Scattering of electrons from neon atoms

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Scattering of electrons from neon atoms is investigated by the polarized-orbital method. The perturbed orbitals calculated with use of the Sternheimer approximation lead to the polarizability $2.803a_0^3$, in fairly good agreement with the experimental value $2.66a_0^3$. Phase shifts for various partial waves are calculated in the exchange, exchange-adiabatic, and polarized-orbital approximations. They are compared with the previous results. The calculated elastic differential, total, and momentum-transfer cross sections are compared with the experimental results. The polarized-orbital approximation yields results which show general improvement over the exchange-adiabatic approximation.

I. INTRODUCTION

During the last few years, a number of calculations on scattering of electrons from neon atoms have been carried out: An R-matrix calculation by Fon and Berrington,[1] optical potential method by McCarthy *et al.*,[2] exchange-adiabatic approximation by Thomson,[3] Garbaty and La-Bahn,[4] and McEachran and Stauffer[5] to name a few. Ever since the inception of the polarized-orbital method,[6] whose main new element is the presence of exchange-polarization terms (not included in Refs. 3, 4, and 5), it has been found that such terms can have a quantitative important effect. This has been again shown to be so in a previous[7] as well as in the recent calculation[8] on the photoionization of alkali-metal atoms. The cross sections throughout the energy range considered are in good agreement with the results of many-body perturbation and close-coupling calculations, when both the continuum and bound-state functions obtained in the full polarized-orbital (PO) approximation are used in the calculation of the matrix elements. Therefore, we have carried out the present calculations in the PO approximation, in addition to the exchange and exchange-adiabatic approximations. The phase shifts calculated in the above-mentioned three approximations have been used to calculate the elastic differential, total, and momentum-transfer cross sections.

A number of experiments have been carried out on electron scattering by neon atoms. Total cross sections have been measured by Stein *et al.*[9] and Kauppila *et al.*[10] The elastic differential, total, and momentum-transfer cross sections have been measured by Register and Trajmar.[11]

II. THEORY AND CALCULATIONS

The calculations of the scattering functions have been carried out using the polarized-orbital method (POM).[6] The details for $N=10$ target have been given in our recent photoionization paper.[8] Briefly, the wave function of the electron-neon system is given by

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

where ψ_0 is the wave function of the N-electron target, and is given by the Hartree-Fock-Slater determinant. The determinant can be expressed in terms of the orbitals which have been determined by Clementi and Roetti[12] in the frozen-core approximation. The ground state of the target can be improved by adding pseudo orbitals $\overline{3s}$, $\overline{3p}$, and $\overline{3d}$ to $1s$, $2s$, and $2p$ orbitals, as has been done by Fon and Berrington.[1]

The perturbed part $\psi^{\rm pol}$ is determined in the adiabatic approximation, i.e., by assuming that the unperturbed ground state ψ_0 is adiabatically perturbed by the incident electron. In the PO approximation,[6] only the dipole part of the interaction potential between the incident and target electrons is included and it is assumed that the incident electron remains stationary while the target electrons are being perturbed. The adiabatic perturbation is thus given by

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

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

Here $Z=N$ (neutral atomic target). The presence of the step functions $\epsilon(r_1,r_j)$ in Eq. (2b) expresses the physically motivated additional approximation that the interaction is zero when the incident electron is inside the target electrons.[6] The radial parts of the perturbed orbitals are obtained from the Sternheimer approximation of first-order perturbation theory:[13]

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

where u_{nl}, the unperturbed orbital, is perturbed to $u_{nl\to l'}$, l and l' being angular momenta of the unperturbed and perturbed orbitals, respectively. For neonlike systems, the perturbed orbitals are $u_{1s\to p}$, $u_{2s\to p}$, $u_{2p\to s}$, and $u_{2p\to d}$.

