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This research was supported by the National Aeronautics
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ABSTRACT

The problem of low energy atomic scattering of electrons by multi-electron atoms is formulated in the adiabatic exchange approximation. The effects of target distortion by the electric field of the incident charged particle are determined by computing a polarization potential to be included in the total scattering interaction. The polarization potential is obtained through a polarized orbital calculation on atomic systems described by Hartree-Fock type wave functions. Application is made to Na and Li where electron exchange is included in the reduction of the scattering equation, and the phase shifts and total elastic scattering cross sections are obtained through the solution of a set of integrodifferential equations. Exchange effects are noted explicitly by solving the scattering equations neglecting electron exchange and comparing the computed cross sections. The total elastic scattering cross sections for Li and Na agree well with recent measurements over the entire experimental range, and are significantly better than any previously published results.

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I. INTRODUCTION

The theoretical treatment of atomic collision processes has received a great deal of attention by many investigators for the last thirty or more years. One can find a vast amount of literature devoted to almost any phase of the problem. Yet adequate solutions to almost all but the very simplest atomic collision phenomena have yet to be realized. In this paper we will concern outselves with electron-atom collision processes, and more particularly we will consider only the case of electrons of low incident energy on single unbound atoms or ions.

The atomic scattering of electrons presents a very complex problem even in the very simplest systems, the least complicated being that of electron-hydrogen atom scattering. Even in this case, however, complete solutions have not as yet been obtained. The Hamiltonian for this system is essentially the same as that for the helium atom which has, of course, never been solved exactly. Scattering by heavier atoms yields far more complicated Hamiltonians than that of the hydrogen system and, of necessity, presents even more formidable problems in seeking anything approximating an exact solution. It can be said, then, that at the present stage of development in atomic scattering problems, exact solutions are nonexistent, and progress toward an agreement of theory and experiment lies in finding the proper approximations which yield accurate results, and thus more insight into the scattering processes.

For low energy electrons incident on an atomic system, there are two major effects which complicate the problem. These are 1) the exchange interactions between the incident electron and the atomic electrons, and 2) the distortion of the atomic systems by the electric field of the incident charged particle. For certain atomic collision problems both these effects are more pronounced than usual. In the case of the alkali atoms this is particularly true since the valence electron is very loosely bound. Earlier calculations for the alkalis[1-3] have shown the extreme sensitivity of the calculated cross sections to the accuracy of the polarization potential in the total scattering interaction and the exchange effects.[3] In this paper the problem of low energy elastic scattering of electrons by alkali-type atoms is treated with application to atomic lithium and sodium in the energy range from .003 to 25.0 eV. The effects of exchange and target distortion have been calculated here through the use of the adiabatic exchange approximation wherein the target atom is distorted by the static field of the incoming electron. The polarization potential is calculated by a method of polarized orbitals similar to that used by Temkin[4,5] and Callaway,[6] and electron exchange between the incident and the valence electron is included through explicit use of the adiabatic exchange approximation which leads to a set of integrodifferential equations for the free electron wave functions.[3-5]

II. THE POLARIZATION POTENTIAL

In this section the distortion of an atomic system by a slow incident electron and the resulting polarization potential is developed from the application of first order perturbation theory to Hartree-Fock electron orbitals. We note than analogous perturbation calculations on Hartree and Hartree-Fock systems have been carried out heretofore in order to determine atomic dipole polarizabilities (Sternheimer[7]); core polarization due to valence electrons in alkali atoms (Callaway[6]); and the polarization potential for electron scattering (Temkin[4]).

We consider the first order perturbation by a free electron of an atomic system whose unperturbed Hartree-Fock (H.F.) self consistent field wave functions have been determined. Under the influence of the perturbation the H.F. one electron orbitals and the H.F. energy depend on the coordinates of the free electron. The perturbed orbitals ψ_i of the H.F. determinant for the atomic system then satisfy the following equation (in Rydberg units) which depends on the free electron coordinate r_f.[4,6]

$$\left[-\nabla_1^2 + V(\vec{r}_1, \vec{r}_f) - A(\vec{r}_1, \vec{r}_f) + \frac{2}{r_{1f}}\right] \psi_i(\vec{r}_1, \vec{r}_f) = \epsilon_i(\vec{r}_f)\, \psi_i(\vec{r}_1, \vec{r}_f) \qquad (1)$$

where

$$V(\vec{r}_1, \vec{r}_f) = -\frac{2Z}{r_1} + \sum_i \int \left|\psi_i(\vec{r}_2, \vec{r}_f)\right|^2 \frac{2}{r_{12}}\, d\vec{r}_2 \tag{2}$$

and

$$A(\vec{r}_1, \vec{r}_f)\, g(\vec{r}_1, \vec{r}_f) = \sum_i \left(\int \psi_i^*(\vec{r}_2, \vec{r}_f)\, g(\vec{r}_2, \vec{r}_f) \frac{2}{r_{12}}\, d\vec{r}_2\right) \psi_i(\vec{r}_1, \vec{r}_f) \tag{3}$$

In these equations $\vec{r}_1$, $\vec{r}_2$ are the coordinates of bound electrons and $\vec{r}_f$ is that of the free electron. In order to simplify the above equations for the perturbed H.F. orbitals we write $\psi_i(\vec{r}_1, \vec{r}_f)$ in the form

$$\psi_i(\vec{r}_1, \vec{r}_f) = \phi_i(\vec{r}_1) + \chi_i(\vec{r}_1, \vec{r}_f) \tag{4}$$

where $\phi_i(\vec{r}_1)$ is the unperturbed H.F. orbital which satisfies

$$[-\nabla_1^2 + V(\vec{r}_1) - A(\vec{r}_1)]\, \phi_i(\vec{r}_1) = \epsilon_i^0\, \phi_i(\vec{r}_1) \tag{5}$$

with

$$V(\vec{r}_1) = -\frac{2Z}{r_1} + \sum_i \int \left|\phi_i(\vec{r}_2)\right|^2 \frac{2}{r_{12}}\, d\vec{r}_2 \tag{6}$$

and

$$A(\vec{r}_1)\, g(\vec{r}_1) = \sum_i \left[\int \phi_i(\vec{r}_2)\, g(\vec{r}_2) \frac{2}{r_{12}}\, d\vec{r}_2\right] \phi_i(\vec{r}_1). \tag{7}$$

Our objective is to determine the first order perturbations χ_i of the single electron orbitals ψ_i of the Hartree-Fock determinant for the bound atomic system. In this calculation the term $2/r_{1f}$ is treated as a perturbation on the atomic system and the perturbations χ_i are determined from first order perturbation theory.[4,6,7] The integro-differential equations for the first order perturbation $\chi_i(\vec{r}_1, \vec{r}_f)$ of the H. F. orbitals may be determined from equation (1). These have been written down explicitly by Callaway,[6] but are too complicated to solve in any reasonable time. However, if all the perturbed Coulomb and exchange integrals are dropped from the equations for the first order perturbation of the H.F. orbitals, the resulting differential equations are more tractable. The effect of omitting these integrals is discussed by Callaway[6] and is shown to be reasonably small.

The presence of the unperturbed exchange integrals $A(r_1)$ which are retained in the equations for the perturbed Hartree-Fock orbitals still leave the equations in a very complicated form. However, these terms can be replaced very conveniently and with reasonable accuracy by an average exchange potential by the method given by Slater.[8] In the simplest form of Slater's method, the exchange term of equation (7) is replaced by the function

$$A_s(r_1)\, g(r_1) = 6\left[\frac{3}{8\pi} \sum_i \phi_i^*(\vec{r}_1)\, \phi_i(\vec{r}_1)\right]^{1/3} g(r_1). \tag{8}$$

The summation in this expression is carried over all occupied orbitals of both spins. With this substitution and with the omission of the perturbation terms in the Coulomb and exchange integrals, the resulting equation for the perturbation χ_i of a H.F. orbital becomes:

$$[-\nabla_i^2 + V(\vec{r}_1) - A_s(\vec{r}_1) - \epsilon_i^0]\, \chi_i(\vec{r}_1, \vec{r}_f) = \left[\int \left|\phi_i(\vec{r}_1)\right|^2 \frac{2}{r_{1f}}\, d\vec{r}_1 - \frac{2}{r_{1f}}\right] \phi_i(\vec{r}_1) \tag{9}$$

In this equation we expand the perturbation term $2/r_{1f}$ which appears in the two terms on the right side, by the multipole expansion

$$\frac{2}{r_{1f}} = \frac{2}{r_1} + \frac{2r_f}{r_1^{\,2}} \cos\theta + \frac{2r_f^{\,2}}{2r_1^{\,3}} (3\cos^2\theta - 1) + \cdots \qquad (r_1 > r_f)$$

$$\frac{2}{r_{1f}} = \frac{2}{r_f} + \frac{2r_1}{r_f^{\,2}} \cos\theta + \frac{2r_1^{\,2}}{2r_f^{\,3}} (3\cos^2\theta - 1) + \cdots \qquad (r_f > r_1), \tag{10}$$

where θ is the angle between r_1 and r_f. Substituting (10) into the two terms in the brackets on the right of (9) we note that all but the spherically symmetric term in the integral will vanish. Dropping the quadrupole and higher order terms the bracket expression then becomes

$$\left[\int \left|\phi_i(\vec{r}_1)\right|^2 \frac{2r_<}{r_>^{\,2}}\, d\vec{r}_1 - \frac{2}{r_<} - \frac{2r_<}{r_>^{\,2}} \cos\theta\right]$$

where $r_<$ is the lesser and $r_>$ the greater of r_1, r_f. We note that for large values of r_1 the first and second terms in this expression will cancel each other leaving only the dipole term $\frac{2r_<}{r_>^2} \cos\theta$. Also noting that for smaller values of r_1 the spherically symmetric term of the potential will be small as compared to the Coulomb term, we make the dipole approximation and retain only the dipole term in the bracketed expression.

To obtain the first order perturbation of each of the atomic electron orbitals Φ_i we thus have the following pair of differential equations to solve:

$$[-\nabla_1^2 + V(r_1) - A_s(r_1) - \epsilon_1^{o}]\, \chi_i(\vec{r}_1, \vec{r}_f) = -\frac{2r_1}{r_f^{\,2}} \cos\theta\ \Phi_i(\vec{r}_1), \quad \text{for } r_f > r_1 \tag{11_a}$$

$$[-\nabla_1^2 + V(r_1) - A_s(r_1) - \epsilon_1^{o}]\, \chi_i(\vec{r}_1, \vec{r}_f) = -\frac{2r_f}{r_1^{\,2}} \cos\theta\ \Phi_i(\vec{r}_1), \quad \text{for } r_1 > r_f \tag{11_b}$$

These equations must be solved in the "inner" region where $r_f < r_1$ and in the "outer" region where $r_f > r_1$ and the solutions matched at the boundary $r_f = r_1$.

