PHYSICAL REVIEW A VOLUME 10, NUMBER 5 NOVEMBER 1974

Independent-particle-model study of the elastic scattering of low-energy electrons by positive ions

P. P. Szydlik,* G. J. Kutcher, and A. E. S. Green
Department of Physics and Astronomy, University of Florida, Gainesville, Florida 32611

(Received 15 May 1974)

The elastic scattering by positive ions of electrons with energies below 2 Ry was investigated theoretically using the independent-particle-model (IPM) potentials of Green, Sellin, and Zachor to represent the electron-ion interaction. Parameters were determined from minimization of the total energy of the bound system consisting of the electron plus target ion, or in some cases from fits to the single-electron eigenvalues of this same system. Potentials of the former type are generally the stronger of the two. The IPM phase shifts versus energy are qualitatively similar to, but usually larger than, those obtained using Hartree-Fock-Slater potentials. For energies below 1 Ry there is excellent agreement between the differential cross sections for Na^+ obtained from the IPM and those computed from semiempirical quantum-defect methods. For this same ion the IPM differential cross sections likewise resemble those computed from Hartree-Fock potentials and lie between the Hartree-Fock results obtained with and without local exchange contributions. Phase shifts are computed using the independent-particle model for all positive ions of nitrogen and oxygen, species of atmospheric interest.

INTRODUCTION

Studies of the interaction of low-energy electrons with positive ions are necessary for a thorough understanding of processes occurring in the upper atmosphere and in plasmas, and of processes producing astrophysical phenomena. Studies of elastic electron scattering are important in providing the directional information necessary to describe the transport of electrons through ionized gases. While investigations of excitation and ionization of positive ions by electron impact are rather extensive, treatments of elastic scattering are much less so and no experimental results are available. Theoretical investigations are generally centered on hydrogenlike ions[1-4] (especially He^+) or on singly charged positive ions.[5-7] There is sufficient information in Seaton's quantum-defect calculations[7] to compute low-energy phase shifts for a few of the more highly ionized species.

The intent of the present investigation is to assess the applicability of the simple atomic independent-particle models (IMP) of Green, Sellin, and Zachor[8] (GSZ) to the study of the elastic scattering of electrons from positive ions. In particular, the validity of methods for choosing the parameters of this IPM potential will be examined. Special attention will be given to the *ab initio* procedure of Bass, Green, and Wood,[9] where the potential parameters are those which minimize the total energy of an atom. This method has been extended recently to ions by Szydlik and Green[10] with a large measure of success. Indeed, in both of these works the total energies are in excellent agreement with Hartree-Fock values. For purposes of comparison, potential parameters derived from phenomenological fits to experimental bound-state data will also be employed.[11]

The current study will explore mainly the region below 2 Ry (27 eV) where inelastic and reactive processes are not expected to be significant. Comparison will be made between results computed from the GSZ independent-particle model and those obtained using semiempirical quantum-defect methods, Hartree-Fock-Slater and Hartree-Fock calculations. For purposes of comparison with the last model, a few IPM computations will be performed at energies higher than 2 Ry. The method will be applied to the ions of nitrogen and oxygen because of their interest to us as atmospheric gases.

METHOD OF CALCULATION

Phase shifts and differential cross sections

Because we are concentrating on low energies, the method of partial waves may be applied conveniently. The target ion is treated strictly as a local spherically symmetric potential with a residual Coulomb tail appropriate to the charge on the ion. The form of this potential and the methods for choosing the parameters of this potential will be described in detail in the following section. The target is thus assumed to be essentially structureless and the theory considers the effects of neither the total angular momentum of the target nor the spin of the electron. The calculation cannot distinguish, for example, between the triplet and singlet partial waves for scattering from singly charged ions of the noble gases.

Methods for computing phase shifts and differential cross sections for scattering from such "modified" (by a short-range interaction) Coulomb potentials are well known and will be described only briefly here. The reader is referred to standard works[12] for a more detailed treatment.

In the region where the target potential can be regarded as entirely Coulombic the wave function for an outgoing electron with orbital angular momentum l has the asymptotic form

$$U_l \sim F_l + A_l (G_l + iF_l) , \tag{1}$$

where $F_l = F_l(\gamma, \rho)$ and $G_l = G_l(\gamma, \rho)$ are, respectively, the regular and irregular Coulomb functions, with $\rho = kr$ and $\gamma = -\eta/E^{1/2}$, where η is the ionicity of the target and E is the electron energy (Rydberg atomic units will be used throughout). The partial-wave amplitude A_l is given by

$$A_l = (e^{2i\delta_l} - 1)/2i , \tag{2}$$

where δ_l is the phase shift due to the short-range interaction. To obtain the partial-wave amplitude (and the phase shift) the Schrödinger equation is integrated outward (the Cowell-Numerov method[13] was used here) to some matching radius r_m at which the short-range interaction is negligible. The logarithmic derivative at r_m of the numerically computed U_l is equated to that calculated from the asymptotic form. From the resulting equation the partial-wave amplitude and the short-range phase shift can be obtained.