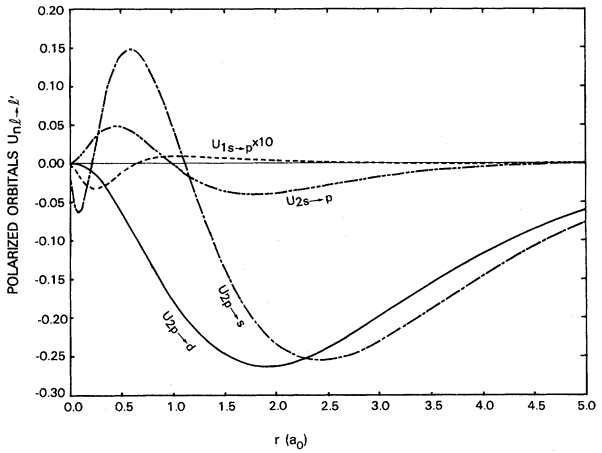

FIG. 1. Polarized orbitals $u_{1s\to p}$, $u_{2s\to p}$, $u_{2p\to s}$, and $u_{2p\to d}$ obtained using Sternheimer approximation (Ref. 13).

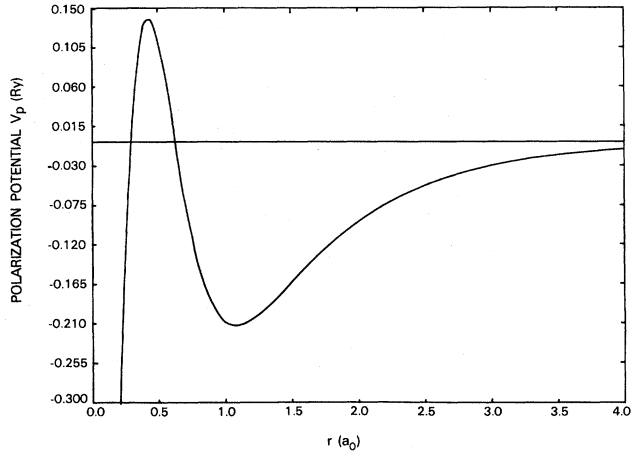

FIG. 2. Polarization potential V_p obtained by using the orbitals shown in Fig. 1.

The perturbed orbitals are orthogonalized to the unperturbed orbitals of the same angular symmetry. In the Sternheimer approximation this is equivalent to Schmid orthogonalization to the unperturbed orbitals. These orbitals are shown in Fig. 1 and it can be seen that the $u_{1s\to p}$ orbital is very small in magnitude compared to other orbitals. Therefore, its contribution is retained only in the direct polarization potential and not in the exchange-polarization terms. It should be pointed out that these perturbed orbitals are much smaller in magnitude than the unperturbed orbitals.

The individual contributions to the total polarizability from these orbitals are $\alpha_{1s\to p}=0.0008a_0^3$, $\alpha_{2s\to p}=0.0495a_0^3$, $\alpha_{2p\to s}=0.6025a_0^3$, and $\alpha_{2p\to d}=2.1504a_0^3$. The polarizability α is, therefore, $2.8032a_0^3$, which is in fairly good agreement with the experimental value $2.66a_0^3$

TABLE I. s- and p-wave phase shifts (rad, modπ) in three approximations. E-A denotes the exchange-adiabatic approximation.

