The elastic scattering of electrons from inert gases II. Neon

W C Fon† and K A Berrington

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland

Received 16 June 1980

Abstract. The *R*-matrix calculations of Fon *et al* on electron-helium elastic scattering are extended to consider the elastic scattering of electrons from neon in which the Ne ground-state wavefunction is coupled with a ¹P pseudo-state to include the full static dipole polarisability. Phaseshifts, differential, integral and momentum transfer cross sections for electrons elastically scattered from neon are reported for the impact energy range of 4 to 200 eV. A search has also been carried out for the 'critical energy' and 'critical angle' where maximum spin polarisation of the incident electrons may be expected after scattering from neon in the elastic scattering channel. Satisfactory agreement between the present calculation and experimental measurements is achieved.

1. Introduction

This paper is the second of a series which studies phaseshifts, integral, differential and momentum transfer cross sections of electrons elastically scattered from inert-gas atoms by using the R-matrix method described in paper I (Fon et al 1981).

The scattering of slow electrons by noble gases has attracted considerable theoretical and experimental interest in recent years. This is partly due to recent developments in inert-gas lasers and partly to new developments in the experimental and theoretical investigation of the spin polarisation of electrons following elastic scattering from atoms. It was pointed out by Mott (1929, 1932) that unless the velocity v of the incident electrons is comparable with the velocity of light c, the polarisation effects would be extremely small. Hence work on spin polarisation was centred mainly on high-energy scattering where relativistic effects complicate the scattering calculation, and the targets selected for the scattering were usually heavy atoms where L.S coupling effects become significant. Recent studies show that significant spin polarisation can be observed at much lower electron impact energies (E < 100 eV) and with much lighter atomic targets (e.g. neon) where both the relativistic and $L \cdot S$ coupling effects are not yet dominant. As discussed by Bühring (1968) and Kollath and Lucas (1979) total spin polarisation occurs at electron energies and electron scattering angles close to the electron energy where a cross section minimum attains its smallest value (the critical energy and critical angle). In addition, because of their relatively simple atomic structure, inert gases have been the subject of extensive investigation. The breaking of the excited 'n-level' states degeneracy in these atoms reduces the theoretical structure due to very long range forces, while the relatively large energy separation between the

[†] Commonwealth Fellow on sabbatical leave from the Department of Mathematics, University of Malaya, Kuala Lumpur, Malaysia.

elastic and inelastic channels significantly reduces the effects due to the coupling with inelastic channels. The dominant feature of the interactions emerges in the form of a long-range polarisation potential and a short-range exchange potential.

Although accurate low-energy elastic calculations for hydrogen and helium already exist (Schwartz 1961, Armstead 1968, O'Malley et al 1979, Nesbet 1979), a calculation of comparable accuracy for the elastic scattering of electrons from neon is yet to be performed. In general, the exchange interaction between electrons is treated by explicit antisymmetrisation of the total wavefunction; however, the treatment of polarisation effects has been more subtle. One approach has been based on the polarised-orbital approximation (Temkin 1957, 1959). Elastic calculations for neon have been carried out by Thompson (1971), Garbaty and LaBahn (1971) and Yau et al (1978) with considerable success. 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. In the low-energy elastic scattering region this may indeed by a realistic approximation. However, it is not clear how this line of argument can be carried over to the intermediate impact energy region well beyond the first excitation threshold. In addition there is no allowance for the loss of flux through the open channels when the incident energy exceeds the first excitation threshold. The problem involving loss of flux may be particularly serious in the intermediate energy range (see paper I).

McCarthy et al (1977) carried out elastic calculations for inert gases (including neon) by using an optical model potential in which two parameters are involved; the strength W of the imaginary potential (to allow for loss of flux through open channels) which is determined by fitting the experimental total non-elastic cross section, and the measured static polarisability. Although considerable success has been achieved in getting agreement with experimental measurements by this method, it is not clear that these two physical quantities are well known without uncertainty and one must not compare this calculation in the same light as those ab initio calculations like the close-coupling or R-matrix methods.

