Scattering of Slow Electrons by Neon and Argon

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Total elastic scattering cross sections have been computed for the scattering of electrons by neutral neon and argon in the energy range 0–1 Ry. These results were obtained by the polarized-orbital method wherein a polarization potential accounts for the distortion of the atomic electron distribution by the scattering electron. The polarization potentials are determined using perturbed orbitals obtained by the Sternheimer and Hartree-Fock-Slater (HFS) approximations. Dipole polarizabilities are also calculated. The results are used to evaluate total scattering cross sections by the two approximations and evaluate their capabilities by comparison with experimental data. The HFS-based approximation works very well for neon giving substantially improved cross sections over earlier Sternheimer-based calculations by Thompson. However, little improvement is obtained in either case for argon.

I. INTRODUCTION

Recently Matese and LaBahn[1] calculated the photo-ionization cross section for lithium, wherein they successfully applied the method of polarized orbitals to account for core-polarization effects. Their approach was a logical extension of the application by LaBahn and Callaway[2,3] of the polarized-orbital method to the analysis of elastic scattering of electrons from helium. A similar approach suggested itself for the case of the heavier alkali metals, the next two being sodium and potassium. The complementary problem, which will give some indication of the validity of a polarized-orbital calculation on equivalent electronic core configurations, is the analysis of elastic scattering of electrons by neon and argon. The purpose of this paper is to present the results of calculations on the elastic scattering of electrons by neon and argon by the polarized-orbital method.

It has been understood for about 40 years that the problem of slow-electron scattering by rare-gas atoms requires consideration of both exchange and polarization effects. Exchange effects have generally been accounted for by assuming the wave function for the system to be of a properly antisymmetrized form. Polarization effects avoided a simple analysis until about 15 years ago when the method of polarized orbital was developed.[4] This method, which is applied in this paper, determines a polarization potential that accounts for the polarization of the atom by the scattering electron.

In 1966, Thompson[5] analyzed the elastic scattering of electrons by neon and argon incorporating both exchange and polarization effects. He used a variant of the polarized-orbital method known as the adiabatic-exchange approximation. His results were in good agreement with experiment near zero energy and maintained relatively good agreement to an energy of 1 Ry.

With the availability of greater computer capacity it has been possible to extend Thompson's treatment of the problem. In particular, he considered only the $np \rightarrow d$ transition, while we have examined all the excitations from the outermost orbital for which $\Delta l = \pm 1$. Calculations were made in either an unnormalized or normalized manner, depending on whether or not the calculated polarizability was close to the experimental value.

Thompson obtained his polarization potential by determining the polarized orbital using the Sternheimer approximation. In this paper the Sternheimer procedure was also utilized and in addition, an alternative one based upon the Slater-averaged-exchange approximation was developed. A comparison of our total cross-section results for both procedures is made with those of Thompson and some recent experiments.

The derivation of the pertinent equations, up to the point of applying either the Sternheimer or Slater approximation is given in Sec. II. The formalism of the Sternheimer and Slater approximations appears in Sec. III. Section IV contains the results and discussions.

II. PERTURBATION THEORY FORMALISM

In the method of polarized orbitals one seeks to find the first-order correction to the atomic orbitals arising from the perturbation by the electric field of the scattering electron. The only orbitals considered to be perturbed are the outer ones which correspond to the least tightly bound electrons. The extension of the Hartree-Fock (HF) formalism[6] for an unperturbed atom or ion to first-order perturbation theory yields for the form of the one-electron HF equation

$$[h(1) + \lambda h' - \epsilon_i]\chi_i(1) = 0, \quad i = 1, 2, \ldots, N \tag{1}$$

where the spin orbitals χ_i are orthonormal; that is,

$$\langle \chi_i | \chi_j \rangle = \delta_{ij}, \quad i,j = 1, 2, \ldots, N . \tag{2}$$

