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The multiconfiguration Hartree-Fock method of Saha, Pindzola, and Compton [Phys. Rev. A **38**, 128 (1988)] applied to photoionization of atoms has been extended in order to consider elastic scattering of electrons from neon atoms. The dynamical polarization and the electron-correlation effects, which are very important in this case, have been taken into account more accurately in the *ab initio* method through the configuration-interaction procedure. Phase shifts, and differential, integral, and momentum-transfer cross sections for electrons elastically scattered from neon atoms are reported for the impact-energy range from 0.136 to 70 eV. The calculated results are compared with experimental and other theoretical results. It is found that the present multiconfigurational self-consistent-field method yields high-quality results which show excellent agreement with experiment and compare well with other theoretical results.

I. INTRODUCTION

This paper presents results of studies of phase shifts, and integral, differential, and momentum-transfer cross sections of electrons elastically scattered from neon atoms by using the multiconfigurational self-consistent-field method of Saha *et al.*[1] extended to apply to scattering problems.

In recent years the scattering of slow electrons by inert-gas atoms has attracted considerable theoretical and experimental interest partly due to the continuous developments in the experimental and the theoretical investigation of the spin polarization of electrons following elastic scattering from atoms. In addition, inert gases have been the subject of extensive investigation because of their relatively simple atomic structure. The important feature of the interactions in these problems is the long-range polarization and the short-range correlation effects.

During the last few years calculations on low-energy elastic scattering of electrons from neon atoms have been performed by many authors using a different method of approximations. The main aim of these calculations was how to take the polarization effects of the target due to the scattering electrons more accurately in the calculation. One approach has been based on the polarized-orbital approximation of Temkin.[2] Dasgupta and Bhatia[3] investigated elastic scattering of electrons from neon atoms by this polarized-orbital method. They calculated elastic differential, total, and momentum-transfer cross sections using phase shifts for various partial waves obtained in the polarized-orbital approximation. McEachran and Stauffer[4] employed the adiabatic-exchange approximation to examine the effects of the polarization potential and the treatment of exchange in the low-energy elastic scattering of electrons from neon atoms. Fon and Berrington[5] applied the R-matrix method to calculate phase shifts, and differential, integral, and momentum-transfer cross sections for electrons elastically scattered from neon atoms in which the neon ground-state wave function is coupled with a ^1P pseudostate to include the static-dipole polarizability. Among other theoretical calculations, elastic calculations for neon have been carried out by Thomson[6] and Garbaty and LaBahn[7] using a simplified polarized-orbital method. This method assumes that the velocity of the incident electron is substantially less than that of the atomic electrons, so that the electronic configuration of the atom can readjust itself instantaneously. McCarthy *et al.*[8] carried out elastic calculations for inert gases by using an optical model potential. Thirumalai and Truhlar[9] reported different model-potential calculations of the elastic and absorption cross sections for e^--Ne scattering at a few intermediate energies. In all the above-mentioned calculations the main effort was given to take the polarization effects more realistically.

A great deal of experimental work has been done on electron scattering by neon atoms. Total cross sections have been measured by Stein *et al.*,[10] Wagenaar and de Heer,[11] Kauppila *et al.*,[12] and Nickel *et al.*[13] Differential cross sections have been measured by Brewer *et al.*,[14] DuBois and Rudd,[15] and Register and Trajmar.[16] Robertson[17] has presented results for the momentum-transfer cross sections. The elastic differential, total, and momentum-transfer cross sections have been measured by Register and Trajmar.[16]

In the quantum-mechanical calculations of electron-atom scattering in the low-energy range there is difficulty in taking into account the dynamical-polarization effects accurately. One realistic approach, the close-coupling method, is to expand the total wave function in terms of eigenstates of the target. A modification of the method is the R-matrix method, where the total wave function was expanded in terms of target pseudostates.

The multiconfiguration self-consistent-field (MCSCF) method which has been applied earlier to calculate photoionization of sodium atoms[1] was found to be more accurate in taking into account the dynamical core polarization effects using *ab initio* methods. In this paper we have applied the MCSCF method which has been extended[18] to consider the dynamical polarization and the electron-correlation effects more accurately and realistically in the *ab initio* method through the configuration-interaction procedure, to the calculation of the low-energy elastic scattering of electrons by neon atoms. The distortion of the target orbitals due to the presence of the projectile carrying different kinetic energy will be different. In this new approach, polarization which is energy dependent and produces a dynamical effect, called the dynamical polarization, is considered through the bound configurations representing the multipole polarization and varying the bound and the continuum orbitals simultaneously for each kinetic energy of the scattered electron. The phase shifts obtained by this method have been used to calculate the elastic differential, total, and momentum-transfer cross sections.

II. THEORY

The multiconfigurational self-consistent-field method described earlier by Saha *et al.*[1] in the calculation of photoionization of sodium atoms has been extended to calculate the scattering wave functions of the electrons elastically scattered from neon atoms. The MCSCF wave function for a scattering state could be expressed in terms of a correlated target coupled with a scattering electron and the other bound-state contributor. Briefly, the wave function of the electron-neon system is given by

$$\Psi(\gamma LS;N+1)=\sum_{j}^{m_t} a_j\Phi(\gamma_j L_t S_t;N)\phi_{kl} + \sum_{i}^{m} c_i\Phi(\gamma_i LS;N+1) , \qquad (1)$$

where the first term represents 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 total energy E_t coupled to a scattering wave function ϕ_{kl} with orbital angular momentum l, to yield an antisymmetric configuration state for the $(N+1)$-electron system, with final term value LS and configuration $\gamma_j kl$. In the second term $\Phi(\gamma_i LS;N+1)$ are $(N+1)$ electron bound configurations which are eigenstates with the same L and S and which are included to allow for polarization and electron-correlation effects.

The above wave function is defined in terms of a set of radial functions $P_i(r)$, $i=1,2,\ldots,m$. In the MCSCF method all the radial functions describing the target are assumed to be fixed with the mixing coefficients a_j. Other bound-state radial functions may be determined variationally along with the radial function for the scattering electron. In the close-coupling approach, all the radial functions are solutions of equations of the form

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

where the off-diagonal energy parameters $\varepsilon_{ii'}$ are related to Lagrange multipliers that ensure orthogonality assumptions. Bound radial functions satisfy the boundary conditions

$$P_i(r)\underset{r\to 0}{\sim} r^{l+1}, \quad P_i(r)\underset{r\to\infty}{\sim} 0 . \qquad (3)$$

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

$$P_i(r)\underset{r\to 0}{\sim} r^{l+1} , \qquad P_i(r)\underset{r\to\infty}{\sim} A\sin\left[kr-\frac{l\pi}{2}+\delta_l\right] , \qquad (4)$$

where δ_l is the phase shift and $\varepsilon_{ii}=-k^2$. k^2 is the kinetic energy of the scattered electrons in rydbergs. 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 are found to be negligible is reached, which may result in considerably smaller values of r than the asymptotic form given by the boundary condition of Eq. (4).

