Electron scattering and charge cloud polarisation II. He and Ne

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Abstract. The treatment of elastic scattering from atoms which was developed in the preceding paper is applied to helium and neon for incident electron energies of 100–500 eV. Charge cloud polarisation effects, which can triple the differential cross section at small scattering angles, are well described and the agreement with experimental cross sections is generally close to or within experimental error. Calculated total cross sections are also in good agreement with experimental values.

1. Introduction

For incident energies of the order of tens of kilovolts, electron scattering is a powerful probe of gas-phase atomic and molecular properties. Extraction of information from the scattering cross section, however, requires an accurate description of the collision process. As one attempts to extract detailed properties of the target, stringent requirements are placed on the theoretical model. For most applications, a simple Born approximation approach is inadequate while a rigorous calculation is intractable. Polarisation and absorption are two of the effects that must be treated when one goes beyond the Born approximation. While the impetus for this study arose from experiments with 40 kV electrons, this paper treats the intermediate-energy region. The reasons for this choice are that the effects on the elastic scattering are greatly magnified at low energies and there are a wealth of absolute, experimental cross sections for this energy region. A high-energy approach will be used so that the accuracy of the method should increase with increasing energy. Comparisons of calculated and experimental cross sections will establish the range of validity of the approximations used and will provide some new insight into the nature of the polarisation phenomenon.

2. Theory

In the preceding paper (Kohl *et al* 1981), an expression for the elastic scattering amplitude was derived which included coupling between elastic and inelastic channels (approximately) but which neglected exchange, relativistic effects, etc. The differential equation to be solved was

$$(\nabla^2 + k^2 + \langle 0|U|0\rangle)(\exp(ik\hat{\boldsymbol{n}}_0 \cdot \boldsymbol{r}) + F_0(\boldsymbol{r})) = h(\boldsymbol{r}) = D(\boldsymbol{r})\exp(ik\hat{\boldsymbol{n}}_0 \cdot \boldsymbol{r}) \tag{1}$$

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where the energy of the incident electron is $\frac{1}{2}k^2$, $\hat{n}_0\,(\hat{n})$ represents the incident (outgoing) direction and the coulombic interaction, U, is defined in the appendix. The ket $|0\rangle$ denotes the ground state of the target atom which is assumed to be the initial state. The expression for $D(r)$

$$D(r) = (4\pi)^{-1}\int dt\, t^{-1}\exp(i\bar{k}t + ik\hat{n}_0\cdot t)(\langle 0|U(r)U(t+r)|0\rangle - \langle 0|U(r)|0\rangle\langle 0|U(t+r)|0\rangle)$$

(2)

was obtained by describing all inelastic collisions by the Born approximation and then using closure to sum over all atomic states. The quantity $\bar{k}$ is an effective momentum for the inelastically scattered electrons. The evaluation of $D(r)$ is described in the appendix and the result is

$$D(r) = d_0(r) + P_1(\hat{n}_0\cdot\hat{r})d_1(r) + \dots$$

(3)

where $P_n(x)$ is the nth-order Legendre polynomial. The homogeneous form of equation (1), i.e. $h(r) = 0$, can be solved by a partial-wave expansion with the result that

$$F_0^{(0)}(r) = \sum_l (2l+1)i^l L_l(r)P_l(\hat{n}_0\cdot\hat{n})$$

(4)

and $L_l(r)$ is obtained by numerical integration of the differential equation. The scattering amplitude, $f(\hat{n}_0, \hat{n})$, which corresponds to the solution of equation (1) is

$$f = f(0) - (4\pi)^{-1}\sum_l (2l+1)(-i)^l \int dr\, L_l(r)P_l(\hat{n}\cdot\hat{r})D(r)\exp(ik\hat{n}_0\cdot r)$$

(5a)

$$\equiv f^{(0)} + f^{(1)}$$

(5b)

where $f^{(0)}$ is the scattering amplitude corresponding to $F_0^{(0)}$, i.e. the amplitude derived from the static atomic potential, $\langle 0|U|0\rangle$. Substitution of the expression for $D(r)$ into equation (5) leads to

$$f^{(1)} = \sum_l (2l+1)P_l(\hat{n}_0\cdot\hat{n})\int_0^\infty dr\, r^2 L_l(r)[d_0(r)j_l(kr) - id_1(r)(l/kr\,j_l(kr) - j_{l+1}(kr)) + \dots].$$

(6)