With the solutions for the perturbations χ_i of the Hartree-Fock orbitals the dipole polarization potential is then determined from the expression[6,9]

$$V_p(r_f) = \sum_i \int \Phi_i^*(\vec{r}_1) \frac{2r_<}{r_>^2} \cos\theta \, \chi_i(\vec{r}_1, \vec{r}_f) \, d\vec{r}_1 \tag{12}$$

where the sum extends over all occupied orbitals Φ_i.

The reduction of equations (11) into radial equations and (12) into integrals over radial coordinates is accomplished easily by expansion of the functions Φ_i and χ_i in the form

$$\Phi_i(\vec{r}_1) = P_{n\ell}(r_1)/r_1 \; Y_\ell^m(\theta, \phi) \tag{13}$$

and

$$\chi_i(\vec{r}_1, \vec{r}_f) = \sum_{\ell', m'} U_{n\ell\to\ell'}(r_1, r_f)/r_1 \; C^{m\to m'}_{n\ell\to\ell'} \; Y_{\ell'}^{m'}(\theta, \phi) \tag{14}$$

With these substitutions the differential equations (9) separate into the radial equations

$$\left[\frac{d^2}{dr_1^2} - \frac{\ell'(\ell'+1)}{r_1^2} - V(r_1) + A_s(r_1) + \epsilon_1^0\right] U_{n\ell\to\ell'}(r_1, r_f) = \frac{2r_1}{r_f^2} P_{n\ell}(r_1), \quad r_f > r_1 \tag{15$_a$}$$

$$\left[\frac{d^2}{dr_1^2} - \frac{\ell'(\ell'+1)}{r_1^2} - V(r_1) + A_s(r_1) + \epsilon_1^0\right] U_{n\ell\to\ell'}(r_1, r_f) = \frac{2r_f}{r_1^2} P_{n\ell}(r_1), \quad r_1 > r_f \tag{15$_b$}$$

which must be solved and matched at the boundary $r_1 = r_f$. The constants $C^{m\to m'}_{n\to}$ in equation (14) are determined from the Clebsch-Gordon coefficients which occur from the angular integrals. These are tabulated by Sternheimer and are zero unless $\ell' = \ell \pm 1$, where only the upper sign holds for $\ell = 0$. With the solutions to (15) the polarization potential becomes

$$V_p(r_f) = \sum_{n\ell\ell'} V_{n\ell\to\ell'}(r_f) \, ,$$

where

$$V_{n\ell\to\ell'}(r_f) = K_{n\ell\to\ell'} \left[\frac{2}{r_f^2} \int_0^{r_f} P_{n\ell}(r_1)\, r_1\, U_{n\ell\to\ell'}(r_1, r_f)\, d\, r_1 + r_f \int_{r_f}^{\infty} P_{n\ell}(r_1)\, U_{n\ell\to\ell'}(r_1, r_f) r_1^{-2}\, d\, r_1 \right] . \tag{16}$$

The constants $K_{n\ell\to\ell'}$ are numbers which depend on ℓ' and on the number of electrons in an $n\ell$ shell and have been given by Sternheimer. In the limit as $r_f \to \infty$ the polarization potential calculated here should approach $-\alpha/r^4$, where α is the dipole polarizability, thus providing a convenient check on the accuracy of the solutions V_p.

III. THE SCATTERING EQUATION

As mentioned in Section I, both target distortion and electron exchange are extremely important in electron scattering by the alkali atoms and must be dealt with accordingly in the scattering equation. On the other hand, if one wishes to obtain cross sections over a fairly wide energy range as in the present investigation, the scattering equation must be written in a reasonably tractable form, since many partial waves are required in the calculation. In order to achieve these objectives the scattering equation is written as essentially a two electron equation for the free electron and the single valence electron in the field of the perturbed core orbitals with exchange between the incident and valence electrons included explicitly. Exchange with core electrons is accounted for implicitly through the exchange term $A_s(r)$ of equation (7) and core polarization is included directly through $V_{pc}(r)$ which is the polarization potential of the core electrons. The Schroedinger equation may then be written in the form

$$\left[\nabla_1^2 + \nabla_2^2 + E - V(r_1) - V(r_2) + A_s(r_1) + A_s(r_2) + V_{p_c}(r_1) + V_{p_c}(r_2) - \frac{2}{r_{12}}\right]\Psi(\vec{r}_1, \vec{r}_2) = 0, \tag{17}$$

where $\vec{r}_1$ and $\vec{r}_2$ are position vectors for the two electrons, and the terms $V(r)$, $A_s(r)$ are given by equations (6) and (8). $V_{p_c}(r)$ is the polarization potential for the core electron calculated by the method of Section II.

With this scattering equation the adiabatic exchange model is again utilized to express the wave function $\Psi(\vec{r}_1, \vec{r}_2)$ for the free and the bound electron. In this approximation Ψ is written in the form

$$\Psi(\vec{r}_1, \vec{r}_2) = \psi'(\vec{r}_1, \vec{r}_2)\, F(\vec{r}_2) \pm \psi_o(\vec{r}_2)\, F(\vec{r}_1), \tag{18}$$

where ψ_o is the ground state wave function for the valence electron, ψ' is the perturbed ground state function which is perturbed adiabatically by the free electron whose wave function is F, and the perturbation term is $2/r_{12}$.

The plus sign in (16) refers to the symmetric (singlet) state of the two electrons, and the minus sign to the antisymmetric (triplet) state. In the adiabatic exchange approximation adopted here the symmetry of the wave function Ψ is partially destroyed since the unperturbed bound state function ψ_o appears in the second term of (18) rather than the first order perturbed function ψ'. The omission of the first order perturbed term in the exchange wave function means that the function $\Psi(\vec{r}_1, \vec{r}_2)$ is not completely antisymmetric except in the limit of large r_2 where the perturbation becomes zero. This approximation is consistent with the perturbation calculation of H.F. functions in Section II and should have an equally small effect on the accuracy of the scattering equation.[3,10]

The perturbed ground state function ψ' is written, as in Section II, in the form

$$\psi'(\vec{r}_1, \vec{r}_2) = \psi_o(\vec{r}_1) + \chi(\vec{r}_1, \vec{r}_2), \tag{19}$$

and the perturbation χ is determined from equation (9).

Equation (18), with ψ' written as in (19), may be substituted into equation (17) in order to obtain an equation for the free electron function F. With this substitution, equation (17) may be multiplied on the left by $\psi_o^*(\vec{r}_1)$ and the result integrated over $\vec{r}_1$. With the use of equations (5), (9) and (12) the Schroedinger equation becomes

$$\left[\nabla_2^2 + k_o^2 - V_o(r_2) + A_s(r_2) + V_{p_c}(r_2) + V_{p_v}(r_2)\right] F(\vec{r}_2)$$

$$= \pm \int d\tau_1 \, \psi_o^*(\vec{r}_1)\left(k_o^2 - E_o - \frac{2}{r_{12}}\right) F(\vec{r}_1)\, \psi_o(\vec{r}_2) \qquad (20)$$

where the upper and lower signs refer to the singlet and triplet states respectively. Here the term $k_o^2 = E - E_o$ is the kinetic energy of the free electron and E_o is the ground state energy of the bound electron. $V_o(r_2)$ is defined as

$$V_o(r_2) = \left\langle \psi_o \left| \frac{2}{r_{12}} + V(r_2) \right| \psi_o \right\rangle$$

which is the screened Hartree-Fock potential for the neutral atom. The term $V_{p_v}(r_2)$ is the polarization potential due to the perturbed valence electron and is given by

$$V_{p_v}(r_2) = \int \psi_o^*(\vec{r}_1) \left| \frac{2}{r_{12}} \right| \chi(\vec{r}_1, \vec{r}_2)\, d\vec{r}_1$$

which is, in the dipole approximation, just that of equation (12) where χ is to be determined from equation (11). Thus the sum of the two terms $V_{p_c} + V_{p_v}$ is the polarization potential for the core plus the valence electron and is just the polarization potential of equation (12) for the complete atom. This will be denoted by V_p.

By the use of a partial wave expansion of the free electron wave function F(r) equation (20) can be reduced to a radial equation for each partial wave f . Thus we write

$$F(\vec{r}_2) = \sum_{\ell} r^{-1} f_{\ell}(r)\, P_{\ell}(\cos\theta_2) \qquad (21)$$

With this expansion, the equation for the partial wave f becomes

$$\frac{d^2}{dr^2} f_{\ell} + \left[k_o^2 - V_o + V_p + A_s - \frac{\ell(\ell+1)}{r^2} \right] f_{\ell} = \pm U_o \left[(E_o - k^2)\delta_{\ell o} \int_o^{\infty} f_o U_o \, dr \right.$$

$$+ \left\{ \frac{1}{2\ell+1} \right\} \times \left\{ r^{\ell} \int_o^{\infty} f_{\ell} U_o r^{-(\ell+1)} \, dr + r^{-(\ell+1)} \int_o^{r} f_{\ell} u_o r^{\ell} dr \right.$$

$$\left. \left. - r^{\ell} \int_o^{r} f_{\ell}\, \phi_o\, r^{-(\ell+1)} \, dr \right\} \right] \qquad (22)$$

where $u_c = r^{-1} \psi_o$ is the radial part of the normalized ground state wave function for the valence electron.

The integrodifferential equation (20) may be solved in a non-iterative fashion by a procedure used by Marriott,[11] or in an iterative self-consistent calculation as was used in the present work.

If electron exchange is completely ignored between the bound and free electrons, the scattering equation (22) reduces to a homogeneous equation where the right side is identically zero. Solutions to both sets of equations were obtained in order to determine the effect of exchange on the calculated cross sections.

IV. APPLICATION TO Li AND Na

A. Calculated Polarization Potential

In the calculation of the polarization potential, the unperturbed wave functions for the atomic system were taken as the Hartree-Fock-Slater (H.F.S.) wave functions obtained from a slightly modified program originally written by Herman and Skillmann.[12] The output of the program furnished the functions

$V(r)$, $A_s(r)$, ϵ_1^o and $P_{n\ell}(r)$ in equations (15), which could then be solved for the perturbations $U_{n\ell\to\ell'}$ of a given orbital whose radial function is $P_{n\ell}$. For a given value of r_f equations (15) were integrated by the Numerov process for inhomogeneous equations as described by Hartree,[13] over the same r_1 mesh as that of the H.F.S. program which furnished the unperturbed functions. The integration in the inner region was started by noting, as did Sternheimer,[6] that for $r_1 \sim 0$ the inhomogeneous term on the right side of (11) is negligible as compared to the potential terms on the left. The solution may thus be started by a series expansion[13] near the origin and continued by numerical integration. With this procedure there is an arbitrary constant in the starting values, this being the value of $(U_{n\ell\to\ell'}/r^{\ell'+1})_0$. For the inhomogeneous set of equations (11), this parameter in the starting conditions must be determined in order to satisfy the boundary conditions; that the solutions to (11_a) and (11_b) and their derivatives match at $r_1 = r_f$ and that the solution be exponentially decreasing at infinity. The value of $(U_{n\ell\to\ell'}/r^{\ell'+1})_0$ was varied automatically in the coded program until two values were found which enclosed the correct one. The choice was then narrowed by successive solutions until an accuracy of five to six significant figures in the starting value was achieved. The calculations were performed on a Univac 1107 computer at the University of Alabama Research Institute.

