

Scattering of electrons from argon atoms

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The scattering of electrons from argon atoms is studied by the method of polarized orbitals. The $3p \rightarrow d$ perturbed orbital calculated using the Sternheimer approximation gives the polarizability $14.29a_0^3$. The perturbation of the orbitals $1s$, $2s$, $2p$, and $3s$ is taken into account by renormalizing the $3p \rightarrow d$ orbitals to give the experimental value $11.06a_0^3$. Using only the modified orbital in the total wave function, phase shifts for various partial waves have been calculated in the exchange, exchange-adiabatic, and polarized-orbital approximations. They are compared with the results of the previous calculations. The calculated total elastic, differential, and momentum-transfer cross sections are compared with the experimental results. The elastic total cross sections obtained in the polarized-orbital approximation agree very closely with the recently measured cross sections by Jost *et al.* and Nickel *et al.* The critical point (the value of k^2 and θ at which the differential cross section is minimum) is at 0.306 eV and 80° , in good agreement with the measurements of Weyhreter *et al.*

INTRODUCTION

Within the last few years, we have applied the method of polarized orbitals¹ to the scattering of electrons from atoms² and photoionization of atoms.^{3,4} The hallmark of this method is that it projects the exchange polarization terms in addition to direct polarization terms, and it has been shown that these terms can have a quantitatively important effect. This is particularly clear from our recent calculation on photoionization of sodium atoms.⁴ The photoionization cross sections obtained in the polarized-orbital (PO) approximation, where again all terms including exchange polarization are retained, agreed very well with the results obtained by many-body perturbation and close-coupling calculations. We continue these studies to the scattering of electrons from argon atoms and calculate phase shifts in the PO approximation in addition to exchange and exchange-adiabatic approximations. The phase shifts calculated in the above-mentioned three approximations have been used to calculate the elastic differential, total, and momentum-transfer cross sections.

During the last few years, a number of calculations have been carried out on scattering of electrons from argon atoms using different theoretical techniques: An R -matrix calculation by Fon *et al.*⁵ and Bell *et al.*;⁶ an optical-potential method by McCarthy *et al.*,⁷ Amusia *et al.*,⁸ and Walker;⁹ and an exchange-adiabatic approximation by Thomson,¹⁰ Garbaty and LaBahn,¹¹ and McEachran and Stauffer.¹²

At the same time, there have been a number of measurements on argon atoms. The most recent measurements of the total elastic cross sections are by Jost *et al.*,¹³ Nickel *et al.*,¹⁴ Ferch *et al.*,¹⁵ and Wagenaar and de Heer,¹⁶ and of differential cross sections by Weyhreter *et al.*¹⁷ In these experiments measurements have been carried out to very low incident energies. The previous measurements include total cross sections by Charlton

et al.,¹⁸ Golden and Bandel,¹⁹ Guskov *et al.*,²⁰ Kauppila *et al.*,²¹ and Wagenaar and de Heer;²² and differential cross sections by Andrick and Bitsch,²³ DuBois and Rudd,²⁴ Lewis,²⁵ Srivastava *et al.*,²⁶ Williams and Wills,²⁷ and Zhou Qing *et al.*²⁸ Momentum-transfer cross sections have been measured by Frost and Phelps,²⁹ McPherson *et al.*,³⁰ and Milloy *et al.*³¹

THEORY AND CALCULATIONS

The scattering functions have been calculated using the polarized-orbital method.¹ The wave function of the electron-argon system is given by

$$\Psi^A = A \{ u_l(r_1) [\psi_0(2, 3, 4, \dots, N+1) + \psi^{\text{pol}}(1; 2, 3, 4, \dots, N+1)] \}, \quad (1)$$

where ψ_0 is the wave function of the N -electron target, and is given by the Hartree-Fock-Slater determinant. The determinant can be expressed in terms of the orbitals which have been determined by Clementi and Roetti³² in the frozen-core approximation.

The perturbed part ψ^{pol} is determined in the adiabatic approximation,¹ i.e., by assuming that the unperturbed ground state ψ_0 is adiabatically perturbed by the incident electron. In the PO approximation,¹ only the dipole part of the interaction potential between the incident and target electrons is included, and the adiabatic approximation means the perturbation of the target electrons is calculated for each position (r_1) of the incident electron. The adiabatic perturbation is thus given by

$$V_{\text{ad}} = \sum_{j=2}^{N+1} 2/r_{1j} - 2Z/r_1, \quad r_1 > r_j \quad (2a)$$

$$\cong \frac{2}{r_1^2} \sum_{j=2}^{N+1} r_j \cos\theta_{1j} \epsilon(r_1, r_j). \quad (2b)$$