In Eq. (1), $h(1)$ is the one-electron HF operator which for an atom of charge z takes the form

$$h(1) = -\nabla_1^2 - 2Z/r_1 + \sum_{j=1}^{N} 2\langle \chi_j | r_{12}^{-1}(1 - P_{12}) | \chi_j \rangle , \tag{3}$$

and h' represents the perturbation $(2|\vec{r}_1 - \vec{r}_e|^{-1}$ in our case, where $\vec{r}_e$ is the coordinate of the perturbing charge). The operator in the summation in Eq. (3) signifies

$$\langle \chi_j | r_{12}^{-1}(1 - P_{12}) | \chi_j \rangle f(1) = f(1) \int \chi_j^*(2) r_{12}^{-1} \chi_j(2)\, d\tau_2 - \chi_j(1) \int \chi_j^*(2) r_{12}^{-1} f(2)\, d\tau_2 , \tag{4}$$

where $f(1)$ is an arbitrary function of the space and spin coordinates of electron 1.

Introducing a perturbation expansion, one writes

$$\chi_i = \chi_i^0 + \lambda \chi_i' + \cdots , \tag{5}$$

$$\epsilon_i = \epsilon_i^0 + \lambda \epsilon_i' + \cdots , \tag{6}$$

which upon substitution into Eq. (1) yields for the zeroth and first order in λ, respectively,

$$[h^0(1) - \epsilon_i^0] \chi_i^0(1) = 0 , \tag{7}$$

$$[h^0(1) - \epsilon_i^0] \chi_i'(1) + [h' - \epsilon_i'] \chi_i^0(1) + \sum_{j=1}^{N} 2[\langle \chi_j' | r_{12}^{-1}(1 - P_{12}) | \chi_j^0 \rangle + \langle \chi_j^0 | r_{12}^{-1}(1 - P_{12}) | \chi_j' \rangle] \chi_i^0(1) = 0 , \tag{8}$$

where $h^0(1)$ is the zeroth-order HF operator

$$h^0(1) = -\nabla_1^2 - 2Z/r_1 + \sum_{j=1}^{N} 2\langle \chi_j^0 | r_{12}^{-1}(1 - P_{12}) | \chi_j^0 \rangle . \tag{9}$$

This operator has solutions χ_i^0 which are the usual HF orbitals and obey the orthonormality relation

$$\langle \chi_i^0 | \chi_j^0 \rangle = \delta_{ij}, \quad i,j = 1, 2, \ldots, N . \tag{10}$$

The first-order equation (8) will yield ϵ_i', once χ_i' is found, by multiplication on the left-hand side by $\chi_i^0(1)$ and integrating over the coordinates of electron 1. This first-order coupled HF equation has been solved by Langhoff, Karplus, and Hurst, [7] who report the effort to be very time consuming. The problem of finding a satisfactory approximation to the solution can be expedited by neglecting all of the terms which represent essentially small effects but add considerable complication.

One of the simplest uncoupling procedures, first suggested by Dalgarno, [8] is to neglect in Eq. (8) all terms in the sum over j. This results in the equation

$$[h^0(1) - \epsilon_i^0] \chi_i'(1) + [h' - \epsilon_i'] \chi_i^0(1) = 0 . \tag{11}$$

Another uncoupling procedure which is equally convenient was suggested by Langhoff, Karplus, and Hurst. [7] We first rearrange Eq. (8) and write it in the form

$$[h_i^0(1) - \epsilon_i^0] \chi_i'(1) + [h' - \epsilon_i'] \chi_i^0(1) + \sum_{j=1}^{N} (j \neq i) 2[\langle \chi_j' | r_{12}^{-1}(1 - P_{12}) | \chi_j^0 \rangle + \langle \chi_j^0 | r_{12}^{-1}(1 - P_{12}) | \chi_j' \rangle] \chi_i^0(1) = 0 , \tag{8'}$$

where the operator $h_i^0(1)$ acting on χ_i' is

$$h_i^0(1) = -\nabla_1^2 - 2Z/r_1 + \sum_{j=1}^{N} (j \neq i) 2\langle \chi_j^0 | r_{12}^{-1}(1 - P_{12}) | \chi_j^0 \rangle . \tag{12}$$

One should note that Eqs. (8) and (8′) are equivalent, since in Eq. (8) the term $j = i$ in the explicit sum over j cancels the self-potential term $j = i$ in $h^0(1)$. The terms with $j \neq i$ in Eq. (8′), known as the first-order self-consistency correction, are now dropped to simplify the equation. This will eliminate all the terms involving first-order functions χ_j' other than the one being calculated (χ_i'), thus uncoupling the equation and leaving the expression

$$[h_i^0(1) - \epsilon_i^0] \chi_i'(1) + [h' - \epsilon_i'] \chi_i^0(1) = 0 . \tag{13}$$

This differs from Eq. (11) in having a modified operator $h_i^0(1)$ [Eq. (12)].