In the present calculation the total polarization potential was taken to be that contributed by electrons in the two outermost shells of the alkali atom. For Li both the core and valence electrons are in s-states. In Sternheimer's notation these undergo s → p perturbations and the radial equations must be solved for the perturbation $U_{1,0\to1}$ and $U_{2,0\to1}$. In the case of Na the 2s and 3s electrons experience s → p excitations similar to Li. However, for the 2p electrons, two modes of excitation 2p → d and 2p → s are possible and the perturbation $U_{2,1\to2}$ and $U_{2,1\to0}$ are required.

The solutions to the pair of differential equations (11) for the perturbations $U_{n\ell\to\ell'}(r, r_f)$ exhibit a behavior very similar to the simpler solutions obtained by

Sternheimer. Thus the nodes of the radial function $U_{n\ell\to\ell'}$ correspond in number to the orbital next higher in energy than $n\ell$ having ℓ' angular momentum. Also the contributions ns → p and np → s are opposite in sign as found in Sternheimer's calculations and tend to cancel each other in their contribution to V_p. (Sternheimer supports this behavior with a reasonable physical and mathematical argument.) The solutions to equations (11) are of course more complicated than those of Sternheimer since his equations correspond to those only in the asymptotic region of r_f where only one of equations (11) holds. As the free electron moves in toward the nucleus, the pair of equations must be solved for each value of r_f. In the actual solution the equations were solved over a 441 point mesh on r_1 and for 110 values of r_f. As one would expect from physical arguments, the amplitude and to some extent the shape of the perturbation $U_{n\ell\to\ell'}(r, r_f)$ of an $n\ell$ orbital depends on the position r_f of the free electron. The perturbation is small for large r_f, largest when $r_f \sim r_o$, where r_o is the position of the largest maximum of the unperturbed function, and small again for $r_f \sim 0$. This is clearly shown in Fig. 1 where the unperturbed radial function $P_{3s}(r)$ for sodium and the perturbation $U_{3,0\to1}(r, r_f)$ for three values of r_f are shown.

We have so far considered the core polarization as being due only to the electric field of the incident electron. However, since the valence electron is strongly polarized by the field of the incident particle, there is an induced field acting on the core due to the polarized valence electron orbital.[14] This field tends to induce a moment of opposite sign in the core orbitals, thus decreasing the effective polarization of the core. An estimate of the size of this effect can be obtained by calculating the electric field at the nucleus $\Delta E_{val}(0)$ due to the perturbation of the valence electron wave functions. The z-component of this field is given by[14]

$$\Delta E_{val,z}(0, r_f) = e \int_0^\infty \rho_{ind}\, r^{-2} \cos\theta \, dv \qquad (23)$$

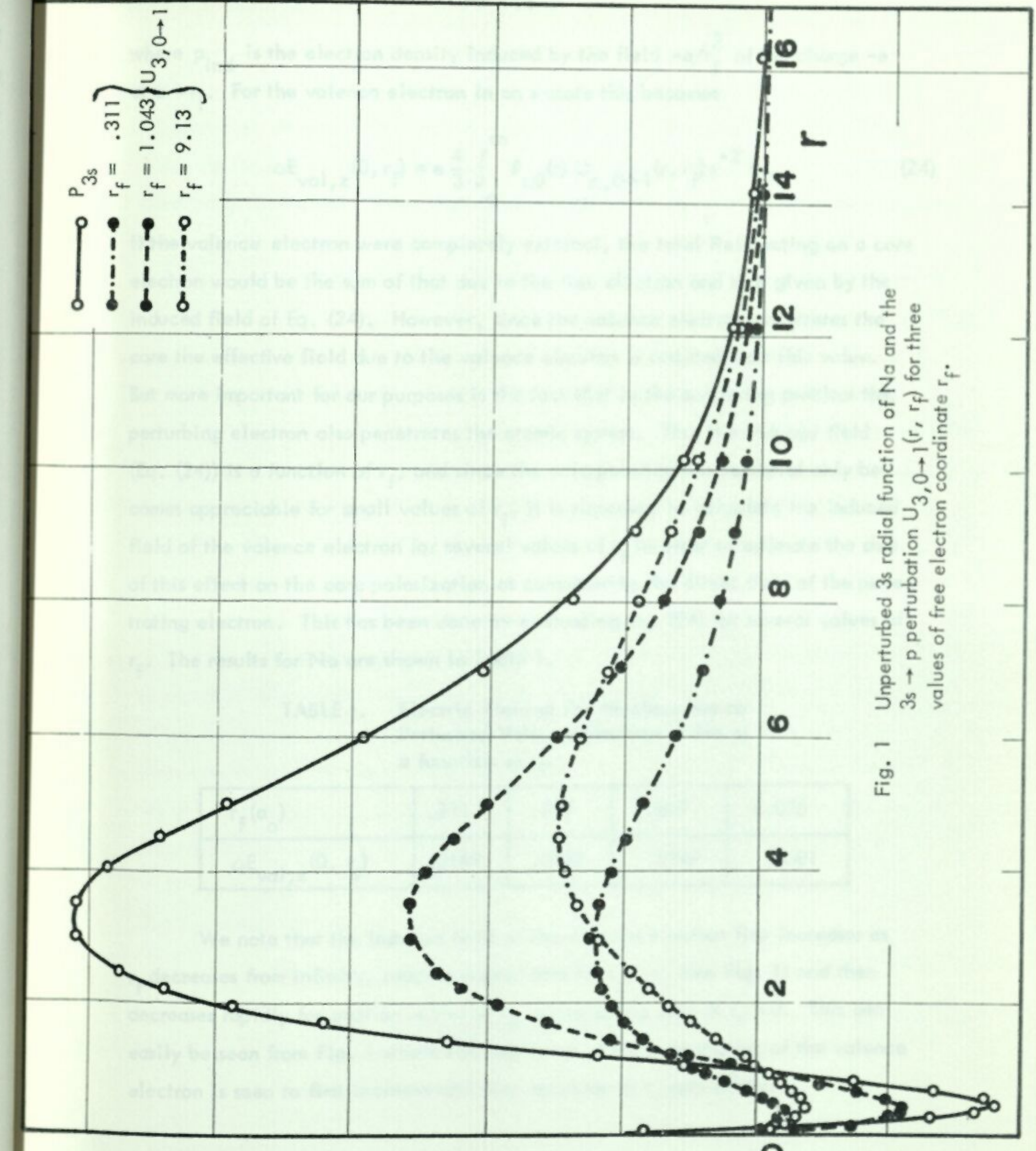

Fig. 1 Unperturbed 3s radial function of Na and the $3s \to p$ perturbation $U_{3,0\to 1}(r, r_f)$ for three values of free electron coordinate r_f.

where ρ_{ind} is the electron density induced by the field $-e/r_f^2$ of the charge $-e$ at $z = r_f$. For the valence electron in an s-state this becomes

$$\Delta E_{val,z}(0, r_f) = e\,\frac{4}{3}\int_0^\infty P_{n0}(r)\, U_{n,0\to 1}(r, r_f)\, r^{-2}\, dr. \qquad (24)$$

If the valence electron were completely external, the total field acting on a core electron would be the sum of that due to the free electron and that given by the induced field of Eq. (24). However, since the valence electron penetrates the core the effective field due to the valence electron is reduced from this value. But more important for our purposes is the fact that in the scattering problem the perturbing electron also penetrates the atomic system. Thus the induced field (Eq. (24)) is a function of r_f, and since the core polarization potential only becomes appreciable for small values of r_f, it is necessary to calculate the induced field of the valence electron for several values of r_f in order to estimate the size of this effect on the core polarization as compared to the direct field of the penetrating electron. This has been done by evaluating Eq. (24) for several values of r_f. The results for Na are shown in Table 1.

TABLE I. Electric Field at the Nucleus due to Perturbed Valence Electron of Na as a function of r_f.

$r_f(a_o)$	.211	.597	3.017	6.075
$\Delta E_{val,z}(0, r_f)$	.0169	.0372	.0949	.0501

We note that the induced field of the valence electron first increases as r_f decreases from infinity, reaches a maximum for $r_f \sim r_o$ (see Fig. 1) and then decreases rapidly for smaller values of r_f, approaching zero at $r_f = 0$. This can easily be seen from Fig. 1 where the amplitude of the perturbation of the valence electron is seen to first increase and then decrease as r_f gets smaller.

In order to estimate the effect of this interaction on the calculated polarization potential, we show separately in Fig. 2 the polarization potential from the valence electron and from the core electrons as calculated from Eq. (16). Then note that for values of r greater than $\sim 2a_o$ where the induced field of the valence electron is appreciable, the polarization potential due to the core electrons whether due to the direct terms from the incident particle or from the induced field of the valence electron is essentially negligible as compared to the large valence electron contribution. Furthermore, for small values of r_f where the core polarization potential becomes appreciable, the induced field due to the valence electron becomes small as compared to the perturbing field of the incident electron (down by a factor of six from its maximum (Table I)) and thus can reasonably be neglected in the calculation of V_{p_c}, since this is the only region where V_{p_c} is important. Thus in the present treatment the core and valence contributions to V_p are calculated independently and added (Fig. 2), neglecting the induced effects of one upon the other. The core contribution is almost entirely due to the 2p→d excitation, since the 2p→s and 2s→p contributions cancelled each other almost exactly.

As a check on the accuracy of the calculations one can compare the asymptotic value of the calculated dipole polarization potential with the value which one knows should result, namely $V_p(r_f)\quad \alpha/r^4$ for $r \rightarrow \infty$ where α is the dipole polarizability whose value is available from experiment. Thus, in Table II we give the calculated value of α from the present calculation which is obtained from the equation $\alpha = V_p(r) \cdot r_f^4$ at $r_f = 25\,a_o$. The results are converted to Å^3 in II and compared with experimental values[15] and with other calculations.[14] The agreement with experiment is very good.

