (5) at $r \approx 0.95 r_0$, which would give the least interference with the core potential.

II. MOLECULES

Properties of the solutions to the diatomic-molecule problem are much the same as the solutions to the atomic problem, which are often used as basis functions for approximate molecular solutions. And, what was said about zeros and inflection points for the atomic problem is formally true for the molecule. That is to say, that the higher energy molecular orbitals (MO) will have inflection points near the exterior of the molecular electron distribution and the molecular scattering solutions of the same symmetry as the MO's will have inflection point zeros near the inflection points of the MO's and on the interior of the charge distribution will take on the functional character of the MO's, completely in analogy with the atomic case. Then, if an imaginary spherical surface is drawn symmetrically about the molecule at a radius outside any reasonable MO charge density, the far field potential will be, to first order, the classical polarization form and centered at the molecular center of mass. However, the actual polarization charge forms two dipoles whose axes of

²⁰ L. Biermann and H. Harting, *Z. Astrophys.* **22**, 87 (1942).

²¹ H. J. Bruder and S. Borowitz, *Phys. Rev.* **120**, 2053 (1960).

symmetry intersect the interatomic axis between, but near the nuclei. This is suggested by Van Vleck's²² observation that the molecular polarizability is approximately equal to the sum of the constituent atomic polarizabilities.²³ However, if α , α_{\parallel} , and α_{\perp} are the atomic polarizability, polarizability parallel to and perpendicular to the axis of symmetry of the diatomic molecule, respectively, then it is usually true that α_{\parallel} is slightly larger and α_{\perp} is slightly smaller than 2α . Radial integration outward along the axis of symmetry for $L=0$ will yield an inflection-point zero in the molecular orbital near the exterior inflection point of the highest energy σ orbital. This zero will occur, relative to the nearest nucleus, at nearly the same relative point as the zero occurs in the atomic problem. That is to say, that the wave function along the internuclear axis will be given by $\phi(r) \cong \phi_A(r-R)$, where ϕ is the molecular orbital, ϕ_A is the atomic orbital, R is half the internuclear distance, and r is the distance from the molecular center of mass and is larger than R . Then, any variation in the molecular wave function exterior to that point that differs with the atomic wave function will be due to the difference in the surface electron fields and polarization fields. This is primarily the near doubling of the polarization field which becomes apparent outside of some distance large with respect to interatomic distance so the inverse-fourth-power potentials centered on each atom are about the same. Presumably, this distance will be far enough such that the contribution to the scattering length in the exterior region is negligible. At some large value of r , the molecular potential approaches spherical symmetry and along with it so does the wave function, i.e., $\phi(r) \rightarrow \phi_A(r-R)$ for values of r that are off the

internuclear axis. The far field behavior of $\phi(r)$ is $\sin(kr - kR + \delta)/k$, which gives a phase shift $\delta' = -kR + \delta$, or, equivalently, changes the scattering length by $-R$. Examining the form for δ given by Levy and Keller,¹⁷ one would expect the low-energy scattering to behave with a scattering length $R + A_A$, where A_A is the atomic scattering length, and with the influence of twice the atomic polarizability. That is

$$\sigma \sim 4\pi \left[-(R + A_A) - \frac{1}{3}\pi(2\alpha)k \right]^2 \quad (6)$$

should give the low-energy behavior. That this is not the case, can be seen from Fig. 2, curve c, which gives half the momentum-transfer cross section for N_2 . The experimental scattering length²⁴ for N_2 is about $0.65 a_0$ and the polarizability average is about $15.3 a_0^3$ which would give a different σ from the observed one in which the apparent values of A and $\alpha(N_2)$ are $2A_A$ and $\alpha(N)/2$ or $A_A/2$ and $2\alpha(N)$. The problem appears to be due to two things, the neglect of the effect of molecular over the atomic polarizability on the scattering length and the corrections, according to Levy and Keller,¹⁷ to the scattering length and to the term of the order of k in Eq. (6) due to the electric quadrupole field. The neglect of the quadrupole interaction is quite serious for the elastic scattering, but may not be as serious in the calculation of bound free matrix elements for inelastic processes where the free function is constructed as suggested here.

