

***Ab initio* calculation of scattering length and cross sections at very low energies for electron-helium scattering**

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The multiconfiguration Hartree-Fock method for continuum wave functions has been used to calculate the scattering length and phase shifts over extremely low energies ranging from 0 to 1 eV very accurately for electron-helium scattering. The scattering length is calculated very accurately with wave functions computed exactly at zero energy, resulting in an upper bound of 1.1784. The electron correlation and polarization of the target by the scattering electron, which are very important in these calculations, have been taken into account in an accurate *ab initio* manner through the configuration-interaction procedure by optimizing both bound and continuum orbitals simultaneously at each kinetic energy of the scattered electron. Detailed results for scattering length, differential, total, and momentum-transfer cross sections obtained from the phase shifts are presented. The present scattering length is found to be in excellent agreement with the experimental result of Andrick and Bitsch [J. Phys. B **8**, 402 (1975)] and the theoretical result of O'Malley, Burke, and Berrington [J. Phys. B **12**, 953 (1979)]. There is excellent agreement between the present total cross sections and the corresponding experimental measurements of Buckman and Lohmann [J. Phys. B **19**, 2547 (1986)]. The present momentum-transfer cross sections also show remarkable agreement with the experimental results of Crompton, Elford, and Robertson [Aust. J. Phys. **23**, 667 (1970)].

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I. INTRODUCTION

The scattering of electrons from noble gases has been the subject of continuing interest to both experimentalists and theoreticians as they have produced much detailed information from measurements. In particular, the study of low-energy elastic scattering of electrons from atoms has been an important field of experimental and theoretical endeavor. Among all the rare gases electron-helium scattering has been the subject of extensive investigation in recent years because of its simple structure.

Cross sections of electron-atom collisions at thermal energies are determined by the scattering length. Generally cross sections at low energies vary very rapidly, and as a result extrapolation of the experimental data at extremely low energy is difficult and cannot be regarded as reliable. Therefore, to obtain correct cross sections at thermal energies extremely accurate calculations are necessary. However, at zero and very low energies the electron correlation and polarization are large and the calculations are made more difficult. In general, the scattering length is determined by computing phase shifts at lower energies with sufficient accuracy and then extrapolating ($\tan\delta_0/k$) to zero energy. But this does not always guarantee the accuracy of the result.

In the past few years there have been a number of experimental measurements [1–6] on electron-helium scattering. In the low-energy region considered here, only Williams [1] has performed a phase-shift analysis of his experimental angular distribution of electrons elastically scattered from the ground state of He and has obtained *s*-, *p*-, and *d*-wave phase shifts. Although accurate total cross-section measurements in helium are available,

they are mainly confined to energies above 1 eV, the measurements below 1 eV in helium being those of Ferch, Raith, and Schröder [2], Kennerly and Bonham [3], and Buckman and Lohmann [4]. An alternative source of information on very low-energy electron scattering is provided by the analysis of swarm measurements. The cross section from such measurements [5], the momentum-transfer cross section, has been obtained in helium as low as 8 meV.

Ferch, Raith, and Schröder [2] determined the absolute total cross sections in helium from transmission measurements made with an electron time-of-flight spectrometer in the energy range 0.02–2 eV. Kennerly and Bonham [3] measured the absolute total cross sections for electron scattering from He over the energy range 0.5–50 eV employing the time-of-flight method. Later Jones and Bonham [6] improved the earlier work of Kennerly and Bonham [3] and reported absolute total cross sections from 0.8 to 50 eV. Buckman and Lohmann [4] made a measurement of absolute total cross sections in helium for impact energies from 0.1 to 20 eV utilizing the time-of-flight electron spectrometer. Crompton, Elford, and Robertson [5] determined the energy-dependent momentum-transfer cross sections for energies between 0.008 to 6 eV from a measurement of drift velocities of electrons in helium at 77 K. This swarm measurement is considered to be the most accurate momentum-transfer cross section.

