Accurate *ab initio* calculations on elastic scattering of low-energy electrons by argon atoms

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The multiconfiguration Hartree-Fock method has been applied to study low-energy scattering of electrons from argon atoms. The polarization of the argon atoms due to the scattered electron and the electron-correlation effects that are very important in the calculation are taken into account in the *ab initio* way more accurately through the configuration-interaction procedure. Phase shifts for various partial waves calculated in this approximation have been used to calculate elastic differential, total elastic, and momentum-transfer cross sections. The present results are compared with the experimental and other theoretical results. It is found that the present results are in very good agreement with the experimental results and compare well with the other theoretical results.

I. INTRODUCTION

In recent years, the scattering of electrons from inert gases has attracted considerable theoretical and experimental interest. This is due to the fact that with the rapid developments in rare-gas-halide high-power lasers, accurate measurements are possible for these gases providing an adequate test of the theoretical models. In particular, elastic scattering of low-energy electrons by argon atoms has received considerable theoretical and experimental study for many years. A lot of theoretical and experimental data are available for total elastic, momentum-transfer cross sections and of differential cross sections. There is still considerable disagreement existing between different sets of experimental results, between different theoretical calculations, and between theory and experiment.

Recently, we have applied the multiconfiguration Hartree-Fock (MCHF) method to the scattering of electrons from atoms.[1,2] The beauty of the method is that it takes into account the electron correlation and the polarization effects very accurately in the *ab initio* way through the configuration-interaction procedure. It has been found that phase shifts and cross sections calculated for the elastic scattering of electrons from neon and helium atoms[1,2] were in excellent agreement with experiment and the other theoretical results. In this paper we continue these studies with the scattering of electrons from argon atoms. The phase shifts for partial waves calculated in the MCHF method have been used to calculate the elastic differential, total, and momentum-transfer cross sections.

During the past few years, there have been a number of measurements on scattering of electrons from argon atoms. The recent measurements of the total elastic cross sections are made by Furst *et al.*,[3] Buckman and Lohmann,[4] Jost *et al.*,[5] Nickel *et al.*,[6] Ferch *et al.*,[7] and Wagenaar and deHeer,[8] and of differential cross sections by Weyhreter, Berzick, and Linder.[9] They carried out experiments to very low incident energies. The measurements made earlier include total cross sections by Charlton *et al.*,[10] Golden and Bandel,[11] Guskov, Savvov, and Slobodyanyuk,[12] Kauppila *et al.*,[13] and Wagenaar and deHeer,[14] and differential cross sections by Andrick,[15] Dubois and Rudd,[16] Lewis,[17] Srivastava *et al.*,[18] Williams and Willis,[19] and Zhou Qing, Beerlage, and van der Wiel.[20] Momentum-transfer cross sections have been measured by Frost and Phelps,[21] McPherson, Feeney, and Hooper,[22] and Milloy *et al.*[23] Derived phase shifts have been given by Andrick,[15] Srivastava *et al.*[18] and Williams.[24]

There are also a number of theoretical calculations carried out on elastic scattering of electrons from argon atoms using different kinds of approximations. The most recent reliable theoretical calculations in this case are by Dasgupta and Bhatia,[25] Bell, Scott, and Lennon,[26] McEachran and Stauffer,[27] Fon *et al.*,[28] and Amusia *et al.*[29] Dasgupta and Bhatia[25] studied the scattering of electrons from argon atoms by the polarized orbital method due to Temkin.[30] They calculated phase shifts for various partial waves in the polarized orbital approximation and used them to calculate total elastic, differential, and momentum-transfer cross sections. Bell, Scott, and Lennon[26] used the R-matrix method for the elastic scattering of electrons by argon atoms in the impact energy range 0–19 eV. The calculation is based on a single configuration atomic ground-state wave function coupled to a ^1P pseudostate. They calculated phase shifts that had been used to calculate differential, total, and momentum-transfer cross sections. McEachran and Stauffer[27] calculated phase shifts, differential, total elastic, and momentum-transfer cross sections for low-energy elastic scattering of electrons from argon atoms. They used the exchange-adiabatic approximation which includes both polarization and exchange potentials. But they did not include the polarized exchange terms which, as shown by Dasgupta and Bhatia,[25] are of significance at these low energies. Fon *et al.*[28] carried out calculations on the elastic scattering of electrons from argon atoms using the R-matrix method in which polarization and exchange were included by coupling a ^1P pseudostate to the argon ground state. Their calculation was performed for impact energies ranging from 3 to 150 eV excluding the region of Ramsauer-Townsend minimum. They reported results for phase shifts, differential, integral, and momentum-transfer cross sections for these energies. Amusia *et al.*[29] employed many-body perturbation theory and the simplified random-phase approximation with exchange to obtain an optical potential to study the elastic scattering of electrons from argon atoms. In principle their approach gives a complex nonlocal potential since exchange, nonadiabatic, and absorption effects are included. McCarthy *et al.*[31] used the optical potential method and Walker[32] employed the relativistic approximation. Thomson[33] and Garbaty and LaBahn[34] used a simplified polarized orbital approximation to examine the effects of polarization in the scattering cross section of electrons elastically scattered from argon atoms. Their method includes nonadiabatic effects only approximately and makes no allowance for inelastic effects which occur at high energies and which become increasingly important for heavier atoms.

In this paper we perform an independent accurate *ab initio* calculation to compare with the above-mentioned absolute measurements and the available theoretical results. In our earlier papers[1,2] the MCHF method extended to apply to the calculation of elastic scattering of electrons from neon and helium atoms produced results in excellent agreement with experiment. In this paper, the MCHF method, which takes into account the polarization and the correlation effects in the *ab initio* way more accurately than any other methods and has been applied to study elastic scattering of electrons from argon atoms, is expected to be more reliable from the physical point of view. In our calculation we shall assume that the spin-orbit interaction and other relativistic effects are not significant in the elastic scattering of electrons on neutral argon. In the MCHF method, the polarization, electron correlation, and absorption effects are considered in a natural way through the configuration-interaction procedure.