	s wave			p wave		
k (a.u.)	Exchange	E-A	PO	Exchange	E-A	PO
0.1000	−0.1065	−0.0440	−0.0400	−0.0012	0.0038	0.0040
0.2000	−0.2134	−0.1200	−0.1158	−0.0092	0.0077	0.0086
0.3000	−0.3209	−0.2137	−0.2067	−0.0282	0.0024	0.0030
0.4000	−0.4291	−0.3171	−0.3079	−0.0597	−0.0163	−0.0141
0.5000	−0.5376	−0.4258	−0.4190	−0.1022	−0.0487	−0.0452
0.6000	−0.6459	−0.5369	−0.5296	−0.1533	−0.0924	−0.0846
0.6062	−0.6530	−0.5442	−0.5367	−0.1567	−0.0954	−0.0876
0.7000	−0.7535	−0.6484	−0.6395	−0.2102	−0.1442	−0.1356
0.8000	−0.8596	−0.7589	−0.7506	−0.2702	−0.2011	−0.1919
0.8573	−0.9199	−0.8218	−0.8130	−0.3051	−0.2350	−0.2255
0.9000	−0.9636	−0.8674	−0.8586	−0.3313	−0.2605	−0.2511
1.0000	−1.0652	−0.9733	−0.9645	−0.3920	−0.3206	−0.3108
1.1000	−1.1639	−1.0761	−1.0670	−0.4513	−0.3799	−0.3700
1.2000	−1.2594	−1.1754	−1.1670	−0.5085	−0.4377	−0.4271
1.2124	−1.2716	−1.1880	−1.1787	−0.5154	−0.4447	−0.4341
1.3000	−1.3518	−1.2712	−1.2620	−0.5632	−0.4932	−0.4821
1.4000	−1.4408	−1.3634	−1.3548	−0.6150	−0.5464	−0.5363
1.5000	−1.5264	−1.4520	−1.4434	−0.6641	−0.5968	−0.5866
1.6000	−1.6087	−1.5370	−1.5280	−0.7103	−0.6444	−0.6344
1.7000	−1.6877	−1.6186	−1.6100	−0.7539	−0.6895	−0.6799
1.8000	−1.7635	−1.6968	−1.6890	−0.7949	−0.7321	−0.7225
1.9000	−1.8363	−1.7718	−1.7640	−0.8335	−0.7722	−0.7629
1.9170	−1.8489	−1.7848	−1.7764	−0.8399	−0.7788	−0.7696
2.0000	−1.9063	−1.8438	−1.8360	−0.8699	−0.8100	−0.8012
2.1433	−2.0021	−1.9424	−1.9346	−0.9185	−0.8606	−0.8524
2.1688	−2.0186	−1.9592	−1.9515	−0.9266	−0.8691	−0.8611
2.1941	−2.0347	−1.9758	−1.9683	−0.9348	−0.8775	−0.8695
2.2682	−2.0810	−2.0233	−2.0160	−0.9577	−0.9015	−0.8939

(quoted in Ref. 14). The resultant polarization potential V_p, which behaves as $-\alpha/r^4$ for $r\to\infty$, is shown in Fig. 2. It is seen to have a repulsive part at short distances. This behavior has also been seen for electron-Li and electron-Na^+ polarization potentials;[15,8] in the former case, it should be emphasized, the polarized orbital was modified because of the large polarizability of the alkali-metals, so as effectively to include the nonadiabatic effects.

The scattering equation is obtained by projecting with ψ_0 on the left of $(H_{N+1}-E)\Psi^A=0$, a basic aspect of POM:[16]

$$\int Y_{l0}(\Omega_1)\chi_{1/2}(\sigma)\psi_0^*(2,3,4,\ldots,N+1) \times(H_{N+1}-E)\Psi^A dr_1^{-1}=0 . \quad (4)$$

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

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

The expression for direct and exchange potential contained in $V_c u(r)$, the polarization potential $V_p u(r)$, and the exchange polarization terms $Wu(r)$ are given in Ref. 8. The exchange and exchange-adiabatic approximations are obtained by neglecting $V_p u(r)$ and $Wu(r)$ terms, and $Wu(r)$ terms, respectively. In the PO approximation, all terms are retained in Eq. (5). The phase shifts are obtained from the asymptotic form of the solutions of Eq. (5) and k^2 is the scattering energy in Ry:

$$\lim_{r\to\infty} u_{kl}(r)=\sin\left[kr-\frac{l\pi}{2}+\delta_l\right] . \quad (6)$$

III. RESULTS

The phase shifts (mod π) for $l=0$ and 1 partial waves at various incident energies are given in Table I in all

