J. Phys. B: At. Mol. Opt. Phys. 26 (1993) 1727–1741. Printed in the UK

Elastic electron scattering from the noble gases including dynamic distortion

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Received 3 November 1992, in final form 9 March 1993

Abstract. We present calculations for the elastic cross sections for electron scattering from neon, argon and krypton which include the effects of dynamic distortion. The improvement in the agreement between our theoretical calculations and the experimental measurements in the cases of argon and krypton indicates the importance of including the effects of dynamic distortion in scattering calculations. However, less successful results for neon emphasize the fact that accurate values for the coefficients of the long-range parts of the interaction potential are necessary in order to obtain theoretical results of high accuracy.

1. Introduction

Previous calculations of the elastic scattering of electrons from neon, argon and krypton using the polarized-orbital approximation (McEachran and Stauffer 1983, 1984, 1985) (referred to in this paper as adiabatic-exchange or AE results) have produced results which were generally in good agreement with the extensive experimental data available and with other theoretical treatments of these processes. However, as meticulous experimental measurements continue to be made for these systems, it has become apparent that there are discrepancies between the previous polarized-orbital calculations and experiment.

One possible explanation for this discrepancy, at least for the heavier atoms, is the fact that relativistic effects were not included in the original calculations. We have tested this hypothesis by carrying out these calculations in a relativistic framework. This led to a marked improvement in the agreement between theory and experiment for the position of the Ramsauer minimum in the case of xenon (McEachran and Stauffer 1987) but not for krypton (McEachran and Stauffer 1988). Another possible cause for these differences is the neglect of the effect of the kinetic energy of the incident electron. The usual polarized-orbital approximation (Temkin 1957, 1959, Temkin and Lamkin 1961) is an adiabatic one in that the kinetic energy operator is neglected in calculating the interaction of the incident particle with the atomic system. LaBahn and Callaway (1966) and Callaway *et al* (1968) proposed an extension of the polarized-orbital approximation which includes these so-called dynamic distortion effects. We have used this approach consistently in the case of electron scattering from helium (McEachran and Stauffer 1990, hereafter referred to as I) and have obtained results which are definitely in better agreement with experimental data than were our previous AE calculations.

In this paper we have extended our calculations to include the dynamic distortion (DD) effects in the elastic scattering of electrons from neon, argon and krypton. The formulae that

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0953-4075/93/111727+15$07.50

we have used were presented in I and further details of the calculations are given in Mimnagh (1991). The major difference from our calculations on helium is that the heavier noble gases have more than one electron shell so that the calculation of the dynamic distortion potential is consequently more complex. In the case of krypton we have used a frozen-core version for the polarized-orbital calculation (McEachran *et al* 1980) in which only the 3d, 4s and 4p orbitals were polarized. At each energy phaseshifts were calculated for angular momentum values up to the point at which they agreed with the effective range results of Fraser (1993) whose values were then used for the higher partial waves. Phaseshifts for angular momenta up to 100 were used to calculate the cross sections given in this paper.

The noble gases have been a popular system for study both experimentally and theoretically. The earlier work in this field at low to moderate electron impact energies has been reviewed in our previous publications mentioned above. Since that time further experimental work has been carried out for neon by Kumar *et al* (1987) and Nickel *et al* (1985) who measured total cross sections and Wagenaar *et al* (1986) who made differential cross section measurements for small scattering angles. In argon, differential cross sections have been measured by Furst *et al* (1989) and Weyhreter *et al* (1988) who also carried out a phaseshift analysis of their data. Buckman and Lohmann (1986), Ferch *et al* (1985) and Subramanian and Kumar (1987) have reported results for total cross sections and Nakamura and Kurachi (1988) have deduced momentum transfer cross sections from drift velocity and longitudinal diffusion measurements. Danjo (1988) has made measurements of the differential cross sections for krypton while Buckman and Lohmann (1987), Ferch (1992), Kanik *et al* (1992) and Subramanian and Kumar (1987) have all measured total cross sections for this atom. In addition, England and Elford (1988), Hunter *et al* (1988), Koizumi *et al* (1986) and Suzuki *et al* (1989) have reported values for the momentum transfer cross section for krypton. Very recently Brennan and Ness (1993) have performed a more detailed experimental investigation of this quantity.