Here $Z = N$ (neutral atomic target). The presence of the step function $\epsilon(r_1, r_j)$ in Eq. (2b) expresses the physically motivated additional approximation that the interaction is zero when the incident electron is inside the target electrons.¹ (This has more recently been called the "non-penetrating" approximation and has been particularly used in electron-molecule scattering.³³) The radial part of the perturbed orbitals are obtained from the Sternheimer approximation of first-order perturbation theory,³⁴

$$\left[\frac{d^2}{dr^2} - \left(\frac{1}{u_{nl}} \frac{d^2}{dr^2} u_{nl} \right) + \frac{l(l+1) - l'(l'+1)}{r^2} \right] u_{nl \rightarrow l'}(r) = r u_{nl}(r), \quad (3)$$

where u_{nl} , the unperturbed orbital, is perturbed to $u_{nl \rightarrow l'}$, l and l' being angular momenta of the unperturbed and perturbed orbitals, respectively. For argonlike systems, the perturbed orbitals are $u_{ns \rightarrow p}$ for $n=1, 2$, and 3 , $u_{np \rightarrow s}$ and $u_{np \rightarrow d}$ for $n=2$ and 3 . We have calculated only the perturbed orbital $u_{3p \rightarrow d}$ here, giving the polarizability $\alpha_{3p \rightarrow d} = 14.29 a_0^3$. It is assumed that this is due to the Sternheimer approximation. This perturbed orbital $u_{3p \rightarrow d}$ is then renormalized to give the experimental³⁵ polarizability $\alpha = 11.06 a_0^3$. It is assumed that by normalizing to the experimental polarizability the perturbed orbital $u_{3p \rightarrow d}$ takes into account³⁶ (obviously only in an approximate way) the perturbation of other orbitals as well. The unnormalized perturbed and unperturbed orbitals, $u_{3p \rightarrow d}$ and u_{3p} , are shown in Fig. 1 and it can be seen that the perturbed orbital is much smaller than the unperturbed orbital throughout the range.

The resultant potential V_p , which behaves as $-\alpha/r^4$ for $r \rightarrow \infty$, is shown in Fig. 2. It is seen to have a repulsive part at short distances. This behavior has also been seen for electron-Li, electron- Na^+ , and electron-Ne polarization potentials,^{37,4,2} in the first case, it should be emphasized, the polarized orbital and hence the polarization potential was modified because of the large polarizability of alkali-metal atoms, so as effectively to include nonadiabatic effects.³⁷

The scattering equation is obtained by projecting with

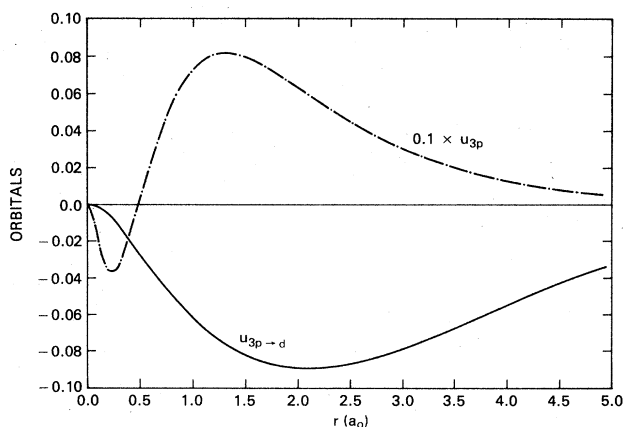


FIG. 1. Perturbed orbital $u_{3p \rightarrow d}$ and unperturbed orbital u_{3p} .

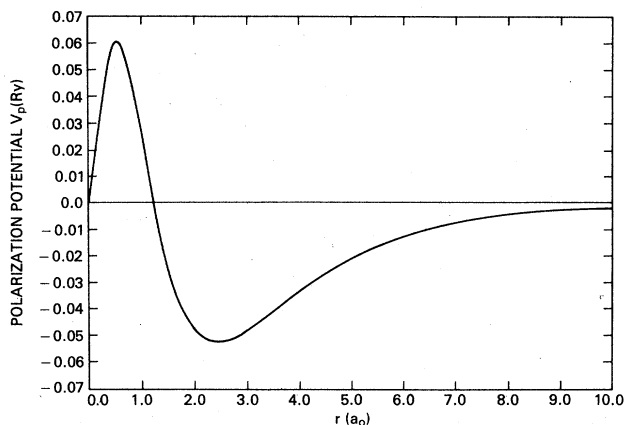


FIG. 2. Polarization potential V_p obtained by normalizing $u_{3p \rightarrow d}$.

ψ_0^* on the left of $(H_{N+1} - E)\Psi^A = 0$, as a basic aspect of POM:³⁸

$$\int Y_{l0}(\Omega_1) \chi_{1/2}(\sigma) \psi_0^*(2, 3, 4, \dots, N+1) \times (H_{N+1} - E) \Psi^A \prod_{i=2}^{N+1} dr_i = 0. \quad (4)$$

H_{N+1} and E are the total Hamiltonian and energy of the electron-argon system. The equation satisfied by the continuum function is derived from Eq. (4):

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right] u_{kl}(r) = [V_c(r) + V_p(r) + W] u_{kl}(r). \quad (5)$$

The expression for direct and exchange potential contained in $V_c u(r)$, the polarization potential $V_p u(r)$, and the exchange polarization terms $W u(r)$ are given in the Appendix and are similar to those given in Ref. 4 (but it is emphasized that we are retaining only the contribution of $u_{3p \rightarrow d}$ terms here). The exchange and exchange-adiabatic approximations are obtained by neglecting $V_p u(r)$ and $W u(r)$ terms, and $W u(r)$ terms, respectively. In the PO approximation, all terms are retained in Eq. (5). The phase shifts are obtained from the asymptotic form of the solutions of Eq. (5) and k^2 is the scattering energy in Ry:

$$\lim_{r \rightarrow \infty} u_{kl}(r) = \sin(kr - l\pi/2 + \eta_l). \quad (6)$$