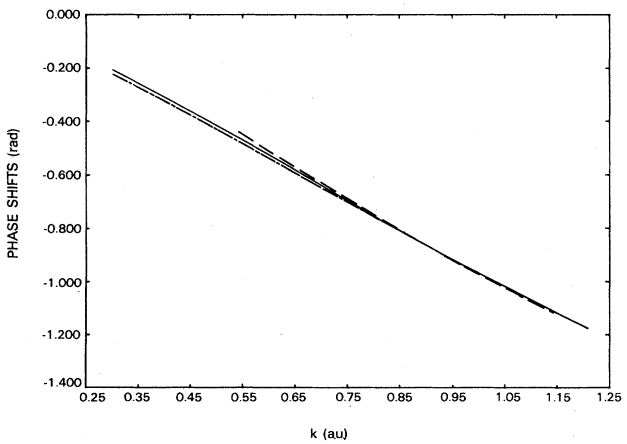

FIG. 3. s-wave phase shifts (modπ): ——, PO; —·—·—·, McEachran and Stauffer (Ref. 5); — — —, Fon and Berrington (Ref. 1).

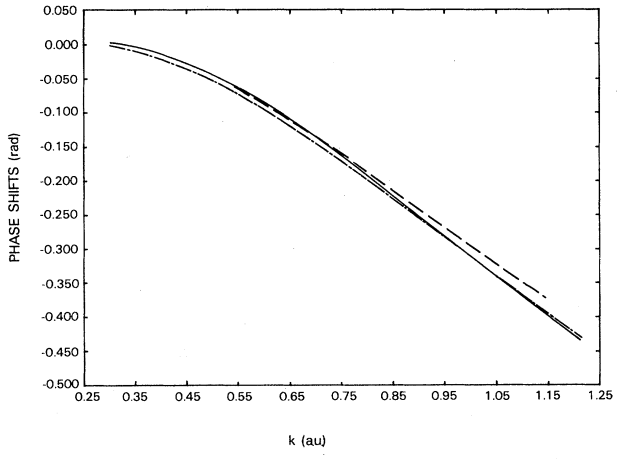

FIG. 4. p-wave phase shifts (modπ): notation as in Fig. 3.

three approximations. The phase shifts for s and p waves go to 2π and π, respectively, as $k^2\to 0$, because of the two filled $1s$ and $2s$ shells, and one $2p$ shell in the neon atoms. We see that the exchange-polarization terms $Wu(r)$ do make a significant contribution, especially at low energies. The relative change is greater for the p wave than the s wave. The phase shifts for s and p waves obtained by McEachran and Stauffer[5] in the exchange-adiabatic approximation are lower (less attractive) than our exchange-

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

	l				
k	2	3	4	5	6
0.1000	0.0008	0.0003	0.0001	0.0001	0.0001
0.2000	0.0030	0.0012	0.0005	0.0003	0.0002
0.3000	0.0080	0.0025	0.0011	0.0006	0.0004
0.4000	0.0140	0.0045	0.0020	0.0011	0.0007
0.5000	0.0230	0.0071	0.0032	0.0017	0.0010
0.6000	0.0340	0.0102	0.0046	0.0024	0.0015
0.6062	0.0354	0.0104	0.0047	0.0025	0.0015
0.7000	0.0490	0.0140	0.0063	0.0034	0.0020
0.8000	0.0670	0.0185	0.0082	0.0044	0.0026
0.8573	0.0797	0.0214	0.0094	0.0051	0.0030
0.9000	0.0890	0.0238	0.0104	0.0056	0.0034
1.0000	0.1140	0.0297	0.0129	0.0069	0.0041
1.1000	0.1420	0.0363	0.0157	0.0083	0.0051
1.2000	0.1730	0.0438	0.0186	0.0099	0.0060
1.2124	0.1773	0.0447	0.0190	0.0101	0.0061
1.3000	0.2060	0.0520	0.0219	0.0116	0.0071
1.4000	0.2410	0.0609	0.0254	0.0134	0.0080
1.5000	0.2770	0.0705	0.0293	0.0155	0.0093
1.6000	0.3130	0.0808	0.0334	0.0176	0.0105
1.7000	0.3498	0.0916	0.0377	0.0198	0.0119
1.8000	0.3850	0.1029	0.0424	0.0222	0.0134
1.9000	0.4200	0.1147	0.0473	0.0247	0.0149
1.9170	0.4260	0.1167	0.0482	0.0252	0.0151
2.0000	0.4530	0.1267	0.0523	0.0273	0.0163
2.1433	0.4986	0.1445	0.0599	0.0312	0.0186
2.1688	0.5063	0.1477	0.0614	0.0320	0.0190
2.1941	0.5137	0.1509	0.0627	0.0327	0.0195
2.2682	0.5350	0.1603	0.0669	0.0348	0.0208