On the theoretical side at the low energies considered, there have been a few accurate calculations [7,8,10,11] on the electron scattering from helium, each of which is based on a particular set of assumptions. Nesbet [7] carried out calculations for the elastic scattering of electrons from helium atoms for energies less than 19 eV using the

matrix variational method. He made variational calculations for s - and p -wave phase shifts and estimated phase shifts for $l > 1$ using the partial-wave Born approximation. The s - and p -wave phase shifts were then corrected for residual errors. The results agree very well with the available experimental measurements [1,3,5]. At the same time O'Malley, Burke, and Berrington [8] made an R -matrix calculation and computed the s - and p -wave phase shifts for e^- -He scattering from 0 to 16.5 eV and estimated the partial-wave phase shifts for $l > 1$ from the Born formula [9]. They used the multiconfiguration He ground state and pseudo- P and $-D$ states constructed from optimized $1s$ through to $4f$ pseudo-orbitals. Their best estimates for cross sections agree very well with the momentum-transfer and total cross-section measurements. McEachran and Stauffer [10] performed calculations in the exchange-adiabatic approximation and obtained the scattering length. They examined the effects of the polarization potential in their investigation. They have not included exchange-polarization terms which may have a significant contribution, especially at low energies. Polarized orbital calculations have been made by LaBahn and Callaway [11], who calculated the differential cross sections at 1 eV.

Even now measurements of the angular distribution or the differential cross section of very low-energetic electrons scattered from helium atoms are not available to check the theoretical work. Moreover, there are also still discrepancies between the different experimental measurements of the total cross sections. It would be useful to provide an accurate calculation over a broad energy range to compare with the available experimental measurements as well as to stimulate interest for future measurements where experimental data are not available.

Although there are a few accurate calculations available which agree very well with the existing measurements, these rely on extrapolation through the Born formula or the generation of pseudo-orbitals. In no calculation are the electron correlation and polarization taken into account in a natural way completely in the *ab initio* manner. Because of the importance of these effects at very low energies, their proper inclusion can strongly affect the result of the calculation. Very recently we applied the multiconfiguration Hartree-Fock (MCHF) method [12] to calculate the scattering length and phase shifts for electron-neon [13] and electron-argon [14] scattering at very low energies. In these calculations, electron correlation and polarization which are very important were taken into account by optimizing both bound and continuum orbitals at each kinetic energy of the scattered electron through the configuration-interaction procedure. This *ab initio* calculation more accurately takes these effects into account than any other method. The results for neon and argon were found to be in excellent agreement with accurate experimental measurements. The MCHF method was also used to calculate [15] the differential, elastic-integral, and momentum-transfer cross sections for elastic electron-helium scattering for energies from 0.58 to 50 eV. These calculations were found to be in excellent agreement with accurate experimental results.

TABLE I. Comparison of scattering length (in a_0) with experiments and other theories.

Scattering length (units of a_0)	
Theory	
Present work	1.1784
Nesbet (Ref. [7])	1.1835
O'Malley <i>et al.</i> (Ref.[8])	1.177
McEachran and Stauffer (Ref. [10])	1.1575
Experiment	
Buckman and Lohmann (Ref. [4])	1.16
Crompton <i>et al.</i> (Ref. [5])	1.19
Andrick and Bitsch (Ref. [16])	1.172
Ferch <i>et al.</i> (Ref. [2])	1.195

The main purpose of the present investigation is to see how accurately the present MCHF method can predict the upper bound for the scattering length and cross section in the case of electron-helium scattering. Moreover, the elastic scattering of electrons from helium atoms is the simple and dominant process which can be handled accurately both theoretically and experimentally. If the elastic differential cross section for this process at very low energies is known accurately this could be used as a standard to normalize the data obtained from other cross-section measurements. As the calculation at very low energies is extremely difficult and, in addition, since a greater quantity of information is contained in the scattering length and differential cross section, in this paper we use the MCHF method to calculate accurately and completely in the *ab initio* manner the scattering length, differential, integral, and momentum-transfer cross sections through an energy range from 0 to 1 eV, an extremely difficult region for *ab initio* calculations. A quantitative comparison of our results with experiments and other theoretical calculations will justify the accuracy of the present MCHF method. At zero and very low energies the polarization of the target by the scattering electron and the electron correlation effects are very large and must be taken into account very carefully. The polarization effect, which is different for each different kinetic energy of the projectile, is considered through the bound configurations which represent the multipole polarization and by varying the bound and the continuum orbitals simultaneously at each kinetic energy of the pro-

TABLE II. The rate of convergence of the scattering length (in units of a_0) with respect to the configurations generated by the orbitals representing the multipole polarization.