On the theoretical side Basu *et al* (1987) have used a model-potential approach to calculate scattering from krypton while Bell *et al* (1984, 1988) have employed the *R*-matrix method for argon and krypton, respectively. Czuchaj *et al* (1987) have studied all the noble gases via a pseudopotential approach and the polarized-orbital method was used by Dasgupta and Bhatia (1984, 1985) for neon and argon, respectively. The Kohn–Sham theory was applied to electron scattering from all the noble gases by Haberland *et al* (1986). Calculations for argon were carried out by Nahar and Wadehra (1987) with a semi-empirical local potential and Saha (1989, 1991) has performed calculations for neon and argon, respectively, within a multiconfiguration Hartree–Fock approach. Sienkiewicz and Baylis (1987, 1992) have used the Dirac equations with a model polarization potential to produce cross sections for argon and krypton, respectively. Yousif and Matthew (1986) have applied a local density approximation to all the noble gases while Yuan (1988) and Yuan and Zhang (1989) have employed a correlation-polarization potential for scattering from neon, argon and krypton.

2. Results

As explained in I the νth multipole component of the interaction potential between the incident particle and the target atom contributes an attractive term to the polarization potential which behaves asymptotically as $x^{-(2\nu+2)}(\nu > 0)$ where x is the position of the incident particle. Its contribution to the distortion potential is a repulsive term which behaves as $x^{-(2\nu+4)}(\nu > 0)$. The $\nu = 0$ terms for both the polarization and distortion potentials go

to zero exponentially and thereby do not contribute to the asymptotic behaviour. It is the asymptotic behaviour of the polarization-distortion potential which is of prime importance since the static potential, which dominates at small distances, falls off exponentially at large distances. Thus in order to maintain consistency, if we include multipole contributions up to order ν for the distortion potential, we must include contributions up to order $\nu+1$ in the polarization potential. The potential which includes contributions to these orders (including the monopoles) is denoted by $V_{dp}^{\nu\nu+1}$. The coefficients of these various asymptotic terms are given in table 1. For the $\nu = 1$ term the coefficient is just the dipole polarizability α_1 of the atom while for the other terms it is written as $\alpha_\nu - 6\beta_{\nu-1}$. The values of α_ν are those given in McEachran *et al* (1979). Our values for β_1 are approximately 20% below those recommended by Dalgarno *et al* (1968).

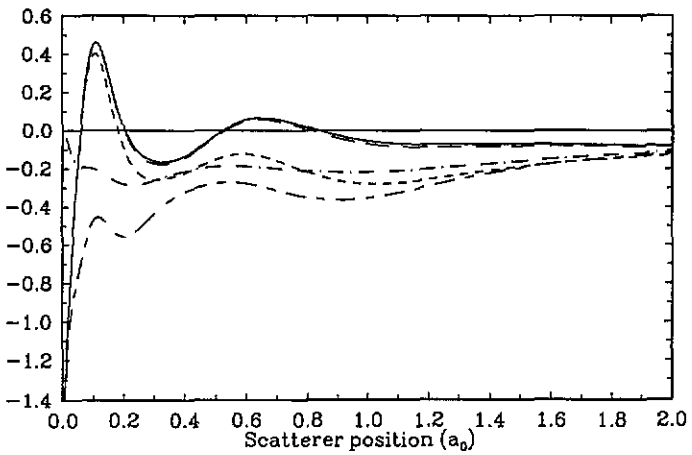

Figure 1. Various multipole contributions to the polarization distortion potential for argon: — · —, V_{dp}^{12}; – – –, V_{dp}^{23}; — — —, V_{dp}^{34}; ——, V_{dp}^{45}; — · —, dipole polarization (AE) potential.