II. THEORY

A. The MCHF wave function for a scattering state

The scattering functions have been calculated using the multiconfiguration Hartree-Fock method.[1,2] The MCHF wave function of the electron-argon system may be expressed in terms of a single scattering orbital coupled to the wave function for an N-electron target and the other bound $(N+1)$-electron configuration states.

Let

$$\Psi(\gamma_t L_t S_t;N)=\sum_j^{m_t} a_j \Phi(\gamma_j L_t S_t;N) \tag{1}$$

be a wave function describing an N-electron target that is an eigenstate of L_t and S_t, in terms of N-electron bound configuration states $\Phi(\gamma_j L_t S_t;N)$ with configuration γ_j and term $L_t S_t$, mixing coefficients a_j, and the total energy E_t. Then a MCHF wave function for a scattering state with label γ, energy E, and the term LS may be expressed in a series of the form

$$\Psi(\gamma LS;N+1)=\sum_j^{m_t} a_j \Phi(\gamma_j L_t S_t;N)\phi_{kl} + \sum_i^{m} c_i \Phi(\gamma_i LS;N+1) , \tag{2}$$

where ϕ_{kl} is a one-electron, scattering orbital with orbital angular momentum l and

$$\Phi(\gamma_j L_t S_t;N)\phi_{kl}$$

represents the coupling of the N-electron target configuration with a single scattering electron to yield an antisymmetric configuration state for the $(N+1)$-electron system with the final term value and configuration $\gamma_j kl$.

A set of radial functions $P_i(r)$, $i=1,\ldots,m$ represents the above $(N+1)$-electron wave function for the electron-argon system. All the radial functions are solutions of the second-order coupled integro-differential equations of the form

$$\left[\frac{d^2}{dr^2}+\frac{2z}{r}-\frac{l(l+1)}{r^2}\right]P_i(r) =\frac{2}{r}[Y_i(r)P_i(r)+X_i(r)+I_i(r)]+\sum_{i'}\varepsilon_{ii'}P_{i'}(r) , \tag{3}$$

where the off-diagonal energy parameters $\varepsilon_{ii'}$ are related to Lagrange multipliers that ensure orthogonality assumptions (for a detailed discussion of these equations see Ref. 1). In this MCHF method the radial function for the scattering electron is determined variationally along with the bound-state radial functions, except those describing the target are kept fixed along with the mixing coefficients, a_j. The boundary conditions satisfied by the bound radial functions are

$$P_i(r) \underset{r\to 0}{\sim} r^{l+1} \quad \text{and} \quad P_i(r) \underset{r\to\infty}{\sim} 0 .$$

In this case the diagonal energy parameter ε_{ii} is an eigenvalue of the integro-differential equation, which must be determined. The radial functions for the scattering orbital satisfy the conditions

$$\begin{aligned} &P_i(r) \underset{r\to 0}{\sim} r^{l+1} , \\ &P_i(r) \underset{r\to\infty}{\sim} \sin(kr-l\pi/2+\delta_l) , \end{aligned} \tag{4}$$

where δ_l is the phase shift and $\varepsilon_{ii}=-k^2$, k^2 being the kinetic energy of the scattering electron. In the multiconfiguration (MC) self-consistent-field (SCF) method the bound and the scattering radial functions are determined by solving the above set of coupled second-order integro-differential equations under the proper boundary conditions. The scattering radial function is normalized by fitting the computed values at two adjacent points to the regular and irregular Bessel functions as soon as the region where the direct and the exchange potentials vanishes is reached, which may be at considerably smaller values of r than the asymptotic form given by the boundary condition of Eq. (4).

TABLE I. Comparison of phase shifts with experiments and other theories for electron-argon scattering.

k (a.u.)	Reference	δ_0	δ_1	δ_2	δ_3
0.4696	This work	−0.4526	−0.1257	0.1342	0.0270
	25	−0.4813	−0.1052	0.1302	0.0256
	26	−0.5057	−0.1329	0.1111	0.0267
	28	−0.4866	−0.1480	0.1131	0.0264
	27	−0.4724	−0.1171	0.1279	0.0248
	18	−0.548	−0.140	0.125	0.035
	15	−0.493	−0.142	0.120	0.025
	24	−0.457	−0.134	0.142	0.021
	3	−0.488	−0.124	0.102	0.025
0.6062	This work	−0.6935	−0.2595	0.2920	0.0466
	25	−0.7209	−0.2459	0.2580	0.0442
	26	−0.7575	−0.2901	0.2316	0.0453
	28	−0.7320	−0.2984	0.2440	0.0427
	27	−0.7092	−0.2570	0.3127	0.0434
	18	−0.747	−0.256	0.254	0.102
	15	−0.733	−0.277	0.260	0.044
	24	−0.685	−0.255	0.317	0.041
	3	−0.770	−0.277	0.228	0.044
0.7425	This work	−0.9291	−0.4169	0.5508	0.0715
	25				
	26				
	28	−0.9668	−0.4565	0.4732	0.0632
	27	−0.9405	−0.4104	0.6805	0.0696
	18	−1.051	−0.398	0.491	0.125
	15	−0.958	−0.429	0.535	0.071
	24	−0.919	−0.405	0.620	0.066
0.8573	This work	−1.1189	−0.5490	0.9403	0.1011
	25	−1.1438	−0.5376	0.7539	0.0999
	26	−1.186	−0.6063	0.6610	0.0960
	28	−1.1554	−0.5865	0.7568	0.0849
	27	−1.1279	−0.5410	1.1049	0.0987
	18	−1.243	−0.430	0.805	0.171
	15	−1.143	−0.562	0.840	0.100
	24	−1.098	−0.528	0.936	0.093
	3	−1.08	−0.650	0.720	0.071
1.05	This work	−1.4218	−0.7616	1.5040	0.1705
	25	−1.4422	−0.7567	1.1961	0.1645
	26				
	28	−1.4519	−0.7889	1.3114	0.1347
	27	−1.4229	−0.7515	1.6321	0.1628
	18	−1.365	−0.506	1.593	0.200
	15	−1.443	−0.782	1.390	0.145
	24	−1.394	−0.750	1.451	0.154
	3	−1.44	−0.830	1.24	0.119
1.2124	This work	−1.6636	−0.9535	1.7348	0.2648
	25	−1.6743	−0.9300	1.4484	0.2334
	26				
	28				
	27	−1.6529	−0.9176	1.8376	0.2309
	18	−1.818	−0.871	1.679	0.262
	15	−1.683	−0.962	1.670	0.232
	24	−1.653	−0.935	1.747	0.241
	3	−2.09	−1.485	1.071	0.129