TABLE III. Differential cross sections at various energies.

θ (deg)	k^2 (eV) 5	10	20	50
0.0	0.5034	0.7851	1.9246	6.8582
5.0	0.6426	0.9059	1.7440	5.5000
10.0	0.7561	1.0226	1.6681	4.6057
15.0	0.8690	1.1505	1.6374	3.8401
20.0	0.9771	1.2814	1.6418	3.1967
25.0	1.0765	1.4080	1.6713	2.6677
30.0	1.1639	1.5236	1.7156	2.2424
35.0	1.2365	1.6222	1.7641	1.9072
40.0	1.2924	1.6985	1.8066	1.6455
45.0	1.3301	1.7486	1.8335	1.4395
50.0	1.3488	1.7695	1.8367	1.2717
55.0	1.3484	1.7599	1.8101	1.1263
60.0	1.3296	1.7198	1.7499	0.9910
65.0	1.2933	1.6505	1.6552	0.8573
70.0	1.2415	1.5549	1.5281	0.7209
75.0	1.1761	1.4370	1.3732	0.5816
80.0	1.0998	1.3021	1.1978	0.4426
85.0	1.0152	1.1559	1.0111	0.3101
90.0	0.9253	1.0048	0.8238	0.1919
95.0	0.8330	0.8552	0.6467	0.0970
100.0	0.7410	0.7133	0.4908	0.0345
105.0	0.6518	0.5845	0.3658	0.0125
110.0	0.5677	0.4736	0.2798	0.0375
115.0	0.4904	0.3839	0.2386	0.1136
120.0	0.4213	0.3177	0.2451	0.2420
125.0	0.3611	0.2756	0.2994	0.4206
130.0	0.3104	0.2571	0.3984	0.6443
135.0	0.2689	0.2601	0.5364	0.9049
140.0	0.2361	0.2814	0.7051	1.1916
145.0	0.2113	0.3169	0.8941	1.4917
150.0	0.1934	0.3619	1.0918	1.7912
155.0	0.1811	0.4113	1.2860	2.0758
160.0	0.1732	0.4600	1.4646	2.3315
165.0	0.1685	0.5034	1.6166	2.5453
170.0	0.1660	0.5375	1.7325	2.7065
175.0	0.1648	0.5593	1.8051	2.8067
180.0	0.1645	0.5668	1.8298	2.8406

adiabatic and PO approximation results. The polarizability obtained by them is $2.33a_0^3$, considerably lower than the value obtained in this calculation. They have also not included exchange-polarization terms, which, as stated, is the basic contribution of this paper. We believe that the inclusion of these exchange-polarization terms would change the phase shifts of Ref. 5 in a similar way. The phase shifts obtained by Fon and Berrington[1] in the close-coupling approximation are higher than the PO results. The PO phase shifts for s and p waves are compared to the results of McEachran and Stauffer,[5] and of Fon and Berrington[1] in Figs. 3 and 4. We present the phase shifts for $l=2$–6 in Table II in the PO approximation and at low energies they follow the phase-shift formula[17]

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

A comparison with the close-coupling[1] results made at common energies $k^2=0.64$, 0.81, 1.0, and 1.44 Ry indicates that the present phase shifts are higher for $l=2$ and lower for higher partial waves than those obtained in Ref. 1.