In figure 1 we display the polarization-distortion potential we have obtained for argon indicating the convergence of the potential as a function of the multipole components retained in the calculation. Thus the combined contribution of the fifth multipole to the polarization potential and the fourth multipole to the distortion potential is negligible in comparison with the sum of the lower order contributions. The distortion potential is always repulsive and dominates over the polarization potential in two regions inside the atom. It also dominates the contribution from the higher multipole components as can be seen by the change of sign in the coefficients in table 1. Similar behaviour is noted for the other noble gases.

2.1. Argon

Turning now to the specific results of our calculations for argon, which were calculated using the converged V_{dp}^{45} potential, in figure 2 we compare our values for the phaseshifts with our previous AE results and the phaseshifts derived from the differential cross sections measured by Andrick and Bitsch (1983), Weyhreter *et al* (1988) and Williams (1979) as well as the calculated values of Bell *et al* (1984), Saha (1991) and Sienkiewicz and Baylis (1987) for the D-wave. Our S- and P-wave phaseshifts are in good agreement with those of Andrick and Bitsch (1983) whereas our previous AE calculations favoured the results of

Table 1. Multipole coefficients of the distortion potential†. Here $\gamma_\nu = \alpha_\nu - 6\beta_{\nu-1}$ is the coefficient of the asymptotic term $x^{-(2\nu+2)}$ in the DD potential.

	Neon			Argon			Krypton		
ν	α_ν	$\beta_{\nu-1}$	γ_ν	α_ν	$\beta_{\nu-1}$	γ_ν	α_ν	$\beta_{\nu-1}$	γ_ν
1	2.377		2.377	1.076(1)		1.076(1)	1.648(1)		1.648(1)
2	6.423	9.679(−1)	6.156(−1)	5.020(1)	6.797	9.422	9.561(1)	1.195(1)	2.390(1)
3	3.427(1)	7.055	−8.065	5.312(2)	8.072(1)	4.689(1)	1.261(3)	1.758(2)	2.058(2)
4	2.675(2)	6.736(1)	−1.366(2)	6.188(3)	1.746(3)	−4.289(3)	1.708(4)	4.825(3)	−1.188(4)
5	3.511(3)	7.808(2)	−1.174(3)	1.234(5)	2.762(4)	−4.228(4)	3.921(5)	8.810(4)	−1.365(5)
6							1.326(7)	2.697(6)	−2.919(6)
7							6.157(8)	1.229(8)	−1.216(8)

† The number in brackets represents the power of ten by which the entry is to be multiplied.