TABLE II. Dipole Polarizabilities From Asymptotic Value of V_p in Present Calculation and From Experiment.[15] Å^3

	Li	Na
Present	22.2	23.9
Measured	20-23	20-25
Sternheimer[a]	24.9	22.9

(a) Ref. 14

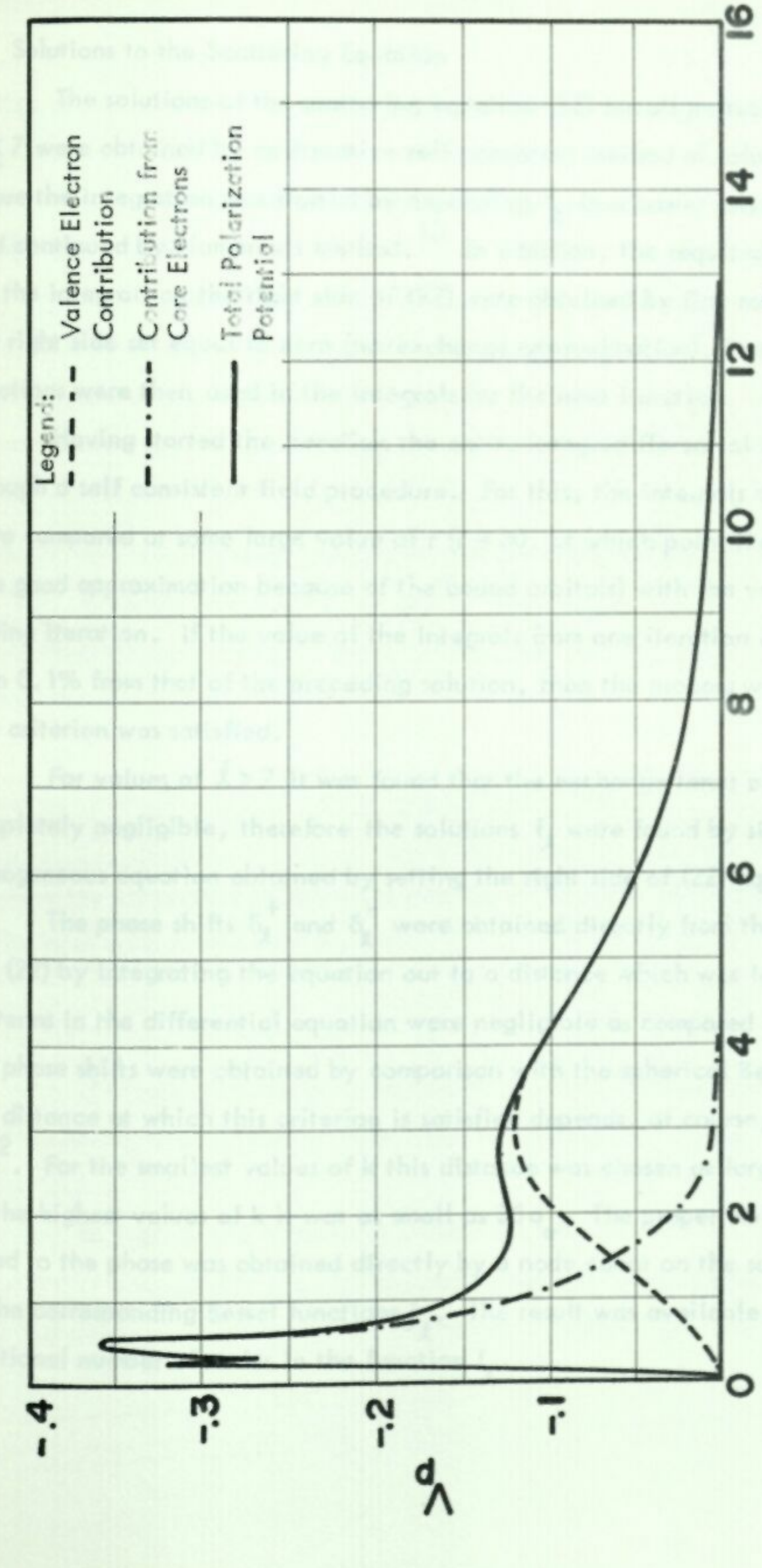

Fig. 2 Polarization potential for Na showing the contribution from the core electrons V_{p_c} and from the valence electron V_{p_v} together with their sum V_p.

B. Solutions to the Scattering Equation

The solutions of the scattering equation (22) for all partial waves f_ℓ having $\ell \leq 7$ were obtained by an iterative self consistent method of solution. In this technique the integration was started by expanding f_ℓ in a power series near the origin and continued by Numerov's method.[13] In addition, the required starting values for the integrals on the right side of (22) were obtained by first solving (22) with the right side set equal to zero (no-exchange approximation). The resulting wave functions were then used in the integrals for the next iteration.

Having started the iteration the entire integrodifferential equation was iterated through a self consistent field procedure. For this, the integrals on the right side were compared at some large value of r (r = 30, at which point the integrands vanish to a good approximation because of the bound orbitals) with the value from the preceding iteration. If the value of the integrals from one iteration differed by more than 0.1% from that of the preceding solution, then the process was repeated until this criterion was satisfied.

For values of $\ell > 7$ it was found that the exchange terms of Eq. (22) were completely negligible, therefore the solutions f_ℓ were found by simply solving the homogeneous equation obtained by setting the right side of (22) equal to zero.

The phase shifts δ_ℓ^+ and δ_ℓ^- were obtained directly from the solutions to Eq. (22) by integrating the equation out to a distance which was large enough that all terms in the differential equation were negligible as compared to k^2 ($< 10^{-4}$). The phase shifts were obtained by comparison with the spherical Bessel functions. The distance at which this criterion is satisfied depends, of course, on the value of k^2. For the smallest values of k this distance was chosen as large as 500 a_o and for the highest values of k it was as small as 35 a_o. The proper multiple of π to be added to the phase was obtained directly by a node count on the solutions f_ℓ and on the corresponding Bessel functions j_ℓ. The result was available directly from the additional number of nodes in the function f_ℓ.

For comparative purposes, the first few phase shifts for Na are shown in Fig. 3 with exchange included and in Fig. 4 with exchange neglected in the scattering equation. The effect of exchange is evident in the plot of the phase shifts. However, in the calculations of the total cross sections the effect is much more pronounced.

The values of the phase shifts for singlet and triplet scattering are listed in Tables A-I and A-II of Appendix I for several energies. In Table A-III are the phase shifts for higher values of ℓ where the triplet and singlet partial waves were indistinguishable. Finally, in Tables A-IV and A-V are listed the phase shifts for Li and Na with exchange effects ignored completely.[16]

V. TOTAL ELASTIC SCATTERING CROSS SECTIONS

With the phase shifts δ_ℓ^+ and δ_ℓ^- determined, the total elastic scattering cross section for the singlet or triplet case may be determined (in units of πa_o^2) from the expression

$$\sigma^{\pm} = \left(\frac{4}{k^2}\right) \sum_{\ell} (2\ell + 1) \sin^2 \delta_\ell^{\pm}$$

where the (+) refers to the singlet and the (–) to the triplet states of the system. The total cross section is then

$$\sigma = \frac{1}{4}\sigma + \frac{3}{4}\sigma^{-} .$$

If electron exchange is neglected the total cross section is given by Eq. where the δ_ℓ 's are those obtained from the homogeneous equation analogous to Eq. (22).

In Figs. 5 and 6 the total elastic scattering cross sections for Li and Na are shown compared to the experimental results of Perel, Englander and Bederson[17] and of Brode.[18] (The results are plotted as a function of $\sqrt{\text{volts}}$ in order to show