Since L_l, d_0 and d_1 are all complex, $f^{(1)}$ is also complex and the cross section is given by

$$d\sigma/d\Omega = |f^{(0)} + f^{(1)}|^2.$$

(7)

3. Results

Although the approach developed here used the same basic ideas, i.e. the Born approximation and closure, that others have employed, there is one essential difference. Only the inhomogeneous term in equation (1), $h(r)$, is influenced directly by these approximations. The solution to equation (1) will approach the correct answer to the extent that $h(r)$ is estimated correctly apart from effects such as exchange which have been excluded. Considering the approximations made in calculating $h(r)$, is it important to solve equation (1) exactly? One approximate method of obtaining the cross section is to replace $L_l(r)$ in equation (5) by $j_l(kr)$, the lth-order spherical Bessel

function. In this case, the scattering amplitude, f, becomes

$$\tilde{f} = f^{(0)} + f_{2B}^{(1)} \tag{8}$$

where $f_{2B}^{(1)}$ is the second Born result. Another approach is to assume that $F_0(r)$ is small, in which case equation (1) becomes

$$(\nabla^2 + k^2 + U_{\text{eff}})(\exp(ikz) + \tilde{F}_0(r)) \simeq 0 \tag{9}$$

where $U_{\text{eff}} = \langle 0|U|0 \rangle + D(r)$. Now the scattering amplitude, $\tilde{f}$, can be obtained from a conventional partial-wave programme if U_{eff} is a spherical potential. The importance of solving the inhomogeneous equation exactly is demonstrated by the results presented in table 1, which compare cross sections calculated from $\tilde{f}$ and $\tilde{f}$ with the cross section calculated from $f = f^{(0)} + f^{(1)}$. Except for small scattering angles, neither $\tilde{f}$ nor $\tilde{f}$ is a good

Table 1. Dependence of the cross section on the method of solving equation (3)[a].

Scattering angle	Helium			Neon		
	$\lvert\tilde{f}\rvert/\lvert f\rvert^{2\text{b}}$	$\lvert\tilde{f}\rvert^2/\lvert f\rvert^{2\text{c}}$	$\lvert f_{BJ}\rvert^2/\lvert f\rvert^{2\text{d}}$	$\lvert\tilde{f}\rvert^2/\lvert f\rvert^{2\text{b}}$	$\lvert\tilde{f}\rvert^2/\lvert f\rvert^{2\text{c}}$	$\lvert f_{BJ}\rvert^2/\lvert f\rvert^{2\text{d}}$
5	1.03	0.96	0.98	1.11	0.88	0.91
10	1.04	0.94	0.93	1.14	0.85	0.86
20	1.06	0.94	0.90	1.19	0.82	0.79
40	1.08	0.92	0.90	1.19	0.78	0.73
60	1.09	0.91	0.91	1.11	0.76	0.71
80	1.09	0.91	0.91	1.10	0.76	0.69
100	1.09	0.91	0.91	1.12	0.75	0.67
120	1.09	0.91	0.92	1.13	0.74	0.65
140	1.09	0.92	0.92	1.14	0.73	0.63
160	1.08	0.91	0.92	1.15	0.73	0.62

[a] All results are for 400 eV electrons with an effective energy loss of 33 eV.
[b] $\tilde{f}$ differs from f in that the second Born approximation is employed to calculate $f^{(1)}$.
[c] See text for the definition of $\tilde{f}$ which is based on an effective potential.
[d] $\lvert f_{BJ}\rvert^2$ is taken from Byron and Joachain (1977c), tables IV and XI. For this comparison $\lvert f_{BJ}\rvert^2$ is the exchange-free cross section.

approximation to f even at 400 eV, and the discrepancy increases with decreasing incident energy. The fall in $\lvert\tilde{f}\rvert^2$ at large angles compared with $\lvert f\rvert^2$ can be traced to the imaginary part of $D(r)$ which corresponds to an absorption. Table 1 also includes a comparison of the present calculations with the results of Byron and Joachain (1977a). There is a marked similarity between $\lvert\tilde{f}\rvert$ and their results. Their cross sections were obtained by solving the scattering problem for an effective potential, and that effective potential is apparently very similar to $\langle 0|U|0 \rangle + D(r)$. Therefore, the essential difference between the present work and that of Byron and Joachain lies in the distinction between equations (1) and (9). Since the latter involves an additional approximation, the present results should be more accurate at large scattering angles. Comparisons with experiment will bear out that conclusion.