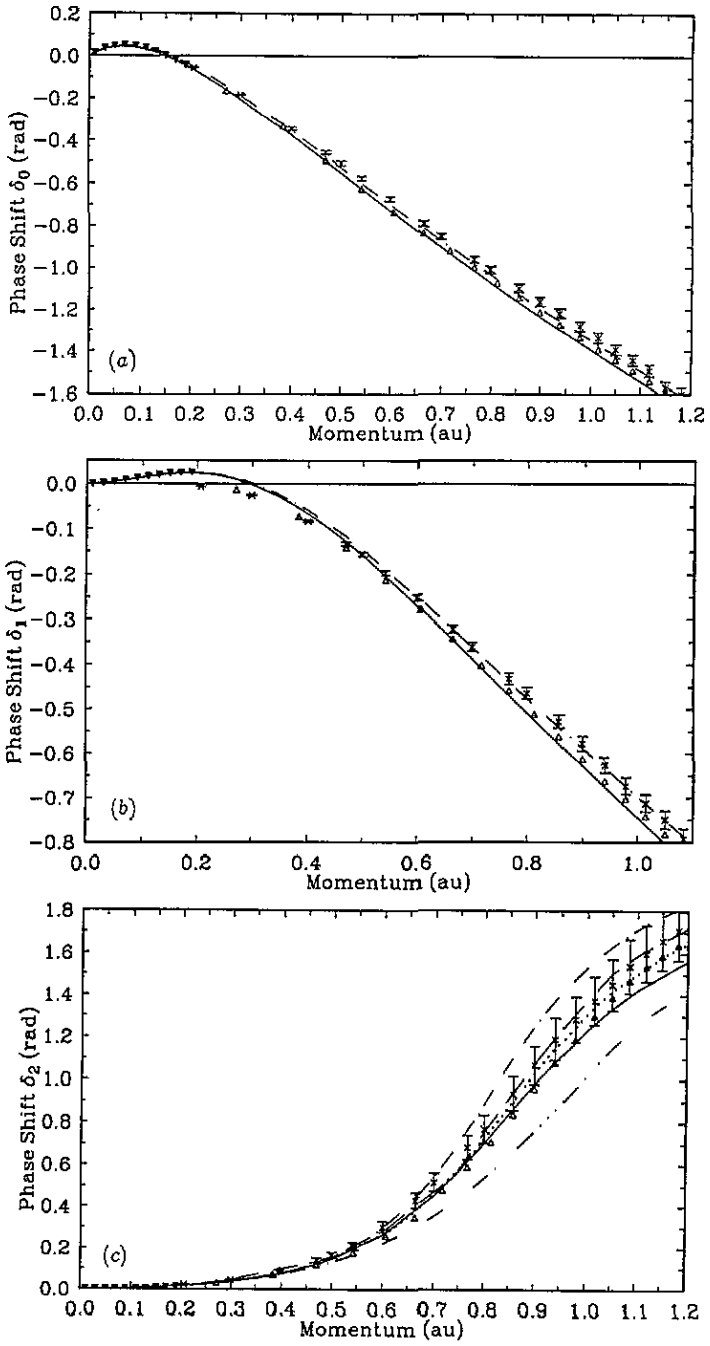

Figure 2. Phaseshifts for elastic scattering from argon: (*a*) S waves; (*b*) P waves; (*c*) D waves. Theoretical results: ——, DD; — · —, AE; — · · · —, Bell *et al* (1984); — — —, Saha (1991); ·····, Sienkiewicz and Baylis (1987). Experimental results: △, Andrick and Bitsch (1983); ×, Williams (1979); ▼, Weyhreter *et al* (1988).

Williams (1979). At lower momenta the results of Weyhreter *et al* (1988) are generally in very good agreement with both our sets of results. At momenta above 0.7 au the present