Langhoff *et al.* [7] have solved these three approximations, including the fully coupled equation (8), and together with yet a fourth approximation have applied the solutions to calculate the dipole and quadrupole polarizabilities and shielding factors of various atoms and ions. Their results show that the approximation represented by Eq. (13) is significantly better than that of Eq. (11) in that it gives values that are in good agreement with those obtained from the fully coupled equation, which are expected to be most accurate.

III. STERNHEIMER AND SLATER APPROXIMATIONS

Equations (11) and (13) are still complex enough to warrant some further approximations that would ease the computational problem. The first approximation we have considered is what is commonly known as the Sternheimer approximation. [9] To exhibit the nature of this approximation it is necessary to be more specific in the representation of the spin orbitals. Hence, let

$$\chi_i^0(1) = [u_{nl}(r_1)/r_1] Y_l^m(\theta, \phi) \sigma(i) , \tag{14}$$

$$\chi_i'(1) = \sum_{l'm'} [u_{nl\text{-}l'}(r_1, R)/r_1] C_{nl\text{-}l'}^{m\text{-}m'} Y_{l'}^{m'}(\theta, \phi) \sigma(i) . \tag{15}$$

The subscripts in $u_{nl\to l'}$ exhibit explicitly that the excitation of the electron is from a state of orbital angular momentum l to one of l'. Simplifying the notation, let the operator

$$h^0(1)-\epsilon_i^0=-\nabla_1^2+V_0-\epsilon_{nl}\ . \tag{16}$$

Operating with this on the unperturbed spin orbital one can separate out the radial equation

$$\left(\frac{-d^2}{dr^2}+\frac{l(l+1)}{r^2}+V_0-\epsilon_{nl}\right)u_{nl}=0\ , \tag{17}$$

from which one can make the association

$$\frac{l(l+1)}{r^2}+V_0\frac{u_{nl}}{u_{nl}}-\epsilon_{nl}=\frac{u_{nl}''}{u_{nl}}\ . \tag{18}$$

Correspondingly, operating on the perturbed spin orbital one obtains for the radial part of Eq. (11)

$$\left(\frac{-d^2}{dr^2}+\frac{l'(l'+1)}{r^2}+V_0-\epsilon_{nl}\right)u_{nl\to l'}=-\frac{2r_<}{r_>^2}u_{nl}\ , \tag{19}$$

where on the right-hand side we have the expression corresponding to a dipole approximation for the perturbation term. Using Eq. (18) one can approximate Eq. (19) as

$$\left(\frac{-d^2}{dr^2}+\frac{l'(l'+1)-l(l+1)}{r^2}+\frac{1}{u_{nl}}\frac{d^2}{dr^2}u_{nl}\right)u_{nl\to l'}=\frac{-2r_<}{r_>^2}u_{nl}\ . \tag{20}$$

In this form the equation is readily solved numerically for $u_{nl\to l'}$, where u_{nl} can be taken to be HF self-consistent field functions tabulated by Clementi.[10]

Now a second approach, which we call the Slater approximation, arises by the use of Eq. (13). Langhoff *et al.*[7] point out that care must be exercised in its application to different systems. For our case of a closed-shell system of $2N$ electrons in N doubly occupied orbitals, Eq. (13) should be replaced with

$$[f_i^0(1)-\epsilon_i^0]\psi_i'(1)+[h'-\epsilon_i']\psi_i^0(1)=0\ , \tag{21}$$

TABLE I. Contributions to the dipole polarizability for neon.