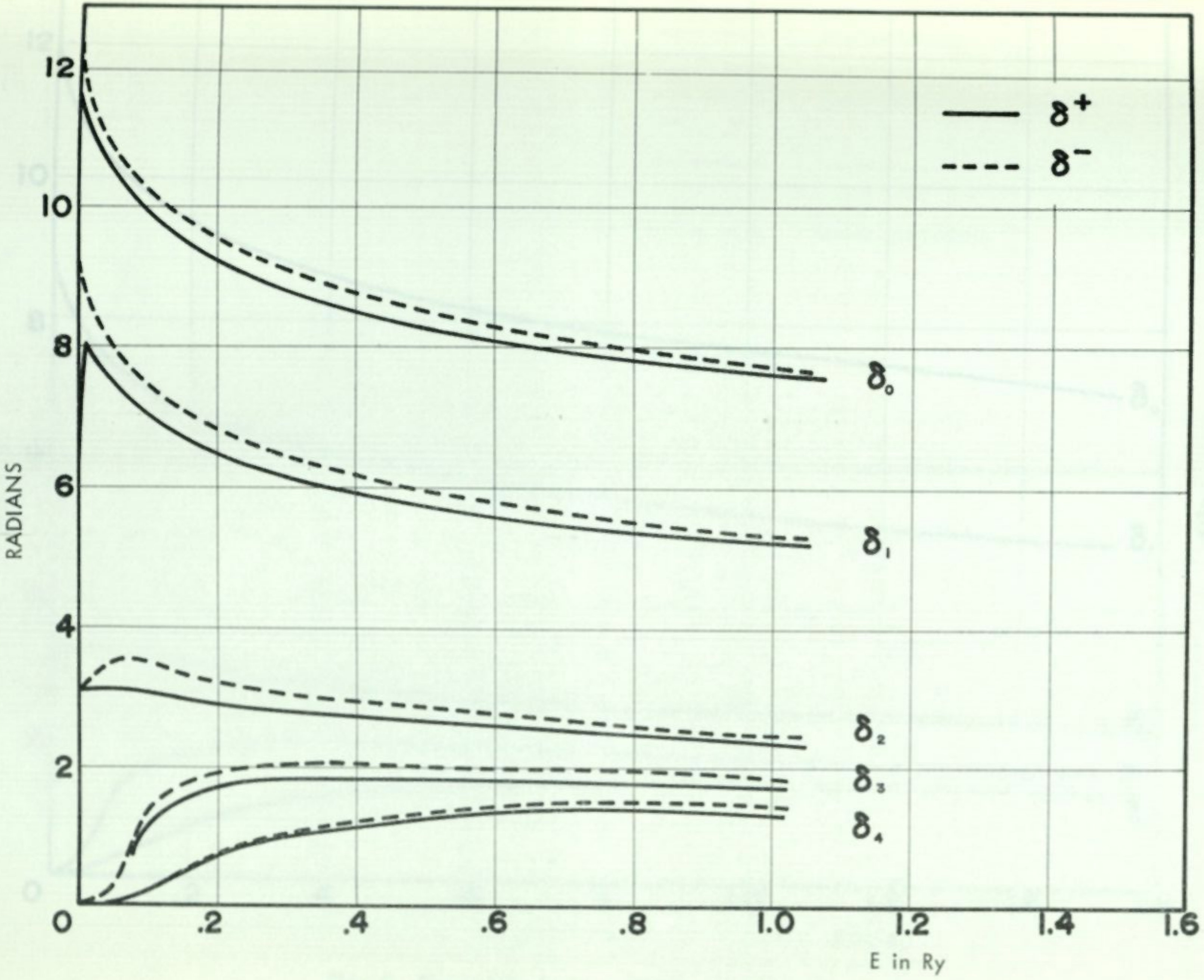

Fig. 3 Phase shifts for Na including electron exchange

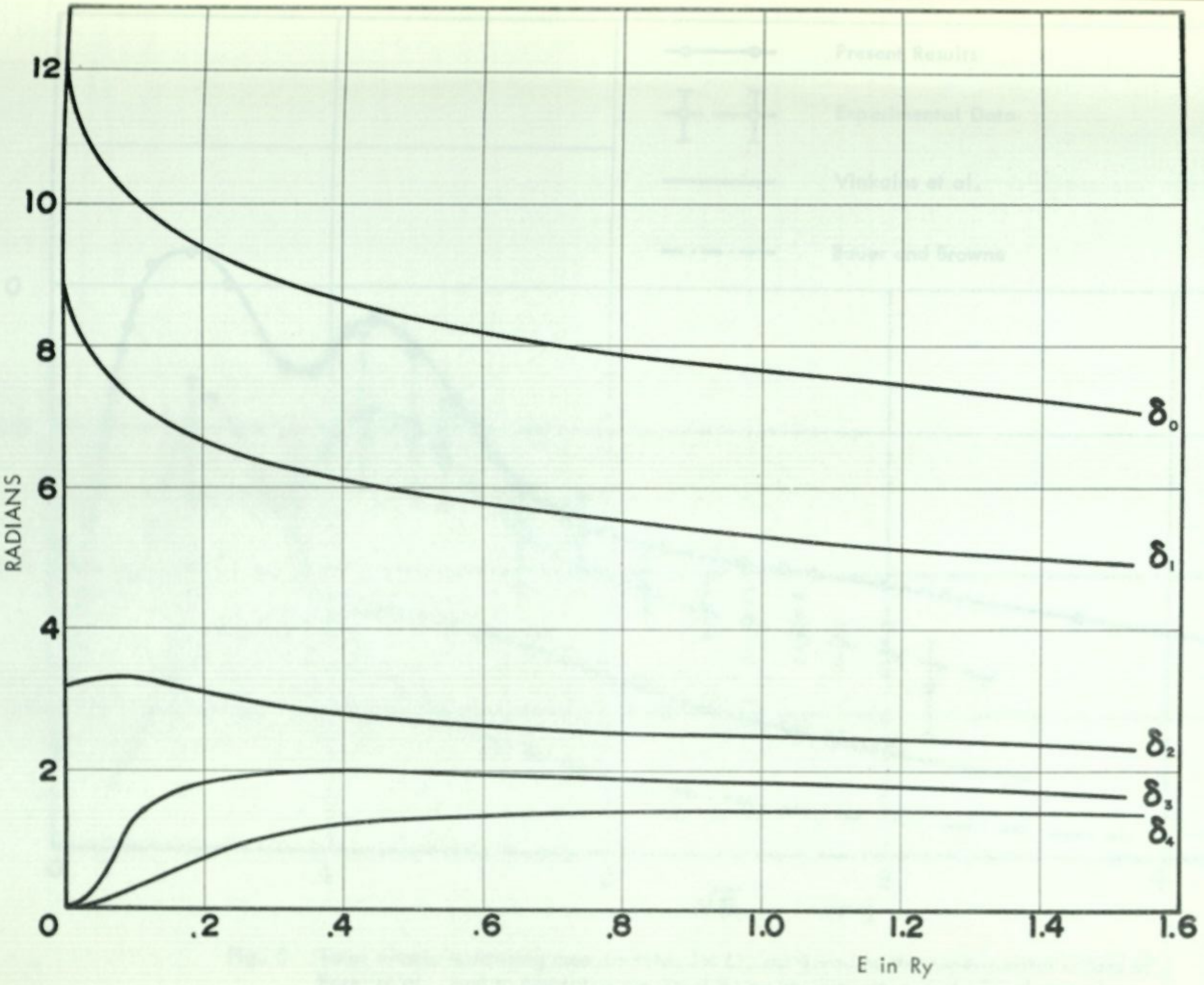

Fig. 4 Phase shifts for Na neglecting exchange effects.

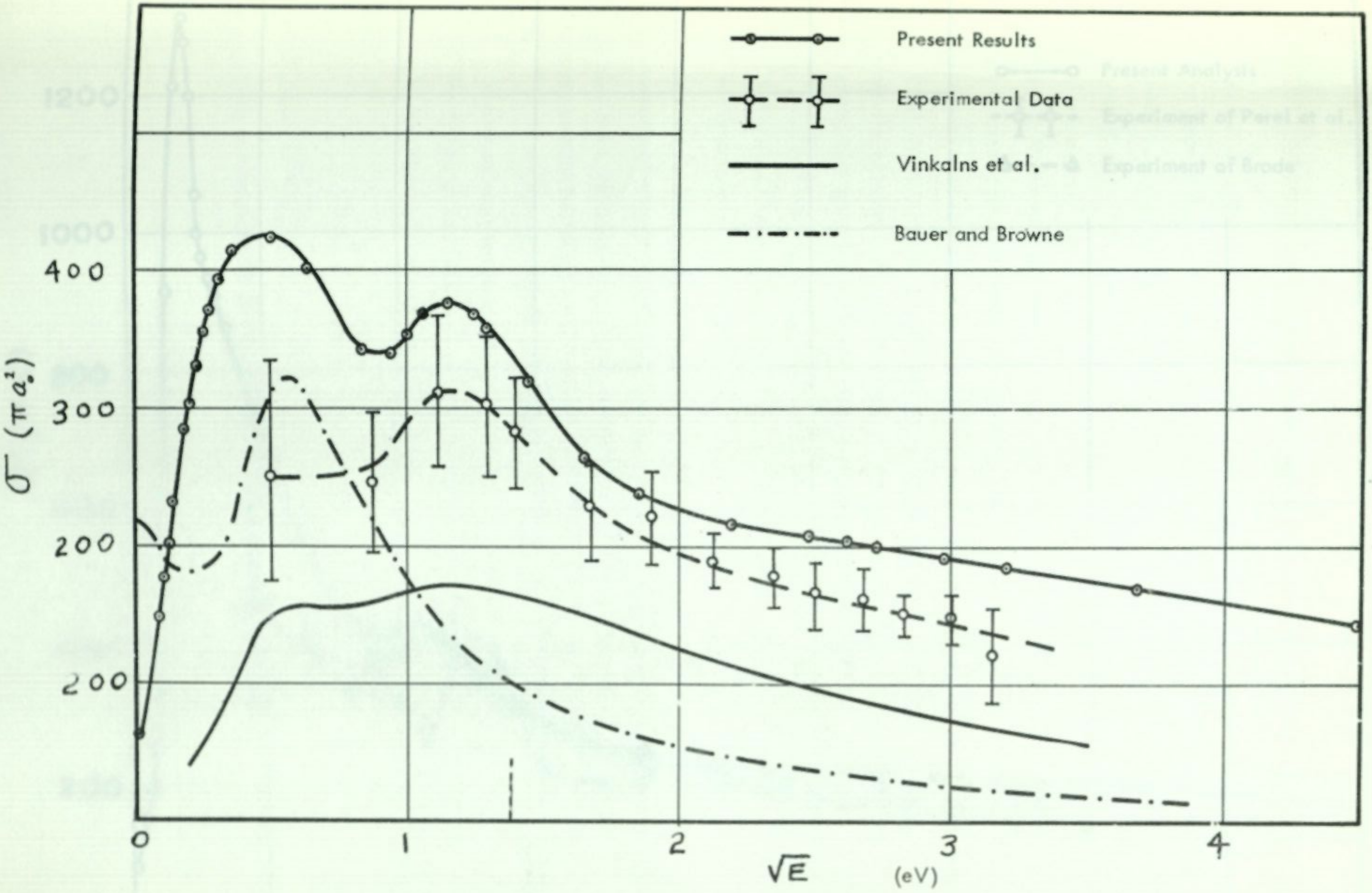

Fig. 5 Total elastic scattering cross sections for Li, compared to the experimental values of Perel et al., and to computed results of Bauer and Browne and of Vinkalns et al.

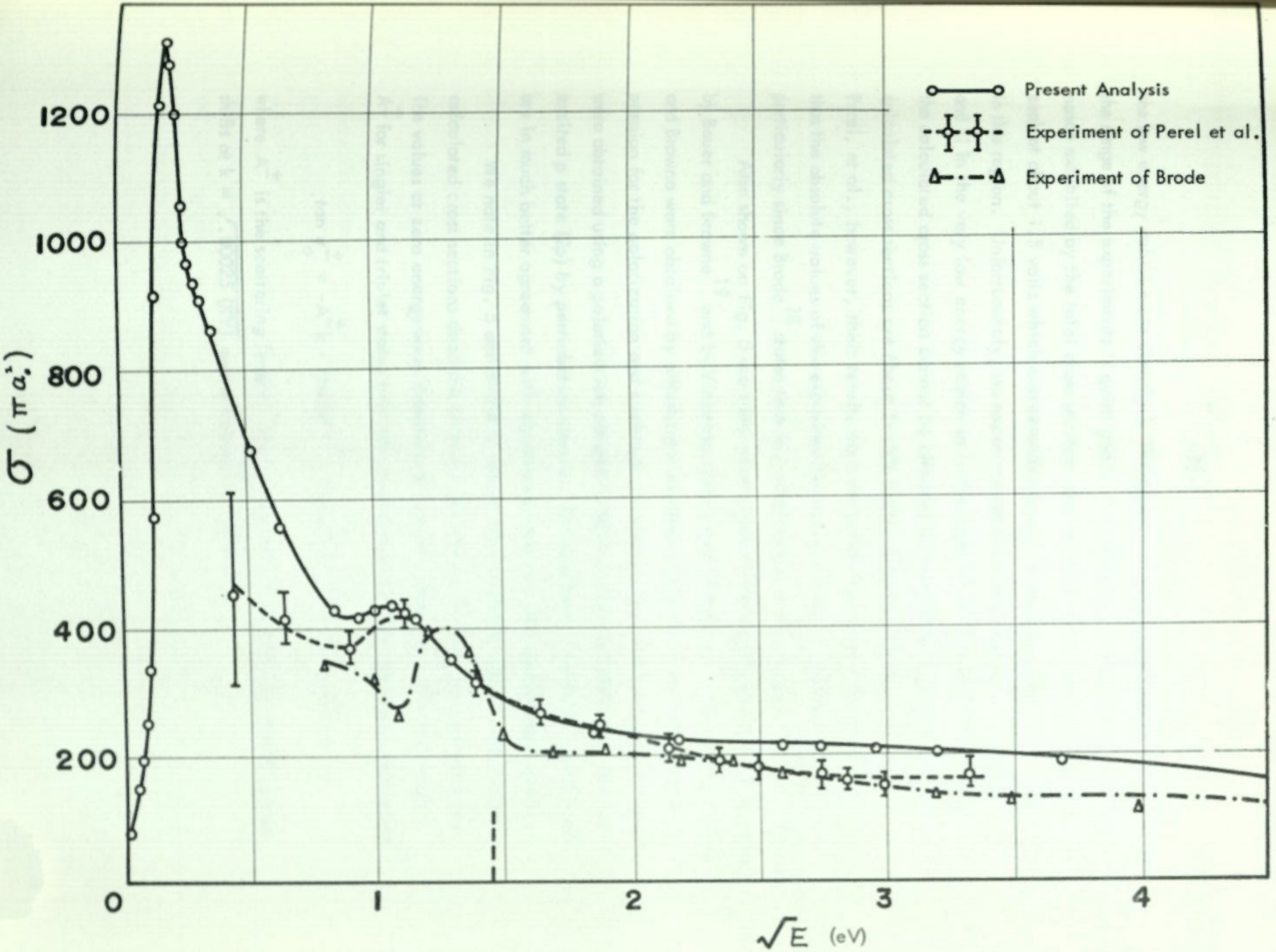

Fig. 6 Total elastic scattering cross sections for Na, with the experimental data of Brode and of Perel et al.