The scattering amplitude $f(\theta)$ is the sum of two parts: $f_s(\theta)$, that due to the short-range interaction, and $f_c(\theta)$, that resulting from the Coulomb potential. The equations for these are, respectively,

$$f_s(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) A_l e^{2i\sigma_l} P_l(\cos\theta) , \tag{3}$$

$$f_c(\theta) = -\frac{\gamma}{2k\sin^2(\theta/2)} \exp\{-i\gamma \ln[\sin^2(\theta/2)] + 2i\sigma_0\} , \tag{4}$$

where

$$\sigma_l = \arg\Gamma(1+i\gamma) + \sum_{s=1}^{l} \tan^{-1}(\gamma/s) \tag{5}$$

is the Coulomb phase shift and other symbols have their usual meanings. The differential cross section is merely

$$\frac{d\sigma}{d\Omega}(\theta) = |f(\theta)|^2 = \frac{d\sigma_c}{d\Omega} + 2\,\mathrm{Re} f_c^*(\theta) f_s(\theta) + |f_s(\theta)|^2 , \tag{6}$$

where $d\sigma_c/d\Omega$ is the Rutherford cross section. The analyses to follow focus on calculating phase shifts and differential cross sections. Where emphasis is to be on the short-range behavior of the potential, the ratio of the differential to the Rutherford cross sections will be discussed. Infinities at $\theta = 0$ produced by the residual Coulomb interaction cause both the total elastic and the momentum-transfer cross sections to diverge.

Form of the potential and its parameters

The form of the potential representing the ion-electron interaction is that of the GSZ independent-particle model appropriately modified for ions,[10] viz.,

$$V(r) = -(2/r)[(Z-\eta)\Omega(r) + \eta] , \tag{7}$$

where

$$\Omega(r) = \frac{1}{H(e^{r/d} - 1) + 1} . \tag{8}$$

Here Z is the atomic number of the target ion, η is the degree of ionization or ionicity, r is the distance of the projected electron from the nucleus of the target ion, and H and d are adjustable parameters. This potential is seen to be divisible into the appropriate "short-range" and Coulombic parts. The parameter d determines the range of the short-range interaction. With no significant error this part of the potential is taken as effectively zero beyond 20 Bohr radii.

Since the long-range behavior of the interaction is dominated by the Coulomb potential, core polarization effects were neglected. Such effects may still be appreciable for the less highly ionized species with "soft" outer-shell electrons. Because of the low energies being investigated, imaginary terms in the potential are also ignored. However, these are found to have little effect on the elastic scattering from neutral atoms[14] even at energies much higher than those considered here.

The energies of the incoming electrons treated here are lower than, or of the order of the kinetic energies of the electrons in the target. Thus, in determining the parameters of our IPM potentials it is assumed that the time spent by the incident electron in the vicinity of the target is sufficient to produce a rearrangement of the target electrons to one characteristic of the bound composite system of electron plus target ion. Sometimes the charge distribution of the target is considered to be "frozen" and the projected electron produces no redistribution. Such an approach would be more valid at energies higher than those investigated here.

To treat accurately the low-energy elastic scattering of electrons it is important to include the effects of exchange.[15,16] This is often represented approximately through a local exchange potential, such as that of Slater[17] or Gaspar,[18] which is proportional to the one-third power of the electronic density. There the interaction of an electron with a "hole" of constant charge density is computed and averaged over the momentum of all the occupied states. Mittleman and Watson[19] maintain there is little justification for such an averaging procedure since the momentum of the incident particle is unrelated to the momenta within the Fermi sea, i.e., the momenta of the electrons in the occupied states. They have obtained a local density form for the exchange potential which is momentum dependent. However, their exchange potential is applicable only at momenta much greater than the Fermi momentum.

The Hartree-Fock-Slater potential as used by Herman and Skillman[20] has the form

$$V_{\mathrm{HS}}(r) = \frac{-2Z}{r} + \frac{2}{r}\int_0^r \sigma(t)\,dt + 2\int_r^\infty \frac{\sigma(t)\,dt}{t} - 6\left(\frac{3}{8\pi}\rho(r)\right)^{1/3}, \qquad (9)$$

where Z is the atomic number and $\rho(r) = \sigma(r)/4\pi r^2$ is the spherically averaged total electronic charge density (both spins). The last term is the free-electron exchange potential. The Gaspar-Kohn-Sham[18] form of the exchange potential is $\frac{2}{3}$ that of the last term in Eq. (9). It is here maintained that the GSZ potential implicitly incorporates the effects of exchange because of the methods employed in determining the potential parameters. Quite evidently the effects of exchange are incorporated in the GSZ potential if its parameters are derived from empirical fits to atomic energy levels. The variational technique of determining the potential parameters (and the potential's eigenfunctions) from minimization of the total energy also results in the inclusion of exchange since the total Hamiltonian, the expectation of which is minimized, includes exchange explicitly. However, the admonition of Mittleman and Watson regarding exchange obtains here as well. In addition the "exchange" portion of the GSZ potential is assigned the same spatial dependence as the direct part. Perhaps the GSZ potential might be improved in future work through the inclusion of a distinct local exchange term proportional to $\rho^{1/3}$. Taking the usual GSZ potential as a starting point, the electronic charge density can be computed from Poisson's equation and is given by the expression

$$\rho(r) = \frac{(Z-\eta)He^{-r/d}}{4\pi r d^2 w^2(r)}\left(\frac{2H}{w(r)} - 1\right), \qquad (10)$$