An approximate evaluation of $D(r)$ given in the preceding paper suggested that the spherical part of $D(r)$, i.e. $d_0(r)$, would have the form

$$d_0(r) \propto [\tfrac{1}{2}r^{-2}(k - \bar{k}) + ir^{-3}] \tag{10}$$

Table 2. The long-range dependence of $d_0(r)$. The target atom is helium, the incident energy is 1000 eV, the effective energy loss is 30 eV and the corresponding values of k and $\bar{k}$ are 8.58 au and 8.45 au, respectively. The values of r and $d_0(r)$ are given in atomic units.

r	Real part $100\,r^{2.2}d_0$	Imaginary part $100\,r^{3.3}d_0$
3	−0.41	−6.6
5	−0.41	−7.2
10	−0.41	−6.9
15	−0.37	−5.0
20	−0.30	−2.3
25	−0.22	+0.4
30	−0.14	+2.2
35	−0.07	+2.9
40	−0.03	+2.4

in the region where r is large but $(k - \bar{k})r < 1$. Table 2 gives the calculated values of $r^n d_0(r)$ for electrons of energy 1000 eV incident on helium with an effective energy loss of 30 eV. For this case, the real part of d_0 is roughly proportional to $r^{-2.2}$ for $r < 20$ au. The imaginary part of d_0 undergoes a sign change so that a simple representation of its long-range behaviour is not possible; it is, however, approximately proportional to $r^{-3.3}$ for $r < 15$ au. As predicted by equation (10) the imaginary part of d_0 is considerably larger than the real part. In other words, the 'potential' d_0 bears little resemblance to the adiabatic r^{-4} potential. For a real polarisation potential, the Born approximation estimate of $f^{(1)}$ would be real. The real (and the imaginary) parts of d_0 contribute to both the real and the imaginary parts of $f^{(1)}$; it is, however, the imaginary part of $f^{(1)}$ which is responsible for the large increase in the small-angle cross section, i.e. the charge cloud polarisation phenomenon.

The expression (6) for the scattering amplitude, f, depends on two functions, d_0 and d_1. Since the calculated cross sections turned out to be very insensitive to d_1 this term was eventually dropped and all results given correspond to the first term in equation (6) only.

An effective outgoing wavevector, $\bar{k}$, for the inelastic channels was employed in the derivation of the expression for the scattering amplitude. The prescription for choosing $\bar{k}$ was based on the following argument. The total, inelastic differential cross section, I_{inel}, in the Born approximation is

$$I_{\text{inel}} = \sum_{n \neq 0} (k_n/k)\,(1/4\pi)^2 \left| \int d\boldsymbol{r}\, \exp(\mathrm{i}\,\boldsymbol{s}_{0n} \cdot \boldsymbol{r}) \langle n|U|0\rangle \right|^2 \tag{11}$$

where $\boldsymbol{s}_{0n} = k\hat{\boldsymbol{n}}_0 - k_n\hat{\boldsymbol{n}}$. If an effective value $\bar{k}$ is adopted for k_n, then

$$I_{\text{inel}} = (\bar{k}/k)S(\bar{s})/\bar{s}^4 \tag{12}$$

where $\bar{s} = k\hat{\boldsymbol{n}}_0 - \bar{k}\hat{\boldsymbol{n}}$ and $S(s)$ is the inelastic scattering factor. With this approximation, the total inelastic cross section, σ_{inel}, is

$$\sigma_{\text{inel}} = (2\pi/k^2) \int_{k-\bar{k}}^{k+\bar{k}} ds\, S(s)/s^3. \tag{13}$$

If the same value of $\bar{k}$ is used to calculate the eleastic scattering amplitude, then

$$\sigma_{\text{elast}} = \int d\Omega |f|^2 \tag{14}$$

$$\sigma_{\text{tot}} = (4\pi/k)\, \text{Im}\, f(0°) \tag{15}$$

and σ_{elast} plus σ_{inel} should agree with σ_{tot} if the approximations are consistent. The total cross section was calculated for helium and for neon for incident energies of 100–500 eV for various values of the effective energy loss. A comparison of σ_{tot}, equation (14), with σ_{elast} plus σ_{inel} led to the choice of an effective energy loss of 30 eV for helium and 40 eV for neon. Byron and Joachain (1977a) adopted values of 33 and 41 eV, respectively, using a different criterion. Tables 3 and 4 show the results for the elastic and total cross sections with an estimate of the dependence of the answer on the choice of the energy loss used to calculate $\bar{k}$. Considering the variations in the experimental values, the calculated values are in general agreement with the experimental cross sections. The following comparisons of differential cross sections will provide a much more sensitive test of the calculations.