The differential cross sections at $k^2=5$, 10, 20, and 50 eV are given in Table III from 0° to 180°. The contribution of $l=7$–500 has been added by using the effective range formula (7) though the differential cross sections seem to converge by $l=50$. The convergence is very slow in the forward direction and we use[18]

$$\begin{aligned}\left[\frac{d\sigma}{d\Omega}\right]_{\theta=0^0} &= \left|\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l\right|^2 \\ &= \left[\frac{d\sigma}{d\Omega}\right]_{\theta=0^0}^{l<l_0} \\ &\quad + \left[\frac{\pi\alpha l_0}{4l_0^2-1}\right]\sum_{l=0}^{l_0-1}(2l+1)\sin2\delta_l \\ &\quad + \left[\frac{\pi\alpha l_0 k}{4l_0^2-1}\right]^2 ,\end{aligned} \tag{8}$$

where Eq. (7) has been used for $l\geq 7$ to derive this formula and here $l_0=7$. It should be pointed out that instead of Eq. (7) McEachran and Stauffer[5] include α^2 and quadrupole terms[19] in Eq. (7). In our opinion it is not consistent to include only the adiabatic portion of the r^{-6} potential,

TABLE IV. Total and momentum-transfer cross sections (a_0^2).

k	Total cross sections	Momentum-transfer cross sections
0.1000	2.0736	2.4518
0.2000	4.2816	4.8576
0.3000	5.9380	6.0720
0.4000	7.3528	6.7342
0.5000	8.7857	7.2111
0.6000	9.8934	7.5101
0.6062	9.9753	7.5448
0.7000	10.8966	7.8088
0.8000	11.7824	8.2397
0.8573	12.2022	8.5266
0.9000	12.4590	8.7186
1.0000	12.9306	9.2006
1.1000	13.2091	9.6327
1.2000	13.3222	9.9938
1.2124	13.3283	10.0350
1.3000	13.2882	10.2315
1.4000	13.1863	10.3805
1.5000	12.9751	10.3939
1.6000	12.6968	10.2844
1.7000	12.3884	10.0934
1.8000	12.0269	9.8023
1.9000	11.6557	9.4518
1.9170	11.5939	9.3887
2.0000	11.2610	9.0463
2.1433	10.6953	8.4226
2.1688	10.5939	8.3072
2.1941	10.4906	8.1916
2.2682	10.1970	7.8524