In the present approximation, the coefficients c_i are to be determined and they are the 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 are solutions of the system of equations

$$\sum_{i'}^{m}\langle\Phi_i|H-E|\Phi_{i'}\rangle c_{i'}+\sum_{j}^{m_t}\langle\Phi_i|H-E|\Phi_j\rangle a_j=0 , \quad i=1,\ldots,m , \qquad (5)$$

where

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

and

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

In the present work the MCSCF method for scattering states is used to compute the phase shifts δ_l of various partial waves for a range of low and intermediate energies. The differential cross section[19] in atomic units (a_0^2/sr) is given by

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

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

$$f(\theta)=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}(\sin\delta_l)P_l(\cos\theta) . \qquad (7)$$

The total cross section in units of a_0^2 is given by

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

and the momentum-transfer cross section is

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

k (a.u.)	Reference	δ_0	δ_1	δ_2	δ_3
0.3	This work	−0.2086	0.0004	0.0700	0.0022
	3	−0.2067	0.0030	0.0080	0.0025
	4	−0.2210	−0.0011	0.0068	0.0021
	5				
	16				
	22				
	14				
	20	−0.2080	0.0000	0.0070	
	21	−0.212	−0.002	0.0040	
0.4	This work	−0.3082	−0.0177	0.0130	0.0033
	3	−0.3079	−0.0141	0.0140	0.0045
	4	−0.3235	−0.0204	0.0128	0.0038
	5				
	16				
	22				
	14				
	20	−0.3100	−0.0190	0.0130	
	21	−0.310	−0.0190	0.0110	
0.6062	This work	−0.5254	−0.0913	0.0340	0.0094
	3	−0.5367	−0.0876	0.0354	0.0104
	4	−0.5440	−0.0974	0.0346	0.0090
	5	−0.514	−0.089		
	16	−0.5220	−0.0911	0.0344	0.0070
	22	−0.5181	−0.1065	0.0359	0.0099
	14				
	20				
	21				
0.8573	This work	−0.7931	−0.2176	0.0817	0.0201
	3	−0.8130	−0.2255	0.0797	0.0214
	4	−0.8156	−0.2302	0.0848	0.0191
	5	−0.811	−0.217		
	9	−0.8374	−0.2715	0.0808	0.0171
	16	−0.7867	−0.2202	0.0787	0.0190
	22	−0.7981	−0.2335	0.0874	0.0197
	14	−0.8054	−0.2340	0.0873	
	20				
	21	−0.800	−0.220	0.076	
1.05	This work	−0.9890	−0.3203	0.1369	0.0289
	3				
	4	−1.0156	−0.3390	0.1423	0.0303
	5	−1.022	−0.322		
	16	−0.9961	−0.3263	0.1356	0.0290
	22	−1.0031	−0.2523	0.1490	0.0297
	14	−0.9518	−0.3241	0.1364	0.0223
	20				
	21	−0.992	−0.328	0.137	
1.2124	This work	−1.1443	−0.4025	0.1946	0.0410
	3	−1.1787	−0.4341	0.1773	0.0447
	4	−1.1753	−0.4277	0.2013	0.0424
	5				
	16	−1.1478	−0.4132	0.1909	0.0347
	22	−1.1631	−0.4293	0.2099	0.0396
	14	−1.163	−0.4294	0.2056	0.0407
	20				
	21	−1.140	−0.423	0.196	

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

The MCSCF method we employed here to calculate the scattering of electrons from neon atom is basically the same as the one previously used for photoionization of sodium atoms.[1] The MCSCF code was modified[18] further to take into account the dynamical polarization and the electron-correlation effects very efficiently and to determine phase shifts for different values of the orbital angular momentum of the scattering electron. Since several of the bound-state orbitals for neon have nodes very close to the origin, we found it necessary to the solution of the 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 order to achieve the desired accuracy.

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

III. COMPUTATIONAL METHOD

The ground-state wave function of the target neon atom is calculated by the multiconfiguration Hartree-Fock (MCHF) wave-function expansion over the 170 configuration states coupled to form a ^1S term. These configurations are generated by the single and double re-

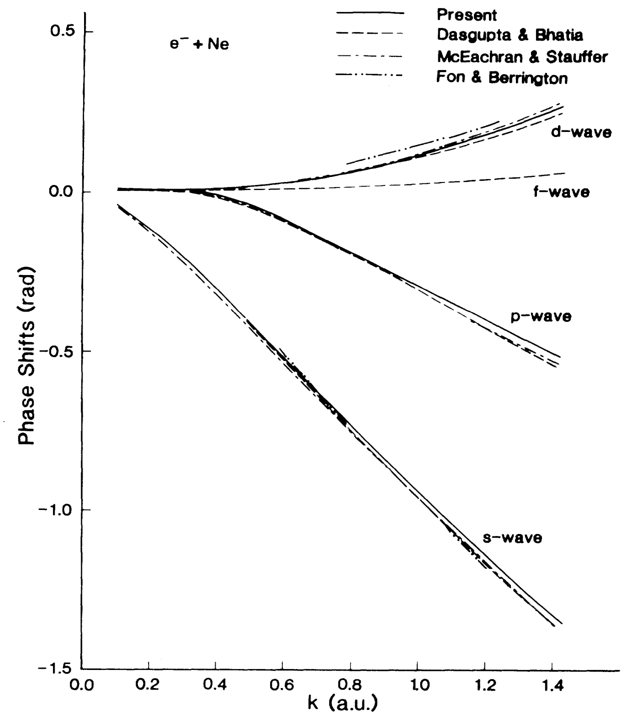

FIG. 1. s-, p-, d-, and f-wave phase shifts (modπ) for the elastic scattering of electrons from neon atoms. ——, MCSCF (present); — — —, Dasgupta and Bhatia (Ref. 3); ----, McEachran and Stauffer (Ref. 4); — · · — · · —, Fon and Berrington (Ref. 5).