Table 3. Total elastic cross sections. The cross sections (in atomic units) were obtained by integrating the differential cross sections numerically. The uncertainties given in parentheses reflect only the sensitivity of the result to the choice of the effective energy loss.

Energy (eV)	He	Ne
100	2.2 (0.1)	10.1 (0.1)
200	0.93 (0.02)	5.6 (0.1)
300	0.580 (0.005)	4.12 (0.03)
400	0.420 (0.004)	3.35 (0.03)
500	0.328 (0.003)	2.90 (0.02)

Absolute measurements of the elastic differential cross sections for the rare gases have been reported by many groups (Bromberg 1964, Jansen *et al* 1976, Crooks 1972, Du Bois and Rudd 1976, Kurepa and Vuskovic 1975, Oda *et al* 1972, Williams and Crow 1975). The most extensive calculations were carried out by Byron and Joachain (1977a), who included exchange contributions. Also, Bonham and Konaka (1978) reported small-angle cross sections. There is general agreement between the various experimental and theoretical results, so a sensitive comparison is afforded by examining ratios of cross sections. Since the experimental uncertainties in the absolute scale are a few per cent, and since no matching of scales was done, variations of a few per cent from unity in the ratios are to be expected.

Table 5 compares the results for helium in the small-angle region while table 6 gives the results for a wide range of scattering angles. Except for the 100 eV case, the ratio of the experimental data to the present calculations is nearly constant and the deviations from unity lie close to, or within, the experimental uncertainties. One can readily see the size of the polarisation effects by noting the column labelled KA/static which corresponds to $|f^{(0)} + f^{(1)}|^2/|f^{(0)}|^2$. For example, at 5° and 100 eV, the presence of $f^{(1)}$ increases the cross section by a factor of four, which is hardly a small perturbation.

Table 4. Total cross sections (elastic plus inelastic) in atomic units.

		Helium						
	Theoretical[a]			Experimental				
Energy (eV)	Present work[b]	Byron and Joachain		Normand (1930)	Jansen (1975)	deHeer and Jansen (1975)	Blaauw *et al* (1980)	
		(1977b)	(1977c)					
100	4.2 (0.7)	4.63	6.16	3.43	5.3	4.05	3.90	
200	2.8 (0.3)	2.92	3.37	2.14	—	2.68	2.53	
300	2.0 (0.3)	2.15	2.38	1.37	2.3	2.03	1.93	
400	1.7 (0.2)	1.71	1.86	0.93	—	1.66	1.57	
500	1.4 (0.1)	1.43	1.54	—	1.5	1.39	1.32	

		Neon				
	Theoretical[a]		Experimental			
Energy (eV)	Present work[b]	Byron and Joachain (1977c)	Normand (1930)	Jansen (1975)	deHeer and Jansen (1975)	
100	13.0 (1.5)	14.2	9.4	10.2	11.3	
200	9.0 (1.0)	9.64	6.96	—	7.94	
300	7.0 (1.0)	7.53	5.38	6.1	6.4	
400	6.0 (0.5)	6.29	4.52	—	5.49	
500	5.5 (0.5)	5.45	—	3.6	4.77	

[a] Total cross sections were calculated from the optical theorem.
[b] The uncertainties given in parentheses reflect only the sensitivity of the result to the choice of the effective energy loss.

Table 5. Ratios of theoretical and experimental cross sections to the present calculations for electrons elastically scattered from helium. The second column lists the differential cross sections in units of a_0^2. Theoretical: KA, this work; BJ, Byron and Joachain (1977a); BK, Bonham and Konaka (1978). Experimental: B, Bromberg (1964).

θ (deg)	500 eV				300 eV			200 eV		
	KA	$\frac{B}{KA}$	$\frac{BJ}{KA}$	$\frac{BK}{KA}$	KA	$\frac{B}{KA}$	$\frac{BJ}{KA}$	KA	$\frac{B}{KA}$	$\frac{BJ}{KA}$
0.0	1.538	—	1.29	1.21	2.043	—	1.21	2.438	—	1.23
1.0	1.489	—		1.06	1.988	—		2.392	—	
2.0	1.357	1.04		1.00	1.840	1.01		2.266	1.02	
2.5	1.273	1.00			1.744	1.02		2.182	1.02	
3.0	1.184	1.04			1.640	1.03		2.089	1.04	
3.5	1.097	1.04			1.535	1.02		1.991	1.02	
4.0	1.014	1.06			1.433	1.03		1.893	1.02	
4.5	0.939	1.07			1.337	1.04		1.791	1.00	
5.0	0.874	1.08	1.07		1.250	1.05	1.12	1.703	1.02	1.16

Table 6. Ratios of theoretical and experimental cross sections to the present calculations for electrons elastically scattered from helium. The second column shows the differential cross sections calculated in this work in units of a_0^2. Theoretical: KA, this work; BJ, Byron and Joachain (1977a). Experimental: B, Bromberg; J, Jansen *et al* (1976). Static refers to the differential cross sections computed for $(0|U|0)$ alone, i.e. $|f^{(0)}|^2$.