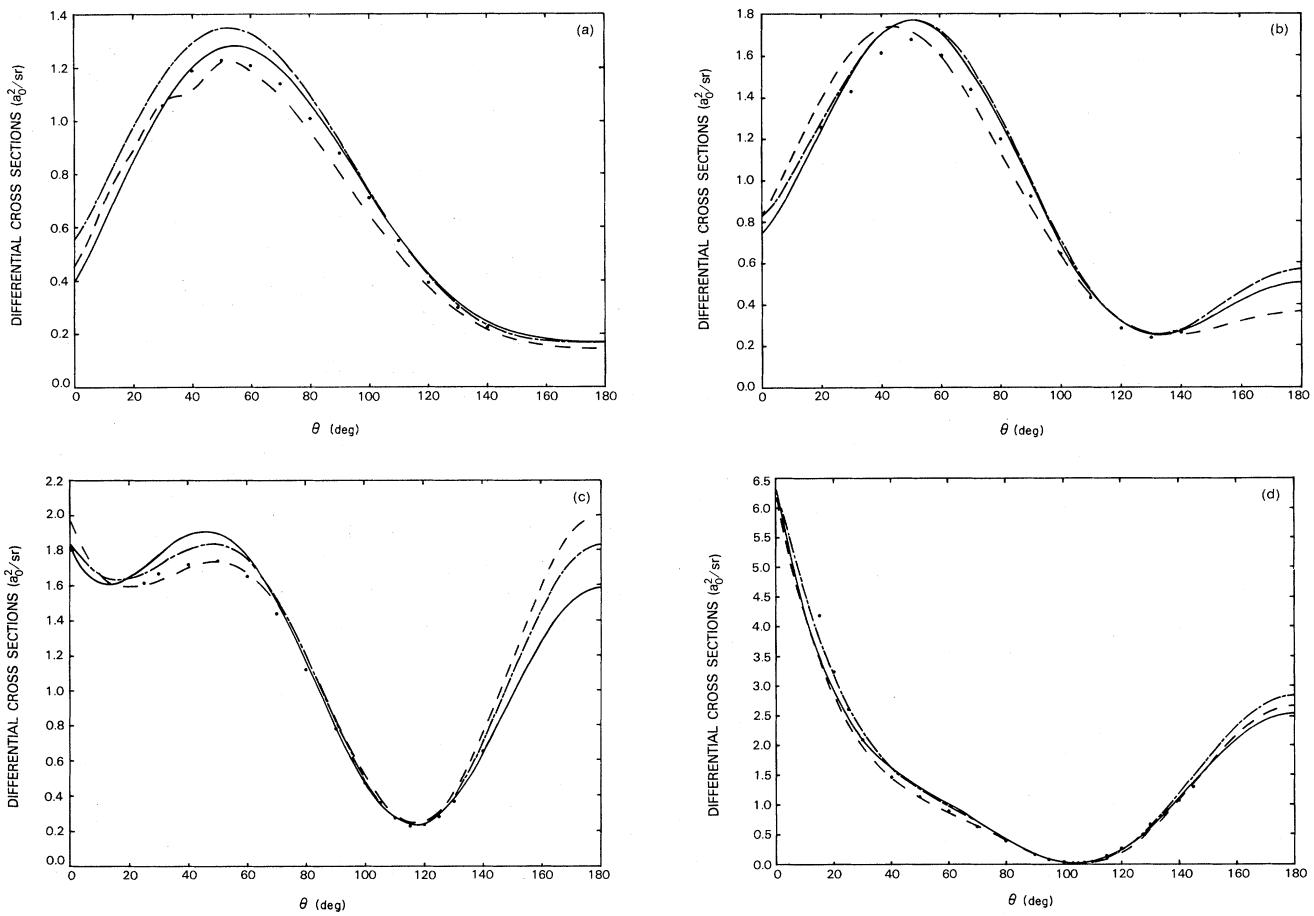

FIG. 5. Differential cross sections: (a) 5 eV; (b) 10 eV; (c) 20 eV; (d) 50 eV. ——, PO; —·—·—·, McEachran and Stauffer (Ref. 5); — — —, Fon and Berrington (Ref. 1); ●, Register and Trajmar (Ref. 11).

because that term has a nonadiabatic contribution[20] which in the case of e-H is actually larger than the adiabatic contribution and of the opposite sign. In the adiabatic description of POM only the dipole potential is retained. Therefore, for consistency, we have not included the higher-order corrections to Eq. (7).

A comparison of the differential cross sections at 5, 10, 20, and 50 eV with the theoretical values obtained by McEachran and Stauffer,[5] Fon and Berrington,[1] and the experimental results of Register and Trajmar[11] is given in Fig. 5. The theoretical results differ from each other but the present results are in good agreement with the experimental values which have an estimated error[11] of 7%. Our exchange-adiabatic cross sections (not shown in Fig. 5) are higher than the PO results. On the whole we believe our results agree better with experiment than the exchange-adiabatic[5] results. This indicates the importance of the exchange-polarization terms which have been ignored in all the previous calculations on noble gases. At 20 eV for $\theta=20°$–$60°$, the present results are higher than the experimental values.[11] A comparison with other experiments has been given in detail in Ref. 5 but for clarity has been omitted here.