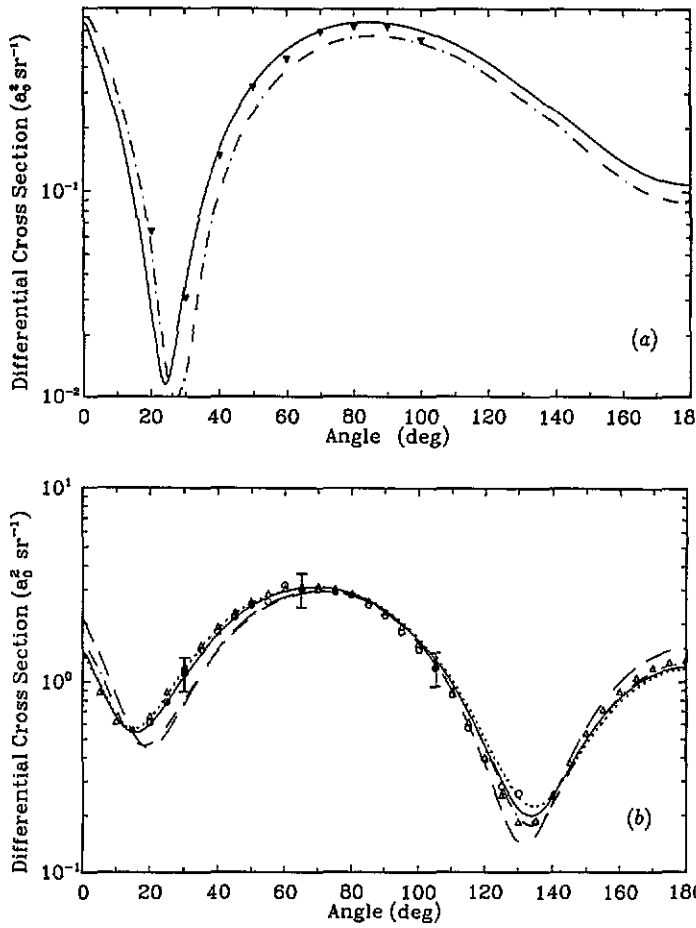

Figure 3. Differential cross sections for elastic scattering from argon: (*a*) 1 eV; (*b*) 3 eV; (*c*) 10 eV; (*d*) 20 eV. Theoretical results: ——, DD; — · —, AE; — — —, Saha (1991); ·····, Sienkiewicz and Baylis (1987). Experimental results: △, Andrick and Bitsch (1983); ●, Dubois and Rudd (1976); ○, Srivastava *et al* (1981); ▼, Weyhreter *et al* (1988); □, Williams and Willis (1975).

results begin to fall below the experimental values. The DD results are for the most part in good agreement with the calculations of Sienkiewicz and Baylis (1987) and Bell *et al* (1984) while those of Saha (1991) are closer to the AE results. The biggest differences occur for the D-wave which dominates for the higher momenta. The AE results were significantly above the experimental ones at the higher momenta while the DD results lie close to the values of Andrick and Bitsch (1983) and at the lower end of the error bars on the data of Williams (1979). The calculations of Bell *et al* (1984) lie significantly below the other results while those of Saha (1991) and Sienkiewicz and Baylis (1987) lie between the DD and AE values for momenta above about 0.5 au.

In figure 3 we present differential cross sections at various energies. For an electron energy of 1 eV the experimental values of Weyhreter *et al* (1988) are in very good agreement with our DD results at almost all angles. This is also the case at 0.4 and 0.5 eV (not shown). At lower energies (i.e., at or below the energy of the minimum in the integral cross section, cf figure 4) the experimental results are in better agreement with the AE

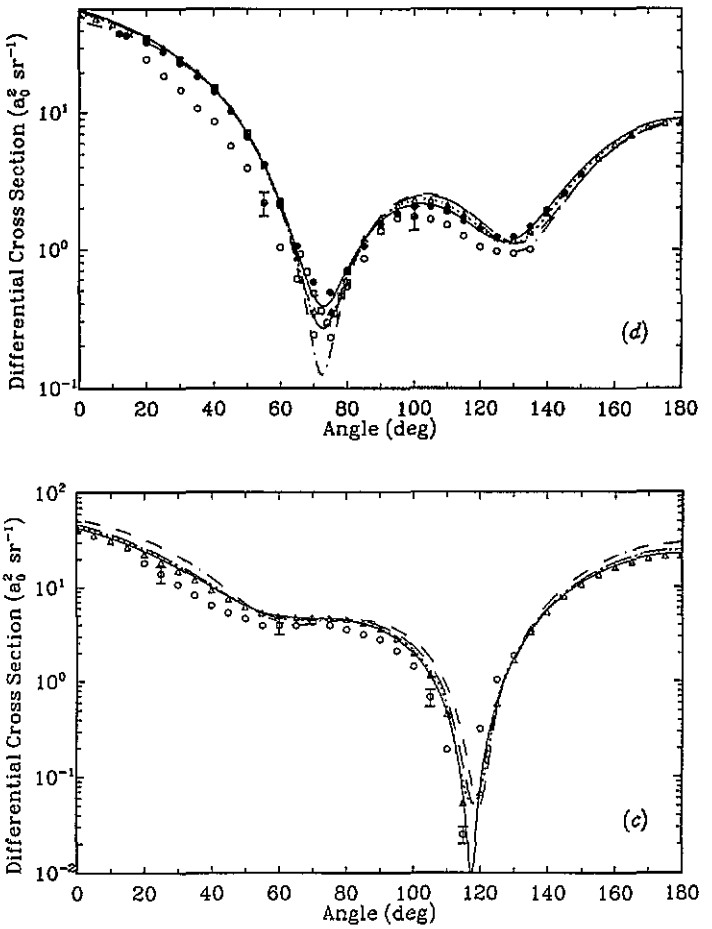

Figure 3. (Continued)