III. METHOD OF COMPUTATION

The central charge distributions used were the PSHF, self-consistent to 1.0%, as described elsewhere,¹⁸ and the analytic H distributions calculated by Strand and

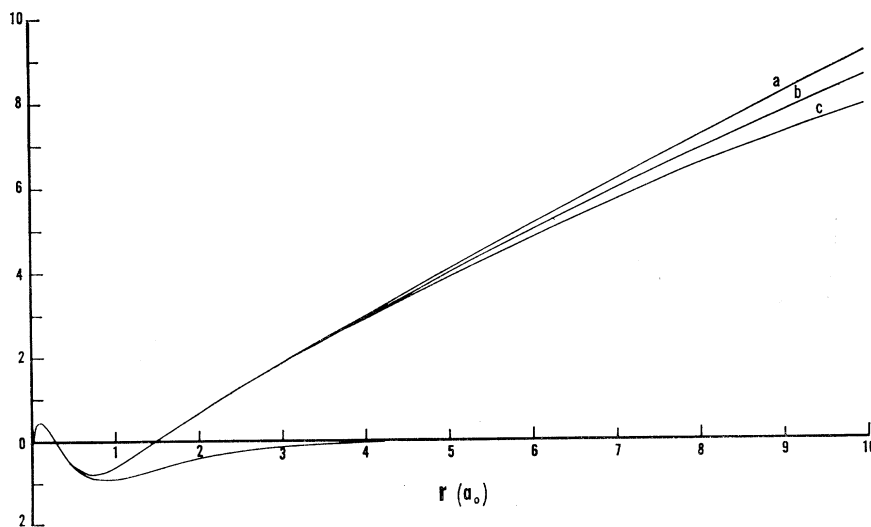


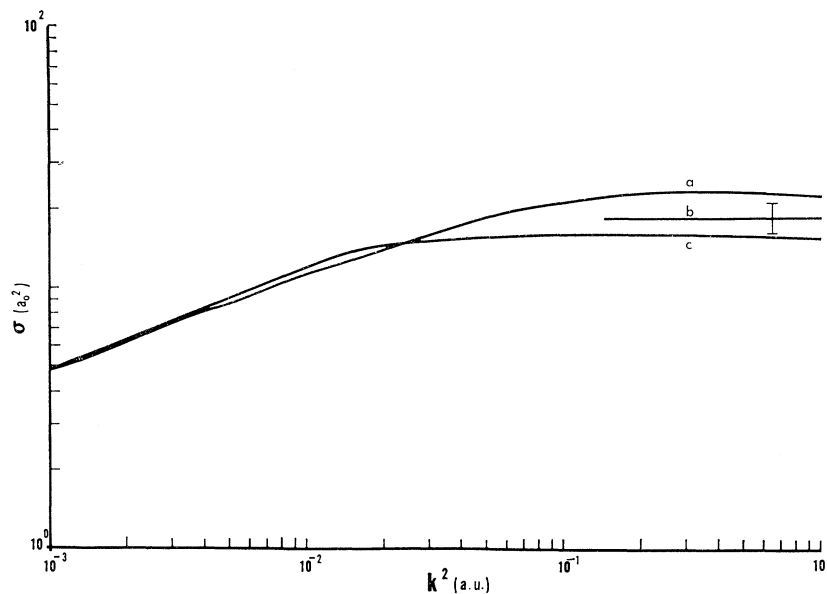
FIG. 1. Shown are the 2s function of O I and the s waves a, b and c with $k^2=0.001$, 0.005 and 0.01, respectively. The nearly common second zeros are 1.4938, 1.4930 and 1.4921, respectively.

²² J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities* (Oxford University Press, London, 1932), p. 82.

²³ This appears to work better when the principal contribution to the atomic polarizability is from the continuum rather than excited bound states as in nitrogen as opposed to hydrogen.

²⁴ L. S. Frost and A. V. Phelps, *Phys. Rev.* **127**, 1621 (1962).

FIG. 2. Cross sections for N I. Curve a is the result of this work, b is a straight line drawn through the higher energy values of Ref. 28 and c is one half the N_2 momentum-transfer cross section from Ref. 32. Partial-wave sum to $l=4$.