TABLE II. Elastic scattering phases shifts δ_l for neon.

k (a.u.)	δ_0	δ_1	δ_2	Phase shifts δ_3	δ_4	δ_5	δ_6
0.10	−0.0448	0.0034	0.0008	0.0002	0.0001	0.0001	0.0001
0.30	−0.2086	0.0004	0.0070	0.0022	0.0010	0.0006	0.0004
0.40	−0.3082	−0.0177	0.0130	0.0033	0.0018	0.0009	0.0007
0.50	−0.4118	−0.0482	0.0215	0.0063	0.0030	0.0016	0.0009
0.6062	−0.5254	−0.0913	0.0340	0.0094	0.0043	0.0024	0.0014
0.70	−0.6259	−0.1358	0.0486	0.0125	0.0057	0.0032	0.0019
0.80	−0.7327	−0.1872	0.0683	0.0167	0.0074	0.0041	0.0024
0.8573	−0.7931	−0.2176	0.0817	0.0201	0.0085	0.0047	0.0028
0.90	−0.8374	−0.2405	0.0926	0.0214	0.0093	0.0052	0.0031
1.00	−0.9393	−0.2939	0.1211	0.0267	0.0111	0.0061	0.0039
1.05	−0.9890	−0.3203	0.1369	0.0289	0.0124	0.0065	0.0043
1.20	−1.1334	−0.3964	0.1898	0.0398	0.0170	0.0090	0.0057
1.2124	−1.1443	−0.4025	0.1946	0.0410	0.0176	0.0093	0.0058
1.40	−1.3236	−0.5072	0.2658	0.0569	0.0242	0.0128	0.0076
1.60	−1.4958	−0.5948	0.3450	0.0645	0.0314	0.0159	0.0094
1.80	−1.6786	−0.7027	0.3822	0.0868	0.0401	0.0200	0.0105
1.9170	−1.7698	−0.7425	0.4303	0.1010	0.0420	0.0230	0.0114
2.00	−1.8189	−0.7688	0.4629	0.1117	0.0476	0.0258	0.0129
2.1433	−1.9059	−0.8104	0.5162	0.1318	0.0499	0.0293	0.0153
2.1688	−1.9147	−0.8173	0.5254	0.1356	0.0512	0.0301	0.0161
2.1941	−1.9198	−0.8240	0.5344	0.1395	0.0521	0.0308	0.0167
2.2682	−1.9722	−0.8427	0.5612	0.1519	0.0581	0.0326	0.0174

placements of the two outermost orbitals $2s$ and $2p$ of the neon atom by the excited orbitals $3s$, $3p$, $3d$, $4s$, $4p$, $4d$, $4f$, $5s$, $5p$, $5d$, $5f$, $5g$, and $6g$. The eigenenergy of the ^1S state of neon atom was found to be $-128.841\,102$ a.u. The $1s$, $2s$, and $2p$ wave functions are obtained from the HF calculation of $2s^22p^6\,{}^1S$ ground state. These wave functions are used as an input in the calculation of the scattering wave functions and the phase shifts for various partial waves.

As the polarization of the $2s^22p^6$ target atom by the scattering electron is very important in the low-energy e^--Ne scattering calculations, it has been taken into account very accurately through the configuration-interaction procedure. Polarization is nothing but the distortion of the $2s$ and $2p$ orbitals of the neon atom due to the presence of the electric field of the scattering electron. It is found that only dipole polarization of the target is important in this case of the e^--Ne scattering problem. The bound configurations which will account for the dipole polarization of the $2s$ and $2p$ target orbitals are generated by the replacements $2s \rightarrow np$ and $2p \rightarrow nd$ and ns. All the configurations generated in this way are considered in the expansion of the scattering wave functions. The bound radial functions ns, np, and nd were varied simultaneously along with the radial function kl of the scattering electron for each kinetic energy of the projectile. This procedure includes the dynamical polarization of the target more accurately in the *ab initio* way.

IV. RESULTS

In the present paper we calculate phase shifts, differential, integral elastic, and momentum-transfer

TABLE III. Differential cross sections for elastic electron-neon scattering at $k^2=5$ eV (in units of a_0^2/sr).

θ	Theory				Experiment
(deg)	Present	Ref. 3	Ref. 4	Ref. 5	Ref. 16
0	0.4271	0.3959	0.558	0.461	
5	0.5352	0.4992	0.643	0.556	
10	0.6483	0.6113	0.755	0.693	
15	0.7631	0.7281	0.869		
20	0.8740	0.8436	0.977	0.891	
25	0.9764	0.9525	1.076		
30	1.0664	1.0505	1.164	1.070	1.064
35	1.1412	1.1339	1.237		
40	1.1989	1.2002	1.292	1.114	1.186
45	1.2381	1.2476	1.330		
50	1.2585	1.2754	1.349	1.221	1.225
55	1.2603	1.2834	1.348		
60	1.2442	1.2722	1.329	1.188	1.207
65	1.2114	1.2432	1.293		
70	1.1637	1.1980	1.242	1.095	1.136
75	1.1033	1.1389	1.176		
80	1.0325	1.0687	1.100	0.961	1.007
85	0.9542	0.9903	1.015		
90	0.8710	0.9064	0.925	0.804	0.878
95	0.7854	0.8200	0.833		
100	0.7000	0.7337	0.741	0.646	0.711
105	0.6171	0.6498	0.652	0.571	
110	0.5385	0.5704	0.568	0.501	0.550
115	0.4659	0.4971	0.490	0.436	
120	0.4007	0.4312	0.421	0.379	0.393
125	0.3437	0.3733	0.361	0.329	
130	0.2952	0.3239	0.310	0.286	0.296
135	0.2553	0.2828	0.269		
140	0.2235	0.2498	0.236	0.221	0.225
145	0.1990	0.2240	0.211		
150	0.1811	0.2046	0.193	0.181	
155	0.1685	0.1907	0.181		
160	0.1601	0.1811	0.173	0.158	
165	0.1548	0.1748	0.169		
170	0.1517	0.1710	0.166	0.148	
175	0.1501	0.1690	0.165		
180	0.1496	0.1684	0.164	0.145	

cross sections for the following process:

$$e^- + \mathrm{Ne}(^1S) \rightarrow e^- + \mathrm{Ne}(^1S) ,$$

at electron energies ranging from 0.136 to 70 eV.

A. Phase shifts

In Table I, the phase shifts for $l=0-3$ partial waves at few energies are compared with experiments and other theoretical results. At energies $k=0.30$ and 0.40 a.u., the s-wave phase shifts are found to be in excellent agreement with the experimental results of O'Malley and Crompton[20] and of Williams,[21] and the theoretical results of Dasgupta and Bhatia.[3] O'Malley and Crompton[20] obtained s-wave phase shifts from the experimentally determined electron drift velocities which are fitted directly with a three-parameter modified effective-range theory measurement. According to them, the uncertainty in δ_0 (the phase shift for $l=0$) is about $\pm 2\%$. Williams[21] derived phase shifts from his experimentally measured absolute differential elastic cross section. Dasgupta and Bhatia[3] used the polarized-orbital method of Temkin[2] to obtain their phase shifts. They have included both direct and exchange polarization terms into their calculations. The s-wave phase shift at energy $k=0.6062$ a.u. is, on the other hand, in excellent agreement with the experimental results of Register and Trajmar[16] and of An-

TABLE IV. Differential cross sections for elastic electron-neon scattering at $k^2=10$ eV (in units of a_0^2/sr).