the low energy values more clearly.) The agreement with experimental values over the range of the experiments is quite good. In particular we note the double resonance exhibited by the total cross section, one at about 1/4 volt and another smaller peak at about 1.5 volts which corresponds exactly in energy to the experimental peak in this region. Unfortunately, no experimental cross sections are available for Na and Li in the very low energy region as in the case of Cs, thus the second peak in the calculated cross section cannot be checked against experiment at present. The calculated cross sections are about 5-15% higher than the experimental values of Perel, et al., however, their results were normalized to those of Brode at 2 eV, thus the absolute values of the experimental curve may be in error by this amount, particularly since Brode[18] states that his values below 4 eV are uncertain to $\pm$ 15%.

Also shown on Fig. 5 are some recent theoretical cross sections for Li obtained by Bauer and Browne[19] and by Vinkalns, Karule and Obedkov.[20] The results of Bauer and Browne were obtained by adjusting a variable parameter in an approximate expression for the polarization and exchange potential. The results of Vikalns, et al., were obtained using a polarization potential obtained from coupling with the first excited p state (2p) by perturbation theory. The results of the present calculations are in much better agreement with experiment than any of the prior calculations.

We note in Fig. 5 and 6 that in the present results for both Li and Na the calculated cross sections decrease to relatively small values at very low energies. The values at zero energy were determined by calculating the scattering lengths $A^{\pm}$ for singlet and triplet states from the modified effective range theory expansion[21]

$$\tan \sigma_o^{\pm} = -A^{\pm} k - (\pi a/3)\, k^2 - (4a A^{\pm}/3)\, k^2 \ln (1.23 \sqrt{ak}) + \cdots$$

where $A^{\pm}$ is the scattering length. The values of A were obtained from the phase shifts at $k = \sqrt{.00025 \text{ (RY)}}$ and are shown in Table VI.

TABLE III. Scattering Lengths for Li and Na

Li		Na	
A^+	A^-	A^+	A^-
7.554	2.088	6.511	1.634

It is worthwhile to compare the scattering lengths of Table III with those calculated for electron-hydrogen scattering by various methods. In the case of hydrogen the singlet scattering length is $A^+ = 6a_o$ and the triplet $A^- = 2a_o$ (Resenberg, Spruch and O'Malley[22] give upper bounds of $6.23a_o$ and $1.91\ a_o$ respectively for A^+ and A^-; other calculations agree well with these results.[23]) We note from the results of Table III that both the singlet and triplet scattering lengths of Li and Na are very little different from those of hydrogen. This is significant for two reasons. First, though the alkali atoms are much more complicated than hydrogen, they retain hydrogen-like characteristics and polarization and exchange effects are similarly important as in the hydrogen atom. Second, and perhaps more important for comparison purposes, is the fact that the negative ions of Li and Na are estimated to have approximately the same binding energy as that of the hydrogen atom (roughly .7-.8 eV).[24] Thus, heuristically one would predict that the singlet and triplet scattering lengths for these alkalis should resemble those for hydrogen, which is true in the present calculation.

The present results for zero energy differ quite drastically from those of other calculations for alkali atoms. The results of Vinkalns, Karule, and Obedkov[20] for Li are $A^+ = -4.8$ and $A^- = -10.4$ and those of Salmona and Seaton[25] for Na are $A^+ = 9$ and $A^- = -12$. Both these results are very much different from those for hydrogen and from the present results, being exactly opposite in relative magnitude and yielding much larger values of σ for $E = 0$. The present results also differ greatly from those for Cs by Crown and Russek,[26] $A^+ = -20$ and $A^- = 360a_o$ which yield very large cross sections at zero energy. Though no experimental data is available for comparison at very low energies, the present results seem more reasonable from the above argument. Also the results at higher energies are much better in the present calculation than in any of the previous alkali atom calculations, which lends some support to the present low energy results.

Finally in Figures 7 and 8 are plotted the total elastic scattering cross sections for Li and Na neglecting electron exchange. The results are compared with those having exchange included, thus exhibiting the effect of the Pauli principle on the calculated cross sections. The results at low energy are, as expected, strongly effected by exchange effects. This is especially true for Na where the figure shows that the results differ by an order of magnitude. Thus one can conclude that computed electron scattering cross sections for the alkalis are completely unreliable at energies below one volt in the no-exchange approximation, a fact which has earlier been demonstrated in the case of Cs.[3]

VI. CONCLUSIONS

From the results obtained in the present calculations it seems that the method of polarized orbitals and the adiabatic exchange approximation is capable of describing low energy electron scattering from more complicated atomic systems, these being represented by H.F. type wave functions. In the calculation of the polarization potential for the alkali atoms, the approximation used in earlier calculations,[4,6,10] that only the outer region of the perturbation equations be included, seems to be inadequate. Since the valence electron is very weakly bound, the wave function of the valence orbital has an appreciable amplitude over a rather large distance, and the inclusion of the inner and outer regions in the equations for the perturbed radial functions gives a strong dependence of the amplitude and the shape of the perturbation $U_{n\ell \rightarrow \ell'}$ on the free electron position. With the strong dependence of the scattering cross sections on the shape of the polarization potential in the region near the atomic radius, this behavior should not be ignored in the calculation of V_p.

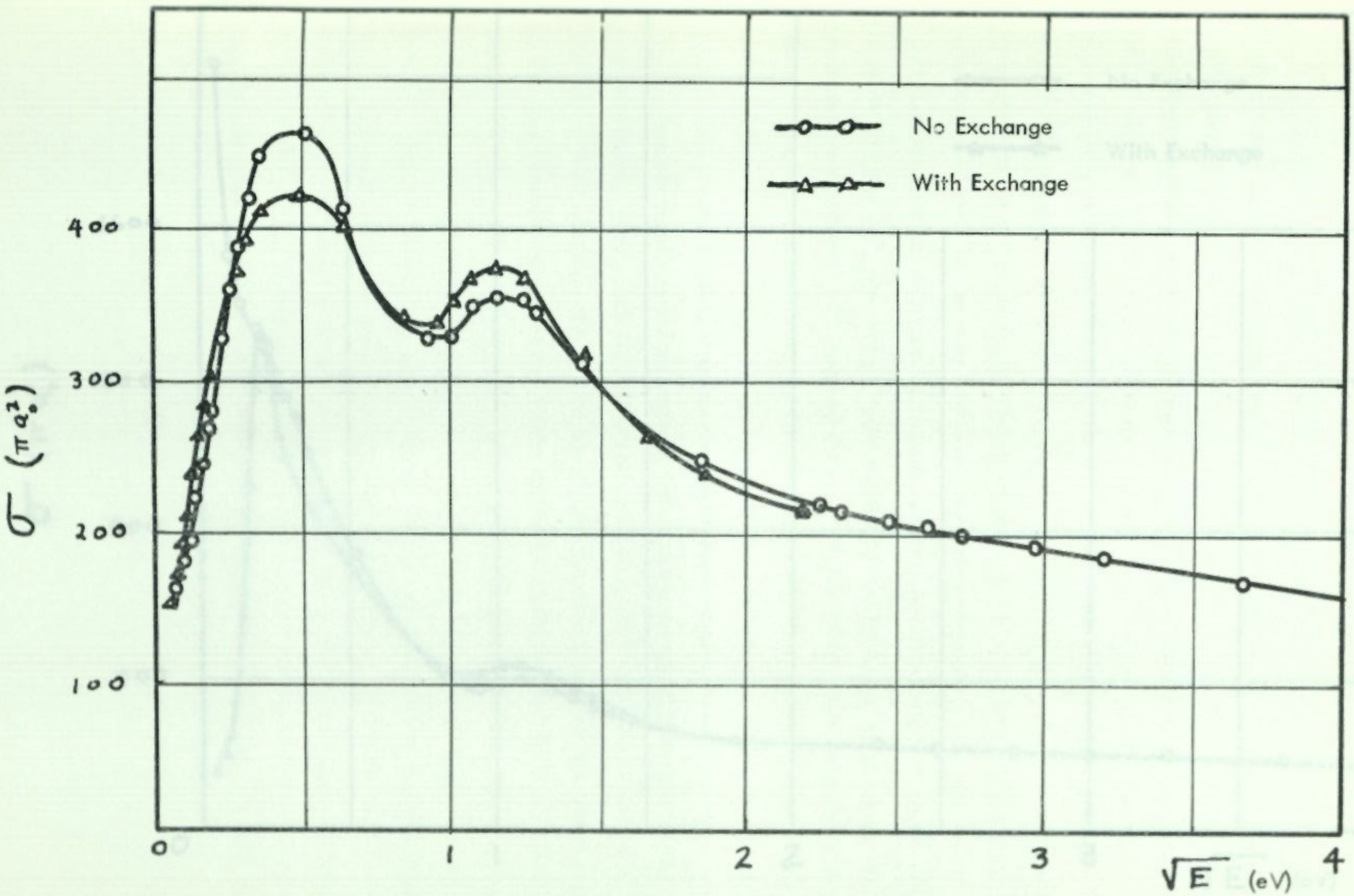

Fig. 7 Total elastic cross section for Li with and without exchange.