RESULTS

The phase shifts (module π) for $l=0$ and 1 partial waves at various incident energies are given in Table I in all three approximations. The phase shifts for s and p waves should go to 3π and 2π , respectively, as $k^2 \rightarrow 0$ because of the three filled $1s$, $2s$, and $3s$ shells and two $2p$ shells in the argon atoms. The exchange-adiabatic and exchange polarization results differ substantially from each other and exchange approximation results. Our s -wave PO phase shifts are lower than exchange-adiabatic results of McEachran and Stauffer¹² (except for $k=0.1$) while the p -wave phase shifts are higher for low k and lower for

TABLE I. s - and p -wave phase shifts in three approximations: the exchange (Exch.), exchange-adiabatic (Ex.-ad.), and polarized-orbital (PO) approximations.

k (a.u.)	s wave			p wave		
	Exch.	Ex.-ad.	PO	Exch.	Ex.-ad.	PO
0.1000	-0.1490	0.0620	0.0447	-0.0044	0.0156	0.0156
0.1500	-0.2243 ^a	0.0286 ^a	0.0090	-0.0137 ^a	0.0364 ^a	0.0249
0.2000	-0.3005	-0.0216	-0.0471	-0.0311	0.0328	0.0291
0.2500	-0.3777 ^a	-0.0875 ^a	-0.1160	-0.0565 ^a	0.0083 ^a	0.0247
0.3000	-0.4559	-0.1637	-0.1930	-0.0894	-0.0198	0.0097
0.4000	-0.6148	-0.3291	-0.3600	-0.1758	-0.0309	-0.0470
0.4696	-0.7266	-0.4498	-0.4813	-0.2478	-0.0847	-0.1052
0.5000	-0.7756	-0.5031	-0.5350	-0.2814	-0.1120	-0.1340
0.6000	-0.9363	-0.6784	-0.7100	-0.3979	-0.2125	-0.2390
0.6062	-0.9462	-0.6792	-0.7209	-0.4053	-0.2192	-0.2459
0.7000	-1.0952	-0.8513	-0.8830	-0.5186	-0.3238	-0.3530
0.8000	-1.2507	-1.0198	-0.9500	-0.6391	-0.4396	-0.4710
0.8573	-1.3379	-1.1138	-1.1438	-0.7071	-0.5064	-0.5376
0.9000	-1.4018	-1.1826	-1.2120	-0.7569	-0.5559	-0.5872
0.9500	-1.4747 ^a	-1.2607 ^a	-1.2905	-0.8136 ^a	-0.6131 ^a	-0.6451
1.0000	-1.5476	-1.3389	-1.3670	-0.8702	-0.6703	-0.7015
1.0500	-1.6177 ^a	-1.4137 ^a	-1.4422	-0.9243 ^a	-0.7258 ^a	-0.7567
1.1000	-1.6878	-1.4885	-1.5157	-0.9784	-0.7812	-0.8117
1.2000	-1.8220	-1.6314	-1.6572	-1.0811	-0.8880	-0.9172
1.2124	-1.8383	-1.6487	-1.6743	-1.0934	-0.9009	-0.9300
1.3000	-1.9504	-1.7677	-1.7920	-1.1785	-0.9901	-1.0182
1.4000	-2.0729	-1.8975	-1.9207	-1.2706	-1.0877	-1.1143
1.5000	-2.1899	-2.0212	-2.0431	-1.3580	-1.1807	-1.2057
1.6000	-2.3016	-2.1391	-2.1598	-1.4408	-1.2693	-1.2928
1.7000	-2.4082	-2.2516	-2.2710	-1.5194	-1.3537	-1.3758
1.8000	-2.5100	-2.3591	-2.3772	-1.5941	-1.4343	-1.4549
1.9000	-2.6074	-2.4617	-2.4787	-1.6653	-1.5111	-1.5305
1.9170	-2.6235	-2.4788	-2.4956	-1.6771	-1.5238	-1.5428
2.0000	-2.7005	-2.5590	-2.5759	-1.7333	-1.5846	-1.6027

^aInterpolated.

higher values of k when compared to the results of McEachran and Stauffer.¹² The polarizability used in their calculation³⁹ is $\alpha = 10.76a_0^3$ and they have not included exchange polarization terms in their calculations, i.e. theirs is an exchange-adiabatic calculation. The PO phase shifts for s , p , and d waves are compared to the results of McEachran and Stauffer¹² and Bell *et al.*⁶ in Figs. 3, 4, and 5. The agreement between the three calculations is good for s - and p -wave phase shifts but d -wave phase

shifts of Ref. 12 for $k > 0.5$ are higher than the results of the two other calculations. This indicates the importance of exchange polarization terms, which have not been included in Ref. 12. At low energies most of the contribution to phase shifts for $l \geq 2$ comes from the polarization potential, but at higher energies exchange terms contribute most. This seems to be particularly true for d -wave phase shifts.