where

$$w(r) = H + (1-H)e^{-r/d}.$$

As previously mentioned, two techniques were used to determine the IPM potential parameters. In the first of these the parameters chosen are those which minimize the total energy of the bound target-ion–electron system. Such techniques were found to give total binding energies in excellent agreement with Hartree-Fock results. It should again be remarked that our IPM does not distinguish among the terms of a multiplet. In the case of oxygen, for example, the total energy obtained is the "center of gravity" of the energies of the ^3P, ^1D, and ^1S states, all of which have the same electronic configuration. This is borne out in the calculation, where the energy minimum found for oxygen using the GSZ independent-particle model is extremely close to that of the Hartree-Fock energy of these three states averaged over S and L as described in Ref. 10.

When the GSZ potential is fit to the experimental excited levels of an atom or ion (such as are given in Ref. 21), it is assumed that the core is undisturbed and that the single-electron energies of the IPM are to be identified with the energies of the appropriate excited states. In addition, averaging techniques are employed similar to those used in assessing the results of the energy-minimization procedure. For example, for oxygen, levels were averaged over total angular momentum as well as over the triplet and quintet spin states. For neon and argon the doublet and quartet spin states were averaged. Because of difficulties encountered in computing accurately the energy of the valence level, this was given ten times the weight of the others in the fitting procedure. Where single-particle levels of the core are included in the fit, these were taken from the ESCA[22] compilation.

For the species studied here many of the experimental levels and higher-lying excited levels are available and either technique for determining the potential parameters could be employed. The energy-minimization technique was favored since it is *ab initio* and may be used when no empirical data are available. Moreover, as exemplified in Table I, in computing the energies of the core levels, this procedure is as accurate as other methods. Only in computing the energy of the $2p$ valence level of atomic oxygen is the fitting scheme significantly more accurate than that of energy minimization.

RESULTS AND DISCUSSION

Comparison of IPM results with those from Hartree-Fock and quantum-defect methods

In terms of the number of target species studied, one of the most wide-ranging investigations of the

TABLE I. Experimental and theoretical single-electron bound spectrum (in Ry) for neutral oxygen.

Level	Experiment[a]	IPM_1[b]	IPM_2[c]	Hartree-Fock[d]	Herman-Skillman	HFS-Xα[e]
1*s*	39.4	38.3	39.4	41.4	39.5	38.1
2*s*	2.35	2.24	2.09	2.50	2.14	1.90
3*s*	0.315	0.311	0.300			0.289
4*s*	0.127	0.127	0.124			0.121
5*s*	0.0690	0.0688	0.0678			0.0666
6*s*	0.0432	0.0431	0.0426			0.0420
7*s*	0.0296	0.0296	0.0293			0.0295
8*s*	0.0216	0.0215	0.0213			0.0211
2*p*	1.000	1.157	1.012	1.233	1.041	0.841
3*p*	0.202	0.201	0.195			0.190
4*p*	0.0952	0.0948	0.0930			0.0914
5*p*	0.0544	0.0553	0.0545			0.0537
6*p*	0.0358	0.0362	0.0358			0.0354
3*d*	0.1129	0.1126	0.1118			0.1112
4*d*	0.0634	0.0633	0.0629			0.0626
5*d*	0.0405	0.0405	0.0402			0.0400
6*d*	0.0281	0.0281	0.0279			0.0278
7*d*	0.0206	0.0206	0.0205			0.0204

[a] Values from Ref. 21 averaged over total angular momentum and spins.

[b] IPM with potential parameters from energy minimization.

[c] IPM with potential parameters from fits to experimental spectrum.

[d] Values from E. Clementi, IBM J. Res. Dev. Suppl. 9, 2 (1965), averaged over ^3P, ^1S, and ^1D levels of the ground-state configuration using $(2S+1)(2L+1)$ weighting factors.

[e] J. C. Slater, Adv. Quantum Chem. 6, 1 (1972). The value of α was set at 0.75, which slightly overbinds neutral oxygen. Values with $\alpha = \frac{2}{3}$ were somewhat poorer. The latter technique [Phys. Rev. 99, 510 (1955)] was used to obtain the Coulomb potential at large distances.

elastic scattering of electrons from singly charged ions is that of Manson.[5] His study is very much in the spirit of the present analysis. There the phase shifts for the elastic scattering of electrons from positive ions are computed using unrelaxed Hartree-Fock-Slater[20] (HFS) potentials of the form given in Eq. (9) and characteristic of an electron in the neutral atom. Results obtained in the present study for the *s*-, *p*-, and *d*-wave phase shifts (the *f*-wave phase shifts at 2 Ry and below are negligible except for argon) are compared with Manson's in Figs. 1–3, respectively. Table II contains the parameters of the IPM potentials used to obtain the results displayed in these figures. Manson's results for the *s* waves and *p* waves are very similar to those obtained here. In most cases the phase shifts calculated from the atomic IPM are slightly higher than those obtained from Manson's HFS potential, although for He^+ and Na^+ the two sets are virtually indistinguishable. Since Manson considers targets at most one electron away from a closed shell, he presents no results for N^+ or O^+, and thus avoids the difficulty of treating target species with several closely spaced levels of the ground-state configuration.