Polarized orbitals	Number of configurations	Scattering length (units of a_0)
$2p$	2	1.4238
$+ 3p, 3d$	6	1.1967
$+ 4p, 4d, 4f$	15	1.1803
$+ 5p, 5d, 5f$	30	1.1784

TABLE III. Comparison of phase shifts with experiment and other theories.

E (eV)		Present	Other theories				Expt. Williams (Ref. [1])
			Nesbet (Ref. [7])	OBB (Ref. [8])	SN (Ref. [18])	MS (Ref. [10])	
0.136 06	δ_0	3.014 5	3.0134	3.0141	3.0164	3.016 8	
	δ_1	0.003 054	0.0031	0.0031	0.0032	0.003 056	
	δ_2	0.000 385	0.0004		0.0004	0.000 396	
0.544 23	δ_0	2.878 3	2.8761	2.877	2.8822	2.883 1	
	δ_1	0.012 814	0.0131	0.0128	0.0131	0.013 286	
	δ_2	0.001 637	0.0017		0.0016	0.001 594	
0.58	δ_0	2.869 5	2.8672				2.868
	δ_1	0.013 695	0.0140				0.015
	δ_2	0.001 746	0.0018				0.0014

jectile. The scattering length and the phase shifts for partial waves computed in the MCHF method have been used to calculate the differential, total elastic, and momentum-transfer cross sections. In principle, an infinite number of partial waves should be used. In practice, however, at the low energies considered, the first few partial waves usually contain the dominant terms in the cross section, and the higher phases may be treated with acceptable accuracy using the Born effective range theory [9].

II. THEORY

The MCHF method is discussed in Refs. [13,15]. In brief, it optimizes both the bound and the continuum wave functions simultaneously at each incident energy. The optimized bound orbitals take into account the polarization effects in the *ab initio* manner very accurately, resulting in an accurate phase shift. To obtain the scattering length we solved the coupled integro-differential equations for both bound and continuum wave functions for zero incident energy and zero angular momentum. In the present calculation, the MCHF method for scattering wave functions is used to calculate the scattering length for zero energy and the phase shifts δ_l for various partial waves for very low energies. The

method of constructing the scattering length and the phase shifts for various partial waves involves the solution of coupled integro-differential equations for the radial functions of the form

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

where $(2/r)Y_i(r)$ is the screening function, $(2/r)X_i(r)$ is the exchange function, and $(2/r)I_i(r)$ represents terms arising from interactions between configuration states. $\epsilon_{ii'}$ are the off-diagonal energy parameters related to Lagrange multipliers that ensure orthogonality assumptions. These equations are solved by an iterative method as described in detail earlier with the boundary conditions for the bound radial functions,

$$P_i(r) \sim r^{l+1}, \quad P_i(r) \sim 0 \quad \text{as } r \rightarrow \infty \quad (2)$$

and those for scattering wave functions

$$P_i(r) \sim r^{l+1}, \quad P_i(r) \sim A \sin(kr - l\pi/2 + \delta_l) \quad \text{as } r \rightarrow \infty \quad (3)$$

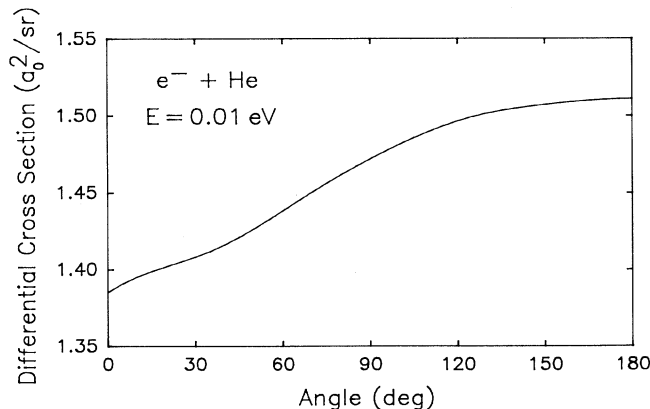


FIG. 1. Differential cross sections at 0.01 eV.