We present phase shifts for $l = 2-6$ in Table II in the

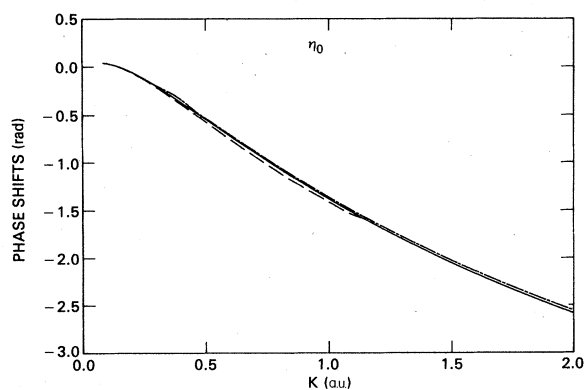


FIG. 3. s -wave phase shifts (modulo π): —, PO; ---, McEachran and Stauffer (Ref. 12); - · -, Bell *et al.* (Ref. 6).

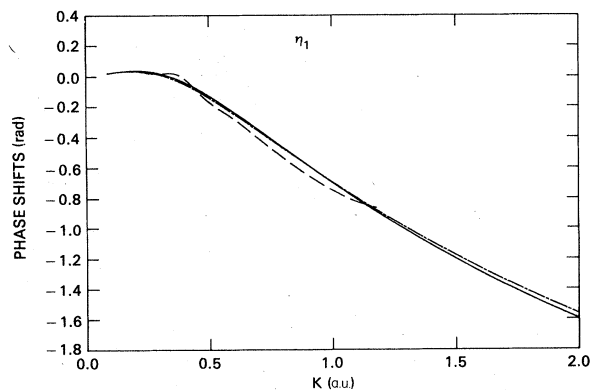


FIG. 4. p -wave phase shifts (modulo π): notation as in Fig. 3.

PO approximation and at low energies they follow the phase-shift formula⁴⁰

$$\tan\eta_l = \frac{\pi\alpha k^2}{(2l-1)(2l+1)(2l+3)} \quad (7)$$

The present results for $l > 3$, though slightly higher, are in good agreement with the results of Ref. 12. A comparison with the close-coupling results of Bell *et al.*⁶ indicates that the present phase shifts in PO approximation are in good agreement with the close-coupling results.

The differential cross sections at $k^2 = 0.136, 0.306, 0.544, 1.424, 3, 5, 10, 20,$ and 50 eV are given in Table III from 0° to 180° . The contribution of $l = 7-500$ has been added by using the effective range formula (7). The convergence is very slow in the forward direction and we use²

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega} \right)_{\theta=0^\circ} &= \left| \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\eta_l} \sin\eta_l \right|^2 \\ &= \left(\frac{d\sigma}{d\Omega} \right)_{\theta=0^\circ}^{l < l_0} + \left(\frac{\pi\alpha l_0}{4l_0^2 - 1} \right) \sum_{l=0}^{l_0-1} (2l+1) \sin(2\eta_l) + \left(\frac{\pi\alpha l_0 k}{4l_0^2 - 1} \right)^2, \end{aligned} \quad (8)$$

where Eq. (7) has been used for $l \geq 7$ to derive this formula and here $l_0 = 7$. As pointed out previously,² since only the dipole potential is retained in the description of the

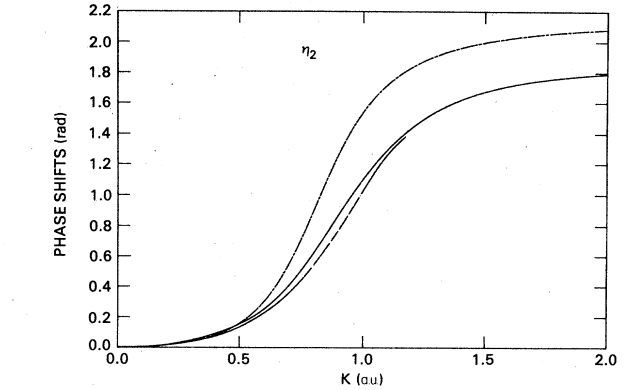


FIG. 5. d -wave phase shifts (modulo π): notation as in Fig. 3.

PO method, we also do not include the higher-order corrections to Eq. (7). The angles at which the differential cross section has a minimum value are also indicated

TABLE II. $l = 2-6$ partial-wave phase shifts (rad) in PO approximation.

k (a.u.)	2	3	4	5	6
0.1000	0.0034	0.0011	0.0005	0.0003	0.0001
0.1500	0.0086	0.0025	0.0011	0.0006	0.0004
0.2000	0.0167	0.0044	0.0020	0.0011	0.0006
0.2500	0.0293	0.0070	0.0031	0.0017	0.0010
0.3000	0.0448	0.0100	0.0045	0.0024	0.0015
0.4000	0.0893	0.0182	0.0081	0.0043	0.0026
0.4696	0.1302	0.0256	0.0114	0.0060	0.0036
0.5000	0.1525	0.0290	0.0126	0.0067	0.0040
0.6000	0.2502	0.0432	0.0184	0.0098	0.0058
0.6062	0.2580	0.0442	0.0187	0.0099	0.0060
0.7000	0.4029	0.0615	0.0253	0.0133	0.0079
0.8000	0.6152	0.0845	0.0334	0.0175	0.0104
0.8573	0.7539	0.0999	0.0388	0.0201	0.0119
0.9000	0.8598	0.1125	0.0430	0.0222	0.0132
0.9500	0.9803	0.1285	0.0484	0.0249	0.0147
1.0000	1.0939	0.1459	0.0542	0.0276	0.0163
1.0500	1.1961	0.1645	0.0604	0.0306	0.0181
1.1000	1.2876	0.1844	0.0670	0.0337	0.0199
1.2000	4.4334	0.2276	0.0815	0.0406	0.0237
1.2124	1.4484	0.2334	0.0835	0.0414	0.0242
1.3000	1.5390	0.2747	0.0977	0.0480	0.0280
1.4000	1.6137	0.3247	0.1155	0.0564	0.0325
1.5000	1.6670	0.3765	0.1348	0.0654	0.0376
1.6000	1.7057	0.4291	0.1555	0.0752	0.0430
1.7000	1.7342	0.4813	0.1774	0.0858	0.0488
1.8000	1.7555	0.5326	0.2003	0.0970	0.0551
1.9000	1.7715	0.5819	0.2240	0.1089	0.0617
1.9170	1.7738	0.5901	0.2281	0.1110	0.0629
2.0000	1.7835	0.6289	0.2483	0.1214	0.0688