values. At 3 eV our DD results are in very good agreement with the experimental results of Andrick and Bitsch (1983) and Srivastava *et al* (1981) and are noticeably superior to both our previous AE calculations and those of Saha (1991). The calculations of Sienkiewicz and Baylis (1987) lie very close to the DD values. At 10 eV our DD results are again superior to our previous AE calculations, being in excellent agreement with the measurements of Andrick and Bitsch (1983) and just outside the error bars of Srivastava *et al* (1981). At this energy the calculations of Saha (1991) and Sienkiewicz and Baylis (1987) are very close to our DD results. For 20 eV the four sets of theoretical calculations begin to deviate for scattering angles greater than 70 ° where the DD data are in better overall agreement with the experiments. Thus it appears that the DD approximation gives consistently reliable results in this energy range.

The integral elastic cross sections are given in figure 4 along with a selection of more recent experimental measurements and theoretical calculations. Given the spread among the experimental measurements it is difficult to make a definitive choice between the AE and DD approximations. Overall the AE results seem to be more reliable in the region of the Ramsauer minimum while the DD results are definitely superior in the region of the peak of the cross section. The theoretical values of Bell *et al* (1984) and Saha (1991) generally lie outside the range of the experimental results while those of Sienkiewicz and Baylis

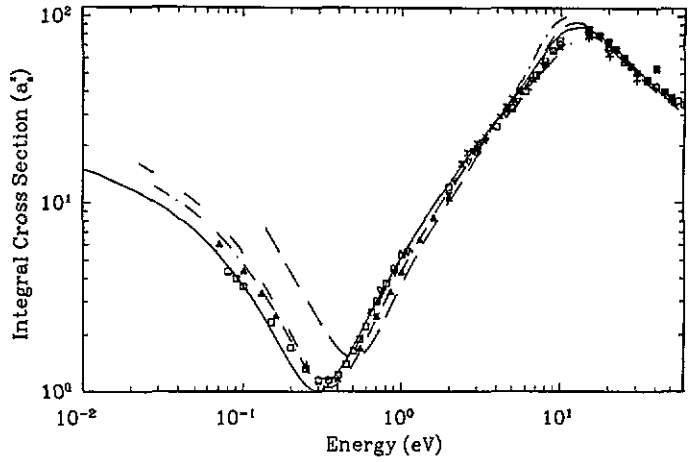

Figure 4. Integral cross sections for elastic scattering from argon. Theoretical results: ——, DD; — · —, AE; — ··· —, Bell *et al* (1984); — — —, Saha (1991). Experimental results: ∗, Charlton *et al* (1980); ▲, Ferch *et al* (1985); ◊, Furst *et al* (1989); □, Jost *et al* (1983); +, Kauppila *et al* (1981); ▽, Subramanian and Kumar (1987); ■, Wagenaar *et al* (1980).

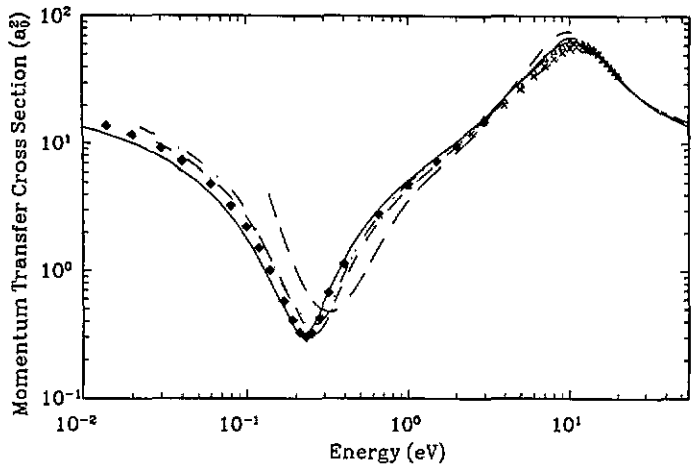

Figure 5. Momentum transfer cross section for argon. Theoretical results: ——, DD; — · —, AE; — ··· —, Bell *et al* (1984); — — —, Saha (1991). Experimental results: △, Andrick and Bitsch (1983); ♦, Milloy *et al* (1977); ×, Nakamura and Kurachi (1988).