θ (deg)	500 eV					300 eV					200 eV					100 eV			
	KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{B}{KA}$	KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{B}{KA}$	KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{B}{KA}$	KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$
5	0.8735	1.53	1.07	1.04	1.08	1.250	2.10	1.12	1.02	1.05	1.703	2.81	1.16	0.99	1.02	2.527	4.08	1.27	0.92
10	0.5496	1.22	1.02	1.00	1.04	0.7680	1.51	1.10	1.02	1.05	1.065	1.95	1.17	1.01	1.05	1.929	3.28	1.26	0.88
15	0.3456	1.11	1.03	1.03		0.5120	1.27	1.08	1.05		0.7194	1.55	1.16	1.03		1.415	2.62	1.26	0.88
20	0.2168	1.05	1.03	1.06	1.04	0.3529	1.17	1.06	1.03	1.04	0.5085	1.35	1.13	1.04	1.04	1.041	2.15	1.24	0.90
25	0.1376	1.03	1.02	1.06	1.04	0.2427	1.10	1.05	1.02		0.3679	1.24	1.10	1.05	1.03	0.7716	1.82	1.23	0.92
30	0.0880	1.01	1.01	1.06	1.04	0.1683	1.06	1.04	1.00	1.05	0.2672	1.16	1.09	1.05	1.03	0.5816	1.59	1.21	0.94
35	0.0575	0.99	1.01	1.06		0.1185	1.03	1.03	1.02		0.1968	1.10	1.07	1.04		0.4458	1.43	1.19	0.95
40	0.0390	0.98	1.01	1.06	1.05	0.0844	1.01	1.02	1.05	1.05	0.1463	1.06	1.06	1.03	1.04	0.3467	1.30	1.17	0.95
45	0.0274	0.98		1.04		0.0616	0.99		0.98		0.1106	1.03		1.03		0.2741	1.22		0.96
50	0.0196	0.96	0.99	1.04	1.03	0.0459	0.97	1.01	0.98	1.05	0.0848	1.00	1.04	1.04	1.05	0.2201	1.15	1.11	0.98
60	0.0110	0.96	0.98		1.03	0.0271	0.95	1.00			0.0526	0.96			1.06	0.1483	1.05	1.06	
80	0.004 45	0.95	0.97		1.01	0.0117	0.93	0.98			0.0245	0.92			1.07	0.0798	0.95	0.99	
100	0.002 30	0.94	0.97		1.00	0.006 40	0.92	0.97			0.0141	0.90			1.03	0.0519	0.91	0.96	
120	0.001 44	0.93	0.96			0.004 15	0.91	0.96			0.0096	0.89				0.0389	0.89	0.96	
140	0.001 05	0.93	0.96			0.003 10	0.91	0.95			0.0074	0.88				0.0324	0.88	0.98	
160	0.000 88	0.93	0.95			0.002 62	0.90	0.94			0.0063	0.88				0.0292	0.87	1.00	

Table 7. Ratios of theoretical and experimental cross sections to the present calculations for electrons elastically scattered from neon. The second column shows the differential cross sections calculated in this work in units of a_0^2. Theoretical: KA, this work; BJ, Byron and Joachain (1977a). Experimental: B, Bromberg, J, Jansen et al (1976); DR, Dubois and Rudd (1976); WC, Williams and Crowe (1975). Static refers to the differential cross sections computed for $\langle 0|U|0\rangle$ alone, i.e. $|f^{(0)}|^2$.