The coefficients c_i which need to be determined are solutions of the system of equations derived from the condition that $\langle \psi | H - E | \psi \rangle$ be stationary with respect to variations in the coefficients, where H is the Hamiltonian for the $(N+1)$-electron system and $E = E_t + k^2/2$ (in atomic units).

The coefficients c_i are solutions of the system of equations

$$\sum_{i'}^{m} \langle \Phi_i | H - E | \Phi_{i'} \rangle c_{i'} + \sum_{j}^{m_t} \langle \Phi_i | H - E | \Phi_j \rangle a_j = 0 \; , \qquad (5)$$

where

$$\Phi_j \equiv \Phi(\gamma_j L_t S_t ; N) \phi_{kl}, \quad j = 1, \ldots, m_t$$

$$\Phi_i \equiv \Phi(\gamma_i LS ; N+1), \quad i = 1, \ldots, m \; .$$

The MCHF method for the scattering states will be applied here to study low-energy elastic scattering of electrons from argon atoms.

B. MCHF theory of elastic scattering

In the present paper we will be concerned mainly with low-energy elastic scattering of electrons from argon atoms. The elastic differential cross sections $\sigma(\theta)$ in atomic units a_0^2/sr is given by[35]

$$\sigma(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \; , \qquad (6)$$

where the scattering amplitude $f(\theta)$ is

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)[\exp(2i\delta_l) - 1] P_l(\cos\theta) \; . \qquad (7)$$

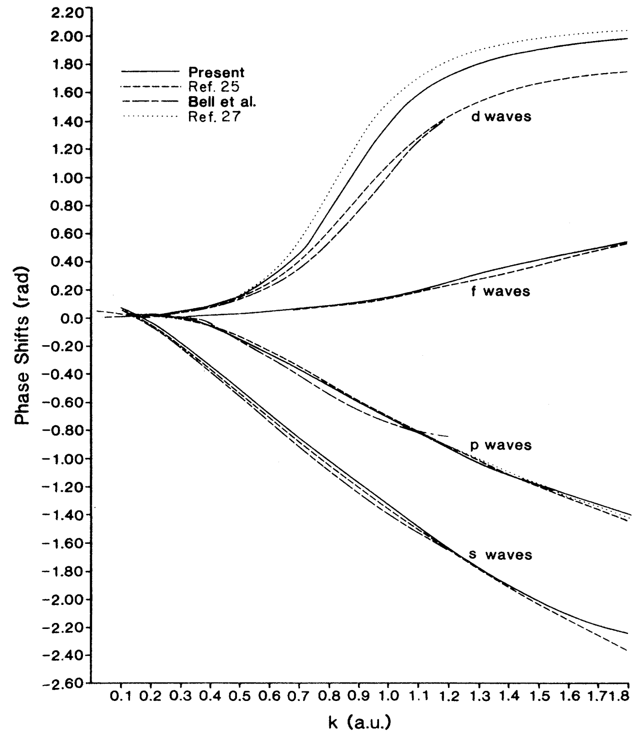

FIG. 1. s-, p-, d-, and f-wave phase shifts (mod π) for the elastic scattering of electrons from argon atoms. ——, MCHF (present); — — —, Dasgupta and Bhatia (Ref. 25); —-—, Bell, Scott, and Lennon (Ref. 26); · · · ·, McEachran and Stauffer (Ref. 27).

TABLE II. Phase shifts (in rad) for elastic scattering of electrons from argon atoms.

k (a.u.)	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0.1000	0.0740	0.0163	0.0042	0.0012	0.0006	0.0003	0.0002
0.1500	0.0378	0.0268	0.0098	0.0028	0.0013	0.0007	0.0005
0.2000	−0.0185	0.0301	0.0177	0.0050	0.0020	0.0012	0.0007
0.2500	−0.0857	0.0240	0.0288	0.0079	0.0034	0.0020	0.0011
0.3000	−0.1632	0.0073	0.0434	0.0113	0.0050	0.0029	0.0016
0.4696	−0.4526	−0.1257	0.1342	0.0270	0.0124	0.0069	0.0042
0.5000	−0.5065	−0.1455	0.1602	0.0314	0.0142	0.0079	0.0047
0.6062	−0.6935	−0.2595	0.2920	0.0466	0.0210	0.0114	0.0072
0.7425	−0.9291	−0.4169	0.5508	0.0715	0.0313	0.0167	0.0115
0.8000	−1.0255	−0.4835	0.7549	0.0857	0.0366	0.0199	0.0122
0.8573	−1.1189	−0.5490	0.9403	0.1011	0.0427	0.0228	0.0138
0.9500	−1.2574	−0.6520	1.2343	0.1300	0.0526	0.0278	0.0177
1.000	−1.3410	−0.7071	1.3725	0.1505	0.0587	0.0303	0.0195
1.0500	−1.4218	−0.7616	1.5040	0.1705	0.0645	0.0345	0.0211
1.1000	−1.4940	−0.8162	1.5901	0.1911	0.0712	0.0388	0.0231
1.2124	−1.6636	−0.9535	1.7348	0.2648	0.0917	0.0470	0.0291
1.4000	−1.9027	−1.1425	1.8767	0.3652	0.1255	0.0674	0.0392
1.6000	−2.1168	−1.2673	1.9453	0.4663	0.1638	0.0817	0.0493
1.8000	−2.2510	−1.3901	1.9900	0.5422	0.1970	0.1065	0.0592
1.9170	−2.3744	−1.4850	2.0214	0.6011	0.2207	0.1150	0.0657
2.0000	−2.4647	−1.5427	2.0308	0.6350	0.2453	0.1245	0.0710

Here δ_l is the real phase shift, $P_l(\cos\theta)$ is the lth Legendre polynomial, and k is the electron momentum in atomic units.