TABLE III. Differential cross sections at various energies.

θ (deg)	k^2 (eV)									
	0.136	0.306	0.544	1.424	3	5	10	20	50	
0	1.896	1.672	1.468	1.255	2.093	6.106	35.660	58.920	67.122	
5	1.696	1.394	1.130	0.811	1.336	4.569	31.040	52.841	52.282	
10	1.514	1.149	0.847	0.479	0.832	3.421	26.617	46.851	40.251	
15	1.347	0.934	0.614	0.247	0.551	2.629	22.451	40.893	30.619	
20	1.194	0.748	0.426	0.102	0.462	2.156	18.610	34.953	22.895	
25	1.055	0.589	0.280	0.032	0.532	1.962	15.174	29.114	16.738	
30	0.928	0.455	0.169	0.026	0.729	2.004	12.217	23.517	11.885	
35	0.812	0.344	0.091	0.069	1.016	2.231	9.789	18.323	8.123	
40	0.707	0.253	0.039	0.150	1.360	2.590	7.909	13.682	5.273	
45	0.612	0.181	0.010	0.258	1.726	3.024	6.557	9.716	3.183	
50	0.527	0.124	0.001	0.380	2.083	3.478	5.675	6.500	1.728	
55	0.452	0.080	0.005	0.507	2.402	3.897	5.175	4.055	0.802	
60	0.386	0.048	0.021	0.630	2.660	4.235	4.943	2.352	0.312	
65	0.329	0.025	0.044	0.739	2.839	4.453	4.859	1.309	0.171	
70	0.279	0.011	0.071	0.830	2.927	4.525	4.803	0.811	0.289	
75	0.236	0.003	0.100	0.897	2.920	4.437	4.677	0.718	5.575	
80	0.200	0.000	0.128	0.937	2.820	4.190	4.406	0.880	0.941	
85	0.168	0.001	0.153	0.951	2.635	3.800	3.954	1.157	1.307	
90	0.141	0.004	0.175	0.939	2.380	3.296	3.326	1.434	1.605	
95	0.118	0.009	0.193	0.902	2.073	2.718	2.564	1.628	1.789	
100	0.098	0.015	0.206	0.845	1.736	2.112	1.747	1.695	1.835	
105	0.081	0.021	0.214	0.773	1.391	1.529	0.975	1.635	1.739	
110	0.067	0.026	0.218	0.689	1.062	1.017	0.367	1.482	1.522	
115	0.055	0.032	0.218	0.599	0.767	0.622	0.036	1.301	1.216	
120	0.045	0.036	0.214	0.508	0.525	0.378	0.088	1.171	0.869	
125	0.038	0.040	0.207	0.420	0.348	0.309	0.584	1.172	0.531	
130	0.031	0.044	0.198	0.339	0.241	0.423	1.574	1.376	0.251	
135	0.026	0.047	0.188	0.267	0.207	0.714	3.044	1.827	0.069	
140	0.022	0.049	0.177	0.206	0.239	1.161	4.942	2.542	0.008	
145	0.019	0.050	0.166	0.156	0.329	1.730	7.169	3.498	0.075	
150	0.016	0.051	0.156	0.117	0.460	2.377	9.592	4.639	0.255	
155	0.014	0.051	0.147	0.088	0.617	3.050	12.051	5.878	0.519	
160	0.013	0.051	0.139	0.067	0.779	3.696	14.374	7.109	0.824	
165	0.011	0.051	0.133	0.054	0.929	4.263	16.392	8.220	1.124	
170	0.011	0.051	0.128	0.045	1.050	4.705	17.955	9.104	1.376	
175	0.010	0.051	0.126	0.042	1.128	4.985	18.943	9.672	1.543	
180	0.010	0.051	0.125	0.040	1.154	5.081	19.281	9.868	1.601	