The phase shifts computed using an IPM potential obtained from fits to the single-electron levels (performed only for $Z = 7, 8, 10$, and 18) are usually smaller than those from an IPM potential whose parameters have been determined from the minimization of the total energy. The single exception is nitrogen. Evidently, the non-Coulombic portion of the IPM determined from energy minimization is of longer range than that of the fitted IPM. These ranges can be compared through their *d* parameters given in Table II.

Differences among the three methods, energy-minimization IPM, fitted IPM, and HFS, are particularly marked for the low-energy *d*-wave phase shifts for Ar^+. However, all three methods indicate a low-energy *d*-wave resonance although for the energy-minimization IPM, the $\pi/2$ phase shifts occurs at lower energy than for the other two models. Above approximately 1 Ry, the three models are in substantially better agreement. This is particularly true of the fitted-IPM and HFS results.

Peixoto[6] has utilized Hartree-Fock potentials to compute differential cross sections for the scattering of electrons from Na^+. Analytic Hartree-Fock functions were used to obtain the charge distribution from which the interaction potential was computed. To this was added the Gaspar-Kohn-Sham

(GKS) form of the $\rho^{1/3}$ local exchange potential. While from the context of the paper it is believed that the wave functions (and hence the charge distribution and potential) are for Na^+ rather than neutral Na, this fact is not stated explicitly in Peixoto's paper. For reasons already given we favor using the potential for an electron in a neutral atom to describe the scattering of low-energy electrons by singly charged positive ions. The results obtained from calculations with IPM potentials (parameters determined from energy minimization) are compared to Peixoto's Hartree-Fock results in Fig. 4. The differential cross section (in Å^2) for 40-eV electrons scattered from Na^+ is plotted as a function of momentum transfer, $S = 2k \sin\frac{1}{2}\theta$ (in Å^{-1}), where k is the wave number and θ the scattering angle. The cross section computed from the GSZ-IPM potential characteristic of an electron in neutral sodium generally lies between those of the Hartree-Fock (HF) computations with and without exchange. It is interesting that the angular distribution obtained from the IPM has the general features of the HF results with exchange. However, in view of the relative inertness of the target ion (closed in the $2p$ shell) it is disconcerting that the agreement is no better than qualitative. The agreement between the IPM and HF results is improved if the IPM potential is one characteristic of an electron in Na^+ to which the GKS exchange potential [charge density given by Eq. (1)] has been added.

Excellent agreement with the HF differential cross section is obtained if the GKS exchange term is added to the IPM potential characteristic of neutral Na (not shown in Fig. 4). However, such a procedure is redundant since the GSZ potential in this case already includes exchange effects. The significant discrepancies between the IPM and HF results for electron scattering from Na^+ remain unresolved.

In contrast to this there is excellent agreement among the IPM, HFS,[5] and semiempirical quantum-defect methods[7] in computing the differential cross sections for electron scattering from this same ion, i.e., Na^+. In the last-named procedure the positions of the Rydberg states of the neutral atom are used to compute the quantum defects whose

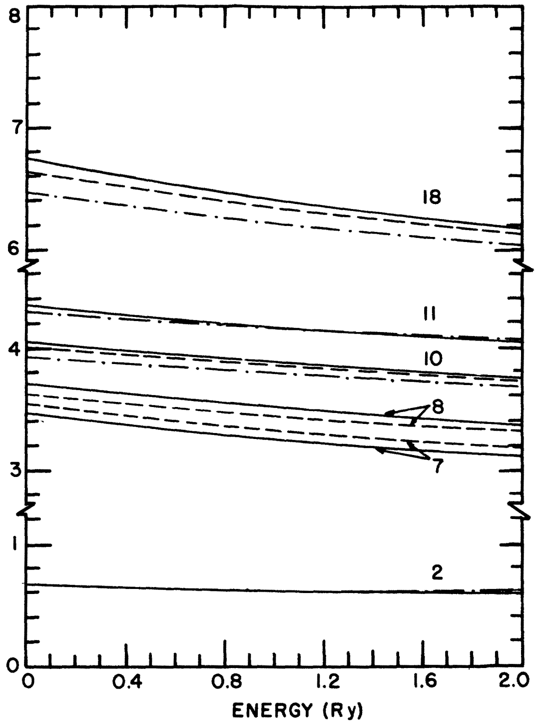

FIG. 1. s-wave phase shifts as a function of energy for electrons elastically scattered from singly charged positive ions. The numbers next to the curves are the target atomic numbers. Curve legend is as follows: solid line, IPM results with potential parameters determined from minimizing the total energy of the neutral atom; dashed line, IPM results with potential parameters determined by fitting the single-electron energies of the neutral atom; long-short dash line, HFS results from Ref. 5.