The total cross section in units of a_0^2 is

$$\sigma_T = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)\sin^2\delta_l \tag{8}$$

and the momentum-transfer cross section is

$$\sigma_M = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1)\sin^2(\delta_l - \delta_{l+1}) \ . \tag{9}$$

Since the polarization of the $3s^2 3p^6$ target by the scattering electron and the electron-correlation effects is very important in the calculation of the phase shifts of the scattering wave function, the most straightforward method to include these effects is to extend the configuration-interaction procedure commonly used for bound-state problems.

III. COMPUTATIONAL PROCEDURE

In this paper a MCHF approach was adopted and the calculations were performed using the MCHF program[36] to study the elastic scattering of electrons from atoms. The MCHF method we employed here to calculate the scattering of electrons from argon atoms is basically the same as the one previously used for neon and helium atoms. Since several of the bound-state orbitals for argon have nodes very close to the origin it was found necessary in the solution of the coupled integro-differential equations for the scattering functions to have a much finer mesh near the origin. The choice of $h = \frac{1}{32}$ in the logarithmic variable $\rho = \ln zr$ was found to be sufficient in or-

TABLE III. Differential cross sections (in units of a_0^2) at various energies for electron-argon scattering.

θ (deg)	3 (eV)	5 (eV)	10 (eV)	20 (eV)	50 (eV)
0	2.1560	7.8018	46.7619	55.4097	57.4222
5	1.3666	5.9422	41.9319	50.7173	44.1344
10	0.8379	4.4660	36.8952	45.9389	33.8859
15	0.5384	3.3490	31.7232	40.9487	25.8873
20	0.4492	2.5997	26.6192	35.7549	19.6295
25	0.5400	2.2016	21.7860	30.4344	14.7128
30	0.7714	2.1146	17.4040	25.1118	10.8285
35	1.0983	2.2789	13.6123	19.9435	7.7421
40	1.4750	2.6233	10.4984	15.1046	5.2883
45	1.8596	3.0736	8.0958	10.7736	3.3638
50	2.2175	3.5602	6.3857	7.1082	1.9122
55	2.5219	4.0217	5.3000	4.2207	0.9013
60	2.7537	4.4068	4.7283	2.1574	0.3008
65	2.9006	4.6743	4.5278	0.8900	0.0663
70	2.9554	4.7933	4.5384	0.3204	0.1327
75	2.9164	4.7441	4.5998	0.2976	0.4159
80	2.7863	4.5199	4.5713	0.6416	0.8213
85	2.5731	4.1287	4.3501	1.1678	1.2547
90	2.2899	3.5947	3.8857	1.7142	1.6342
95	1.9553	2.9581	3.1880	2.1537	1.8976
100	1.5924	2.2733	2.3272	2.4062	2.0070
105	1.2273	1.6033	1.4243	2.4405	1.9491
110	0.8861	1.0130	0.6342	2.2727	1.7352
115	0.5923	0.5618	0.1237	1.9596	1.3993
120	0.3643	0.2939	0.0480	1.5896	0.9954
125	0.2138	0.2404	0.5305	1.2694	0.5911
130	0.1454	0.4114	1.6464	1.1067	0.2584
135	0.1571	0.7998	3.4122	1.1908	0.0610
140	0.2412	1.3818	5.7802	1.5747	0.0421
145	0.3851	2.1191	8.6391	2.2639	0.2163
150	0.5725	2.9605	11.8203	3.2132	0.5667
155	0.7838	3.8445	15.1102	4.3329	1.0475
160	0.9980	4.7028	18.2680	5.5034	1.5918
165	1.1933	5.4653	21.0478	6.5926	2.1222
170	1.3500	6.0664	23.2228	7.4749	2.5635
175	1.4516	6.4519	24.6096	8.0484	2.8535
180	1.4880	6.5880	25.0926	8.2459	2.9470
$\theta_{\min}$	20, 130	30, 125	65, 120	75, 130	65, 140

der to achieve the desired accuracy. The extended programs[36] were vectorized and optimized according to the architecture of the supercomputer CRAY-YMP. All calculations were performed on the CRAY-YMP.

First of all, an accurate wave function for the ground state of the argon atom was calculated in the multiconfiguration Hartree-Fock approximation.[37] The $1s$, $2s$, $2p$, $3s$, and $3p$ wave functions were obtained from the Hartree-Fock (HF) calculation of the $3s^2 3p^6\,{}^1S$ ground state of the argon atom. The excited wave functions $4s$, $4p$, $4d$, $4f$, $5s$, $5p$, $5d$, $5f$, and $5g$ were calculated from the MCHF wave-function expansion over the 112 configuration states coupled to form the ${}^1S$ term. The ground-state energy is $-527.056\,899$ a.u. These bound-state wave functions were then used as an input to calculate the phase shifts for various partial waves. As the polarization is very important in this case, its effect has been taken into account very accurately in the *ab initio* way through the configuration-interaction procedure. It was found that the dipole polarization is very important in this case. The contributions from higher multipoles were not seen to be very important. Configurations were generated by the single replacement of the target $3s$ and $3p$ orbitals by the excited orbitals which represent the dipole polarization effect. About more than 100 configurations were used to calculate scattering wave functions for the various partial waves over a range of impact energies considered. The bound orbitals that are responsible for the dipole polarization of the target atom were varied simultaneously along with the scattering electron in order to obtain accurate dynamical polarization of the target. For each partial wave different sets of configurations were used. For a particular partial wave, the same set of configurations was used for various kinetic energies of the scattering electron. Since the dipole polarization of the target is different for different energies of the scattering electron, both bound and scattering electron orbitals were varied simultaneously at each kinetic energy of the scattering electron.