θ	Theory				Experiment	
(deg)	Present	Ref. 3	Ref. 4	Ref. 5	Ref. 16	Ref. 14
0	0.6922	0.7444	0.829	0.812		
5	0.7835	0.8399	0.906	0.928		
10	0.8986	0.9626	1.022	1.075		
15	1.0290	1.1027	1.152			
20	1.1644	1.2485	1.282	1.368	1.257	1.26
25	1.2958	1.3897	1.408			1.40
30	1.4158	1.5173	1.524	1.601	1.428	1.52
35	1.5179	1.6239	1.622			1.63
40	1.5971	1.7039	1.698	1.725	1.614	1.71
45	1.6498	1.7534	1.748			1.77
50	1.6737	1.7705	1.770	1.725	1.678	1.79
55	1.6678	1.7548	1.760			1.78
60	1.6322	1.7074	1.720	1.609	1.603	1.73
65	1.5684	1.6308	1.651			1.66
70	1.4792	1.5288	1.555	1.406	1.443	1.57
75	1.3686	1.4064	1.437			1.44
80	1.2416	1.2692	1.302	1.151	1.200	1.30
85	1.1039	1.1233	1.156			1.15
90	0.9616	0.9750	1.005	0.885	0.921	1.00
95	0.8206	0.8301	0.855			0.844
100	0.6866	0.6940	0.713	0.644	0.646	0.696
105	0.5647	0.5716	0.585	0.542		0.566
110	0.4590	0.4666	0.474	0.454	0.432	0.455
115	0.3728	0.3818	0.384	0.382		0.375
120	0.3080	0.3189	0.318	0.327	0.286	0.296
125	0.2651	0.2781	0.276	0.288		
130	0.2436	0.2584	0.257	0.264	0.243	
135	0.2415	0.2579	0.260			
140	0.2558	0.2735	0.281	0.255	0.268	
145	0.2830	0.3015	0.317			
150	0.3187	0.3377	0.362	0.280		
155	0.3585	0.3777	0.411			
160	0.3980	0.4172	0.460	0.319		
165	0.4332	0.4524	0.503			
170	0.4608	0.4800	0.538	0.351		
175	0.4785	0.4976	0.559			
180	0.4848	0.5039	0.566	0.364		

drick,[22] and the theoretical results of Dasgupta and Bhatia[3] and of Fon and Berrington.[5] Register and Trajmar[16] obtained phase shifts by fitting their measured angular distributions at few impact energies. Fon and Berrington[5] calculated phase shifts by the R-matrix method. They carried out calculations by coupling the neon ground-state wave function with a ^1P pseudostate to include the full ground-state static dipole polarizability. They used the Hartree-Fock neon ground-state wave function from Clementi's tables[23] and the ^1P pseudostate is formed by the HF orbitals $1s$, $2s$, and $2p$, and the pseudo orbitals $\overline{3s}$, $\overline{3p}$, and $\overline{3d}$ given by Hibbert *et al.*[24] Again at energy $k=0.8573$ a.u. the present s-wave phase shift is found to be in excellent agreement with the experimental results of Andrick,[22] Register and Trajmar,[16] Brewer *et al.*,[14] and of Williams.[21] Brewer *et al.*[14] derived phase shifts from the experimentally measured differential cross sections. The present s-wave phase shifts are also in excellent agreement with the experimental results of Williams,[21] Register and Trajmar,[16] and of Andrick[22] at energy $k=1.05$ a.u., whereas at $k=1.2124$ a.u. this phase shift is in best agreement with the experimental results of Register and Trajmar[16] and of Williams.[21] The present s-wave phase shifts at these energies are also in very good agreement with the theoretical results of Dasgupta and Bhatia,[3] Fon and Berrington,[5] and McEachran and Stauffer.[4] McEachran and Stauffer[4] obtained phase shifts in the adiabatic exchange approximation. They have not included the exchange polarization terms in their calculation.

The present p-wave phase shift at $k=0.30$ a.u. is very small and compares well with the experimental result of O'Malley and Crompton[20] and of Williams,[21] and the theoretical result of McEachran and Stauffer.[4] These phase shifts at energies $k=0.6062$ and 0.8573 a.u. are in excellent agreement with the experimental results of Register and Trajmar,[16] and agree very well with the theoretical results of Fon and Berrington[5] and of Dasgupta and Bhatia.[3] At energy $k=1.05$ a.u., the p-wave phase shift is again in excellent agreement with the experimental results of Register and Trajmar,[16] Brewer *et al.*,[14] and of Williams,[21] and the theoretical result of Fon and Berrington.[5] This phase shift at $k=1.2124$ a.u. also agrees very well with the experimental results of Register and Trajmar,[16] Andrick,[22] Brewer *et al.*,[14] and of Williams,[21] and the theoretical result of McEachran and Stauffer.[4] It is seen from Table I, that the d-wave phase shifts at energies $k=0.30$ and 0.40 a.u. show excellent agreement with the experimental results of O'Malley and Crompton,[20] and the theoretical results of Dasgupta and Bhatia[3] and of McEachran and Stauffer.[4] At energy $k=0.6062$, this phase shift is, on the other hand, in excellent agreement with the experimental result of Register and Trajmar[16] and the theoretical result of McEachran and Stauffer,[4] whereas at $k=0.8573$ a.u., this phase shift agrees very well with the experimental phase shift of Register and Trajmar,[16] and the theoretical phase shifts of Thirumalai and Truhlar[9] and of Dasgupta and Bhatia.[3] Thirumalai and Truhlar[9] used model potentials; in particular, the static-exchange nonadiabatic polarization potential, in their calculations in order to obtain phase shifts. At energy $k=1.05$ a.u., this d-wave phase shift again shows excellent agreement with the experimental results of Register and Trajmar,[16] Brewer *et al.*,[14] and of Williams.[21] The present d-wave phase shift at energy $k=1.2124$ a.u., also shows excellent agreement with the experimental results of Register and Trajmar[16] and of Williams,[21] and is very close to the experimental results of Andrick[22] and of Brewer *et al.*,[14] and the theoretical result of McEachran and Stauffer.[4]

The present f-wave phase shifts at energies $k=0.30$ and 0.40 a.u. agree very well with the results obtained by McEachran and Stauffer.[4] This phase shift also agrees very well with theoretical result of Dasgupta and Bhatia[3] at $k=0.30$ a.u. At energy $k=0.6062$ a.u., this phase shift is in excellent agreement with the experimental result of Andrick[22] and the theoretical result of McEachran

TABLE V. Differential cross sections for elastic electron-neon scattering at $k^2=15$ eV (in units of a_0^2/sr).