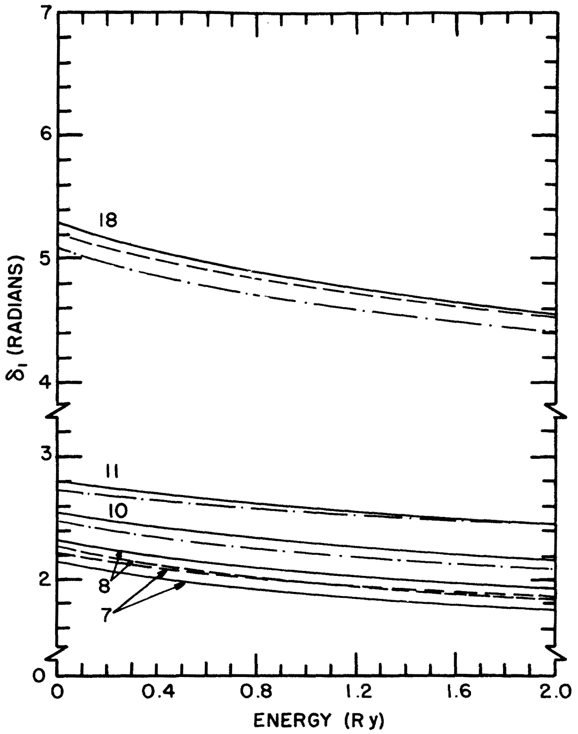

FIG. 2. p-wave phase shifts as a function of energy for electrons elastically scattered from singly charged positive ions. See caption to Fig. 1 for explanation of curve legend.

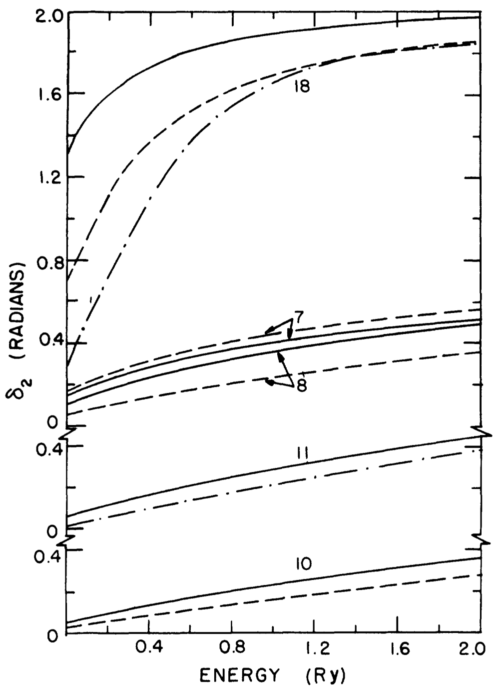

FIG. 3. *d*-wave phase shifts as a function of energy for electrons elastically scattered from singly charged positive ions. See caption to Fig. 1 for explanation of curve legend.

values at zero energy are simply related to the zero-energy phase shift of the same angular momentum. Rational approximations in powers of k^2 justified by analytic continuation properties are then used to compute phase shifts at low positive energies. In Fig. 5 the ratio of the differential cross section to the Rutherford cross section is plotted as a function of the scattering angle. Except for one curve to be explained later these cross sections were computed from only s- and p-wave contributions. To within the accuracy with which data could be obtained from the graphs in Manson's[5] and Seaton's[7] papers, the agreement among the three methods at $k=0.25$ (inverse Bohr radii) is excellent. The agreement is equally good (if not better) at $k=0.50$ and $k=0.75$ (curves not shown.) At $k=1.00$ the quantum-defect results above 90° depart significantly from those obtained using IPM and HFS potentials. An energy of 1 Ry may be above the region of validity of the expansions used to compute the phase shifts in the quantum-defect prescription, although the abrupt deterioration in the quality of the agreement between $k=0.75$ and $k=1.00$ is surprising. The additional curve at $k=1.00$ was computed using the IPM and

TABLE II. GSZ independent-particle-model potential parameters used in computing phase shifts for elastic scattering of electrons from singly charged positive ions.

Ion	Type of parameters [a]	Potential parameters d (a.u.)	H
He^+	EM	0.3807	0.6746
N^+	EM	0.8480	1.9250
N^+	FS	0.8585	1.8324
O^+	EM	0.7348	1.7731
O^+	FS	0.5745	1.2608
Ne^+	EM	0.5575	1.5131
Ne^+	FS	0.4619	1.1216
Na^+	EM	0.5840	1.6644
Ar^+	EM	1.0450	3.6554
Ar^+	FS	0.8407	2.6967

[a] EM means the parameters are those which minimize the total energy of the neutral atom. FS means the parameters are those which provide the best fits to the single-electron levels of the neutral atom.