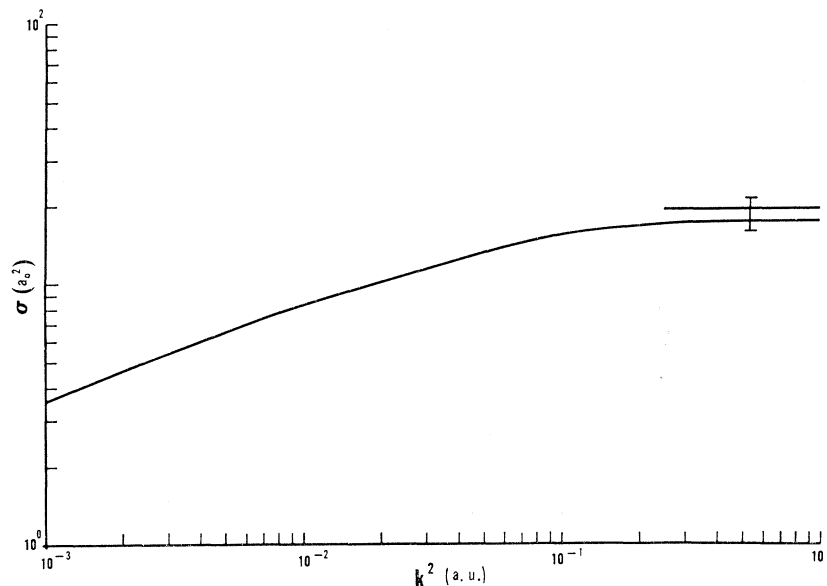


Bonham.²⁵ The polarizabilities were taken from Dalgarno²⁶ for Ar I and calculated for N I and O I by $\alpha_x = \alpha_{Ne}(Z_{Ne}/Z_x)^3$, where α_{Ne} is the polarizability of neon and the Z 's are the nuclear charges of the elements involved. Agreement with experimental values²⁷ is rather good, see Table II which cites Ref. 28. The Schrödinger equation was integrated outward using the Numerov²⁹ method to a point $r_{max} = 2\lambda_0 + r_m$, where

λ_0 is the wavelength of the lowest energy considered and r_m is the point where the central charge potential is less than 0.005. This was always several hundred Bohr radii. The radial intervals used were: $\Delta r = 0.005$ for $0 \leq r \leq 0.5$; $\Delta r = 0.02$ for $0.5 \leq r \leq 2.5$ and $\Delta r = 0.1$ for $2.5 \leq r \leq r_{max}$.

The solutions were normalized to k^{-1} at the closest maximum to r_{max} and the phase shift $\delta_i(k)$ was evalu-

FIG. 3. Elastic scattering cross section for O I with the experimental value from Ref. 33. Partial wave sum to $l=4$.



²⁵ T. G. Strand and R. A. Bonham, *J. Chem. Phys.* **40**, 1686 (1964).

²⁶ A. Dalgarno, *Advan. Phys.* **11**, 281 (1962).

²⁷ R. A. Alpher and D. R. White, *Phys. Fluids* **2**, 153 (1959).

²⁸ T. F. O'Malley, *Phys. Rev.* **130**, 1020 (1963).

²⁹ B. Numerov, *Publ. Observ. Astrophys. Cent. Rusie* **11** (Moscow, 1923); Ref. 30, p. 71.

³⁰ D. R. Hartree, *The Calculation of Atomic Structures* (John Wiley & Sons, Inc., New York, 1957).