θ (deg)	500 eV KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{B}{KA}$	$\frac{DR}{KA}$	300 eV KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{B}{KA}$	200 eV KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{B}{KA}$	$\frac{DR}{KA}$	$\frac{WC}{KA}$	100 eV KA	$\frac{KA}{static}$	$\frac{BJ}{KA}$	$\frac{J}{KA}$	$\frac{WC}{KA}$
5	8.116	1.64	1.00	0.93	0.98	0.98	10.00	2.32	0.97	0.86	0.90	11.87	3.15	0.93	0.80	0.82	0.81		13.44	4.52	0.90	0.77	
10	4.886	1.28	0.95	0.94	0.96	0.87	5.993	1.66	0.96	0.92	0.91	7.394	2.22	0.96	0.84	0.87	0.86		10.40	3.72	0.89	0.75	
15	2.941	1.14	0.90	0.92	0.93	0.88	3.752	1.36	0.91	0.92	0.92	4.721	1.72	0.92	0.87		0.93	0.91	7.461	2.95	0.88	0.77	0.90
20	1.723	1.05	0.86	0.93	0.91	0.89	2.372	1.20	0.85	0.92	0.89	3.070	1.45	0.87	0.90	0.92	1.00	0.94	5.198	2.36	0.86	0.80	0.93
25	1.006	0.99	0.84	0.95	0.91	0.91	1.481	1.10	0.80	0.94	0.89	2.004	1.27	0.80	0.91		1.02	0.96	3.605	1.92	0.80	0.82	0.99
30	0.6048	0.96	0.82	0.96	0.93	0.94	0.9277	1.03	0.76	0.95	0.90	1.305	1.15	0.74	0.92	0.90	1.03	0.97	2.510	1.61	0.73	0.84	0.93
35	0.3834	0.93	0.81	0.96	0.93		0.5916	0.97	0.73	0.96	0.93	0.8548	1.06	0.69	0.92		1.04	1.00	1.768	1.39	0.63	0.85	0.89
40	0.2590	0.92	0.81	0.95	0.95	1.03	0.3903	0.93	0.71	0.98	0.94	0.5683	0.99	0.64	0.94	0.95	1.09	1.02	1.268	1.24	0.53	0.87	0.95
45	0.1867	0.91		0.96	0.97		0.2702	0.91		1.01	0.98	0.3873	0.94		0.96				0.9222	1.13		0.89	
50	0.1428	0.90	0.83	0.98	0.97	1.03	0.1978	0.90	0.72	1.03	0.99	0.2733	0.91	0.60	1.00	1.00	1.10	1.09	0.6794	1.06	0.37	0.93	0.99
60	0.0953	0.90	0.84		0.96	1.01	0.1248	0.89	0.75		1.02	0.1529	0.90	0.62			1.16	1.16	0.3710	0.99	0.33		1.10
80	0.0585	0.90	0.80		0.97	0.95	0.0814	0.89	0.73		0.99	0.0787	0.92	0.73			1.13	1.24	0.0713	1.06	0.97		1.66
100	0.0452	0.89	0.77		0.94	0.98	0.0792	0.88	0.67		0.97	0.0892	0.89	0.60			0.98	1.27	0.0345	1.06	0.84		1.09
120	0.0394	0.89	0.80			0.98	0.0923	0.87	0.66			0.1520	0.86	0.52			0.91	1.16	0.2648	0.95	0.18		1.05
140	0.0366	0.89	0.85			1.03	0.1099	0.86	0.68			0.2401	0.86	0.53			0.93	1.14	0.6753	0.95	0.29		1.07
160	0.0353	0.89	0.89				0.1243	0.86	0.70			0.3159	0.85	0.56					1.064	0.95	0.38		

Despite the enormous correction involved, the calculated cross section is within ten per cent of the experiment.

Table 7 presents the results for neon for a wide angle range with incident energies of 100–500 eV. The present results tend to be about ten per cent higher than the experimental values and the disagreement worsens at the smallest angles. However, the agreement is satisfactory for medium and large angles where the calculations of Byron and Joachain differ greatly from experiment. This large-angle discrepancy between the present results and those of Byron and Joachain was also noted in the results in table 1. Their results, in the absence of exchange corrections, could be reproduced by approximating f by $\tilde{f}$ (see equation (9) for the definition of $\tilde{f}$). When exchange corrections are added, the results of Byron and Joachain move closer to the experimental values; however the disagreement is still a factor of two or more for neon. This seems to establish the superiority of the present method and demonstrates the importance of solving the inhomogeneous differential equation, equation (1), without approximation.

4. Conclusions

The use of the term 'charge cloud polarisation' in the text and in the title follows common usage; the formalism used here, however, never makes any explicit use of the conceptual picture of an induced distortion of the target. When one includes the inelastic channels in the total wavefunction, the phenomenologically different concepts of polarisation and absorption appear in a natural fashion but not as separate effects. Were it not for the established terminology in the literature, the titles of these two papers would not have included the term 'charge cloud polarisation'. Although it may be useful for qualitative discussion to consider effective polarisation and absorption potentials, the present results show that a potential scattering approach can lead to serious discrepancies with experiment.