θ	Theory		Experiment	
(deg)	Present	Ref. 4	Ref. 16	Ref. 14
0	1.0982	1.227		
5	1.0956	1.235		
10	1.1405	1.277		
15	1.2183	1.349		
20	1.3153	1.439		1.31
25	1.4197	1.538	1.471	1.41
30	1.5211	1.637	1.578	1.51
35	1.6113	1.727		1.59
40	1.6833	1.799	1.711	1.66
45	1.7316	1.848		1.71
50	1.7524	1.868	1.796	1.73
55	1.7429	1.853		1.72
60	1.7015	1.804	1.728	1.68
65	1.6283	1.720		1.60
70	1.5254	1.605	1.532	1.49
75	1.3965	1.462		1.36
80	1.2475	1.299	1.250	1.21
85	1.0856	1.124		1.05
90	0.9191	0.945	0.932	0.883
95	0.7568	0.772		0.721
100	0.6071	0.615	0.600	0.574
105	0.4777	0.480		0.445
110	0.3749	0.374	0.364	0.342
115	0.3033	0.304	0.311	0.272
120	0.2655	0.271	0.264	0.239
125	0.2620	0.275	0.275	0.216
130	0.2913	0.315	0.307	
135	0.3500	0.387		
140	0.4330	0.485	0.468	
145	0.5341	0.601		
150	0.6458	0.727		
155	0.7593	0.853		
160	0.8668	0.971		
165	0.9603	1.073		
170	1.0327	1.151		
175	1.0786	1.200		
180	1.0949	1.216		

and Stauffer;[4] on the other hand, at $k = 0.8573$ a.u., this phase shift shows excellent agreement with the experimental results of Andrick,[2] and of Register and Trajmar,[16] and the theoretical result of McEachran and Stauffer[4] and of Dasgupta and Bhatia.[3] This phase shift at $k = 1.05$ a.u. agrees best with the experimental results of Register and Trajmar[16] and of Andrick,[22] whereas at $k = 1.2124$ a.u., the present phase shift is also in excellent agreement with the experimental results of Andrick[22] and of Brewer *et al.*,[14] and the theoretical results of McEachran and Stauffer[4] and of Dasgupta and Bhatia.[3]

The MCSCF phase shifts of *s*, *p*, *d*, and *f* waves are compared to the results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] and Fon and Berrington[5] in Fig. 1. Agreements are very good.

We present the phase shifts for $l = 0-6$ in Table II calculated in the MCSCF approximation for a range of energies from $k^2 = 0.136-70$ eV. At low energies they follow the phase shift formula,[25]

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

where α is the dipole polarizability.

B. Differential cross section

The differential cross sections at $k^2 = 5$, 10, 15, 20, and 50 eV are compared in Tables III–VII from 0° to 180°. The contribution of phase shifts for $l = 7-500$ has been calculated using the effective-range formula, Eq. (10). The experimental value[26] of the dipole polarizability $\alpha = 2.66a_0^3$ is used in the calculation. It is found that the differential cross sections converge by $l = 60$. Since in the forward direction the convergence is very slow, we use[27]

TABLE VI. Differential cross sections for elastic electron-neon scattering at $k^2 = 20$ eV (in units of a_0^2/sr).

θ	Theory				Experiment	
(deg)	Present	Ref. 3	Ref. 4	Ref. 5	Ref. 16	Ref. 14
0	1.7238	1.8296	1.840	1.971		
5	1.5652	1.6828	1.744	1.790		
10	1.4824	1.6179	1.668	1.663		
15	1.4562	1.6127	1.637			
20	1.4720	1.6489	1.642	1.590		1.65
25	1.5152	1.7092	1.671		1.614	1.68
30	1.5727	1.7778	1.716	1.625	1.668	1.72
35	1.6324	1.8409	1.764			1.77
40	1.6836	1.8869	1.806	1.699	1.714	1.82
45	1.7176	1.9072	1.833			1.84
50	1.7276	1.8956	1.837	1.741	1.739	1.84
55	1.7086	1.8490	1.810			1.81
60	1.6578	1.7667	1.750	1.671	1.650	1.74
65	1.5744	1.6506	1.655			1.65
70	1.4604	1.5052	1.528	1.492	1.443	1.52
75	1.3199	1.3370	1.373			1.37
80	1.1593	1.1542	1.198	1.198	1.114	1.20
85	0.9870	0.9664	1.011			1.02
90	0.8125	0.7834	0.824	0.845	0.786	0.829
95	0.6459	0.6150	0.647			0.654
100	0.4972	0.4700	0.491	0.519	0.479	0.492
105	0.3756	0.3565	0.366	0.391	0.364	0.364
110	0.2889	0.2802	0.280	0.300	0.279	0.275
115	0.2427	0.2450	0.239	0.255	0.232	0.229
120	0.2400	0.2523	0.245	0.259	0.243	0.232
125	0.2813	0.3008	0.299	0.314	0.286	
130	0.3641	0.3872	0.398	0.418	0.371	
135	0.4837	0.5057	0.536			
140	0.6328	0.6489	0.705	0.750	0.654	
145	0.8023	0.8081	0.894			
150	0.9817	0.9736	1.092	1.1752		
155	1.1595	1.1353	1.286			
160	1.3245	1.2834	1.465	1.5980		
165	1.4659	1.4090	1.616			
170	1.5743	1.5047	1.733	1.901		
175	1.6426	1.5647	1.805			
180	1.6667	1.5860	1.829	2.004		

$$\left(\frac{d\sigma}{d\Omega}\right)_{\theta=0^\circ} = \left|\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l\right|^2$$
$$= \left(\frac{d\sigma}{d\Omega}\right)_{\theta=0^\circ}^{l<l_0} + \left(\frac{\pi\alpha l_0}{4l_0^2-1}\right)\sum_{l=0}^{l_0-1}(2l+1)\sin 2\delta_l + \left(\frac{\pi\alpha l_0 k}{4l_0^2-1}\right)^2, \quad (11)$$

where $l_0=7$ and the effective-range formula Eq. (10) has been used for $l \geq 7$ to derive this formula.

A comparison of the differential cross sections at 5 eV with the theoretical values obtained by Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] Fon and Berrington,[5] and the experimental results of Register and Trajmar[16] is given in Table III. At this energy the present differential cross sections agree remarkably well with the experimental results of Register and Trajmar[16] and the theoretical results of Fon and Berrington.[5] The present results also agree well with the results obtained by Dasgupta and Bhatia.[3] Although there is little variation in magnitude among the various theoretical sets of data at this energy, there is general agreement about the positions of the peak of the cross sections.