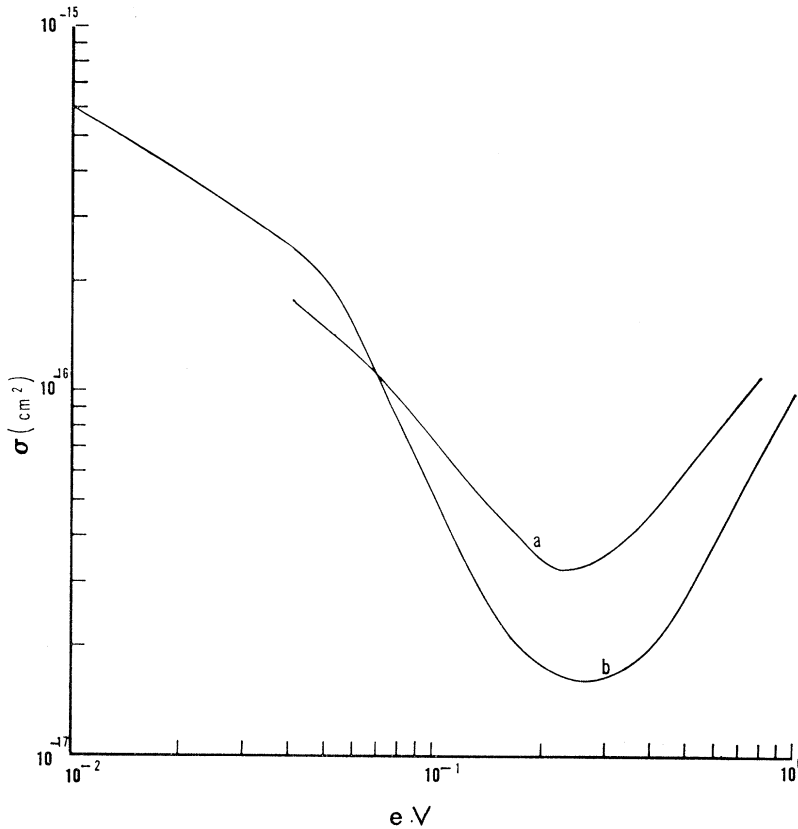


FIG. 4. Cross section for Ar I near the Ramsauer minimum. Curve a is the result of this work and b is the momentum transfer cross section of Ref. 37. Partial wave sum to $l=4$.

ated from the nearest zero to r_{\max} as $\tan\delta_l(k) = j_l(kX)/n_l(kX)$ where X is the value of r where the solution crosses the r axis as given by linear extrapolation from the points on either side of the axis and the $j_l(kX)$ and $n_l(kX)$ are the spherical Bessel functions. This is the best way to obtain the phase shift because it avoids curve fitting by making use of the linear property of the solutions in the neighborhood of an inflection-point zero.

The scattering cross section is then expressed as

$$\sigma = \sum_{l=0}^M \sigma_l = \frac{4\pi}{k^2} \sum_{l=0}^M (2l+1) \sin^2[\delta_l(k)], \quad (7)$$

where M is determined as the value of l for which the

TABLE II. Cutoff radius, polarizability, and scattering length from this calculation compared to other values. Quantities are given in atomic units.

	r_0	α^b	α_{exp}^c	A^a	A
N	6.75	7.65	7.65	0.257	0.333 ^b
O	5.90	5.20	5.20	0.305	0.300 ^b
Ne	...	2.65	2.65	...	0.240 ^b
Ar	4.5	...	11.0	-1.60	-1.70 ^d

^a Calculated here.

^b Power relation.

^c Dalgarno, Ref. 26.

^d O'Malley, Ref. 28.

ratio of that partial cross section to the sum including that partial cross section is less than 0.01 for two successive waves.

Figure 1 presents some wave functions of O I, and cross sections for N I, O I, and Ar I are presented in Figs. 2-4, respectively.

The computer program was checked by calculating the square-well problem and gave results agreeing with the analytical solution evaluated by use of a standard table.³¹

IV. DISCUSSION OF RESULTS

This simple model appears to predict the general behavior, with energy, of the low-energy-electron elastic-scattering cross section for atoms and by the simple extension for molecules also. Also, the cross section reported here for³² N I is enhanced in the upper range because the PSHF produces an exchange interaction with an extra $\frac{1}{2}$ electron because the number of electrons for N I is odd. The agreement with experiment for O I is good in the range where data is available.³³

³¹ P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 1926.

³² R. H. Neynaber, L. L. Marino, E. H. Rothe, and S. M. Trujillo, *Phys. Rev.* **123**, 148 (1961).

³³ R. H. Neynaber, L. L. Marino, E. H. Rothe, and S. M. Trujillo, *Phys. Rev.* **129**, 148 (1961).

Considering the approximate power-rule³⁴ transformation properties of solutions to the atomic problem, it would be expected that the cross section for N I would be more like that for O I in behavior with energy and not begin to decrease at as high an energy as 4–5 eV, as reported.³² This behavior in the measurement may be caused by the interference of the inelastic process which dominates the N₂ cross section in the 1–5 eV range.^{32,35} The corresponding inelastic cross section does not occur in³⁶ O₂ and thus would not effect the reported measurement in O I.