Approximation	Sternheimer[a]	Sternheimer[b]	Slater	Slater $\times\frac{2}{3}$
$2s\to p$	1.526	1.330	1,088	0.980
$2p\to s$	0.162	−0.700	−0.917	−1.342
$2p\to d$	2.465	2.148	2.264	2.150
Total	4.153	2.778	2.435	1.788
Experimental[a]	2.687	(units a_0^3)		

[a]S. Kaneko, Ref. 13.
[b]This calculation.

where ψ is the spatial part of the atomic orbitals [$\chi_i=\psi_i\sigma(i)$], and the new operator has the form

$$f_i^0(1)=-\nabla_1^2-2Z/r_1+\sum_{j=1}^{N}(j\neq i)2\langle\psi_j^0|r_{12}^{-1}(2-P_{12})|\psi_j^0\rangle+2\langle\psi_i^0|r_{12}^{-1}(1+2P_{12})|\psi_i^0\rangle\ . \tag{22}$$

An expansion of the sum and recombination of the terms permits one to express the form of the operator as

$$f_i^0(1)-\epsilon_i^0=-\nabla_1^2+V'+A_s-\tfrac{3}{2}A_s''-\epsilon_{nl}\ , \tag{23}$$

where

$$V'=-2Z/r_1+\sum_j'\int|\psi_j^0(2)|^2(4/r_{12})\,d\tau_2\ , \tag{24}$$

$$A_s(1)g(1)=6[\tfrac{3}{8}\pi^{-1}\textstyle\sum_j\psi_j^*(1)\psi_j(1)]^{1/3}g(1)\ . \tag{25}$$

The single prime implies that one excludes from the sum the electron that is in the orbital being perturbed. The double prime implies that two electrons in the orbital being perturbed are excluded from the sum. A_s is the well-known Slater-averaged-exchange potential originally computed as the exchange correction in a free-electron-gas model.[11] The particular combination that arises in the operator equation (23) stems from the need to preserve spherical symmetry.

Using the operator in the form of Eq. (23) in expression (21) one obtains the radial equation

$$\left(\frac{-d^2}{dr^2}+\frac{l'(l'+1)}{r^2}+V'+A_s-\tfrac{3}{2}A_s''-\epsilon_{nl}\right)u_{nl\to l'}=-\frac{2r_<}{r_>^2}u_{nl}\ , \tag{26}$$

where again the perturbation term on the right-hand side is taken in the dipole approximation. In this form the equation is solved numerically for $u_{nl\to l'}$, with the u_{nl} again taken as the functions tabulated by Clementi.[10]

For a comparison of these two approximations, the respective solutions were used to calculate the dipole polarizabilities and the total elastic scattering cross sections. The dipole polarizability is obtained from the expression

$$\alpha_{nl\to l'}=C_{l\to l'}\int_0^\infty u_{nl}\,u_{nl\to l'}\,r\,dr\ , \tag{27}$$

where $C_{l\to l'}$ accounts for all constants and angular integrations. The results are tabulated in Tables I and II and discussed in Sec. IV.

In order to determine the scattering cross section one needs phase shifts which are obtained from the solution of a scattering equation for the reduced radial wave function of the scattered electron. The scattering equation is, in the form given by Thompson,[5]

$$(L+k^2)F_{kL}(R) = KF_{kL}(R) + \sum_n (k^2+\epsilon_{nl}) \times \int_0^\infty u_{nl}(r')F_{kL}(r')\,dr'\,u_{nl}(R)\,, \quad (28)$$

where the operator L is

$$L = \frac{d^2}{dR^2} + \frac{2Z}{R} - \frac{1}{R}\sum_{nl} 4(2l+1)Y_0(u_{nl},u_{nl}) - \frac{L(L+1)}{R^2} + V_p(R)\,. \quad (29)$$

V_p is the polarization potential and is given by

$$V_p(R) = \sum_j \int \chi_j^0(\vec{r}_1)(2r_<\!/r_>^2)\cos\theta\chi_j'(\vec{r}_1, R)\,d\vec{r}_1\,. \quad (30)$$