In the present calculation only partial waves up to $l=6$ are calculated directly by the MCHF method.[36] The necessary higher partial-wave contributions were added by employing phase shifts derived from the effective range formula[38]

$$\tan\delta_l = \frac{\pi\alpha k^2}{(2l+3)(2l+1)(2l-1)} , \tag{10}$$

where α is the static dipole polarizability. In the energy range considered, the effective range theory provides

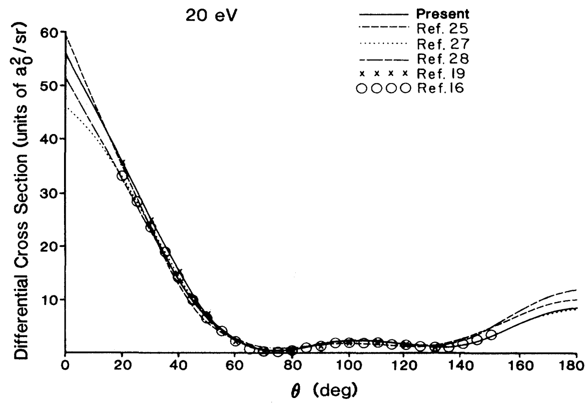

FIG. 3. Differential cross sections at $k^2=20$ eV. ——, MCHF (present); — — —, Dasgupta and Bhatia (Ref. 25); · · · ·, McEachran and Stauffer (Ref. 27); —-—, Fon *et al.* (Ref. 28); × × ×, Williams and Willis (Ref. 19); ○ ○ ○, DuBois and Rudd (Ref. 16).

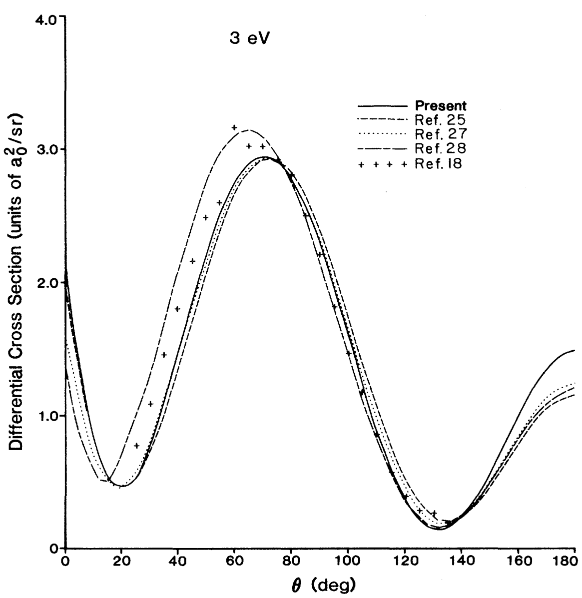

FIG. 2. Differential cross sections at $k^2=3$ eV. ——, MCHF (present); — — —, Dasgupta and Bhatia (Ref. 25); · · · ·, McEachran and Stauffer (Ref. 27); —-—, Fon *et al.* (Ref. 28); + + +, Srivastava *et al.* (Ref. 18).

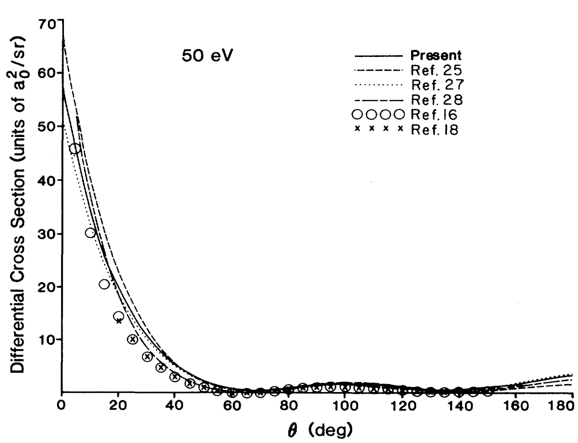

FIG. 4. Differential cross sections at $k^2=50$ eV. ——, MCHF (present); — — —, Dasgupta and Bhatia (Ref. 25); · · · ·, McEachran and Stauffer (Ref. 27); —-—, Fon *et al.* (Ref. 28); ○ ○ ○, DuBois and Rudd (Ref. 16); × × ×, Srivastava *et al.* (Ref. 18).

higher partial-wave phase shifts of adequate accuracy since contributions to the cross sections are in general quite small.

In Sec. IV we compare our results for phase shifts and elastic differential, total elastic, and momentum-transfer cross sections with experimental measurements of these quantities and with other theoretical calculations.

IV. RESULTS AND DISCUSSIONS

We have performed detailed calculations to determine the effects of polarization on the low-energy elastic scattering of electrons from argon atoms. Argon is chosen as the representative of the heavier noble gases. We have calculated phase shifts and integral, elastic differential, and momentum-transfer cross sections for the following process:

$$e^- + \mathrm{Ar}(^1S) \rightarrow e^- + \mathrm{Ar}(^1S) \; .$$

A. Phase shifts

Table I compares our phase shifts for $l=0$, 1, 2, and 3 calculated using the MCHF approximation, with the experimental phase shifts and the other theoretical results for few impact energies.