Until more accurate experimental cross sections are available for helium, it will be difficult to test additional improvements in the calculations. Since the major effect has been accounted for, use of a correlated wavefunction for calculating $D(r)$ and $\langle 0|U|0\rangle$, introduction of exchange, etc, should not alter the basic agreement. For neon, it would be worthwhile to find the source of the discrepancy of roughly ten per cent with experiment. Although the numerical results were not reported here, cross sections for neon were calculated for energies up to 3000 eV. A difference of five per cent between the calculations and the experimental cross sections of Jansen *et al* (1976) persisted up to these higher energies. Since exchange seems to be a likely candidate as the source of this disagreement, an extension of the present work is in progress.

Appendix.   Evaluation of $D(r)$

Consider the evaluation of

$$I(r, t) \equiv \langle 0| U(r) U(t+r)|0\rangle - \langle 0| U(r)|0\rangle\langle 0| U(t+r)|0\rangle \qquad (A.1)$$

where

$$U(r) = Z/r - \sum_{i=1}^{Z} |r - R_i|^{-1} \qquad (A.2)$$

and R_i is the position coordinate of the ith atomic electron. Since the contribution to I from Z/r and $Z/|t+r|$ vanishes

$$I(r, t) = \sum_i \sum_j \langle 0| |r - R_i|^{-1} |t+r - R_j|^{-1} |0\rangle - \sum_i \sum_j \langle 0| |r - R_i|^{-1}|0\rangle\langle 0| |t+r - R_j|^{-1}|0\rangle. \qquad (A.3)$$

The first term on the right-hand side of equation (A.3) involves one- and two-electron integrals which can be expressed in terms of Coulomb and exchange integrals. For a closed-shell atom with N doubly occupied spin orbitals, I can be reduced, in the Hartree–Fock approximation, to

$$I(r,t) = 2 \sum_{\mu} (\langle\mu| |r - R|^{-1}|r+t - R|^{-1}|\mu\rangle - \langle\mu| |r - R|^{-1}|\mu\rangle\langle\mu| |r+t - R|^{-1}|\mu\rangle)$$

$$-4 \sum_{\mu<\nu} \langle\mu| |r - R|^{-1}|\nu\rangle\langle\mu| |r+t - R|^{-1}|\nu\rangle \qquad (A.4)$$

where the summations range over the set of spatial orbitals, $|\mu\rangle$, $\mu = 1, N$.

The expression for $D(r)$, equation (2), is

$$D(r) = (-1/4\pi) \int dt\, t^{-1} \exp(i\bar{k}t + ik\hat{n}_0 \cdot t) I(r, t). \qquad (A.5)$$

Several methods for evaluating $D(r)$ were investigated but most were either slowly convergent or numerically unstable. The following approach proved to be suitable for numerical evaluation. Since each term in $I(r, t)$ contains the factor $|r + t - R|^{-1}$, reverse the order of integration and consider

$$J(q) \equiv (-1/4\pi) \int dt \exp(ikt + ik\hat{n}_0 \cdot t) t^{-1} |q + t|^{-1} \qquad (A.6)$$

where $q = r - R$. Expansion of $|q + t|^{-1}$ in a multipole series leads to

$$J(q) = \int_0^\infty dt\, t \exp(i\bar{k}t) j_0(kt)(t, q)_0 - iP_1(\hat{n}_0 \cdot \hat{q}) \int_0^\infty dt\, t \exp(i\bar{k}t) j_1(kt)(t, q)_1 + \ldots \quad (A.7)$$

where $(t, q)_n = \langle^n/\rangle^{n+1}$ and $<$ and $>$ denote the lesser and greater, respectively, of t and q and $j_n(x)$ is the spherical Bessel function. For large q

$$J(q) = \bar{q}^{-1}(1 - iP_1(\hat{n}_0 \cdot \hat{q}) 2k/\bar{q} + \ldots) \qquad (A.8)$$

where $\bar{q} = q(k^2 - \bar{k}^2)$. For $q \to 0$, the two integrals on the right-hand side of equation