The other terms and symbols in Eqs. (29) and (30) are defined as

$$KF_{kL}(R) = -(1/R)\sum_{nl\lambda}(2l+1)C_{lL\lambda}Y_\lambda(u_{nl},F_{kL})u_{nl}(r)\,, \quad (31)$$

$$Y_\lambda(A,B) = R^{-\lambda}\int_0^R A(r)B(r)r^\lambda\,dr + R^{\lambda+1}\int_R^\infty A(r)B(r)r^{-\lambda-1}\,dr\,, \quad (32)$$

$$C_{lL\lambda} = \int_{-1}^{1} P_l(t)P_L(t)P_\lambda(t)\,dt\,, \quad (33)$$

the P_l being the Legendre polynomials.

In the numerical solution of Eqs. (20), (26), and (29), all iterations were performed using Numerov's method. All integrals were evaluated by means of the trapezoidal rule. The starting values required were obtained by appropriate power-series expansion of the functions. In the iterations a variable mesh size was used that began with $\Delta r = 0.0025$ at the origin and doubled periodically to $\Delta r = 0.16$ at $r = 25.0a_0$ (where a_0 is the Bohr radius), remaining at this value for all larger r. The phase shifts were determined by employing a procedure given by Burgess,[12] with the iteration extended until the value converged to within 5×10^{-5} rad. This occurred usually in the neighborhood of $r = 35a_0$. Having determined the phase shifts, the total elastic scattering cross section is calculated from the expression

TABLE III. Argon scattering lengths by various approximations (in a.u.)

Approximation	Polarizability	Scattering length
Slater (unnorm)	18.48	−8.062
Sternheimer (unnorm)	16.51	−5.819
Slater $\times\frac{2}{3}$ (unnorm)	12.40	−2.327
Sternheimer (norm)	11.00	−1.946
Slater (norm)	11.00	−1.898
Slater $\times\frac{2}{3}$ (norm)	11.00	−1.689
Slater $\times0.594$	11.00	−1.608
Thompson (Ref. 5)	11.00	−1.60
Golden and Bandel (expt) (Ref. 15)		−1.647

$$Q = (4/k^2)\sum_L (2L+1)\sin^2\eta_L\,. \quad (34)$$

The range of the partial-wave sum for neon was $L = 0, 1, 2$ and for argon $L = 0, 1, 2, 3$. Some of the partial-wave shifts and scattering cross-section results are presented in Sec. IV.

IV. RESULTS AND DISCUSSIONS

Contributions to the dipole polarizability from the outermost occupied level are listed for neon in Table I and for argon in Table II. They are compared with earlier calculations by Kaneko,[13] who used the Sternheimer approximation and experiment. Our Sternheimer results for neon are in better agreement with experiment than those of Kaneko. In additon, the Sternheimer components calculated by Montgomery and LaBahn[14] in an independent calculation agree with the present calculations.

Results for argon were not as satisfying in that no significant change in the values of the polarizabilities in Sternheimer approximation were obtained from those of Kaneko[13] or Montgomery and LaBahn.[14] The change in the total polarizability through use of the Slater approximation also went the wrong way and did not yield the desirable reduction that occurred for neon.

The additional sets of values listed correspond to some of the modifications made to the Slater approximation. The nature of these modifications

TABLE II. Contributions to the dipole polarizability for argon.

Approximation	Sternheimer[a]	Sternheimer[b]	Slater	Slater $\times\frac{2}{3}$	Slater $\times0.594$
$3s\rightarrow p$	5.598	5.888	5.070	4.224	4.076
$3p\rightarrow s$	−3.282	−3.374	−3.467	−6.255	−7.075
$3p\rightarrow d$	13.883	13.998	16.875	14.435	14.000
Total	16.199	16.512	18.478	12.404	11.001
Experimental[a]	11.000	(units a_0^3)			

[a]S. Kaneko, Ref. 13.

[b]This calculation.

TABLE IV. Neon scattering lengths by various approximations (in a.u.).