Blum and Burke (1975) have carried out a two-state R-matrix calculation for elastic scattering of electrons from neon similar to that described in paper I on helium. The Hartree-Fock neon ground state used and the pseudo-state were formed by Hartree-Fock orbitals 1s, 2s, 2p and pseudo-orbitals $\overline{3}$ s, $\overline{3}$ p and $\overline{3}$ d determined by Burke and Mitchell (1974) in which the exponent radial coefficients were fixed at $2\cdot0$ au for all the pseudo-orbitals. The phaseshifts obtained by Blum and Burke (1975) are systematically lower than those calculated by Thompson (1971) and the experimental phaseshifts (Naccache and McDowell 1974). There is also considerable uncertainty in the convergence of the R-matrix calculation to the Born effective range theory (ERT) for higher angular momentum at low energy and no systematic search for the pseudo-resonances in the intermediate energies. Since the calculation of Blum and Burke, the R-matrix program has undergone considerable improvement and a new version of the R matrix has been published (Berrington et al 1978). In view of the limitations of this earlier work, there is a need to look at this problem again.

2. R-matrix calculation

In this paper we extend the earlier calculations on helium (paper I) to consider the elastic scattering of electrons from neon for a similar impact energy range. We adopt

the R-matrix radius, a=10.0 au and the number of continuum orbitals included for each angular momentum is twenty. The calculations were carried out by coupling the Ne ground-state wavefunction with a ¹P pseudo-state to include the full ground-state static dipole polarisability. While the Hartree-Fock (HF) neon ground-state wavefunction is given in Clementi's table (1965), the ¹P pseudo-state is formed by the HF orbitals 1s, 2s, 2p and pseudo-orbitals $\overline{3s}$, $\overline{3p}$ and $\overline{3d}$ given by Hibbert et al (1977). The HF ground-state energy is -128.5405 au while the CI wavefunction for ¹P gives the pseudo-threshold at -127.7578 au. The ground-state static dipole polarisability obtained by coupling the ground state to the ¹P pseudo-state is 2.555 au.

In the present calculation, only partial waves up to L=13 are calculated directly by the R-matrix program; for $L \ge 14$, the T-matrix elements converge well (see table 1) to those obtained by the Born ERT formula of Rosenberg *et al* (1961);

$$T_L = 2(\tan \delta_L)^2 - 2i \tan \delta_L \tag{1}$$

where

$$\tan \delta_L = \frac{\pi \alpha k^2}{(2L+3)(2L+1)(2L-1)}$$
 (2)

and α is the dipole polarisability. For energies of 100 eV or above, a few more partial waves $(L \ge 14)$ are extrapolated to give smooth convergence to the *T*-matrix elements obtained by equation (1). The highest partial wave included is L = 150 for $E \ge 20$ eV.

Pseudo-resonances due to the (N+1)-electron correlation terms appear over the energy range from 35 eV to 120 eV. The T-matrix elements for impact energies in this region of pseudo-resonances were extracted by an averaging technique described in a previous paper (Burke $et\ al\ 1981$).

k^2 (R	yd)	$\boldsymbol{\delta}_{0}$	δ_{i}	δ_2	δ_3	δ_4	δ_5
0.64	(a)	-0.745	-0.186	0.0975	0.0161	0.00737	0.00416
	(b)	-0.735	-0.173	0.0752	0.0175	0.00746	0.00388
	(c)	-0.748	-0.192	0.0746	0.0188		
	(d)	-	_		0.0163	0.00743	0.00400
0.81	(a)	-0.859	-0.240	0.1251	0.0204	0.00928	0.00514
	(b)	-0.842	-0.229	0.1013	0.0232	0.00943	0.00493
	(c)	-0.854	-0.244	0.1000	0.0249		_
	(d)				0.0207	0.00940	0.00506
1.00	(a)	-0.969	-0.295	0.153	0.0255	0.0113	0.00632
	(b)	-0.946	-0.285	0.132	0.0292	0.0122	0.00609
	(c)	-0.958	-0.296	0.129	0.0322		
	(d)	_			0.0255	0.0116	0.00625
1.44	(a)	-1.175	-0.401	0.212	0.0384	0.0164	0.00897
	(b)	-1.147	-0.398	0.205	0.044	0.0178	0.00925
	(c)	-1.155	-0.397	0.198	0.0501		
	(d)			_	0.0368	0.0167	0.00900

Table 1. Comparison of phaseshifts with theories.