At 10 eV, the present differential cross sections are compared with the theoretical results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] Fon and Berrington,[5] and the experimental results of Register and Trajmar[16] and Brewer *et al.*[14] in Table IV. The present differential cross sections agree well with the experimental results of

TABLE VII. Differential cross sections for elastic electron-neon scattering at $k^2=50$ eV (in units of a_0^2/sr).

θ	Theory				Experiment	
(deg)	Present	Ref. 3	Ref. 4	Ref. 5	Ref. 16	Ref. 14
0	5.7065	6.3854	6.283	6.203		
5	4.6730	5.1890	5.501	5.196		
10	3.8701	4.2462	4.611	4.257		4.33
15	3.2336	3.4964	3.839		4.182	3.38
20	2.7292	2.9092	3.196	2.857	3.239	2.75
25	2.3282	2.4546	2.668		2.603	2.32
30	2.0082	2.1048	2.242	1.986	2.100	1.96
35	1.7518	1.8347	1.907			
40	1.5444	1.6220	1.645	1.464	1.468	1.37
45	1.3735	1.4474	1.439			
50	1.2270	1.2954	1.272	1.134	1.139	1.05
55	1.0941	1.1538	1.126			
60	0.9656	1.0143	0.991	0.882	0.889	0.812
65	0.8352	0.8720	0.857			
70	0.7004	0.7258	0.721	0.650	0.643	0.604
75	0.5627	0.5780	0.581			
80	0.4268	0.4335	0.443	0.414	0.400	0.384
85	0.2995	0.2993	0.310			
90	0.1883	0.1835	0.192	0.199	0.168	0.211
95	0.1006	0.0941	0.097		0.084	0.121
100	0.0433	0.0388	0.035	0.052	0.035	0.040
105	0.0228	0.0239	0.012	0.023	0.020	0.036
110	0.0444	0.0539	0.038	0.035	0.054	0.065
115	0.1128	0.1309	0.114	0.093	0.150	
120	0.2306	0.2543	0.242	0.201	0.268	0.260
125	0.3979	0.4210	0.421	0.357		
130	0.6109	0.6254	0.644	0.561	0.643	0.657
135	0.8619	0.8596	0.905			
140	1.1387	1.1141	1.192	1.075	1.103	1.17
145	1.4264	1.3776	1.492		1.314	
150	1.7083	1.6383	1.791	1.648		1.74
155	1.9687	1.8840	2.076			
160	2.1947	2.1032	2.332	2.174		
165	2.3769	2.2856	2.545			
170	2.5098	2.4227	2.706	2.539		
175	2.5906	2.5080	2.807			
180	2.6194	2.5388	2.838	2.666		

Register and Trajmar[16] and Brewer *et al.*[14] The results obtained by Dasgupta and Bhatia[3] and McEachran and Stauffer[4] are higher than the present results. From $\theta=20°-80°$, the present results agree best with the experimental results of Register and Trajmar,[16] and from $\theta=90°-120°$ the present results are closer to the experimental results of Brewer *et al.*[14] Again at this energy there is excellent agreement between the theoretical and the experimental results about the position of the maximum, and also there is general agreement between them about the position of the minimum.

The differential cross sections at 15 eV are compared with the experimental results of Register and Trajmar[16] and Brewer *et al.*,[14] and the theoretical results of McEachran and Stauffer[4] in Table V. The present results at this energy are in excellent agreement with the experimental results of Register and Trajmar[16] and Brewer *et al.*[14] The theoretical results obtained by McEachran and Stauffer[4] are higher than the present results. The position of the maximum around 50° agrees extremely well with the theoretical and the experimental results. There is also good agreement about the position of minimum around 120°–125° among four sets of results.

At 20 eV, the present differential cross sections are compared with the theoretical results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] Fon and Berrington,[5] and the experimental results of Register and Trajmar[16] and Brewer *et al.*[14] in Table VI. The present results are in very good agreement with the experimental results of Register and Trajmar[16] and Brewer *et al.*[14] Once again there is general agreement about the positions of maximum around 50° and the minimum around 115°–120° among the comparable theoretical and experimental results.

The differential cross sections at 50 eV are compared with the theoretical results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] Fon and Berrington,[5] and the experimental results of Register and Trajmar[16] and DuBois and Rudd[15] in Table VII. The present results are in good agreement with the experimental results of Register and Trajmar, and DuBois and Rudd. Except for a few angles $\theta=0°-15°$, the present results are close to those of Dasgupta and Bhatia.[3] The results obtained by Fon and Berrington[5] are very close to the present results except for $\theta=0°-10°$. At this energy there is no maximum, all sets of results start decreasing from the angle $\theta=0°$, go to minimum at $\theta=105°$, and then increase.

It is seen from the analysis of the differential cross sections at the energies considered that they reach a maximum around 50°, except at 50 eV. The position of the minimum shifts towards the smaller angles with the increase of the energy, except at the lowest energy, 5 eV, where there appears no minimum.

C. Total cross section

In Table VIII, total cross sections are compared with the theoretical results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] Fon and Berrington,[5] and Thirumalai and Truhlar,[9] and the available experimental results of Nickel *et al.*,[13] Register and Trajmar,[16] Brewer *et al.*,[14] Kauppila *et al.*,[12] Wagenaar and de Heer,[11] Du-

TABLE VIII. Comparison of present total elastic cross sections (in a_0^2) for electron-neon scattering with experiment and other theoretical results.

k^2		Theory				Experiment						
(eV)	Present	Ref. 3	Ref. 4	Ref. 5	Ref. 9	Ref. 13	Ref. 16	Ref. 14	Ref. 12	Ref. 11	Ref. 15	Ref. 20
5	9.6837	9.9753	10.363	9.545		10.153	9.570					
10	11.7082	12.2022	12.408	12.499	13.713	12.295	11.606	12.4±0.6				
15	12.5009		13.258				12.677	12.2±0.6				
20	12.7603	13.3283	13.544	13.474		13.309	12.892	13.6±0.7	13.163			
50	11.2846	11.5939	12.114	11.017	9.76	12.902	11.177		12.723	13.06	11.0	
70	10.1303	10.1970		9.625	9.17	12.134	10.070			12.32		
0.136	2.5688	2.0736										2.482
1.224	6.0294	5.9380										5.999
2.176	7.3772	7.3528										7.464