Approximation	Polarizability	Scattering length
Slater $\times\frac{2}{3}$ (unnorm)	1.79	0.4351
Thompson (Ref. 5)	2.20	0.347
Slater	2.44	0.2757
Slater $\times\frac{2}{3}$ (norm)	2.69	0.0556
Sternheimer	2.78	0.0276
Salop and Nakano (expt) (Ref. 17)		0.30 ± 0.03

will be described later. The seven modifications being reported for which the total scattering cross sections were calculated are listed in Table III. This table gives a comparison of the total polarizability with the zero-energy scattering length for argon. The analogous results for neon are exhibited in Table IV. The scattering lengths were observed to be quite sensitive to the value of the total polarizability.

For the calculation of the total scattering cross section, the energy values investigated were generally 0.0 (0.10)–1.00 Ry, with the exception of one modification, Slater $\times 0.594$, where several additional values were taken in the neighborhood of the maximum and minimum. As was mentioned earlier, all calculations included the three transitions $ns \rightarrow p$, $np \rightarrow s$, and $np \rightarrow d$, where n has the value corresponding to the outermost occupied level. The partial phase shifts are listed for only a few modifications, viz., those for neon in Table V and argon in Table VI.

Let us now consider the nature of the modifications used. When the calculated value of the polarizability was significantly different from the experimental one, a second solution of the scattering equation was made using a polarization potential normalized to the experimental value of the polarizability. The normalizing factors were just the ratio of the experimental to calculated values of the polarizability. The results are labeled appropriately as unnormalized and normalized.

Another modification of the Slater approximation of the exchange term in the potential was made. Slater[11] derived his averaged-exchange potential [Eq. (25)] on the basis of a free-electron-gas model. More recently Kohn and Sham[16] in their consideration of the problem of a homogeneous gas of interacting electrons have obtained the same functional form except reduced by a factor of $\frac{2}{3}$. Slater has apparently found the proper form for the interaction with the value of a multiplicative constant depending on the system being considered. Calculations were made with the factor taken as both 6 and 4, and the corresponding results labeled as Slater and Slater $\times\frac{2}{3}$. One would have hoped that the better agreement with the experimental results would have decided which factor was more correct.

The good agreement of the Slater cross sections for neon with the recent experimental results of Salop and Nakano[17] shown in Fig. 1 would indicate that the factor of 6 is better. Although no improvement was expected, the modifications Slater $\times\frac{2}{3}$ (unnorm) and Slater $\times\frac{2}{3}$ (norm) were calculated for neon to observe the relative behavior when they are applied to argon.

The argon results shown in Fig. 2 imply in contradiction that the factor of 4 will yield results in better agreement with experiment. Argon results for Slater $\times\frac{2}{3}$ are not plotted because they are almost identical with Thompson's above 5 eV and our Sternheimer (norm) below 5 eV. Since the Slater $\times\frac{2}{3}$ modification did not yield the experimental polarizability, it was used in a normalized calculation as described above.

The polarizability obtained from the Slater $\times\frac{2}{3}$ approximation was considerably improved over the value arising from the Slater approximation. This suggested an alternative normalization procedure, that of multiplying the Slater-averaged-exchange

TABLE V. Electron-neon partial-wave phase shifts from the Slater approximation (in modulo π rad).

k (a_0^{-1})	Energy (eV)	η_0		η_1		η_2	
		A[a]	B[b]	A[a]	B[b]	A[a]	B[b]
0.1	0.136	−0.0468	−0.0583	0.0035	0.0022	0.0008	0.0006
0.2	0.544	−0.1217	−0.1374	0.0071	0.0026	0.0030	0.0023
0.3	1.224	−0.2127	−0.2289	0.0030	−0.0057	0.0070	0.0054
0.4	2.176	−0.3131	−0.3285	−0.0128	−0.0259	0.0131	0.0105
0.5	3.400	−0.4189	−0.4330	−0.0409	−0.0579	0.0219	0.0186
0.6	4.896	−0.5273	−0.5404	−0.0797	−0.0999	0.0342	0.0306
0.7	6.664	−0.6364	−0.6490	−0.1264	−0.1491	0.0504	0.0474
0.8	8.704	−0.7450	−0.7573	−0.1785	−0.2030	0.0708	0.0694
0.9	11.016	−0.8520	−0.8643	−0.2337	−0.2594	0.0956	0.0966
1.0	13.600	−0.9566	−0.9692	−0.2901	−0.3168	0.1245	0.1284

[a]A: Calculated in the HFS (unnorm) approximation.