⁽a) R-matrix calculation (present).

⁽b) Thompson (1971).

⁽c) Yau et al (1978).

⁽d) Born ERT phaseshifts.

Finally, it is clear that the present calculation will not show any resonance structure in the excited-state threshold region, apart from that due to the pseudo-state threshold. The results should therefore be treated with caution in the energy range 16 eV to 22 eV.

3. Results and discussion

We calculate phaseshifts, total, integral elastic, differential and momentum transfer cross sections for the following process:

$$e + Ne(^{1}S_{0}) \rightarrow e + Ne(^{1}S_{0})$$

at impact energies ranging from 5 to 200 eV. The present calculations are given in tables 1-5 and figures 1-6, where comparisons between the present calculation and other theoretical calculations and experimental measurements are also made.

3.1. Phaseshifts

In table 1, the present calculation of phaseshifts for $L=0,\,1,\,2,\,3,\,4$ and 5 are compared with the polarised-orbital calculations of Thompson (1971) and Yau et al (1978) at various impact energies. There is good agreement between these calculations. We have also included the phaseshifts calculated from the Born ERT (see equation (2)) for $L\geqslant 3$. The present calculations and those obtained by polarised-orbital methods converge to Born ERT phaseshifts for $L\geqslant 3$ at energies below 20 eV. Any doubt on the validity of the Born ERT approximation (Blum and Burke 1975) for higher angular momentum at low energies seems to be unfounded.

		δ_0	$oldsymbol{\delta}_1$		
Ξ(eV)	Williams (1979)	Present	Williams (1979)	Present	
4.0	-0.456	-0.437	-0.066	-0.062	
4.9	-0.523	-0.507	-0.087	-0.086	
5.0	_	-0.514		-0.089	
6.0	-0.594	-0.584	-0.119	-0.116	
6.66	-0.632	-0.626	-0.135	-0.134	
7.0		-0.647	_	-0.142	
8.0	-0.710	-0.706	-0.171	-0.168	
8.7	-0.745	-0.744	-0.187	-0.186	
9.0	_	-0.760		-0.193	
0.0	-0.800	-0.811	-0.220	-0.217	
1.0	-0.837	-0.858	-0.243	-0.240	
2.0	-0.877	-0.902	-0.265	-0.262	
3.0	-0.913	-0.944	-0.288	-0.283	
4.0	-0.951	-0.984	-0.309	-0.303	
.5.0	-0.992	-1.022	-0.328	-0.322	
6.0	-1.029	-1.058	-0.348	-0.341	
7.0	-1.064	-1.092	-0.367	-0.358	
8.0	-1.092	-1.125	-0.388	-0.375	

Table 2. Comparison of phaseshifts with Williams (1979).

Williams (1979) has performed a phaseshift analysis on his measurements of absolute differential cross sections. We compare, in table 2, the s and p phaseshifts from the present calculation with those derived by Williams (1979). Excellent agreement is observed for impact energies ranging from 4 to 18 eV. We have not included in our discussion the phaseshift analysis of Naccahe and McDowell (1974) which is based mainly on the experiments of McConkey and Preston (1973). These data are now thought to be unreliable (Blum and Burke 1975, Williams and Crowe 1975).

3.2. Integral elastic and momentum transfer cross sections

The present calculations on integral elastic and momentum transfer cross sections for impact energies ranging from 5 to 200 eV are summarised in table 3 and compared with other theoretical calculations and experimental measurements in table 4 and in figure 1.

The present calculation on integral elastic cross sections seems to agree very well with the measurements of Stein et al (1978) and Williams and Crowe (1975) for

Table 3. Integral elastic and momentum transfer	cross sections (present results).
---	---------------------------------	----

E(eV)	$Q_{\rm E}(10^{-16}~{\rm cm}^2)$	$Q_{\rm MT}(10^{-16}~{\rm cm}^2)$		
5	2.673	1.933		
10	3.500	2.218		
20	3.773	3.042		
30	3.557	3.106		
40	3.310	2.817		
50	3.085	2.586		
60	2.853	2.268		
70	2.695	2.078		
100	2.250	1.549		
130	1.924	1.205		
150	1.768	1.041		
170	1.613	0.908		
200	1.449	0.756		

 $Q_{\rm E}$ = Integral elastic cross sections.