At energy $k=0.4696$ a.u., we compare our phase shifts with the theoretical results of Dasgupta and Bhatia,[25] Bell, Scott, and Lennon,[26] Fon *et al.*,[28] and McEachran and Stauffer[27] and the experimental results of Furst *et al.*,[3] Srivastava *et al.*,[18] Andrick,[15] and Williams.[24] The present s-wave phase shift is in excellent agreement with the experimental results of Williams and Furst *et al.* and also agrees very well with the theoretical results obtained by Dasgupta and Bhatia, Fon *et al.*, and McEachran and Stauffer. Srivastava *et al.*,[18] Andrick,[15] and Williams[24] derived phase shifts from their experimental differential cross sections. The present p-wave phase shift at this energy is in excellent agreement with the experimental phase shifts of Furst *et al.*[2] and Williams and the theoretical results of Bell, Scott, and Lennon.[26] The present d-wave phase shift at this energy agrees very well with the experimental result of Williams[24] and Srivastava *et al.*[18] and the theoretical result of Dasgupta and Bhatia[25] and McEachran and Stauffer[27] and the f-wave phase shift is in best agreement with the experimental results of Furst *et al.*[2] and Andrick[15] and the theoretical results of Bell, Scott, and Lennon,[26] Fon *et al.*,[28] and Dasgupta and Bhatia.[25]

At energy $k=0.6062$ a.u. the present s-wave phase shift agrees very well with the experimental phase shift derived by Williams[24] and the theoretical results of McEachran and Stauffer[27] and Dasgupta and Bhatia,[25] and the present p-wave phase shift at this energy is in excellent agreement with the experimental results of Srivastava *et al.*[18] and Williams[24] and the theoretical result of McEachran and Stauffer.[27] The present d-wave phase shift at this energy agrees very well with the experimental results of Williams and the theoretical results of McEachran and Stauffer, and the f-wave phase shift at this energy is also in excellent agreement with the experimental results of Andrick,[15] Furst *et al.*,[2] and Williams[24] and the theoretical results of Dasgupta and Bhatia,[25] Bell, Scott, and Lennon,[26] Fon *et al.*,[28] and McEachran and Stauffer.[27]

The present s-wave phase shift at energy $k=0.7425$ a.u. agrees very well with the experimental results of Williams[24] and Andrick[15] and the theoretical results of Fon *et al.*[28] and McEachran and Stauffer,[27] and the p-wave phase shift is in excellent agreement with the experimental results of Williams, Andrick, and Srivastava *et al.* and the theoretical results of McEachran and Stauffer. The d-wave phase shift at this energy is in remarkably good agreement with the experimental results of Andrick,[15] and the f-wave phase shift at this energy is in excellent agreement with the experimental results of Andrick and the theoretical result of McEachran and Stauffer.

The s-wave phase shift at $k=0.8573$ a.u. is in excellent agreement with the experimental results of Williams[24] and Furst *et al.*,[2] and the theoretical results of McEachran and Stauffer[27] and the p-wave phase shift, on the other hand, agrees very well with the experimental results of Andrick[15] and the theoretical results of McEachran and Stauffer[27] and Dasgupta and Bhatia. The d-wave phase shift at this energy is again in excellent agreement with the experimental results of Williams[24] and the f-wave phase shift at this energy is in excellent agreement with the experimental results of Andrick[15] and the theoretical results of Dasgupta and Bhatia[25] and McEachran and Stauffer.[27]

The s-wave phase shift at energy $k=1.05$ a.u. agrees very well with the experimental results of Andrick,[15] Furst *et al.*,[2] and Williams[24] and the theoretical results of McEachran and Stauffer[27] and Dasgupta and Bhatia[25] and the p-wave phase shift is in best agreement with the experimental results of Williams[24] and Andrick[15] and the theoretical results of Dasgupta and Bhatia,[25] McEachran and Stauffer,[27] and Fon *et al.*[28] The present d-wave phase shift agrees well with the experimental results of Williams[24] and the f-wave phase shift agrees very well with the experimental results of Williams[24] and the theoretical results of Dasgupta and Bhatia[25] and McEachran and Stauffer.[27]

The present s-wave phase shift at energy $k=1.2124$ a.u. is in excellent agreement with the experimental results of Williams[24] and Andrick[15] and the theoretical results of Dasgupta and Bhatia[25] and McEachran and Stauffer.[27] The present p-wave phase shift is in excellent agreement with the experimental results of Andrick[15] and Williams[24] and the theoretical results of Dasgupta and Bhatia.[25] The present d-wave phase shift is again in excellent agreement with the experimental result of Williams[24] and the f-wave phase shift is in excellent agreement with the experimental result of Srivastava *et al.*[18]

The present MCHF phase shifts for s, p, d, and f waves are compared to the results of Dasgupta and Bhatia,[25] Bell, Scott, and Lennon[26] and McEachran and Stauffer[27] in Fig. 1. The agreement among the four calculations is good for s, p, and f waves but d-wave phase shifts differ among the four calculations. The present s-wave phase shift is very close to those obtained by McEachran and Stauffer[27] and the f-wave phase shifts of McEachran and Stauffer are very nearly the same as those obtained by Dasgupta and Bhatia, so the differences could not be shown in the figure. It appears that d-wave phase shifts are very sensitive to the types of approximations used. As the present MCSCF approach takes into account the effect of polarization in the *ab initio* manner more accurately than any other method, we believe that the present d-wave phase shifts are more reliable.

We present phase shifts for $l=0-6$ in Table II in the MCHF approximation for a range of energies considered.

B. Differential cross sections

The elastic differential cross sections at $k^2=3$, 5, 10, 20, and 50 eV are given in Table III from $\theta=0°$ to 180°. The effective range formula (10) is used to calculate contributions of $l=7-500$. In the forward direction the convergence is very slow and we use[2]

$$\left[\frac{d\sigma}{d\Omega}\right]_{\theta=0°}=\left|\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\eta_l}\sin\eta_l\right|^2$$

$$=\left[\frac{d\sigma}{d\Omega}\right]_{\theta=0°}^{l<l_0}+\left[\frac{\pi\alpha l_0}{4l_0^2-1}\right]\sum_{l=0}^{l_0-1}(2l+1)\sin(2\eta_l)+\left[\frac{\pi\alpha l_0 k}{4l_0^2-1}\right]^2,$$

where $l_0=7$ and the effective range formula (10) has been used for $l\geq 7$ to derive this formula. We use the experimental polarizability[39] into our calculation. The angles $\theta_{\min}$ at which the differential cross section has a minimum value are also indicated in Table III.