[b]B: Calculated in the HFS $\times\frac{2}{3}$ (unnorm) approximation.

TABLE VI: Electron-argon partial-wave phase shifts from the Slater approximation (in modulo π rad).

k (a_0^{-1})	Energy (eV)	η_0		η_1		η_2		η_3	
		A[a]	B[b]	A[a]	B[b]	A[a]	B[b]	A[a]	B[b]
0.1	0.136	0.0729	0.0503	0.0158	0.0152	0.0034	0.0034	0.0012	0.0012
0.2	0.544	−0.0039	−0.0374	0.0342	0.0304	0.0143	0.0142	0.0045	0.0045
0.3	1.224	−0.1409	−0.1798	0.0242	0.0142	0.0370	0.0361	0.0100	0.0100
0.4	2.176	−0.3023	−0.3443	−0.0225	−0.0397	0.0820	0.0775	0.0181	0.0180
0.5	3.400	−0.4733	−0.5171	−0.0991	−0.1232	0.1693	0.1535	0.0290	0.0289
0.6	4.896	−0.6467	−0.6917	−0.1955	−0.2256	0.3344	0.2875	0.0435	0.0431
0.7	6.664	−0.8186	−0.8644	−0.3030	−0.3380	0.6238	0.5076	0.0624	0.0613
0.8	8.704	−0.9866	−1.0328	−0.4154	−0.4543	1.0283	0.8181	0.0864	0.0841
0.9	11.016	−1.1492	−1.1956	−0.5288	−0.5707	1.4071	1.1543	0.1163	0.1119
1.0	13.600	−1.3056	−1.3521	−0.6406	−0.6848	1.6611	1.4280	0.1523	0.1447

[a]A: Calculated in the HFS (norm) approximation. [b]B: Calculated in the HFS×0.594 approximation.

potential by an appropriate factor which would yield a polarizability equal to the experimental value. A justification for this procedure stems from the fact that the multiplicative factor is dependent on the type of system that is being described. The factors of 6 or 4 that arise from consideration of systems of a free-electron gas or a homogeneous gas of interacting electrons should not be expected to be correct in describing the electron distribution in an isolated atom. The results of this calculation, labeled Slater×0.594, are in best agreement with experiment, which is represented in Fig. 2 by the open circles. No further improvement on the agreement however was attempted by an arbitrary manipulation of the factor. Thompson's argon results, obtained through a normalized Sternheimer approximation including only the $3p \rightarrow d$ transition, were in excellent agreement with the Slater ×0.594 below 2 eV.

A single curve represents the normalized results of the two approximations (Sternheimer and Slater) since they are in essential agreement. There was a slight deviation in the range 6–10 eV. The normalized Slater×$\frac{2}{3}$ curve for argon was not shown since it essentially paralleled the Slater×0.594 curve, lying above it except for the range between 1 and 5 eV where it dips slightly below.

The behavior of the argon results leads one to conclude that the two different approximations in the normalized modification account for those aspects of the scattering process known as adiabatic-exchange effects. The nature of the disagreement with experiment indicates that some nonadiabatic effects are making an appreciable contribution. The formalism for accounting the nonadiabatic effects has been established and successfully applied to helium.[3] The procedure is known as the extended polarization approximation.