θ_{\min}	80	50	30	20,135	25,125	115	75,120	65,140
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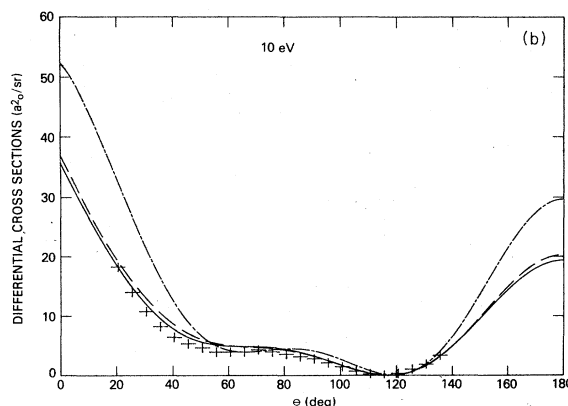
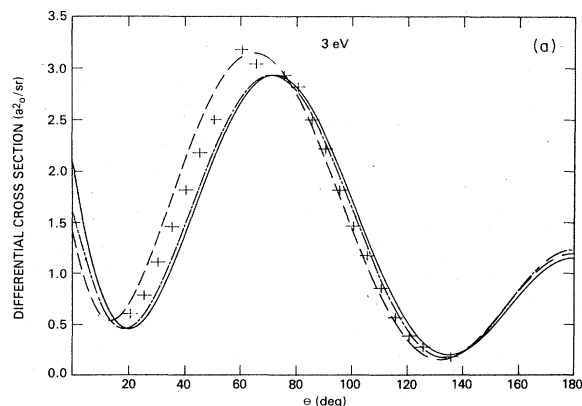


FIG. 6. Differential cross sections: (a) 3 eV, (b) 10 eV, (c) 20 eV. —, PO; ---, McEachran and Stauffer (Ref. 12); - - -, Fon *et al.* (Ref. 5); +, Srivastava *et al.* (Ref. 26); *, DuBois and Rudd (Ref. 24).

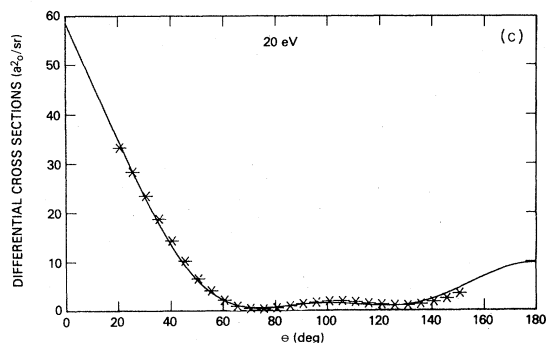


FIG. 6. (Continued).

in Table III.

We find the critical point, i.e., the value of k^2 and θ at which the differential cross section is minimum as $k^2=0.306$ eV and $\theta=80^\circ$, in good agreement with the re-

sults given by Weyhreter *et al.*,¹⁵ as $k^2 \cong 0.25$ eV and $\theta=100^\circ$ for the critical point. There are double minima at $k^2=3, 5, 20,$ and 50 eV, but not at $k^2=10$ eV. The angles $\theta=75^\circ$ and 120° at $k^2=20$ eV for which the differential cross section has double minima agree very well with the experimental values of 75° and 130° of Srivastava *et al.*²⁶ A comparison of the differential cross sections at 3, 10, and 20 eV with the theoretical values obtained by McEachran and Stauffer,¹² Fon *et al.*,⁵ and the experimental results of Refs. 24 and 26 is given in Figs. 6(a)–6(c). The present results are in good agreement with experimental results, but comparison does not really favor any of these calculations. Our exchange-adiabatic cross sections (not shown) are higher than in PO results. On the whole, we believe our PO results agree better with the experimental results than our exchange-adiabatic results. As pointed out previously, this indicates the importance of exchange polarization terms.

TABLE IV. Total elastic cross sections. Units are a_0^2 .

k (a.u.)	E (eV)	Present	Theory			Experiment		$W^{a,g}$
			MS ^{a,b}	$B^{a,c}$	$J^{a,d}$	$N^{a,e}$	$F^{a,f}$	
0.10	0.136	3.51	3.24	3.62	2.76		3.05	
0.15	0.306	1.32		1.18	1.13		1.15	
0.20	0.544	1.99	1.60	1.85	1.84		1.68	
0.25	0.850	4.02		3.93	4.14		3.43	
0.30	1.225	6.71	5.93	6.79	6.61		5.79	
0.40	2.177	13.64	12.80	14.17	13.71		11.41	
0.4696	3.0	19.26	19.11	20.30	19.48		17.30	
0.50	3.401	21.96	23.30	23.19	21.88		19.53	
0.60	4.898	32.01	37.07	33.56	31.79	31.46	30.20	
0.6062	5.0	32.74	37.92	34.24	32.59	32.10	30.87	
0.7	6.667	45.11	61.31	45.05	46.12	45.94	40.79	
0.8	8.708	60.87	84.61	57.92	63.94	63.09	55.74	
0.8573	10.0	69.20	97.28	65.03	74.33	73.47	67.54	
0.9	11.021	74.17	94.89	69.78	80.89	79.16	76.42	
(Inelastic threshold 11.6 eV)								
0.95	12.279	77.99	92.10	74.39	86.96	84.65	83.65	
1.0	12.606	79.69	89.30	77.39	88.07	85.96	85.75	
1.05	15.000	79.36	86.51	78.48	85.16	84.37	85.24	
1.1	16.463	77.67	80.90	77.27	80.44	80.65	83.14	
1.2	19.592	71.83	69.69		70.15	69.32	73.82	70.01
1.2124	20.0	71.01	68.30		68.97	67.97	72.19	68.75
1.3	22.994	65.11	62.24		61.41	61.82		61.39
1.4	26.667	58.80	55.33		54.77	55.85		53.13
1.5	30.613	53.27	48.84		50.22	51.32		48.26
1.6	34.831	48.54	44.76		46.39	47.54		44.96
1.7	39.321	44.49	40.68		42.91	43.76		42.32
1.8	44.083	41.01	37.68		40.13	41.09		38.93
1.9	49.117	37.99	34.85		37.87	38.62		36.93
1.917	50.0	37.51	37.51		37.52	38.20		35.65
2.0	54.423	35.34	32.29		35.94	36.91		35.33

^aInterpolated.