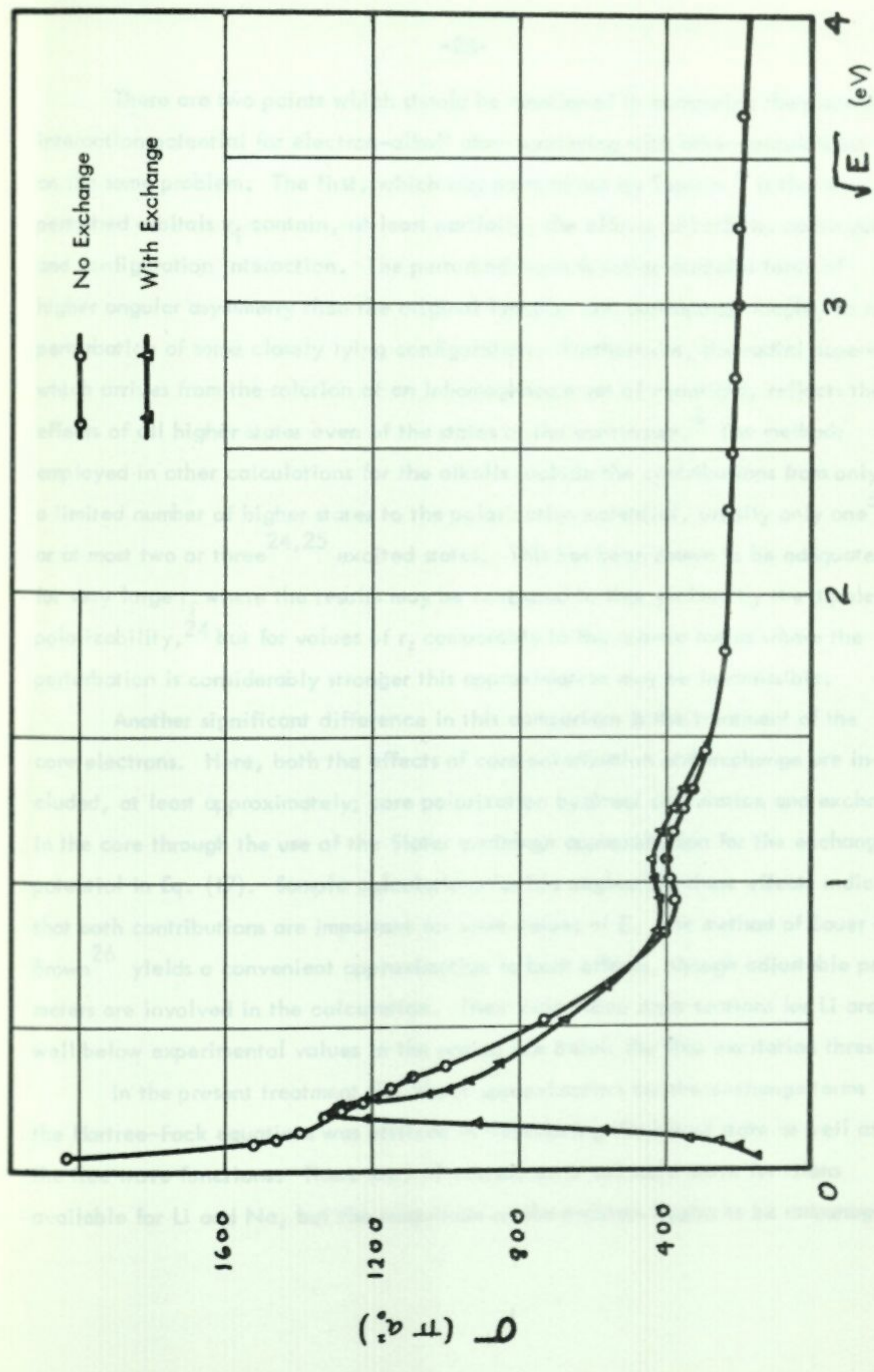

Fig. 8 Total elastic scattering cross section for Na with and without exchange.

There are two points which should be mentioned in comparing the present interaction potential for electron-alkali atom scattering with other calculations on the same problem. The first, which was pointed out by Temkin,[4] is that the perturbed orbitals χ_i contain, at least partially, the effects of both the continuum and configuration interaction. The perturbed wave function contains terms of higher angular asymmetry than the original function and corresponds roughly to a perturbation of some closely lying configuration. Furthermore, the radial dependence, which arrives from the solution of an inhomogeneous set of equations, reflects the effects of all higher states even of the states of the continuum.[4] The methods employed in other calculations for the alkalis include the contributions from only a limited number of higher states to the polarization potential, usually only one[5,23] or at most two or three[24,25] excited states. This has been shown to be adequate for very large r_f where the results may be compared to that yielded by the dipole polarizability,[24] but for values of r_f comparable to the atomic radius where the perturbation is considerably stronger this approximation may be inadmissible.

Another significant difference in this comparison is the treatment of the core electrons. Here, both the effects of core polarization and exchange are included, at least approximately; core polarization by direct calculation and exchange in the core through the use of the Slater exchange approximation for the exchange potential in Eq. (17). Sample calculations for Na neglecting these effects indicate that both contributions are important for some values of E. The method of Bauer and Brown[26] yields a convenient approximation to both effects, though adjustable parameters are involved in the calculation. Their calculated cross sections for Li are well below experimental values in the region just below the first excitation threshold.

In the present treatment the Slater approximation for the exchange terms in the Hartree-Fock equations was utilized in calculating the bound state as well as the free wave functions. There are, of course, more accurate wave functions available for Li and Na, but the magnitude of the problem begins to be unmanagable in the complete H.F. perturbation calculation. The H.F.S. wave functions are, in fact, very close approximations to the H.F. solutions and since exchange polarization terms are neglected in the polarization potential calculations, it seems that little would be gained by using more exact H.F. ground state wave functions in the equations derived here. In fact, the present investigation indicates that a useful criterion for a "good" set of bound state wave functions in a low energy scattering problem where the polarization potential is so important is that set which gives a good value of the polarizability in the polarization potential calculation. The H.F.S. wave functions used here satisfy this requirement very well.

APPENDIX

Tables of phase shifts for Li and Na

TABLE A-I

Singlet and Triplet Phase Shifts for Li

E (Ry)	δ_0^+	δ_1^+	δ_2^+	δ_3^+	δ_4^+	δ_5^+	δ_6^+	δ_0^-	δ_1^-	δ_2^-	δ_3^-	δ_4^-	δ_5^-	δ_6^-
.00025	9.2756	6.2738	3.1426	.000				9.3549	6.2850	3.1426	.000			
.0050	9.2055	6.2548	3.1437	.000				9.3140	6.2857	3.1438	.000			
.00075	9.1501	6.2327	3.1446	.000				9.2796	6.2832	3.1450	.000			
.0010	9.1023	6.2058	3.1452	.001				9.2486	6.2787	3.1461	.001			
.0015	9.022	6.157	3.147	.002				9.195	6.267	3.149	.002			
.0020	8.954	6.111	3.148	.003				9.148	6.253	3.152	.003			
.0025	8.894	6.067	3.149	.004				9.105	6.236	3.155	.004			
.0030	8.840	6.026	3.149	.006	.002			9.066	6.219	3.158	.005	.002		
.0040	8.745	5.952	3.148	.006	.003			8.995	6.184	3.164	.006	.003		
.0050	8.662	5.886	3.147	.008	.003			8.932	6.148	3.170	.008	.003		
.0060	8.588	5.827	3.145	.010	.004			8.375	6.111	3.177	.010	.004		
.075	8.490	5.748	3.142	.013	.005			8.798	6.058	3.188	.013	.005		
.010	8.355	5.636	3.135	.017	.007			8.684	5.975	3.209	.018	.007		
.020	7.955	5.321	3.109	.049	.016	.008		8.345	5.704	3.300	.049	.016	.008	
.030	7.683	5.113	3.089	.100	.027	.012	.007	8.095	5.499	3.380	.101	.027	.012	.007
.050	7.313	4.853	3.065	.270	.064	.025	.013	7.733	5.223	3.448	.282	.063	.025	.013
.065	7.101	4.732	3.043	.451	.102	.038	.018	7.523	5.053	3.458	.486	.103	.038	.018
.075	6.984	4.642	3.027	.590	.133	.048	.022	7.393	4.963	3.451	.650	.134	.048	.022
.085	6.879	4.562	3.011	.734	.167	.061	.027	7.293	4.873	3.436	.827	.168	.061	.027
.100	6.741	4.462	2.989	.922	.223	.081	.036	7.148	4.763	3.402	1.060	.224	.081	.036
.125	6.546	4.302	2.946	1.210	.325	.121	.054	6.939	4.622	3.346	1.410	.329	.122	.054
.150	6.383	4.182	2.902	1.410	.419	.167	.075	6.763	4.482	3.285	1.640	.426	.167	.075
.250	5.909	3.821	2.746	1.662	.776	.353	.174	6.241	4.064	3.061	1.902	.805	.356	.174
.500	5.243	3.328	2.461	1.812	1.200	.710	.419	5.482	3.490	2.676	1.982	1.270	.726	.422
.750	4.837	3.047	2.270	1.767	1.323	.896	.592	5.025	3.117	2.431	1.919	1.398	.924	.600
1.000	4.511	2.857	2.127	1.727	1.357	.993	.704	4.704	2.950	2.254	1.838	1.428	1.028	.718

TABLE A-II

Singlet and Triplet Phase Shifts for Na

ε (Ry)	δ_0^+	δ_1^+	δ_2^+	δ_3^+	δ_4^+	δ_5^+	δ_6^+	δ_0^-	δ_1^-	δ_2^-	δ_3^-	δ_4^-	δ_5^-	δ_6^-
.00025	12.4297	6.3070	3.1430					12.5002	9.4183	3.1430	.000			
.00050	12.3625	6.3460	3.1444	.000				12.4587	9.4017	3.1445	.000			
.00075	12.3090	6.3995	3.1450	.000				12.4237	9.3814	3.1459	.000			
.0010	12.2609	6.4740	3.1451	.000				12.3912	9.3528	3.1454	.0003			
.0015	12.183	6.680	3.147	.001				12.336	9.307	3.148	.001			
.0020	12.116	6.960	3.149	.002				12.288	9.262	3.152	.002			
.0025	12.060	7.283	3.152	.003				12.240	9.219	3.156	.003			
.0030	12.006	7.573	3.153	.004	.000			12.206	9.177	3.159	.004	.000		
.0040	11.913	7.765	3.156	.006	.002			12.133	9.100	3.167	.006	.002		
.0050	11.832	8.113	3.157	.008	.003			12.069	9.031	3.175	.008	.003		
.0060	11.759	8.193	3.158	.010	.004			12.010	8.968	3.183	.011	.004		
.0075	11.663	8.035	3.158	.014	.006			11.931	8.883	3.198	.014	.006		
.010	11.526	8.025	3.157	.021	.009			11.814	8.762	3.224	.021	.009		
.020	11.126	7.845	3.150	.057	.018	.009		11.466	8.415	3.348	.057	.018	.009	
.030	10.855	7.753	3.144	.121	.031	.014	.008	11.216	8.185	3.461	.124	.031	.014	.008
.050	10.475	7.473	3.133	.345	.075	.028	.014	10.835	7.885	3.554	.370	.075	.028	.014
.065	10.259	7.313	3.116	.583	.123	.043	.020	10.615	7.743	3.567	.654	.124	.043	.020
.075	10.137	7.221	3.101	.760	.161	.056	.025	10.495	7.633	3.559	.874	.162	.056	.025
.085	10.028	7.139	3.086	.935	.204	.071	.031	10.382	7.543	3.538	1.100	.205	.071	.031
.100	9.886	7.029	3.065	1.140	.273	.097	.042	10.231	7.413	3.507	1.350	.276	.097	.042
.125	9.683	6.871	3.022	1.420	.397	.146	.064	10.016	7.232	3.445	1.610	.403	.147	.064
.150	9.512	6.738	2.979	1.590	.567	.201	.089	9.833	7.079	3.382	1.712	.519	.202	.090
.250	9.016	6.349	2.833	1.752	.896	.420	.208	9.292	6.626	3.159	2.002	.939	.424	.209
.500	8.305	5.790	2.597	1.842	1.270	.797	.483	8.506	5.975	2.811	2.012	1.360	.819	.488
.750	7.840	5.453	2.464	1.792	1.370	.969	.662	8.028	5.588	2.617	1.928	1.451	1.003	.673
1.000	7.568	5.212	2.383	1.761	1.380	1.049	.766	7.683	5.316	2.497	1.843	1.456	1.088	.783