An analysis of the extended polarization approximation has established that the nonadiabatic effects

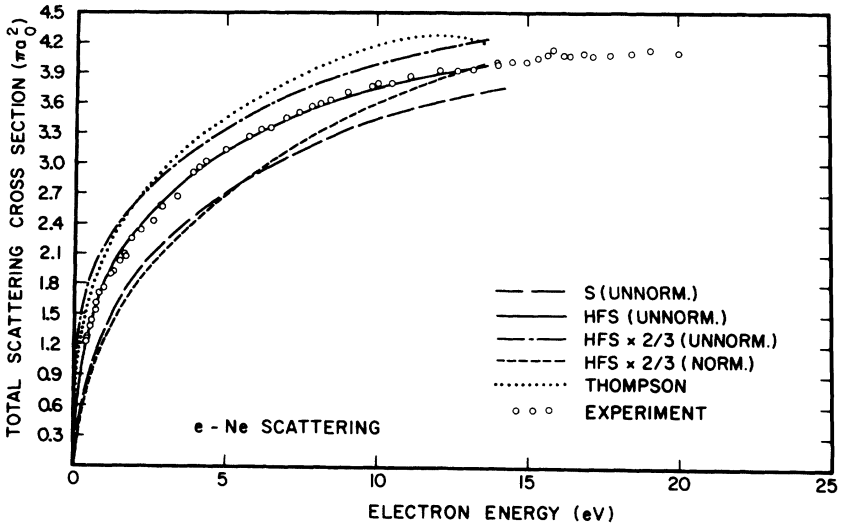

FIG. 1. Total scattering cross sections for neon. Our results obtained from various approximations employed in determining the perturbed orbital are compared with the computation of Thompson and the experimental data of Salop and Nakano. The notations designating the different approximations used are S (unnorm) for Sternheimer, HFS (unnorm) for Slater, and HFS×$\frac{2}{3}$ (unnorm) for Slater ×$\frac{2}{3}$. The HFS×$\frac{2}{3}$ (norm) curve shows the effect of the normalization of the polarization potential obtained from the Slater ×$\frac{2}{3}$ approximation.

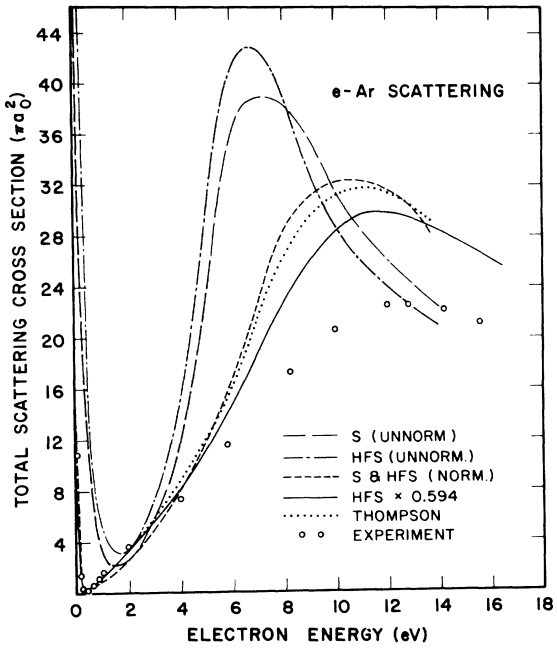

FIG. 2. Total scattering cross sections for argon. Our results obtained from various approximations employed in determining the perturbed orbital are compared with the computation of Thompson and the experimental data of Golden and Bandel. The notations designating the different approximations used are S (unnorm) for Sternheimer, HFS (unnorm) for Slater, and HFS×0.594 for Slater×0.594. The S and HFS (norm) curve shows the almost identical results obtained by normalizing the polarization potential of either the Sternheimer or Slater approximations.

add a repulsive contribution via a distortion potential. This has been shown to be less significant at larger distances than the polarization potential but comparable in the vicinity of the core. Hence, only those scattered electrons that penetrate the core, which are those of the higher energies, will be significantly affected. The agreement of the results at the lower energies and the appreciable deviation at the higher energies suggests that argon would be an ideal system for testing the extended polarization approximation. However, for our ultimate application of this formalism to photoionization of Na and K, the adiabatic-dipole approximation is believed to be sufficiently accurate.

Note added in proof. Very recently, D. G. Thompson [J. Phys. B4, 468 (1971)] improved his earlier calculation for neon and argon (Ref. 5) by using the Pople-Schofield approximation to determine the polarization potentials. His new phase shifts for neon were slightly higher than ours while those for argon were slightly lower. He thus also obtained excellent agreement with the experimental data for neon.

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