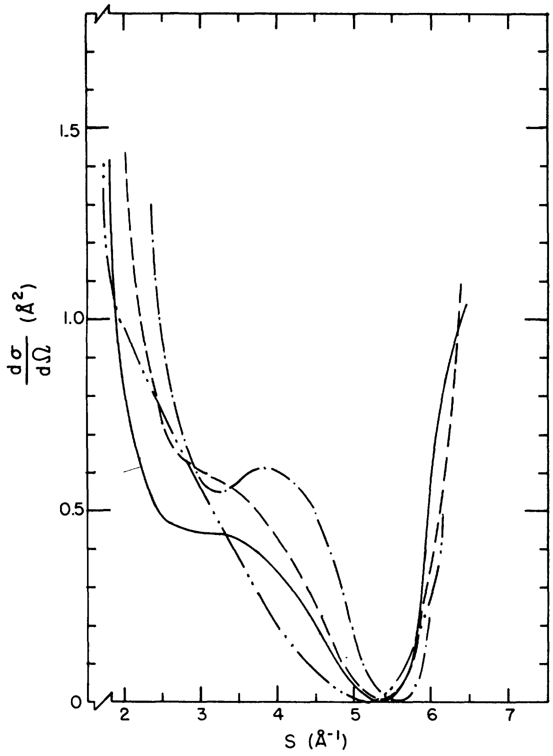

FIG. 4. Differential cross sections as a function of momentum transfer ($s=2k\sin\frac{1}{2}\theta$) for 40-eV electrons scattered from Na^+: solid line, IPM results with potential parameters determined from minimization of the energy of neutral Na; long-dash line, IPM results with potential parameters determined from minimization of the energy of Na^+ and including GKS (Ref. 18) exchange contribution and charge distribution given by Eq. (11); long–double-short dash line, Hartree-Fock computation without exchange from Ref. 6; long-short dash line, Hartree-Fock computation with GKS exchange potential.

10 partial waves, although only those waves with $l \leq 2$ contribute significantly to the differential cross section. The effects of the d-wave contribution at this energy are readily apparent, whereas at $k = 0.25$ they were imperceptible.

Elastic electron scattering from positive ions of nitrogen and oxygen

Having established the reliability of our IPM procedures for computing phase shifts and differential cross sections, the computations are extended to all positive ions of oxygen and nitrogen, species of interest as atmospheric constituents for which there are no scattering data, experimental or theoretical. The phase shifts produced by the short-range interaction for electrons of representative energies, 2 Ry and below, scattering from the ions of nitrogen and oxygen are presented in Tables III and IV, respectively. Phase shifts for the more highly ionized species are virtually energy independent in the range up to about 2 Ry. Because of the general slow variation of phase shifts with energy, sufficient information is contained in these tables to reconstruct accurately the differential cross sections at any energy up to 2 Ry. The required Coulomb phase shifts are easily computable using readily available computer programs. While it is not our purpose to make an exhaustive comparison with results obtainable by the quantum-defect method, an apparent discrepancy in the zero-energy p-wave phase shift for O^{4+} obtained here (about 0.68 rad) and that derivable from Fig. 2 of Seaton[7] (about 0.55 rad) was somewhat disturbing since O^{4+} has the electronic configuration $1s^2 2s^2$ and is thus a reasonable example of a closed-shell ion. However, the energies of the $2p$ and $3p$ Rydberg levels as given in Ref. 21 would indicate that the p-state zero-energy quantum defect rather than being the 0.17 implied by Fig. 2 of Seaton is more nearly 0.225. This latter value gives an O^{4+} zero-energy p-wave phase shift of 0.71 rad, in good agreement with our IPM result.

To emphasize the short-range properties of our IPM potentials, the ratio of the cross section to the Rutherford contribution is plotted in Figs. 6

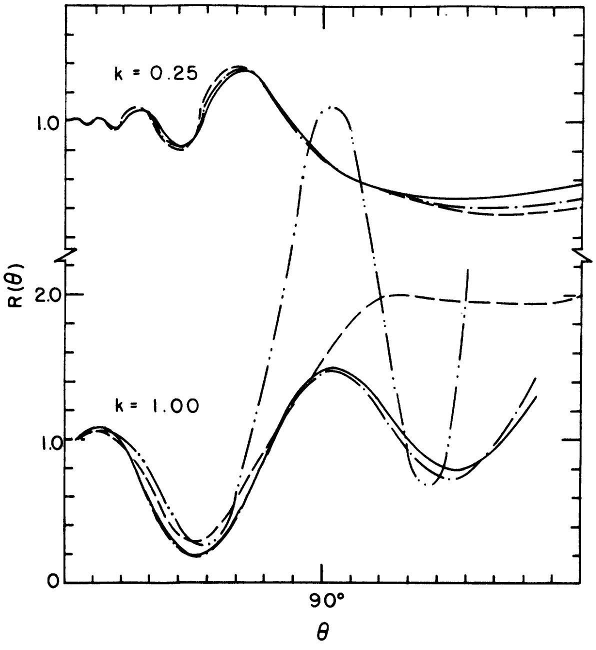

FIG. 5. Ratio of differential to Rutherford cross sections as a function of scattering angle for electrons elastically scattering from Na^+ at $k = 0.25$ and 1.00 (inverse Bohr radii). Except where stated otherwise cross sections are computed from only s- and p-wave contributions: solid line, IPM results with potential parameters from minimization of the energy of neutral Na; long-short dash line, from HFS results of Ref. 5; long-dash line, from quantum-defect method of Ref. 7; long–double-short dash line, IPM results including contributions from all partial waves with $l \leq 9$.