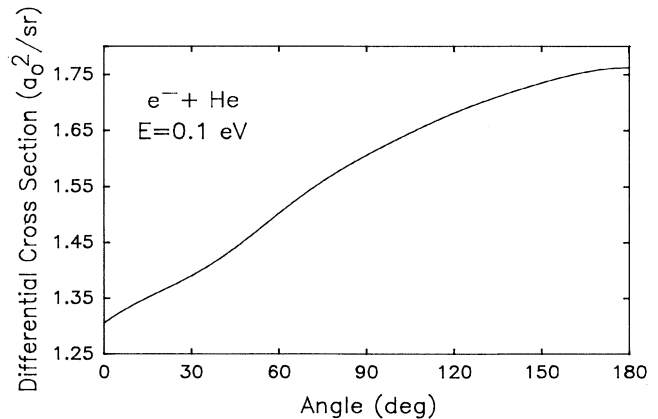


FIG. 2. Differential cross sections at 0.10 eV.

TABLE IV. (Continued).

E (Ry)	E (eV)	Present	Experiments					Other theories				
			BL [4]	KB [3]	AB [16]	CER [5]	GB [19]	Nesbet [7]	OBB [8]	SN [18]	LC [11]	MS [10]
0.029 40	0.400 00	5.938	5.98									
0.033 07	0.450 00	5.964	6.03									
0.036 75	0.500 00	5.985	6.03	6.24				6.092				
0.040 00	0.544 23	6.002						6.103	6.11	5.833		5.795
0.040 42	0.550 00	6.003	6.03									
0.042 63	0.580 00	6.012										
0.044 10	0.600 00	6.018	6.02									
0.047 77	0.650 00	6.030	6.04									
0.051 45	0.700 00	6.040	6.03									
0.055 12	0.750 00	6.048	6.05									
0.058 80	0.800 00	6.054	6.07									
0.062 47	0.850 00	6.059	6.07									
0.066 15	0.900 00	6.062	6.07									
0.069 82	0.950 00	6.064	6.08									
0.073 50	1.000 00	6.065	6.08	6.23		6.09	5.584	6.115		5.836	5.816	

taken into account by the bound configurations generated by the replacement $1s \rightarrow np$, $n \leq 5$. The quadrupole and higher multipole polarization effects are taken into account through the replacements $1s \rightarrow n'd$, and $n''f$, where $n' \leq 5$ and $n'' = 4$. All the configurations generated in this way are retained in the expansion of the scattering wave function. These bound orbitals, which are responsible for the polarization of the target atom, are determined by optimizing both the bound and the scattering electron orbitals kl simultaneously at each kinetic energy of the scattered electron. This procedure, which includes the polarization of the target atom in an *ab initio* manner reproduces this effect more accurately than any other method.

For each partial wave the same set of configurations which represent the electron correlation and polarization effects was used to calculate the scattering wave functions over a range of impact energies considered. As the polarization of the target is energy dependent, both the bound and the scattering electron orbitals are varied simultane-

ously at each kinetic energy of the scattering electron. Since at very low energies not many partial-wave phase shifts contribute to the cross section, partial waves up to $l=0-6$ are calculated directly by the MCHF method and the higher partial-wave contributions were obtained from the effective range formula [9]. The present calculation converges very well for all ranges of energy considered. It is found that higher partial waves do not contribute considerably to the cross sections over the energy range considered. The scattering length and the phase shifts calculated in this way are then used in the standard formulas to obtain the differential, total, and momentum-transfer cross sections.