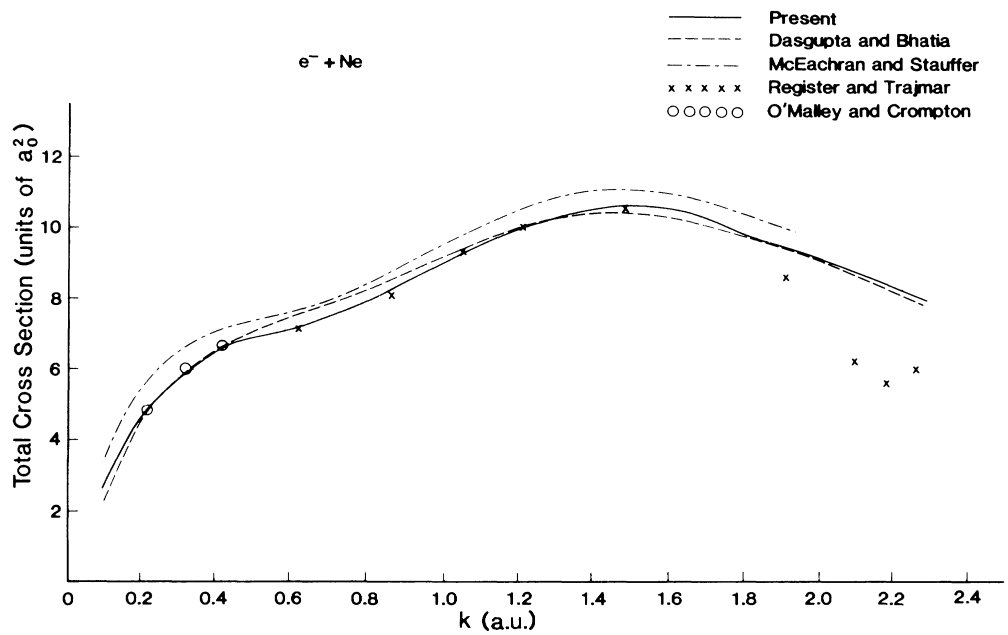

FIG. 2. Total-elastic cross sections (in units of a_0^2) for the low-energy scattering of electrons from neon atoms. ——, MCSCF (present); — — —, Dasgupta and Bhatia (Ref. 3); –·–·–, McEachran and Stauffer (Ref. 4); ×, Register and Trajmar (Ref. 16); ○, O'Malley and Crompton (Ref. 20).

Bois and Rudd,[15] and O'Malley and Crompton.[20] Comparison of present results at the lowest three energies 0.136, 1.224, and 2.176 eV with the experimental results of O'Malley and Crompton,[20] and the theoretical results of Dasgupta and Bhatia[3] shows that the present results at these energies are in remarkably excellent agreement with the experimental results of O'Malley and Crompton.[20] The present results also agree very well with those of Dasgupta and Bhatia.[3] At 5 eV, the present result agrees extremely well with the experimental result of Register and Trajmar,[16] and the theoretical result of Fon and Berrington.[5]

At energies 10 and 20 eV the present results are in extremely good agreement with the experimental results of Register and Trajmar[16] and Brewer *et al.*[14] At energy 20 eV, the present result also shows best agreement with the experimental result of Register and Trajmar[16] and Brewer *et al.*[14] The theoretical results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] and Fon and Berrington[5] are higher than the present result but are close to each other, and agree well with the experimental results of Nickel *et al.*,[13] Brewer *et al.*,[14] and Kauppila *et al.*[12] Nickel *et al.*[13] measured the total electron-scattering cross section from neon atoms utilizing the linear transmission device. Total scattering cross sections have been measured for electrons colliding with neon atoms in the energy range 15–800 eV using a beam transmission technique. The present result at energy 50 eV is found to be in excellent agreement with the experimental result of Register and Trajmar[16] and DuBois and Rudd,[15] and the theoretical results of Fon and Berrington[5] and Dasgupta and Bhatia.[3] DuBois and Rudd[15] measured absolute differential and total elastic cross sections for electron scattering from neon atoms in the energy range 50–800 eV. The result obtained by Thirumalai and Truhlar[9] at this energy is lower than the present, as well as the other theoretical and experimental results. At energy 70 eV the present result shows excellent agreement with the experimental result of Register and Trajmar,[16] and the theoretical result of Dasgupta and Bhatia.[3]

TABLE IX. Present total and momentum-transfer cross sections (in units of a_0^2).

k (a.u.)	Cross sections: Total	Momentum-transfer
0.10	2.5688	2.9356
0.30	6.0294	6.0335
0.40	7.3772	6.6149
0.50	8.5398	6.8829
0.6062	9.6837	7.1840
0.70	10.5552	7.5129
0.80	11.3371	7.9591
0.8573	11.7082	8.2429
0.90	11.9368	8.4653
1.00	12.3545	8.9819
1.05	12.5009	9.2355
1.20	12.7517	9.8894
1.2124	12.7603	9.9304
1.40	12.9785	10.5172
1.60	12.5252	10.5752
1.80	11.6832	9.7561
1.9170	11.2846	9.4466
2.00	11.0189	9.1303
2.1433	10.5196	8.5511
2.1688	10.4451	8.4296
2.1941	10.3759	8.3016
2.2682	10.1303	8.0059

TABLE X. Comparison of present momentum-transfer cross sections (in a_0^2) for electron-neon scattering with experiment and other theoretical results.

k^2	Theory					Experiment			
(eV)	Present	Ref. 3	Ref. 4	Ref. 5	Ref. 9	Ref. 16	Ref. 14	Ref. 17	Ref. 20
5	7.1840	7.5448	7.636	6.903		7.106		7.392	
10	8.2429	8.5266	8.733	7.921	9.178	8.071	8.7±0.5		
15	9.2355		9.799			9.320	8.9±0.5		
20	9.9304	10.0350	10.538	10.863			10.6±0.6		
50	9.4466	9.3887	9.924	9.235	7.321	9.999			
70	8.0059	7.8524		7.421		8.571			
0.136	2.9356	2.4518				5.928			2.868
1.224	6.0335	6.0720							6.035
2.176	6.6149	6.7342							6.642

Figure 2 shows present results of total cross section as well as the theoretical results of Dasgupta and Bhatia[3] and McEachran and Stauffer,[4] and the experimental results of Register and Trajmar[16] and O'Malley and Crompton.[20] The results of Register and Trajmar[16] are calculated from the phase shifts derived from their measured differential cross sections. O'Malley and Crompton[20] obtained their total cross sections by fitting the data of Robertson[17] derived from drift-velocity measurements. From the figure it is found that the present results are in excellent agreement with the experimental results of Register and Trajmar,[16] and O'Malley and Crompton[20] throughout the energy range considered. The theoretical results obtained by Dasgupta and Bhatia[3] agree well from $k = 0.1-0.5$ and $k = 1.4-2.3$ a.u.