^bReference 12.

^cReference 6.

^dReference 13.

^eReference 14.

^fReference 15.

^gReference 16.

TABLE V. Momentum-transfer cross section. Units are a_0^2 .

k (a.u.)	E (eV)	Present	Theory MS ^{a,b}	$B^{a,c}$	Experiment $S^{a,d}$
0.10	0.136	1.46		1.54	
0.15	0.306	0.51		0.50	
0.20	0.544	2.07		1.97	
0.25	0.850	4.28		4.08	
0.30	1.225	6.53		6.24	
0.40	2.177	11.57		11.05	
0.4696	3.0	15.81	15.47	15.49	14.65
0.50	3.401	18.04	19.55	17.81	16.48
0.60	4.898	27.13	32.95	26.92	22.50
0.6062	5.0	27.84	33.78	27.55	22.87
0.70	6.667	39.47	54.84	37.45	34.19
0.80	8.708	51.95	70.25	47.31	46.47
0.8573	10.0	56.42	76.11	51.21	53.60
0.90	11.021	57.70	70.23	52.76	53.60
0.95	12.279	56.90	63.34	53.00	53.80
1.00	12.606	54.02	56.46	51.58	53.60
1.05	15.000	49.93	49.57	48.73	53.60
1.10	15.463	45.31	44.38	44.94	44.36
1.20	19.592	36.46	33.99		25.88
1.2134	20.0	35.48	32.70		23.58
1.30	22.994	29.47	29.12		20.25
1.40	26.667	24.40	25.04		16.45
1.50	30.613	20.78	21.32		13.07
1.60	34.831	18.16	19.67		12.06
1.70	39.321	16.20	18.03		11.05
1.80	44.083	14.68	16.90		10.04
1.90	49.117	13.46	15.87		9.29
1.9170	50.0	13.27	15.68		8.58
2.00	54.423	12.44			8.46

^aInterpolated.^bReference 12.^cReference 6.^dReference 26.

The total elastic cross sections in PO approximations are given in Table IV along with other theoretical and experimental results. We see that the present PO results at low energies are in excellent agreement with the experimental results of Jost *et al.*¹³ The present calculations indicate a minimum in the cross sections at $k^2=0.342$ eV (interpolated) in agreement with the minimum observed by Ferch *et al.*¹⁵ at $k^2=0.345$ eV, and a maximum at $k^2=12.606$ eV in agreement with the observed maximum by Jost *et al.*,¹³ Nickel *et al.*,¹⁴ and Ferch *et al.*¹⁵ The present maximum value of the cross section $79.69a_0^2$ agrees with the close-coupling⁶ result, but differs from the experimental results. The difference from experiment may be attributed to the contribution from the onset of inelastic processes around this energy.

The momentum-transfer cross sections in PO approximation are given in Table V along with the results of the other calculations.^{6,12} There is good agreement between the present calculation and the calculations of Bell *et al.*, and of McEachran and Stauffer, and the results are consistent with the recent experimental results of Srivastava *et al.*²⁶

A more detailed comparison of the elastic differential,

total, and momentum-transfer cross sections between the results of various theories and experiments is given in Ref. 12 but has been omitted here for clarity.

CONCLUSIONS

A polarized-orbital calculation for electron-argon scattering has been carried out. The polarizability of the argon atoms is taken into account by considering only the perturbation of the $3p$ orbital and renormalizing the perturbed orbital to obtain the experimental polarizability. By comparison with exchange-adiabatic calculations using the same perturbed orbital $u_{3p \rightarrow d}$ it is found that the exchange-polarization terms are important in the calculation of phase shifts. The elastic cross sections are in very good agreement with the recent experimental results.

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APPENDIX

We give the explicit expressions for V_c , V_p , and W appearing in Eq. (5):

$$V_c(r) = 4\Gamma^0(1s, 1s; r) + 4\Gamma^0(2s, 2s; r) + 4\Gamma^0(3s, 3s; r) + 12\Gamma^0(2p, 2p; r) + 12\Gamma^0(3p, 3p; r) - \frac{2Z}{r},$$

$$V_p(r) = \frac{-16}{3} \frac{1}{r^4} \int_0^r u_{3p}(x) x u_{3p \rightarrow d}(x) dx,$$

$$W u_{kL}(r) = W_{\text{ex}} u_{kL}(r) + W_{\text{ep}} u_{kL}(r),$$

$$\begin{aligned} W_{\text{ex}} u_{kL}(r) = & -\frac{2}{2L+1} u_{1s}(r) \Gamma^L(1s, kL; r) - \frac{2}{2L+1} u_{2s}(r) \Gamma^L(2s, kL; r) \\ & - \frac{2}{2L-1} u_{3s}(r) \Gamma^L(3s, kL; r) - 3 \sum C_{1L\lambda} \Gamma^\lambda(2p, kL; r) u_{2p}(r) \\ & - 3 \sum C_{1L\lambda} \Gamma^\lambda(3p, kL; r) u_{3p}(r) + \delta_{IL} (k^2 + \epsilon_{nl}) u_{nl}(r) \int_0^\infty u_{kL}(x) u_{nl}(x) dx, \end{aligned}$$