IV. RESULTS AND DISCUSSIONS

In Table I the scattering length obtained by the MCHF method is compared with results derived from experi-

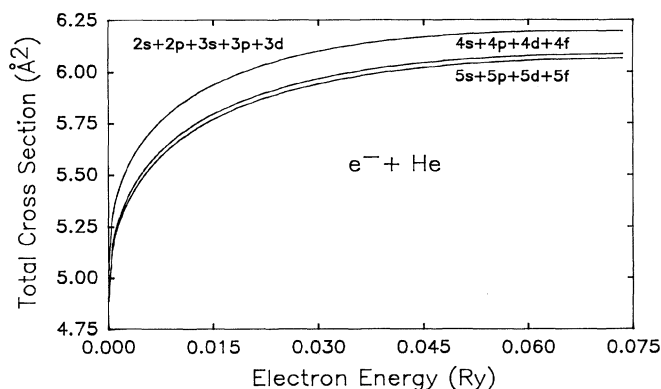


FIG. 4. Rate of convergence of total cross sections with respect to the number of orbitals representing the multipole polarization.

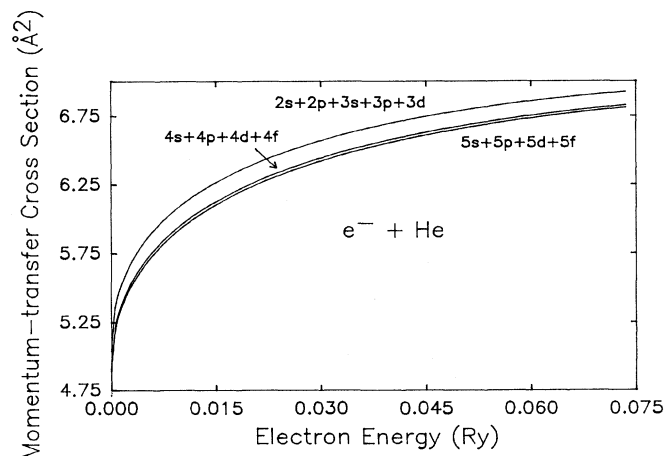


FIG. 5. Rate of convergence of momentum-transfer cross sections with respect to the number of orbitals representing the multipole polarization.

ments and with other theoretical data. The present result is in excellent agreement with the result derived from experiment by Andrick and Bitsch [16]. Andrick and Bitsch [16] measured the angular distribution of electrons scattered elastically from helium atoms in the energy range from 2 to 19 eV. They fitted the experimental data by the effective range formula and obtained the value of the scattering length from coefficients of the best fit. The present result also agrees to within 1.56% with the most recent result derived from experiment by Buckman and Lohmann [4]. Buckman and Lohmann carried out a

measurement of the absolute total cross section for electrons scattered from helium over the energy range 0.1–20 eV. They applied the effective range formula to their experimental data over the energy range 0.1–0.5, yielding a value of $1.16a_0$ for the e^- -He scattering length, which is in excellent agreement with the present result. The scattering lengths obtained from measurements by Crompton, Elford, and Robertson [5] and Ferch, Raith, and Schröder [2] also agree very well with the present result. Crompton, Elford, and Robertson reported $1.19a_0$ for the scattering length obtained from momentum-

TABLE V. Comparison of momentum-transfer cross sections (in units of \AA^2) with experiment and other theories.