Figures 2, 3, and 4 compare differential cross-section data for impact energies $k^2=3$, 20, and 50 eV with experimental and other theoretical results. In Fig. 2, the present differential cross sections at $k^2=3$ eV are compared with the experimental results of Srivastava *et al.*[18] and the theoretical results of Dasgupta and Bhatia,[25] McEachran and Stauffer,[27] and Fon *et al.*[28] There is a double minimum at 20° and 130°. The present results are in very good agreement with those of Dasgupta and Bhatia, McEachran and Stauffer, and Fon *et al.* and are in excellent agreement with the experimental results of Srivastava *et al.*

In Fig. 3, we compare the present differential cross sections for $k^2=20$ eV with the experimental results obtained by Williams and Willis[19] and DuBois and Rudd[16] and the theoretical results of Dasgupta and Bhatia,[25] McEachran and Stauffer,[27] and Fon *et al.*[28] There is substantially good agreement among all four calculations. All exhibit two distinct minima. Two sets of experimental data shown agree reasonably well with each other. The present differential cross sections agree very well with the experimental results of Williams and Willis[19] and DuBois and Rudd.[16]

At 50 eV, the present differential cross sections are compared with the experimental results of DuBois and Rudd[16] and Srivastava *et al.*[18] and the theoretical results of Dasgupta and Bhatia,[25] McEachran and Stauffer,[27] and Fon *et al.*[28] The two sets of experimental results agree very well. The present differential cross sections agree very well with the experimental results of DuBois and Rudd[16] and Srivastava *et al.*[18] and the theoretical results of Dasgupta and Bhatia, McEachran and Stauffer, and Fon *et al.* At this energy also, all sets of results exhibit two distinct minima.

C. Integral elastic and momentum-transfer cross sections

The integral elastic and momentum-transfer cross sections obtained in the MCHF approximation are given in Table IV for impact energies $k^2=0.01$ to 4.0 Ry. In Table V, integral elastic cross sections are compared with other theoretical and experimental results for few in-

TABLE IV. Total elastic and momentum-transfer cross sections (in units of a_0^2) for electron-argon scattering.

k (a.u.)	k^2 (eV)	Total cross section	Momentum-transfer cross section
0.10	0.136	7.3493	4.0788
0.15	0.306	2.3141	0.4790
0.20	0.544	1.5285	1.0031
0.25	0.850	2.7780	2.7023
0.30	1.225	5.2007	4.8423
0.4696	3.00	17.9002	14.5869
0.50	3.401	21.8940	17.9392
0.6062	5.00	35.6421	30.9906
0.7425	7.50	58.2095	51.1206
0.80	8.708	74.5771	63.2117
0.8573	10.00	85.2585	67.6292
0.95	12.279	92.2143	63.3910
1.00	13.606	90.8232	57.3640
1.05	15.00	87.1603	50.6270
1.10	16.463	82.1693	44.3507
1.2124	20.00	72.2547	33.4303
1.40	26.667	57.9708	24.0059
1.60	34.831	47.0176	19.3813
1.80	44.083	39.1703	16.1352
1.9170	50.00	35.6864	15.1124
2.00	54.423	33.6049	14.3573

TABLE V. Comparison of total elastic cross sections (in units of a_0^2) for electron-argon scattering with other theories and experiments.

Reference \ k^2 (eV)	3	5	7.5	10	15	20	50
			Theory				
Present	17.90	35.64	58.21	85.26	87.16	72.25	35.69
25	19.26	32.74		69.20	79.36	71.01	37.51
26	20.29	34.24		65.03	78.48		
27	19.11	37.92	71.89	97.27	86.51	68.30	34.32
28	20.20	34.76		71.60	83.80	68.18	30.77
			Experiment				
8					82.76[a]	68.75	36.65
7	17.28	30.85		67.49		72.14	
6			54.7	73.4	84.3	67.9	38.2
5			53.5	71.4	85.3	68.9	37.5
13					77.0	61.9	35.5
18	19.64	29.99	46.42	64.28	74.99	44.64	21.78
10	20.64	36.76		69.30	78.82	70.78	36.19
24	20.14	36.07		83.35	85.46	70.60	
16						68.4	25.6
15	20.50	34.71	48.21	77.24	85.42	71.14	
3	18.58	33.66		71.29	82.98	66.47	
4	17.72	31.48		71.68	82.33	65.39	

[a] Reference 14.

cident energies. The present cross section at 3 eV is in excellent agreement with the recent experimental results of Buckman and Lohmann and Furst *et al.* The theoretical results obtained by Dasgupta and Bhatia[25] and McEachran and Stauffer[27] and the experimental results of Srivastava *et al.*[18] are very close to the present results. At 5 eV, the integral elastic cross section agrees very well with the experimental results of Charlton *et al.*,[10] Williams,[24] and Andrick[15] and also with Buckman and Lohmann[3] and with the theoretical results obtained by Bell, Scott, and Lennon[26] and Fon *et al.*[28] The present cross section at 7.5 eV is in good agreement with the experimental results of Nickel *et al.*[6] and Jost *et al.*[5] and at 10 eV, it agrees very well with the experimental results of Williams.[24] The present cross section at 15 eV also agrees very well with the experimental results of Jost *et al.*,[5] Williams,[24] and Andrick[15] and the theoretical results of McEachran and Stauffer.[27] The present cross section at 20 eV is in excellent agreement with the experimental results of Ferch *et al.*[7] and Andrick[15] and the theoretical result of Dasgupta and Bhatia,[25] whereas at 50 eV, the present cross section is in excellent agreement with the experimental results of Kauppila *et al.*,[13] Charlton *et al.*,[10] and also of Wagenaar and deHeer.[8] The

TABLE VI. Comparison of momentum-transfer cross sections (in units of a_0^2) for electron-argon scattering with other theories and experiments.