$$W_{\text{ep}} u_{kL}(r) = -r \{ W_{\text{ep}}^0(r) + \delta_{L0} I_{\text{ep}}^0(r) + \delta_{L1} I_{\text{ep}}^1(r) + \delta_{L2} [I_{\text{ep}}^2(r) + J^{3p, 3p \rightarrow d}(r)] \},$$

$$W_{\text{ep}}^0(r) = 8 \sum_\lambda \begin{bmatrix} \lambda & L & 2 \\ 0 & 0 & 0 \end{bmatrix}^2 u_{3p \rightarrow d}(r) r^{\lambda-1} \int_r^\infty \frac{u_{3p}(x) u_{kL}(x) dx}{x^{\lambda+3}},$$

$$\begin{aligned} I_{\text{ep}}^0(r) = & -\frac{8}{5} \frac{u_{3p \rightarrow d}(r)}{r} \left[\left[\int_r^\infty \frac{u_{kL}(x) u_{3p}(x)}{x^2} dx \right] \Gamma^2(3p, 3p; r) + \left[\int_r^\infty \frac{u_{kL}(x) u_{2p}(x)}{x^2} dx \right] \Gamma^2(3p, 2p; r) \right] \\ & + \frac{16}{3} \sum_{n=2,3} \frac{u_{np}(r)}{4} \int_0^\infty \frac{u_{kL}(x) u_{np}(x)}{x^2} dx \int_0^x u_{3p \rightarrow d}(y) u_{3p}(y) g_1(r, y) dy, \end{aligned}$$

$$\begin{aligned} I_{\text{ep}}^1(r) = & -\frac{8}{9} \frac{u_{3p \rightarrow d}(r)}{r} \left[\left[\int_r^\infty \frac{u_{kL}(x) u_{1s}(x)}{x^2} dx \right] \Gamma^1(3p, 1s; r) + \sum_{n=2,3} \left[\int_r^\infty \frac{u_{kL}(x) u_{ns}(x)}{x^2} dx \right] \Gamma^1(3p, ns; r) \right] \\ & + \frac{16}{9} \sum_{n=1,2,3} \frac{u_{ns}(r)}{r} \left[\int_0^\infty \frac{u_{kL}(x) u_{ns}(x)}{x^2} dx \int_0^x u_{3p \rightarrow d}(y) u_{3p}(y) g_1(r, y) dy \right], \end{aligned}$$

$$\begin{aligned} I_{\text{ep}}^2(r) = & \frac{8}{5} \frac{u_{3p \rightarrow d}(r)}{r} \left[\int_r^\infty \frac{u_{kL}(x) u_{3p}(x)}{x^2} dx \right] \\ & \times [2\Gamma^0(1s, 1s; r) + 2\Gamma^0(2s, 2s; r) + 2\Gamma^0(3s, 3s; r) + 6\Gamma^0(2p, 2p; r) + 5\Gamma^0(3p, 3p; r) - \frac{1}{5} \Gamma^2(3p, 3p; r)] \\ & - \frac{8}{5} \frac{u_{3p \rightarrow d}(r)}{r} \left[\int_r^\infty \frac{u_{kL}(x) u_{2p}(x)}{x^2} dx \right] [\Gamma^0(3p, 3p; r) + \frac{1}{5} \Gamma^2(2p, 2p; r)] \\ & + \frac{2}{25} \frac{u_{3p}(r)}{4} \left[\int_0^\infty \frac{u_{kL}(x) u_{3p}(x)}{x^2} dx \right] \left[\frac{59}{3} \int_0^x u_{3p \rightarrow d}(y) u_{3p}(y) g_1(r, y) dy - \frac{36}{7} \int_0^x u_{3p \rightarrow d}(y) u_{3p}(y) g_3(r, y) dy \right] \\ & + \frac{32}{15} \frac{u_{2p}(r)}{r} \left[\int_0^\infty \frac{u_{kL}(x) u_{2p}(x)}{x^2} dx \int_0^x u_{3p \rightarrow d}(y) u_{3p}(y) g_1(r, y) dy \right] \\ & - \frac{8}{25} \frac{u_{2p}(r)}{r} \left[\int_0^\infty \frac{u_{kL}(x) u_{3p}(x)}{x^2} dx \left[\frac{9}{7} \int_0^x u_{3p \rightarrow d}(y) u_{2p}(y) g_3(r, y) dy + 2 \int_0^x u_{3p \rightarrow d}(y) u_{2p}(y) g_1(r, y) dy \right] \right] \\ & - \frac{8}{25} \sum_{n=1,2,3} \frac{u_{ns}(r)}{r} \left[\int_0^\infty \frac{u_{kL}(x) u_{3p}(x)}{x^2} dx \int_0^x u_{3p \rightarrow d}(y) u_{ns}(y) g_2(r, y) dy \right]. \end{aligned}$$

Γ^λ , g_λ , and $J^{nl, nl \rightarrow l'}$ have been defined in Ref. 4;

$$C_{1L\lambda} = \int_{-1}^1 P_l(x) P_L(x) P_\lambda(x) dx,$$

where the P_l are the Legendre polynomials.

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