E (Ry)	E (eV)	Present	Expt. CER [5]	Other theories		
				Nesbet [7]	MS [10]	OBB [8]
0.000 00	0.000 00	4.886	4.983	4.929	4.715	4.97
0.000 59	0.008 00	5.196	5.18	5.249		
0.000 66	0.009 00	5.214	5.19	5.267		
0.000 74	0.010 00	5.226	5.21	5.284		
0.000 95	0.013 00	5.277	5.26	5.330		
0.001 25	0.017 00	5.324	5.31	5.382		
0.001 47	0.020 00	5.357	5.35	5.417		
0.001 84	0.025 00	5.401	5.41	5.468		
0.002 21	0.030 00	5.449	5.46	5.514		
0.002 94	0.040 00	5.515	5.54	5.593		
0.003 68	0.050 00	5.578	5.62	5.661		
0.004 41	0.060 00	5.635	5.68	5.720		
0.005 14	0.070 00	5.685	5.74	5.774		
0.005 88	0.080 00	5.731	5.79	5.822		
0.006 61	0.090 00	5.773	5.83	5.867		
0.007 35	0.100 00	5.811	5.86	5.908		
0.008 82	0.120 00	5.882	5.94	5.983		
0.010 00	0.136 06	5.931		6.036	5.729	6.05
0.010 29	0.140 00	5.944				
0.011 03	0.150 00	5.971	6.04	6.079		
0.011 76	0.160 00	5.998				
0.012 49	0.170 00	6.023				
0.013 23	0.180 00	6.048	6.12	6.161		
0.013 97	0.190 00	6.071				
0.014 70	0.200 00	6.094	6.16	6.210		
0.018 37	0.250 00	6.196	6.27	6.316		
0.022 05	0.300 00	6.278	6.35	6.404		
0.025 72	0.350 00	6.351				
0.029 40	0.400 00	6.414	6.49	6.541		
0.033 07	0.450 00	6.469				
0.036 75	0.500 00	6.518	6.59	6.641	6.363	6.64
0.040 00	0.544 23	6.558		6.676		
0.040 42	0.550 00	6.562				
0.042 63	0.580 00	6.587				
0.044 10	0.600 00	6.602	6.66	6.715		
0.047 77	0.650 00	6.638				
0.051 45	0.700 00	6.670	6.73	6.771		
0.055 12	0.750 00	6.699				
0.058 80	0.800 00	6.726	6.77	6.815		
0.062 47	0.850 00	6.750				
0.066 15	0.900 00	6.772	6.82	6.850		
0.069 82	0.950 00	6.792				
0.073 50	1.000 0	6.810	6.85	6.880		

transfer cross-section data by simple extrapolation, apparently not including the logarithmic term in the effective range formula. Ferch, Raith, and Schröder used the effective range formula of O'Malley [17] to fit their total cross-section data obtained from transmission measurements employing the time-of-flight method. From the fitting coefficient they obtained the value $1.195a_0$ for the scattering length. The present scattering length is in excellent agreement with the best theoretical estimate obtained by O'Malley, Burke, and Berrington [8] using the R -matrix method and that obtained by Nesbet [7] using the matrix variational method. The theoretical result obtained by McEachran and Stauffer [10] is slightly lower than the present result. The present result lies in between those obtained by Buckman and Lohmann [4] and Crompton, Elford, and Robertson [5]. The rate of convergence of the scattering length with respect to the number of orbitals representing the multipole polarization is shown in Table II.

The present phase shifts for partial waves $l=0, 1$, and 2 are compared in Table III with the theoretical results obtained by Nesbet [7], O'Malley, Burke, and Berrington [8], Sinfailam and Nesbet [18], and McEachran and Stauffer [10] at three energies. The present results are in excellent agreement with all of the other theoretical results. There is only one experimental result obtained by Williams [1] for the phase shift available at the energy 0.58 eV. The present s -wave phase shift is in excellent agreement with the experimental results of Williams and the p - and d -wave phase shifts are also in very good agreement.

The elastic differential cross sections for incident energies $E=0.01, 0.1$, and 1 eV are shown in Figs. 1–3. At $E=1$ eV the present results are compared with the theoretical results obtained by LaBahn and Callaway [11]. LaBahn and Callaway [11] calculated the differential cross sections using the extended polarization potential method. Their results qualitatively follow the relative variation of the present data, but there is a constant difference between the present results and those of LaBahn and Callaway at all angles and their results are lower. In Table IV, the present elastic differential cross sections are compared with those obtained by O'Malley *et al.* at $k^2=0.01$ and 0.04 Ry. O'Malley, Burke, and Berrington [8] reported results at $\theta=0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ$, and 150° . The present results are in excellent agreement with the results obtained by O'Malley *et al.*

Figure 4 shows the present total cross sections as a function of incident electron energy from 0.0 to 0.075 Ry. The convergence of the total cross section with respect to the number of orbitals which represent the multipole polarization is also shown. The present results for the total cross section are presented in Table IV at selected energies between 0.0 to 1 eV and compared with the corresponding experimental results of Buckman and Lohmann [4] and Kennerly and Bonham [3] (where available) and the theoretical results of Nesbet [7], O'Malley, Burke, and Berrington [8], Sinfailam and Nesbet [18], and McEachran and Stauffer [10] (where available). At the energies considered there is a remarkably excellent agreement between the present results and the experimental

measurement of Buckman and Lohmann [4]. The present results also agree very well with the available results obtained by Nesbet and O'Malley *et al.* but their results are a little higher. The agreement between the present data and those of McEachran and Stauffer [10] and of Sinfailam and Nesbet [18] (where available) is good, but their results are a little less than the present values.