TABLE A-III

Phase Shifts for Higher ℓ Values

Li and Na $\delta_\ell^+ \sim \delta_\ell^- = \delta_\ell$

	Li									Na								
E	δ_7	δ_8	δ_9	δ_{10}	δ_{11}	δ_{12}	δ_{13}	δ_{14}	δ_{15}	δ_7	δ_8	δ_9	δ_{10}	δ_{11}	δ_{12}	δ_{13}	δ_{14}	δ_{15}
.050	.008									.008								
.065	.011	.007								.012	.008							
.075	.013	.008								.014	.009							
.085	.015	.009								.016	.010							
.100	.019	.012								.021	.013							
.125	.028	.016	.010							.031	.018	.011						
.150	.038	.021	.013							.045	.025	.015						
.250	.095	.054	.032							.114	.064	.037						
.500	.256	.159	.103	.066						.301	.188	.123	.080					
.750	.392	.263	.178	.123	.086	.061	.044	.032		.448	.306	.209	.146	.101	.072	.052	.038	
1.000	.496	.349	.247	.176	.128	.092	.069	.051	.038	.556	.396	.286	.206	.152	.110	.081	.062	.044

TABLE A-IV

Phase Shifts for Lithium (No exchange)

Energy	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6	δ_7
.0005	3π - .142	2π - .008	π + .001					
.00075	3π - .182	2π - .014	π + .003					
.0010	3π - .217	2π - .024	π + .004	.001				
.0015	3π - .279	2π - .048	π + .007	.002				
.0020	3π - .331	2π - .073	π + .010	.003				
.0025	3π - .379	2π - .100	π + .012	.004				
.0030	3π - .422	2π - .127	π + .015	.005				
.0040	3π - .500	2π - .180	π + .019	.007				
.0050	3π - .569	2π - .231	π + .024	.008	.004			
.0060	3π - .631	2π - .279	π + .029	.010	.005			
.0075	3π - .741	2π - .346	π + .036	.013	.006			
.010	3π - .836	2π - .447	π + .048	.019	.008			
.020	3π - 1.197	2π - .750	π + .092	.049	.016	.008		
.030	3π - 1.452	2π - .963	π + .120	.100	.027	.012	.008	
.050	2π + 1.313	2π - 1.231	π + .142	.276	.064	.025	.013	.008
.065	2π + 1.098	2π - 1.397	π + .133	.467	.110	.040	.019	.011
.075	2π + .976	2π - 1.480	π + .120	.602	.130	.047	.022	.013
.085	2π + .867	2π - 1.575	π + .103	.776	.167	.060	.027	.015
.100	2π + .720	π + 1.487	π + .075	.983	.217	.081	.036	.019
.115	2π + .590	π + 1.388	π + .044	1.185	.285	.105	.047	.024
.125	2π + .511	π + 1.328	π + .022	1.300	.327	.121	.054	.029
.150	2π + .335	π + 1.193	π - .031	π - 1.501	.422	.162	.073	.038
.250	2π - .179	π + .805	π - .228	π - 1.368	.790	.354	.174	.095
.350	2π - .530	π + .544	π - .383	π - 1.257	1.033	.519	.276	.156
.400	2π - .673	π + .441	π - .451	π - 1.244	1.118	.593	.330	.190
.450	2π - .798	π + .350	π - .512	π - 1.240	1.184	.660	.379	.224
.500	2π - .913	π + .269	π - .569	π - 1.243	1.237	.718	.421	.257
.550	2π - 1.014	π + .197	π - .620	π - 1.245	1.271	.764	.462	.284
.650	2π - 1.193	π + .072	π - .711	π - 1.263	1.325	.845	.533	.340
.750	2π - 1.347	π - .033	π - .789	π - 1.289	1.357	.910	.593	.390
1.00	π + 1.490	π - .237	π - .950	π - 1.358	1.393	1.010	.711	.496
1.50	π + 1.062	π - .506	π - 1.173	π - 1.491	1.380	1.095	.839	.636
2.00	π + .768	π - .685	π - 1.32	1.561	1.336	1.111	.897	.715

Phase Shifts (contd.) and Cross Sections for Lithium

Energy	δ_8	δ_9	δ_{10}	δ_{11}	δ_{12}	δ_{13}	δ_{14}	δ_{15}	$\sigma\,(a_0^2)$
.0005									504.4
.00075									559.7
.0010									607.5
.0015									693.0
.0020									770.9
.0025									842.3
.0030									873.9
.0040									1030.3
.0050									1131.1
.0060									1214.1
.0075									1310.6
.010									1411.5
.020									1456.9
.030									1289.0
.050									1071.1
.065	.007								1033.3
.075	.008								1031.6
.085	.009								1089.7
.100	.011								1106.6
.115	.014	.009							1103.7
.125	.017	.011							1077.6
.150	.021	.013							969.1
.250	.054	.032							755.3
.350	.091	.056	.035						684.4
.400	.114	.071	.045						662.8
.450	.136	.087	.056						648.7
.500	.159	.103	.066						633.7
.550	.182	.117	.784						617.1
.650	.220	.147	.098	.067					590.5
.750	.261	.177	.122	.085	.061	.043			569.0
1.00	.349	.247	.176	.128	.092	.069	.051	.038	519.1
1.50	.477	.362	.273	.210	.160	.122	.096	.073	440.7
2.00	.562	.444	.348	.278	.219	.172	.140	.110	382.0

TABLE A-V

Phase Shifts for Sodium (No exchange)

Energy	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6	δ_7	δ_8	δ_9
.00075	4π - .178	3π - .295	π + .002							
.0010	4π - .212	3π - .333	π + .003	.0003						
.0015	4π - .273	3π - .397	π + .006	.001						
.0020	4π - .327	3π - .451	π + .009	.002						
.0025	4π - .375	3π - .499	π + .013	.003						
.0030	4π - .418	3π - .542	π + .016	.004	.001					
.0040	4π - .497	3π - .617	π + .023	.006	.002					
.0050	4π - .566	3π - .682	π + .029	.008	.003					
.0060	4π - .629	3π - .741	π + .035	.011	.004					
.0075	4π - .714	3π - .819	π + .045	.014	.006					
.0100	4π - .837	3π - .929	π + .062	.014	.006					
.0200	4π - 1.20	3π - 1.25	π + .133	.057	.018	.009				
.0300	4π - 1.47	3π - 1.47	π + .189	.123	.031	.014	.008			
.0500	3π + 1.29	2π + 1.44	π + .228	.357	.075	.028	.014	.008		
.0650	3π + 1.07	2π + 1.26	π + .225	.616	.124	.043	.020	.012	.008	
.0750	3π + .942	2π + 1.16	π + .213	.810	.162	.057	.025	.014	.009	
.0850	3π + .830	2π + 1.07	π + .197	1.01	.205	.072	.031	.017	.010	
.1000	3π + .679	2π + .954	π + .166	1.23	.275	.097	.042	.021	.013	.009
.1150	3π + .544	2π + .846	π + .134	1.43	.349	.126	.054	.027	.016	.010
.1250	3π + .463	2π + .781	π + .112	1.53	.401	.147	.064	.031	.018	.011
.1500	3π + .281	2π + .637	π + .056	1.56	.514	.202	.090	.045	.025	.015
.2500	3π - .250	2π + .211	π - .135	π - 1.26	.917	.422	.208	.115	.064	.037
.3500	3π - .615	2π - .081	π - .278	π - 1.21	1.15	.609	.330	.190	.111	.070
.4000	3π - .763	2π - .200	π - .337	π - 1.20	1.23	.682	.388	.225	.139	.085
.4500	3π - .894	2π - .305	π - .387	π - 1.21	1.28	.750	.442	.264	.162	.104
.5000	3π - 1.01	2π - .399	π - .433	π - 1.22	1.32	.808	.486	.301	.188	.123
.5500	3π - 1.12	2π - .484	π - .474	π - 1.22	1.35	.852	.531	.331	.215	.139
.6500	3π - 1.31	2π - .634	π - .543	π - 1.25	1.38	.932	.603	.396	.260	.177
.7500	3π - 1.47	2π - .762	π - .599	π - 1.28	1.41	.986	.668	.448	.306	.209
1.000	2π + 1.34	2π - 1.02	π - .702	π - 1.35	1.42	1.07	.775	.556	.396	.287
1.500	2π + .880	2π - 1.38	π - .817	π - 1.47	1.38	1.12	.889	.691	.530	.408

Phase Shifts (contd.) and Cross Sections for Sodium

Energy	δ_{10}	δ_{11}	δ_{12}	δ_{13}	δ_{14}	δ_{15}	δ_{16}	$\sigma\ (a_0^2)$
.00075								4778.0
.0010								4594.1
.0015								4375.6
.0020								4235.2
.0025								4127.7
.0030								4036.5
.0040								3877.5
.0050								3734.4
.0060								3601.6
.0075								3417.2
.0100								3139.1
.0200								2313.9
.0300								1780.6
.0500								1267.2
.0650								1206.7
.0750								1234.7
.0850								1256.2
.1000								1200.6
.1150								1113.0
.1250								1047.5
.1500								914.8
.2500								753.4
.3500	.044							724.8
.4000	.054							712.9
.4500	.067							704.3
.5000	.080							693.0
.5500	.094							679.5
.6500	.118	.080						657.3
.7500	.146	.101	.072	.052				635.0
1.000	.206	.152	.110	.081	.062	.044		575.3
1.500	.313	.243	.188	.145	.114	.086	.070	481.8

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