Table 4. Integral elastic cross sections (in units of a_0^2) for electron-neon scattering.

E(eV)	R-matrix	Williams and Crowe (1975)	de Heer <i>et al</i> (1979)	Dubois and Rudd (1976)	Thompson (1971)	Walker (1971)	
	calculation (Present)					RSE	RSEP
20	13.48	13.40	12.30		13.16	14.63	13.15
30	12.70	12.34	11.32	_	13.28	13.34	13.16
40	11.82	11.68	10.71		12.91	12.18	12.98
50	11.02	11.79	10.82	11.0	12.30	11.19	12.35
60	10.19		10.42		11.62	10.36	11.65
70	9.625		9.987		10.95	9.629	
100	8.036	9.820	8.737	7.90	9.178	7.942	9.162
150	6.314	_	6.196			6.208	7.189
200	5.175	5.642	4.994	5.40		5.167	5.979

 $Q_{\rm MT}$ = Momentum transfer cross sections.

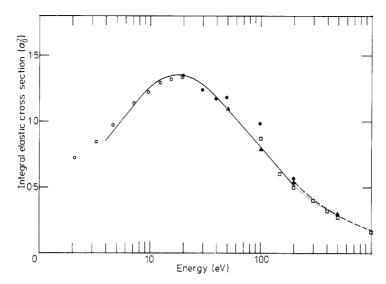


Figure 1. Integral elastic cross sections (in units of a_0^2). Experiment: \bigcirc , Stein *et al* (1978); \bigcirc , Williams and Crowe (1975); \triangle , Dubois and Rudd (1976); \square , Jansen *et al* (1976). Theory: ——, Present *R*-matrix calculation; ——, DWSBA, calculation of Dewangan and Walters (1977); \cdots , static exchange calculation of Dewangan and Walters (1977).

Table 5. Differential cross sections for elastic electron-neon scattering (units of $10^{-19} \, \mathrm{cm^2 \, sr^{-1}}$).