In Fig. 5 the present momentum-transfer cross sections are shown as a function of incident electron energy ranging from 0.0 to 1.0 eV. The results are also presented showing the rate of convergence of the momentum-transfer cross sections with respect to the number of configurations generated with the number of orbitals representing the dipole polarization. In Table V, the present momentum-transfer cross sections are compared with the experimental results of Crompton *et al.* and the theoretical results of Nesbet [7] and O'Malley, Burke, and Berrington [8] and McEachran and Stauffer [10].

TABLE VI. Comparison of differential cross sections ($\text{\AA}^2/\text{sr}$).

$\theta(\text{deg})$	$k=0.1a_0^{-1}$		$k=0.2a_0^{-1}$	
	Present	O'Malley <i>et al.</i> (Ref. [8])	Present	O'Malley <i>et al.</i> (Ref. [8])
0	0.359	0.366	0.292	0.303
5	0.365		0.302	
10	0.370		0.311	
15	0.374		0.320	
20	0.379		0.328	
25	0.382		0.337	
30	0.386	0.399	0.347	0.362
35	0.391		0.358	
40	0.397		0.369	
45	0.403		0.381	
50	0.409		0.394	
55	0.416		0.407	
60	0.423	0.434	0.420	0.430
65	0.429		0.433	
70	0.436		0.444	
75	0.441		0.455	
80	0.447		0.465	
85	0.452		0.475	
90	0.457	0.466	0.485	0.496
95	0.461		0.495	
100	0.466		0.505	
105	0.470		0.515	
110	0.474		0.525	
115	0.478		0.535	
120	0.482	0.491	0.544	0.550
125	0.485		0.553	
130	0.489		0.561	
135	0.492		0.567	
140	0.495		0.573	
145	0.497		0.578	
150	0.500	0.508	0.582	0.585
155	0.503		0.586	
160	0.505		0.589	
165	0.507		0.591	
170	0.508		0.593	
175	0.509		0.594	
180	0.510		0.595	

The present results are seen to be in excellent agreement with the experimental results of Crompton *et al.* and also agree very well with the theoretical results of Nesbet. From 0.0 to 0.02 eV, the present results are a very little higher than the results obtained by Crompton *et al.*, and from 0.025 to 1.0 eV the results of Crompton *et al.* are a little higher. The results obtained by Nesbet are a little higher than the present results and those obtained by Crompton *et al.* except at zero energy, where Nesbet's result is lower than the result obtained by Crompton *et al.* In Table VI, the results of O'Malley *et al.* (where available) are slightly higher than the present results and those obtained by Crompton *et al.* and by Nesbet. On the other hand, the results obtained by McEachran and Stauffer are a little lower than the present results and those of Crompton *et al.* and Nesbet.

V. CONCLUSION

In conclusion it should be mentioned that the scattering length of $1.1784a_0$ is calculated and bounded very accurately in the *ab initio* manner using the MCHF method. This scattering length is calculated with the wave function computed exactly at zero energy. The polarization and the electron correlation effects, which are

very important in this electron-helium scattering, have been taken into account accurately in an *ab initio* manner through the configuration-interaction procedure. The advantage of the present method lies in the fact that both the bound and the scattering electron wave functions are optimized simultaneously for each kinetic energy of the scattering electron to obtain the energy-dependent polarization very accurately. The excellent agreement of the present results with the accurate experimental and theoretical results shows that the present MCHF method produces very accurate values of the scattering length and the cross sections at very low energies, an extremely difficult region for theoretical investigation, which verifies the accuracy and the reliability of the present theoretical method.

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