We tried to find the critical point, i.e., the value of θ and k^2 at which the differential cross section is minimum. We find that at 64, 65.5, and 70 eV the differential cross section has a minimum at $\theta=101.3°$, 101.0°, and 100.2°, respectively. The measured[11] differential cross section has a minimum at $\theta=101.7\pm1.5°$ and $k^2=62.5\pm2.5$ eV. The calculated energy and angle indicating minimum in the

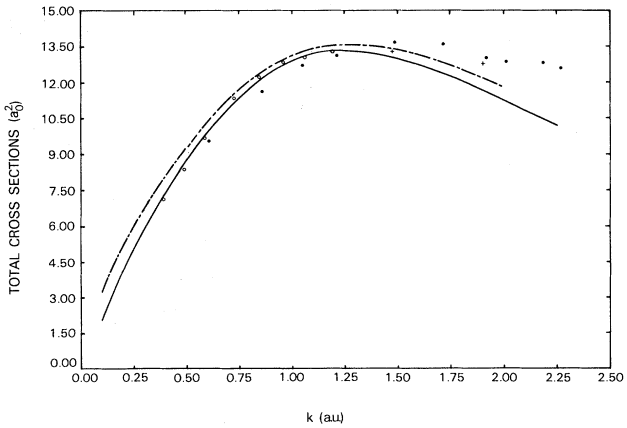

FIG. 6. Total cross sections: ——, PO; —·—·—·, McEachran and Stauffer (Ref. 5); ○, Stein *et al.* (Ref. 9); +, Kauppila *et al.* (Ref. 10); ●, Register and Trajmar (Ref. 11).

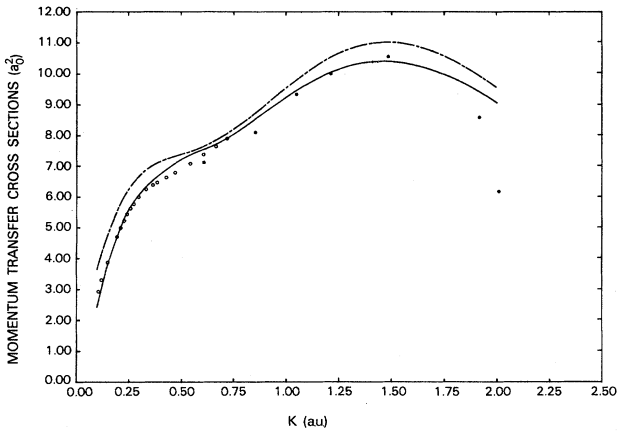

FIG. 7. Momentum-transfer cross sections: ——, PO; —·—·—·, McEachran and Stauffer (Ref. 5); ○, Robertson (Ref. 21); ●, Register and Trajmar (Ref. 11).

differential cross section is within the experimental range.

The total and momentum-transfer cross sections in PO approximation are given in Table IV. The total cross sections are compared to the theoretical results of McEachran and Stauffer[5] and experimental results of Stein *et al.*,[9] Kauppila *et al.*,[10] and Register and Trajmar[11] in Fig. 6. The errors quoted in the latter two experimental values are 5% and 3%, respectively. Stein *et al.*[9] have measured the total cross sections from 2.1—19.08 eV and our results agree with theirs very well. At 30 and 50 eV our results are lower than the results of Kauppila *et al.*[10] The averaged values given by Register and Trajmar[11] are lower than our results below 20 eV and higher above this energy. At 20 eV their result is close to that of Kauppila *et al.*[10]

The momentum-transfer cross sections have been compared with the theoretical results of McEachran and Stauffer[5] and the experimental results of Robertson,[21] and Register and Trajmar[11] in Fig. 7. The cross section at low energies obtained by drift velocity measurements[21] have an accuracy of 3% and they agree very well with the present results given in Fig. 7. Register and Trajmar[11] obtained cross sections between 5 and 50 eV and they agree with our results except at 50 eV, where their result is very much below our value.

IV. CONCLUSIONS

The purpose of this investigation was to gauge the importance of the exchange-polarization terms which heretofore have been omitted. These have been shown to change the phase shifts and hence the cross sections measurably. We look forward to a comparison of the present results with the forthcoming experiments.[22]

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