E(eV))							
θ°	5	10	20	30	40	50	60	70
0	1.290^{2}	2.275^{2}	5·518 ²	8·381 ²	1·339 ³	1·737 ³	2·073 ³	2·363 ³
5	1.556^{2}	2.598^{2}	5.012^{2}	7.360^{2}	1.132^{3}	1.455^{3}	1.729^{3}	1.959^{3}
10	1.941^{2}	3.009^{2}	4.658^{2}	6.544^{2}	9.474^{2}	1.192^{3}	1.400^{3}	1.565^{3}
20	2.494^{2}	3.832^{2}	4.453^{2}	5.576^{2}	6.846^{2}	8.000^{2}	8.908^{2}	9.471^{2}
30	2.995^{2}	4.482^{2}	4.550^{2}	5.036^{2}	5.284^{2}	5.561^{2}	5.689^{2}	5.650^{2}
40	3.120^{2}	4.829^{2}	4.759^{2}	4.626^{2}	4.354^{2}	4.099^{2}	3.780^{2}	3.483^{2}
50	3.420^{2}	4.829^{2}	4.875^{2}	4.192^{2}	3.717^{2}	3.176^{2}	2.652^{2}	2.269^{2}
60	3.327^{2}	4.507^{2}	4.680^{2}	3.652^{2}	3.108^{2}	2.470^{2}	1.912^{2}	1.529^{2}
70	3.067^{2}	3.937^{2}	$4 \cdot 177^{2}$	3.018^{2}	2.417^{2}	1.819^{2}	1.329^{2}	9.970^{1}
80	2.690^{2}	3.223^{2}	3.355^{2}	2.277^{2}	1.636^{2}	1.160^{2}	7.919^{1}	5.565^{1}
90	2.252^{2}	2.479^{2}	2.367^{2}	1.506^{2}	8.807^{1}	5.569^{1}	3.245^{1}	1.997^{1}
100	1.809^{2}	1.804^{2}	1.453^{2}	8.266^{1}	3.418^{1}	1.454^{1}	3·750°	1.244°
105	1.598^{2}	1.517^{2}	1.095^{2}	5.753^{1}	$2 \cdot 152^{1}$	6.528^{0}	5.436^{-1}	1.648^{0}
110	1.402^{2}	1.271^{2}	8.413^{1}	4.238^{1}	$2 \cdot 136^{1}$	9.866^{0}	7·118°	1.035^{1}
115	1.222^{2}	1.070^{2}	$7 \cdot 147^{1}$	4.012^{1}	3.521^{1}	2.614^{1}	2.472^{1}	2.849^{1}
120	1.062^{2}	9.156^{1}	7.256^{1}	5.316^{1}	6.376^{1}	5.617^{1}	5.400^{1}	5.671 ¹
125	9.213^{1}	8.067^{1}	8.781^{1}	8.348^{1}	1.070^{2}	1.001^{2}	9.504^{1}	9.503^{1}
130	8.013^{1}	7.401^{1}	1.170^{2}	1.324^{2}	1.639^{2}	1.570^{2}	1.473^{2}	1.429^{2}
140	6.199^{1}	$7 \cdot 139^{1}$	$2 \cdot 101^{2}$	2.826^{2}	3.099^{2}	3.009^{2}	2.778^{2}	2.619^{2}
150	5·061 ¹	7.850^{1}	3.291^{2}	4.799^{2}	4.754^{2}	4.615^{2}	4.240^{2}	3.949^{2}
160	4.429^{1}	8.935^{1}	4.475^{2}	6.834^{2}	6.289^{2}	6.088^{2}	5.600^{2}	5.139^{2}
170	4.133^{1}	9.843^{1}	5.323^{2}	8.350^{2}	7.364^{2}	$7 \cdot 111^{2}$	6.551^{2}	5.967^{2}
180	4.049^{1}	1.019^{2}	5.611^{2}	8.887^{2}	7.741^{2}	7.466^{2}	6.886^{2}	6.271^{2}
θ^*_{min}			~117°	~113°	~107°	~105°	~104°	~102°

Table 5. (continued)

E(eV)	7	······································				
θ°	100	130	150	170	200	
0	2·815³	2·986³	3·037³	3.050^{3}	3·077³	
5	2.263^{3}	2.325^{3}	2.317^{3}	2.276^{3}	2.223^{3}	
10	1.723^{3}	1.693^{3}	1.644^{3}	1.566^{3}	1.478^{3}	
20	9.323^{2}	8.480^{2}	8.030^{2}	7.472^{2}	6.942^{2}	
3 0	5.061^{2}	4.402^{2}	4.111^{2}	3.748^{2}	3.378^{2}	
40	2.841^{2}	2.349^{2}	$2 \cdot 134^{2}$	1.882^{2}	1.649^{2}	
50	1.655^{2}	1.298^{2}	1.142^{2}	1.002^{2}	8.638^{1}	
60	9.837^{1}	7.396^{1}	6.381^{1}	5.686 ¹	5.108^{1}	
70	5.739^{1}	4.302^{1}	3.854^{1}	3.650^{1}	3.516^{1}	
80	2.994^{1}	2·5111	2.588^{1}	2.693^{1}	2.837^{1}	
85	2.024^{1}	2.014^{1}	2.301^{1}	2.524^{1}	2.736^{1}	
90	1.372^{1}	1.803^{1}	2.239^{1}	2.533^{1}	2.756^{1}	
95	1.077^{1}	1.872^{1}	2.392^{1}	2.689^{1}	2.886^{1}	
100	$1 \cdot 184^{1}$	$2 \cdot 213^{1}$	2.750^{1}	2.990^{1}	$3 \cdot 121^{1}$	
105	1.757^{1}	2.842^{2}	3.320^{1}	3.462^{1}	3.466^{1}	
110	2.853^{1}	3.773^{1}	4.111^{1}	4.118^{1}	3.907^{1}	
115	4.482^{1}	4.985^{1}	5.098^{1}	4.902^{1}	4.433^{1}	
120	6.621^{1}	6.459^{1}	6.243^{1}	5·7621	5.023^{1}	
130	1.233^{2}	1.022^{2}	8.965^{1}	7.758^{1}	6.317^{1}	
140	1.957^{2}	1.480^{2}	1.210^{2}	9.924^{1}	7.617^{1}	
150	2.745^{2}	1.924^{2}	1.512^{2}	$1 \cdot 197^{2}$	8.889^{1}	
160	3.489^{2}	2.290^{2}	1.752^{2}	1.397^{2}	9.989^{1}	
170	4.008^{2}	2.521^{2}	1.882^{2}	1.520^{2}	1.062^{2}	
180	4.181^{2}	2.590^{2}	1.912^{2}	1.544^{2}	1.080^{2}	
$ heta_{\min}^*$	~96°	~91°	~89°	~87°	~87°	