The results for Ar I were quite sensitive to the value chosen for r_0 for the placement of the s -wave cross-section minimum. However, the general behavior with energy remained the same. The p wave seemed little affected by a variation in r_0 , predicting a Ramsauer minimum at about 1.2 eV in comparison to the experimental value 1.1 eV. The resultant scattering length -1.60 is between the value reported by O'Malley²⁸ as -1.90 and the value of about -1.4 at 0.01 eV calculated from Englehardt and Phelps.³⁷

Values of the cross sections for k^2 lower than 0.001 Ry (0.0136 eV) should not be taken too seriously, because the electron's wavelength is becoming on the order of the length of the gas interparticle distance so a collision may not be thought of as a two-body interaction. Indeed, the electron will be interacting with several centers at once.

The behavior of the scattering cross sections in different ranges of energy appears to be attributable to separate interactions. Although the interactions all contribute simultaneously there are energy ranges in which certain interactions dominate the cross section behavior: polarization in about 0.08 to 1 eV, and above that, Coulomb and exchange. It is conceivable that a long-range force such as the quadrupole field would dominate the region below that for the dipole polarization. In any event, partial-wave, two-body analysis is questionable in such a low energy range.

Choice of r_0 was the most indefinite portion of this method. In an effort to establish values for r_0 , excited state functions were generated and the matrix elements $\langle g|r|n\rangle$ were calculated. The contribution to the integral with increasing r was observed and r_0 was expected to be near the region where contributions to the integral became small. The calculation for O I is given in Table III. It has been shown³⁸ that the majority of the polarization for this row atom comes from the low-energy continuum and because of the inward shift of

TABLE III. Contributions to the radial matrix elements of the two lowest states used in Eq. (2).

r (a.u.)	$\Delta\langle 2p r 3s\rangle\times 10$	$\Delta\langle 2p r 3d\rangle\times 10$
0.10	0.0188	
0.20	0.0603	
0.30	-0.0574	
0.40	-0.4332	
0.50	-0.9986	0.0141
1.00	-1.2809	0.0715
1.50	+1.1020	0.1975
2.00	1.2359	0.3523
2.50	2.0949	0.4940
3.00	2.3105	0.5790
3.50	2.0921	0.5983
4.00	1.6885	0.5649
5.00	0.8892	0.4165
6.00	0.3941	0.2586
7.00	0.1574	0.1435
8.00	0.0584	0.0732

the s -free functions the maximum contribution to the polarizability lies inside that of the $3s$ function. The initial guess was³⁹ $r_0=5.5$. The final value was $r_0=5.9$ to give the scattering length in near agreement with the power rule value continued from neon as was done for the polarizability.

Variation of polarizability should be predictable by the power relation within a given nl shell, however, the r_0 value for group IA and IIA atoms will have to be estimated from polarizability calculations. In these cases the principal contribution will come from the lower excited states and should be easily estimated with the PSHF method.

V. CONCLUSION

A simple method for the approximate prediction of low-energy elastic scattering of electrons from atoms has been presented and an extension to homonuclear diatomic molecules has been proposed and appears to give generally good results for the cross sections. The model, I believe, has demonstrated that induced polarization is a perturbative effect and not a strong interaction on the interior of the atom. The interactions used are only the general ones on the assumption that at low energies the electron wavelength is too long to "see" the details of the scattering center's structure.

ACKNOWLEDGMENTS

I would like to acknowledge many discussions on scattering theory and calculations with Fred Roehrs and Stanley Schneider of the Aerospace Corporation. And I would like to express my gratitude to B. A. Troesch and the Corporation's Computation and Data Processing Center for their cooperation in handling the codes involved in this analysis.

³⁹ This is about the region where the polarization charge is entered appreciably as seen in Ref. 4, Fig. 2.

³⁴ This rule comes from the observation that zeros, maxima, matrix elements and eigenvalues are closely predictable by the transformation of the unit of length by the ratio of the nuclear charges: r_1/r_2 (Z_2/Z_1).

³⁵ G. J. Schulz, Phys. Rev. **125**, 229 (1962).

³⁶ G. J. Schulz and J. T. Dowell, Phys. Rev. **128**, 174 (1962).

³⁷ A. G. Engelhardt and A. V. Phelps, Phys. Rev. **133**, A375 (1964).

³⁸ H. P. Kelly and H. S. Taylor, J. Chem. Phys. **40**, 1478 (1964).