(A.7) can be evaluated analytically. Values of $J(q)$ could be represented accurately by

$$J(\boldsymbol{q}) = \sum_{j=1}^{4} (\alpha_{R,j} \exp(-\beta_{R,j}q) + i\alpha_{I,j} \exp(-\beta_{I,j}q))$$

$$-iqP_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{q}}) \sum_{j=1} (\alpha'_{R,j} \exp(-\beta'_{R,j}q) + i\alpha'_{I,j} \exp(-\beta'_{I,j}q)) \tag{A.9}$$

where the set of constants α and β were obtained by least-squares fits to the real (R) and imaginary (I) components. With this judicious choice of a representation for $J(\boldsymbol{q})$, $D(\boldsymbol{r})$ depends on integrals over the atomic orbitals of the form $\langle \mu | q^m \exp(-\beta q) | \nu \rangle$ and $\langle \mu | q^m P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{q}}) \exp(-\beta q) | \nu \rangle$ where $m = 0$ or ± 1. For ns and np orbitals

$$O\langle u | \exp(-\beta q)/q | \nu \rangle = T_0(u, \nu, 0) \tag{A.10}$$

$$O\langle u | P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{q}}) \exp(-\beta q) | \nu \rangle = P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{r}})(rT_0(u, \nu, 0) - T_1(u, \nu, 1)) \tag{A.11}$$

$$O\langle n s | q^{-1} | n's \rangle \langle n s | \exp(-\beta q) | n's \rangle = B_0(ns, n's)(\partial/\partial\beta) T_0(ns, n's, 0) \tag{A.12}$$

$$O\langle n s | q^{-1} | n'p \rangle \langle n s | \exp(-\beta q) | n'p \rangle = \tfrac{1}{3} B_1(ns, n'p)(\partial/\partial\beta) T_1(ns, n'p, 0) \tag{A.13}$$

$$O\langle n p_z | q^{-1} | n'p_z \rangle \langle n p_z | \exp(-\beta q) | n'p_z \rangle$$

$$= B_0(np_z, n'p)(\partial/\partial\beta) T_0(np_z, n'p_z, 0)$$

$$+ \tfrac{4}{125} B_2(np_z, n'p_z)(\partial/\partial\beta) T_2(np_z, n'p_z, 0) \tag{A.14}$$

$$O\langle n p_z | q^{-1} | n'p_x \rangle \langle n p_z | \exp(-\beta q) | n'p_x \rangle = \tfrac{3}{25} B_2(np_z, n'p_x)(\partial/\partial\beta) T_2(np_z, n'p_x, 0) \tag{A.15}$$

$$O\langle n s | q^{-1} | n's \rangle \langle n s | q P(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{q}}) \exp(-\beta q) | n's \rangle$$

$$= P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{r}}) B_0(ns, n's)(-\partial/\partial\beta)(RT_0(ns, n's, 0) - T_1(ns, n's, 1)) \tag{A.16}$$

$$O\langle n s | q^{-1} | n'p \rangle \langle n s | q P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{q}}) \exp(-\beta q) | n'p \rangle$$

$$= \tfrac{1}{3} P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{r}}) B_1(ns, n'p)(-\partial/\partial\beta)(RT_1(ns, n'p, 0) - T_0(ns, n'p, 1)) \tag{A.17}$$

where

$$B_n(u, \nu) = \int_0^{\infty} dR \, R^2 F_u(R) F_\nu(R)(r, R)_n \tag{A.18}$$

$$T_n(u, \nu, m) = \int_0^{\infty} dR \, R^{2+m} F_u(R) F_\nu(R) \, D_m(r, R, \beta) \tag{A.19}$$

$$D_m(r, R, \beta) = \beta I_{m+1/2}(\beta <) K_{m+1/2}(\beta >) \tag{A.20}$$

where $I_{n+1/2}$ and $K_{n+1/2}$ are the modified Bessel functions and $F_u(R)$ is the normalised radial function for atomic orbital u. The operator, O, denotes an orientation average of the z axis of the coordinate system of the atom relative to the incident direction $\hat{\boldsymbol{n}}_0$. This averaging is only relevant for integrals involving p orbitals and it implies that a unique direction in the atom is not induced by the incoming electron. The quantities B_n and T_n were evaluated by numerical integration and the atomic radial functions were obtained from a numerical Hartree–Fock wavefunction. When the sum over all atomic orbitals is carried out, the final result becomes

$$D(r) = d_0(r) + P_1(\hat{\boldsymbol{n}}_0 \cdot \hat{\boldsymbol{r}}) d_1(r) + \ldots \tag{A.21}$$

where $d_0(r)$ and $d_1(r)$ are tabulated at discrete values of r.

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