The superscript denotes the power of ten by which the number should be multiplied.

 $E < 50 \,\mathrm{eV}$. For energies above 50 eV, the present calculation appears to give better agreement with the measurements of Dubois and Rudd (1976) and those measured by Jansen $et\,al$ (1976) (see figure 1). At higher energies, the present calculation converges smoothly to the calculation of Dewangan and Walters (1977) using the static exchange approximation. Comparison with other measurements and theoretical calculations is also given in table 4.

3.3. Differential cross sections

The present calculation on elastic differential cross sections is summarised in table 5. Comparison with other calculations and experimental measurements is made in figures 2-6.

In accordance with the present calculation, the general features of the differential cross section show

- (i) a sharp forward peak and
- (ii) the formation of a deep minimum at all energies of 20 eV or above.

This sharp forward peak derives its contribution from high partial waves. As the incident energy increases, the higher partial waves become more dominant and the forward peak becomes sharper. At low energies (e.g. 5 and 10 eV shown in table 5), where the s and p partial waves dominate, there is a complete absence of a forward

peak. As the impact energy increases a single cross section minimum emerges in the angular distribution above 20 eV, and moves 'monotonically' towards smaller scattering angles, becoming smaller and attaining its smallest value before rising again. The monotonically decreasing behaviour of the cross section minimum as a function of scattering angle enables us to establish the position of the critical energy at 64 eV and the critical angle at 103.6° . Total spin polarisation of the electron can be expected at this critical position (Lucas 1979, Yates 1968). As we have not included the L.S coupling effect, the spin change can only be the result of the exchange between the incident electron and the atomic electron. This exchange effect is not only treated by antisymmetrisation of the total wavefunctions but also by the inclusion of (N+1)-electron correlation terms in the expansion of the total wavefunction. The critical position predicted by the present theory compares very favourably to the observation by Kollath and Lucas (1979) at 73 eV with the critical angle at 103°. The discrepancy between the present calculation and the observation of Kollath and Lucas is probably due to the neglect of L.S coupling.

In figure 2, we compare our calculations at 20 eV with those of Thompson (1971) and the measurement of Williams and Crowe (1975). There is good agreement between the theories and the measurements except perhaps at 20 and 15°. The present calculation confirms the general shape of the angular distribution predicted by Thompson (1971). The latter suggests the formation of a second minimum at around 20° and a forward peak. This is in sharp contrast with the calculation of Blum and Burke (1975) which shows a pronounced maximum and the forward peak is completely absent.

In figure 3, we compare the present results at 30, 40 and 50 eV with the polarised-orbital calculations of Thompson (1971) and the experimental measurements of Williams and Crowe (1975). There is excellent agreement between the calculations and the measurements.

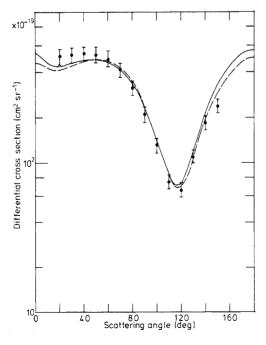


Figure 2. Differential cross section $(cm^2 sr^{-1})$ at 20 eV. Experiment: $\dot{\Phi}$, Williams and Crowe (1975). Theory: —, present R-matrix calculation; —, Thompson (1971) and private communication.