In Table IX, the present total and momentum-transfer cross sections are presented for the energy range from $k = 0.10$ to $k = 2.2682$ a.u. The present momentum-transfer cross sections at few energies are compared with the theoretical results of Dasgupta and Bhatia,[3] McEachran and Stauffer,[4] Fon and Berrington,[5] and Thirumalai and Truhlar[9] (where available), and the experimental results of Register and Trajmar,[16] Brewer *et al.*,[14] Robertson,[17] and O'Malley and Crompton[20] in Table X. At the three lowest energies 0.136, 1.224, and 2.176 eV, the present momentum-transfer cross sections are in excellent agreement with the experimental results of O'Malley and Crompton.[20] The present results at

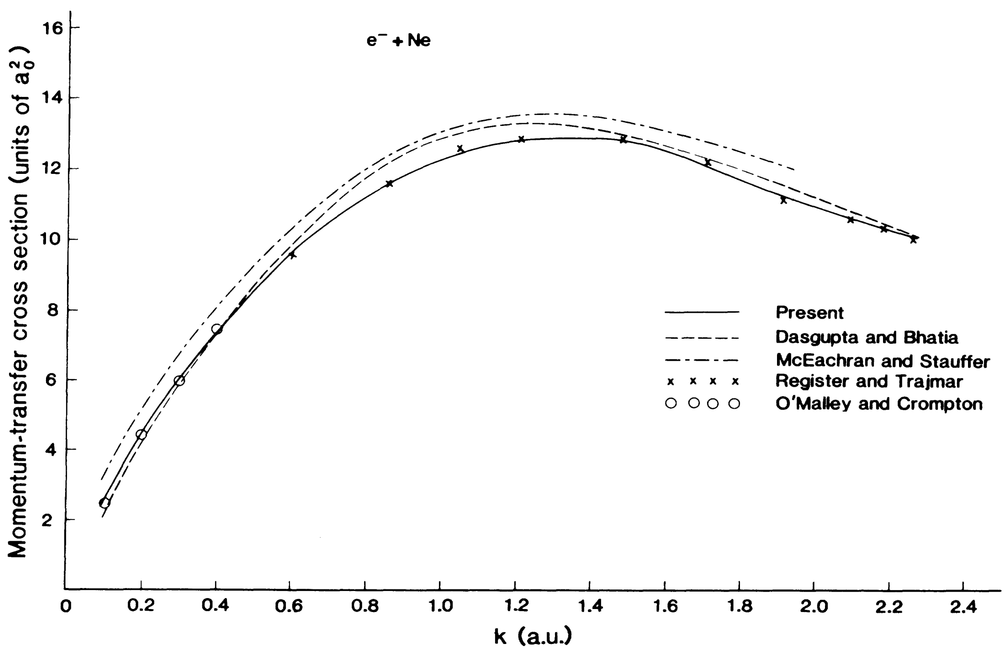

FIG. 3. Momentum-transfer cross sections (in units of a_0^2) for the low-energy scattering of electrons from neon atoms. ——, MCSCF (present); — — —, Dasgupta and Bhatia (Ref. 3); —-—-, McEachran and Stauffer (Ref. 4); ×, Register and Trajmar (Ref. 16); ○, O'Malley and Crompton (Ref. 20).

these energies also agree well with the theoretical results of Dasgupta and Bhatia.[3] At energy 5 eV, the present result shows excellent agreement with the experimental result of Register and Trajmar[16] and Robertson.[17] The present result at this energy also agrees very well with the theoretical result of Fon and Berrington[5] although their result is a little lower than the present result. Robertson[17] derived energy-dependent momentum-transfer cross sections from the analysis of the data obtained from the drift-velocity measurements in neon. The accuracy of the result was estimated to be $\pm 3\%$ for energies between 0.04 and 6.0 eV. The present momentum-transfer cross section at 10 eV agrees very well with the experimental results of Register and Trajmar[16] and Brewer *et al.*,[14] and the theoretical result of Fon and Berrington.[5] The present result at 15 eV agrees extremely well with the experimental results of Register and Trajmar[16] and Brewer *et al.*[14] At 20 eV, the present result shows excellent agreement with the experimental results of Register and Trajmar[16] and Brewer *et al.*,[14] and the theoretical result of Dasgupta and Bhatia.[3] At 50 eV, the present result agrees very well with the theoretical results obtained by Dasgupta and Bhatia[3] and Fon and Berrington,[5] but is higher than the experimental result of Register and Trajmar.[16] The present result at 70 eV also agrees well with the theoretical result of Dasgupta and Bhatia,[3] but is much higher than the experimental result of Register and Trajmar.[16]

Figure 3 shows the present momentum-transfer cross sections, the theoretical result of Dasgupta and Bhatia[3] and McEachran and Stauffer,[4] and the experimental results of Register and Trajmar[16] and O'Malley and Crompton.[20] As indicated earlier, the results of O'Malley and Crompton[20] are derived from the drift-velocity measurement data of Robertson.[17] The present results are in excellent agreement with the experimental results of O'Malley and Crompton[20] and Register and Trajmar,[16] except at higher energies from 50 eV to higher where the experimental results of Register and Trajmar[16] are much lower than the present results. The results obtained by Dasgupta and Bhatia[3] agree well with the present and experimental results, except for the energies from $k = 0.4-1.1$ a.u., where their results are a little higher. The results obtained by McEachran and Stauffer[4] are higher than the present and experimental results throughout the energy region considered. This may be due to the neglect of the exchange polarization terms in their calculations.

V. CONCLUSION

Very extensive and more accurate calculations have been made on the low-energy elastic scattering of electrons from neon atoms. The multiconfiguration Hartree-Fock method for the bound and the continuum wave functions is applied to calculate phase shifts, differential, total-elastic, and momentum-transfer cross sections. The dynamical-polarization and the electron-correlation effects which are very important in these calculations are taken into account more accurately than any other method using the *ab initio* technique through the configuration-interaction procedure. The present phase shifts are in excellent agreement with the experimental results of Register and Trajmar[16] and O'Malley and Crompton.[20] The present results compare very well with other available theoretical results. The differential cross sections at different energies compare very well with the experimental and other theoretical results. The total-elastic and the momentum-transfer cross sections are in best agreement with the experimental results. As the present MCSCF method takes into account the dynamical polarization and the electron correlation effects more accurately than any other methods, we conclude that the present results are more accurate and reliable. Moreover, the present results agree with experiment better than any other methods. Finally, it should be mentioned that the present MCSCF method has wide applications both in the photoionization of atoms and the elastic scattering of electrons from atoms.

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