Reference \ k^2 (eV)	3	5	7.5	10	15	20	50
			Theory				
Present	14.59	30.99	51.12	67.63	50.63	33.43	15.11
25	15.81	27.84		56.42	49.93	35.48	13.27
26	15.49	27.55		51.21			
27	15.47	33.78	64.37	76.11	49.57	32.70	15.65
28	15.20	28.44		57.47	50.76		
			Experiment				
18	14.64	22.85	39.28	53.57	53.57	23.57	8.57
24	16.71	32.43		67.60	51.17	33.64	
15	16.07	29.50	50.71	62.35	51.28	34.78	

theoretical results obtained by Dasgupta and Bhatia[25] and McEachran and Stauffer[27] and the experimental results of Jost *et al.*[5] and Nickel *et al.*[6] are also in very good agreement with the present results.

In Table VI, we compare the present momentum-transfer cross-section results with the other theoretical and the experimental results at few electron energies. The present momentum-transfer cross section at 3 eV is in excellent agreement with the experimental result of Srivastava *et al.*[18] The theoretical results of Dasgupta and Bhatia,[25] Bell, Scott, and Lennon,[26] McEachran and Stauffer,[27] and Fon *et al.*[28] are very close to the present result. At 5 eV, the present result agrees very well with the experimental result of Williams[24] and Andrick[15] and at 7.5 eV it is in excellent agreement with the experimental result of Andrick.[15] At 10 eV the present result is again in excellent agreement with the experimental result of Williams[24] and at 15 eV is in remarkably good agreement with the experimental result of Williams[24] and of Andrick[15] and the theoretical result of Fon *et al.*,[28] Dasgupta and Bhatia,[25] and also of McEachran and Stauffer.[27] At 20 eV, again the present result is in excellent agreement with the experimental result of Williams.[24] The present result is very close to the result of McEachran and Stauffer[27] and the experimental result of Andrick[15] but lies in between the two. The present result at 50 eV agrees very well with that of McEachran and Stauffer.[27]

Figure 5 shows the total cross section as a function of incident electron momentum. The theoretical results of Dasgupta and Bhatia,[25] McEachran and Stauffer,[27] and the experimental results of Wagenaar and deHeer,[8,14] Ferch *et al.*,[7] and Jost *et al.*[5] are included for comparison. The present results are in good agreement with the experimental results of Jost *et al.*,[5] Ferch *et al.*,[7] and Wagenaar and deHeer.[8,14] From $k=1.0$ to 2.0 a.u., the present results and the results obtained by McEachran and Stauffer[27] are very close and agree very well with the experimental results. Over the energy region from $k=1.2$ to 2.0 a.u., the results obtained by Dasgupta and Bhatia[25] are very close to the present results.

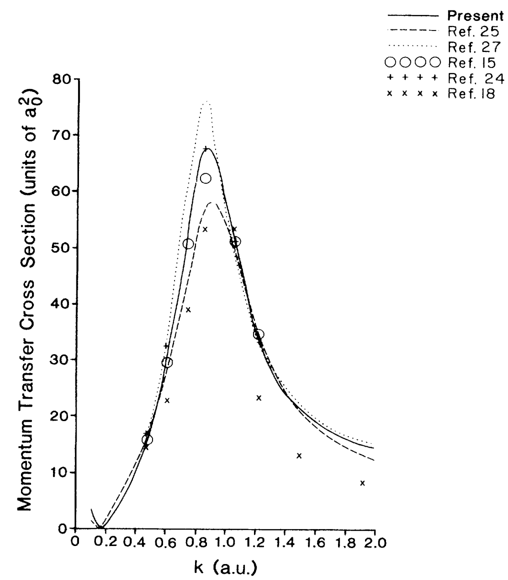

FIG. 6. Momentum-transfer cross sections (in units of a_0^2) for the low-energy scattering of electrons from argon atoms. ——, MCHF (present); — — —, Dasgupta and Bhatia (Ref. 25); · · · ·, McEachran and Stauffer (Ref. 27); ○○○, Andrick (Ref. 15); + + +, Williams (Ref. 24); ×××, Srivastava *et al.* (Ref. 18).

Figure 6 presents the momentum-transfer cross sections as a function of k, the incident electron momentum. The theoretical results of Dasgupta and Bhatia,[25] McEachran and Stauffer[27] and the experimental results of Andrick,[15] Williams,[24] and Srivastava *et al.*[18] are included for comparison. The present results are in excellent agreement with the experimental results of Andrick[15] and Williams.[24]

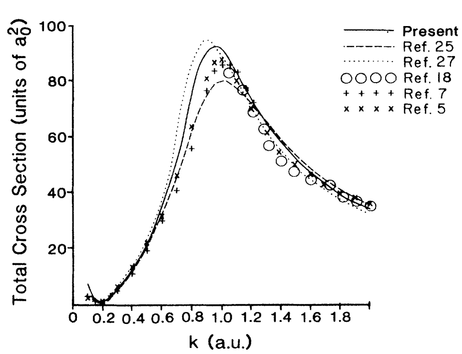

FIG. 5. Total elastic cross sections (in units of a_0^2) for the low-energy scattering of electrons from argon atoms. ——, MCHF (present); — — —, Dasgupta and Bhatia (Ref. 25); · · · ·, McEachran and Stauffer (Ref. 27); ○○○, Wagenaar and deHeer (Ref. 8); + + +, Ferch *et al.* (Ref. 7); ×××, Jost *et al.* (Ref. 5).

V. CONCLUSION

The multiconfiguration Hartree-Fock method extended to carry out calculations on electron-atom scattering has been applied to the low-energy scattering of electrons from argon atoms. The polarization and the electron-correlation effects which are particularly very important in these calculations have been taken into account in an *ab initio* way more accurately than any other methods through the configuration-interaction procedure. The phase shifts, elastic differential, total and momentum-transfer cross sections are calculated for the energy range $k^2=0.01$ to 4 Ry, and compared with other theoretical and the experimental results. The results are in very good agreement with the experiments and compare well with other theoretical results. As the present MCHF method takes into account polarization and the electron-correlation effects in the *ab initio* way more accurately than any other methods, we conclude that the phase shifts and hence the cross sections calculated in this method are more reliable. As there are a number of discrepancies between the different experimental measurements, particularly in the case of momentum-transfer cross section over the energy region considered, we believe that the present accurate calculation will encourage further careful experimental investigations.

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