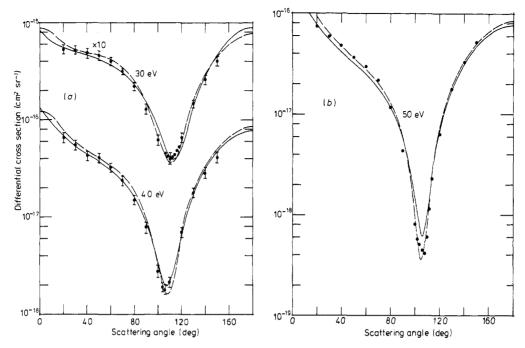


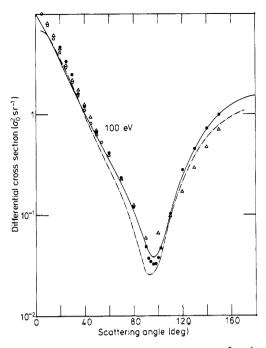
Figure 3. Differential cross section (cm² sr⁻¹) at (a) 30 and 40 eV and (b) 50 eV. The legend for the data is the same as figure 2.

Figures 4 and 5 show the present calculation of differential cross sections at 100 and 150 eV. The present calculation is in good accord with the measurements of Williams and Crowe (1975) and Jansen et al (1976), while the measurements of Gupta and Rees (1975) seem rather low at large scattering angles. Although the optical-model calculations of McCarthy et al (1977) are in good agreement with the present theory for scattering angles of 40° or less, their cross section appears to be rather low at large scattering angles and their minimum is at a smaller angle than the observations of Williams and Crowe indicate.

In figure 6, the present calculation is in excellent agreement with the measurements of Williams and Crowe (1975), Jansen et al (1976) and Bromberg (1974). While there is good agreement between the measurements of Gupta and Rees (1975) with the rest of the experiments at small angles, their measurements seem to underestimate the cross section at large angles. There is general agreement between the present calculation and those of Thompson (1971); however the latter exhibit oscillatory behaviour which may be the result of not including sufficiently high partial waves. The optical-model calculation of McCarthy et al (1977) again appears to underestimate the cross sections.

4. Conclusion

We have demonstrated that the *R*-matrix calculation described by paper I, in which the ground-state wavefunction is coupled only with the ¹P pseudo-state to include the full ground-state dipole polarisability, produces excellent agreement with experiments on phaseshifts, integral, momentum transfer and differential cross sections for the elastic



150 eV

150 eV

150 eV

150 eV

150 eV

150 eV

Figure 4. Differential cross section (units of a_0^2 sr⁻¹) at 100 eV. Experiment: \bullet , Williams and Crowe (1975); \bigcirc , Jansen *et al* (1976); \triangle , Gupta and Rees (1975). Theory: —, present *R*-matrix calculation; — · —, McCarthy *et al* (1977).

Figure 5. Differential cross section (cm² sr⁻¹) at 150 eV. The legend for the data is the same as figure 4 except that the broken curve represents the calculation of Thompson (1971).

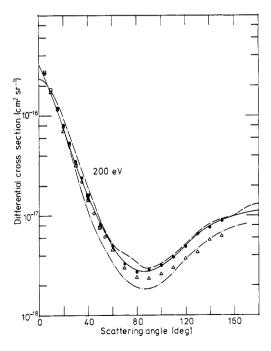


Figure 6. Differential cross section (cm² sr⁻¹) at 200 eV. The legend for the data is the same as in figures 4 and 5 except that □ represents the measurements of Bromberg (1974).

scattering of electrons from neon. A search has also been carried out for the position of critical energy and critical angle (Bühring 1968). The present theory predicts that the critical position occurs at 64 eV and at an electron scattering angle of 103.6° . Further work is in progress on argon and krypton.