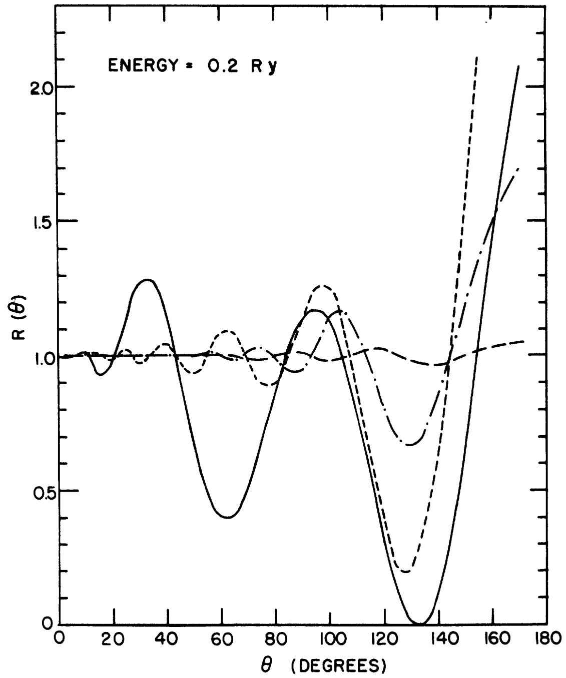

FIG. 6. Results of IPM computation of the ratio of differential to Rutherford cross sections as a function of scattering angle for electrons of energy 0.2 Ry elastically scattered from positive ions of oxygen. IPM potential parameters from minimization of the total energy of bound system of electron plus target ion. Results are as follows: solid line, O^+; short-dash line, O^{3+}; long-short dash line, O^{5+}; long-dash line, O^{7+}.

TABLE III. Phase shifts (δ_l in radians) computed from the GSZ independent-particle model for elastic scattering of electrons from positive ions of nitrogen.

	Potential parameters^a		Energy					
Ion	d (a.u.)	H	(Ry)	δ_0	δ_1	δ_2	δ_3	δ_4
N^+	0.8480	1.9250	0.1	3.45	2.10	0.184	0.015	0.001
			0.8	3.30	1.92	0.371	0.079	0.020
			2.0	3.12	1.76	0.516	0.166	0.061
N^{2+}	0.6300	1.6191	0.1	2.23	1.35	0.250	0.028	0.003
			0.8	2.19	1.29	0.307	0.060	0.012
			2.0	2.12	1.22	0.364	0.103	0.031
N^{3+}	0.4555	1.3478	0.1	1.44	0.818	0.177	0.023	0.002
			0.8	1.42	0.798	0.196	0.035	0.006
			2.0	1.39	0.771	0.219	0.053	0.013
N^{4+}	0.2957	1.0394	0.1	0.856	0.422	0.078	0.008	0.001
			0.8	0.850	0.417	0.084	0.011	0.001
			2.0	0.840	0.410	0.094	0.016	0.003
N^{5+}	0.1524	0.6716	0.1	0.426	0.139	0.014	0.001	...
			0.8	0.423	0.139	0.015	0.001	...
			2.0	0.421	0.139	0.017	0.001	...
N^{6+}	0.0960	0.6864	0.1	0.149	0.030	0.002	...	...
			0.8	0.149	0.030	0.002	...	...
			2.0	0.148	0.030	0.002	...	...

^{a}Potential parameters from minimization of the total energy of the bound system of electron plus target ion.

TABLE IV. Phase shifts (δ_l in radians) computed from the GSZ independent-particle model for elastic scattering from positive ions of oxygen.

	Potential parameters^a		Energy					
Ion	d (a.u.)	H	(Ry)	δ_0	δ_1	δ_2	δ_3	δ_4
O^+	0.7348	1.7731	0.1	3.69	2.28	0.140	0.009	...
			0.8	3.55	2.10	0.322	0.057	0.012
			2.0	3.37	1.94	0.488	0.136	0.045
O^{2+}	0.5958	1.6039	0.1	2.53	1.58	0.268	0.027	0.002
			0.8	2.48	1.51	0.335	0.060	0.011
			2.0	2.41	1.43	0.404	0.106	0.030
O^{3+}	0.4760	1.4361	0.1	1.76	1.07	0.245	0.032	0.003
			0.8	1.74	1.04	0.268	0.049	0.008
			2.0	1.70	1.00	0.297	0.073	0.018
O^{4+}	0.3674	1.2675	0.1	1.18	0.676	0.164	0.024	0.002
			0.8	1.17	0.666	0.174	0.030	0.005
			2.0	1.15	0.650	0.186	0.041	0.009
O^{5+}	0.2454	0.9998	0.1	0.718	0.357	0.071	0.008	...
			0.8	0.714	0.354	0.074	0.010	0.001
			2.0	0.709	0.350	0.080	0.013	0.002
O^{6+}	0.1350	0.6900	0.1	0.366	0.126	0.014	0.001	...
			0.8	0.365	0.126	0.015	0.001	...
			2.0	0.363	0.126	0.016	0.001	...
O^{7+}	0.0800	0.6480	0.1	0.128	0.025	0.002	...	...
			0.8	0.128	0.025	0.002	...	...
			2.0	0.127	0.025	0.002	...	...

^{a}By energy minimization.