Acknowledgments

It is a pleasure to express our gratitude to Professor P G Burke for suggesting this problem and his advice and encouragement throughout the course of this work and to Dr A Hibbert for his advice on running his CIV3 program. We wish to thank Dr D G Thompson for illuminating discussions and his generosity in providing us with his unpublished data and to Professor W E Kauppila for sending us tabulated values of their cross sections. One of us (WCF) would like to acknowledge his gratitude to the Association of Commonwealth Universitites for an award of an Academic Staff Fellowship. Most of the calculations were carried out using a link to the IBM 370/165 ar the Daresbury Laboratory provided by a grant from the Science Research Council.

References

---- 1959 Phys. Rev. 116 358-63

```
Armstead R L 1968 Phys. Rev. 171 91-3
Berrington K A, Burke P G, Le Dourneuf M, Robb W D, Taylor K T and Vo Ky Lan 1978 Comput. Phys.
    Commun. 14 367-412
Blum K and Burke P G 1975 J. Phys. B: Atom Molec. Phys. 8 L410-3
Bromberg J P 1974 J. Chem. Phys. 61 963-9
Bühring W 1968 Z. Phys. 208 286-98
Burke P G, Berrington K A and Sukumar C V 1981 J. Phys. B: Atom. Molec. Phys. 14 289-305
Burke P G and Mitchell J F B 1974 J. Phys. B: Atom. Molec. Phys. 7 665-73
Clementi E 1965 IBM J. Res. Dev. Suppl. 9 2
Dewangan D P and Walters H J 1977 J. Phys. B: Atom. Molec. Phys. 10 637-61
Dubois R D and Rudd M E 1976 J. Phys. B: Atom. Molec. Phys. 9 2657-67
Fon W C, Berrington K A and Hibbert A 1981 J. Phys. B: Atom. Molec. Phys. 14 307-21
Garbaty E A and LaBahn R W 1971 Phys. Rev. A 4 1425-31
Gupta S C and Rees J A 1975 J. Phys. B: Atom. Molec. Phys. 8 417-25
de Heer F J, Jansen R H J and van der Kaay W 1979 J. Phys. B: Atom. Molec. Phys. 12 979-1002
Hibbert A, Le Dourneuf M and Vo Ky Lan 1977 J. Phys. B: Atom. Molec. Phys. 10 1015-25
Jansen R H J, de Heer F J, Luyken H J, Van Wingerden B and Blaauw H J 1976 J. Phys. B: Atom. Molec.
    Phys. 9 185-212
Kollath K J and Lucas C J 1979 Z. Phys. A 292 215-8
Lucas C J 1979 J. Phys. B: Atom. Molec. Phys. 12 1549-58
McCarthy J E, Noble C J, Phillips B A and Turbull A D 1977 Phys. Rev. A 15 2173-85
McConkey J W and Preston J A 1973 Proc. 8th Int. Conf. on Physics of Electronic and Atomic Collisions
    (Belgrade: Institute of Physics) Abstracts p 273
Mott N F 1929 Proc. R. Soc. A 124 425
   - 1932 Proc. R. Soc. A 135 429
Naccahe P F and McDowell M R C 1974 J. Phys. B: Atom. Molec. Phys. 7 2203-22
Nesbet R K 1979 Phys. Rev. A 20 58-70
O'Malley TF, Burke PG and Berrington KA 1979 J. Phys. B: Atom. Molec. Phys. 12 953-65
Rosenberg L, O'Malley T F and Spruch L 1961 J. Math. Phys. 2 491-8
Schwartz C 1961 Phys. Rev. 124 1468-71
Stein T S, Kauppila W E, Pol V, Smart J H and Jesion G 1978 Phys. Rev. A 17 146-54
Temkin A 1957 Phys. Rev. 107 1004-12
```

334 W C Fon and K A Berrington

Thompson D G 1971 J. Phys. B: Atom. Molec. Phys. 4 468-82 Williams J F 1979 J. Phys. B: Atom. Molec. Phys. 12 265-82

Williams J F and Crowe A 1975 J. Phys. B: Atom. Molec. Phys. 8 2233-48

Yates A C 1968 Phys. Rev. 176 173-80

Yau A W, McEachran R P and Stauffer A D 1978 J. Phys. B: Atom. Molec. Phys. 11 2907-22