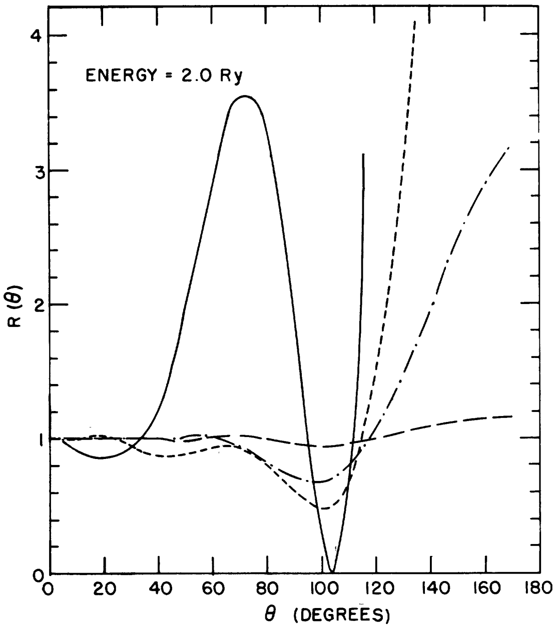

FIG. 7. Results of IPM computation of the ratio of differential to Rutherford cross sections as a function of scattering angle for electrons of energy 2.0 Ry elastically scattered from positive ions of oxygen. See caption to Fig. 6.

and 7 as a function of scattering angle for several ions of oxygen at energies of 0.2 and 2 Ry, respectively. As expected, the greatest departures from pure Coulomb scattering occur for the singly charged O^{+} ion, and the least for O^{7+}, where the departure from Rutherford scattering is negligible. For the other ions there is a significant (much greater than 10%) departure from Coulomb scattering only above 70° at 0.2 Ry and only at the back angles for an energy of 2 Ry.

CONCLUSIONS

Without precise experimental information it is not possible to assess objectively the accuracy of the current IPM analysis of the elastic scattering of electrons from positive ions. For the lower-order partial waves the IPM results are very similar to those obtained using HFS potentials. The IPM potential has the distinct computational advantage of being characterized by only two numbers, namely the H and d parameters. The analytic IPM is potentially of broader applicability than the quantum-defect approach because of the latter's empirical basis. For similar reasons the energy-minimization procedure for selecting the parameters of the IPM potentials has been favored over that of fitting the energies of the single-electron levels. However, the IPM results using these two different approaches are not widely at variance. At no increase in the number of parameters a more realistic $\rho^{1/3}$ exchange term may be included in the IPM potentials and this warrants further investigation.

The present results are sufficiently encouraging to establish the validity of the GSZ independent-particle model for computing cross sections for the scattering of electrons from ions. The intent has been to obtain a convenient and reasonably accurate atomic model for applications. In this respect the investigation has been successful.

ACKNOWLEDGMENTS

We would like to express our thanks to Dr. T. Mo for his helpful assistance. This work was supported in part by the United States Atomic Energy Commission. Computational support was contributed by the Northeast Regional Data Center at the University of Florida.

---

*On sabbatical leave from Department of Physics, State University College, Plattsburgh, New York 12901.

[1] B. H. Brandsden and A. Dalgarno, Proc. Phys. Soc. Lond. A 66, 268 (1953).

[2] Isao Shimamura, J. Phys. Soc. Jap. 31, 217 (1971).

[3] Barry Schneider and Joel I. Krugler, Phys. Rev. A 4, 1008 (1971).

[4] M. J. Jamieson, J. Phys. B 5, L26 (1972).

[5] S. T. Manson, Phys. Rev. 182, 97 (1969).

[6] E. M. A. Peixoto, Phys. Rev. 177, 204 (1969).

[7] M. J. Seaton, Mon. Not. R. Astron. Soc. 118, 504 (1958); see also M. J. Seaton, Proc. Phys. Soc. Lond. 88, 815 (1966).

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

[9] J. N. Bass, A. E. S. Green, and J. H. Wood, Adv. Quantum Chem. 7, 263 (1973).

[10] P. P. Szydlik and A. E. S. Green, Phys. Rev. A (to be published).

[11] For general features of the fitting procedure cf. P. S. Ganas and A. E. S. Green, Phys. Rev. A 4, 182 (1971). For more specific information cf. a companion to the present paper, viz., G. J. Kutcher, P. P. Szydlik, and A. E. S. Green, Phys. Rev. A 10, 842 (1972).

[12] See, for example, N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, 3rd ed. (Oxford U. P., London, 1965), pp. 65 ff.

[13] M. A. Melkanoff, T. Sawada, and J. Raynal, in *Methods in Computational Physics* (Academic, New York, 1966), Vol. 6.

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

[15] H. F. Weiss, Z. Phys. 229, 299 (1969).

[16] A. C. Yates and T. G. Strand, Phys. Rev. 170, 184

(1968).

[17] J. C. Slater, *Quantum Theory of Matter*, 2nd ed. (McGraw-Hill, New York, 1968), pp. 339 ff.

[18] R. Gaspar, Acta Phys. Acad. Sci. Hung. 3, 263 (1954); the same result was derived much later by Kohn and Sham, Phys. Rev. 140, A1133 (1965).

[19] M. H. Mittleman and K. M. Watson, Ann. Phys. (N. Y.) 10, 268 (1960).

[20] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N. J., 1963).

[21] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U. S.) Circ. No. 467 (U. S. GPO, Washington, D. C., 1949), Vol. I.

[22] K. Siegbahn *et al.*, *ESCA Atomic, Molecular, and Solid State Structure Studied by Means of Electron Spectroscopy* (Almquist-Wiksells, Uppsala, 1967), Appendix II.