(1987) are very close to the DD ones. Similar comments hold for the momentum transfer cross sections shown in figure 5 although in this case the DD results seem to give the best agreement at the minimum. Numerical values for the integral and momentum transfer cross sections for argon are presented in table 2.

2.2. *Krypton*

For krypton we have used the converged potential V_{dp}^{67} for our DD calculations. The phaseshifts are displayed in figure 6 from which it is obvious that there is less difference between the DD and AE results than there was for argon and both are close to the results of the relativistic calculation of Sin Fai Lam (1982). As in argon the greatest difference among

Table 2. Integrated total cross sections (TXS) and momentum transfer cross sections (MTXS) for argon and krypton (a_0^2).

Argon			Krypton		
E (eV)	TXS	MTXS	E (eV)	TXS	MTXS
0.01	14.235	12.604	0.01	92.365	86.575
0.02	11.468	9.591	0.02	76.733	69.597
0.05	7.155	5.118	0.05	51.277	42.904
0.10	3.624	1.835	0.10	31.270	23.061
0.20	1.388	0.342	0.20	14.528	8.079
0.22	1.228	0.319	0.30	7.635	2.904
0.25	1.079	0.362	0.40	4.369	0.981
0.27	1.028	0.429	0.50	2.807	0.421
0.28	1.013	0.471	0.53	2.540	0.396
0.29	1.006	0.518	0.60	2.176	0.500
0.30	1.005	0.569	0.63	2.109	0.598
0.31	1.010	0.625	0.65	2.089	0.676
0.32	1.019	0.683	0.66	2.086	0.720
0.35	1.071	0.861	0.67	2.087	0.764
0.40	1.239	1.226	0.68	2.092	0.812
0.50	1.731	1.976	0.69	2.101	0.860
0.66	2.738	3.135	0.70	2.114	0.914
0.78	3.618	3.971	0.78	2.339	1.381
1.00	5.205	5.258	1.00	3.743	3.002
2.18	14.066	11.224	2.18	18.626	15.661
3.00	20.309	16.004	3.00	32.427	28.356
5.00	36.590	31.269	5.00	75.243	68.000
10.00	80.719	63.743	10.00	116.002	74.148
13.61	87.760	55.819	13.61	103.088	51.096
15.00	85.500	50.198	15.00	97.817	44.710
20.00	72.536	34.195	20.00	82.615	29.770
30.00	52.834	21.192	30.00	64.549	16.621
40.00	41.637	16.822	40.00	53.778	11.036

all three calculations occurs for the D-wave. None of the calculations is in particularly good agreement with the experimentally derived values of Srivastava *et al* (1981). The S-wave phaseshifts from the low-energy measurements of Weyhreter *et al* (1988) are somewhat above all of the theoretical results except for those of Bell *et al* (1988) while the P-wave values are in good agreement with all of the theoretical ones.

We show our low-energy differential cross sections in figure 7 in comparison with the AE results, the calculations of Sin Fai Lam (1982) and Sienkiewicz and Baylis (1992) and the measurements of Weyhreter *et al* (1988). Our DD results are consistently closer to the experimental results than the other calculations although the agreement in magnitude is only moderately good. At higher energies the difference between the AE and DD calculations is not large and given the spread in the experimental measurements no definite conclusions can be reached. A typical example is shown in figure 8 for an electron energy of 10 eV. The DD and AE results and the semi-relativistic calculations of Sin Fai Lam (1982) all have very similar values while those of Sienkiewicz and Baylis (1992) exhibit a somewhat different shape. The experimental values show an even wider variation in values.

In the case of the integrated elastic cross sections shown in figure 9, the DD results are in better agreement with the experimental measurements of Buckman and Lohmann (1987), Ferch (1992) and Jost *et al* (1983) than the AE results for energies below the Ramsauer minimum. Above the minimum both theories yield results above the various experimental

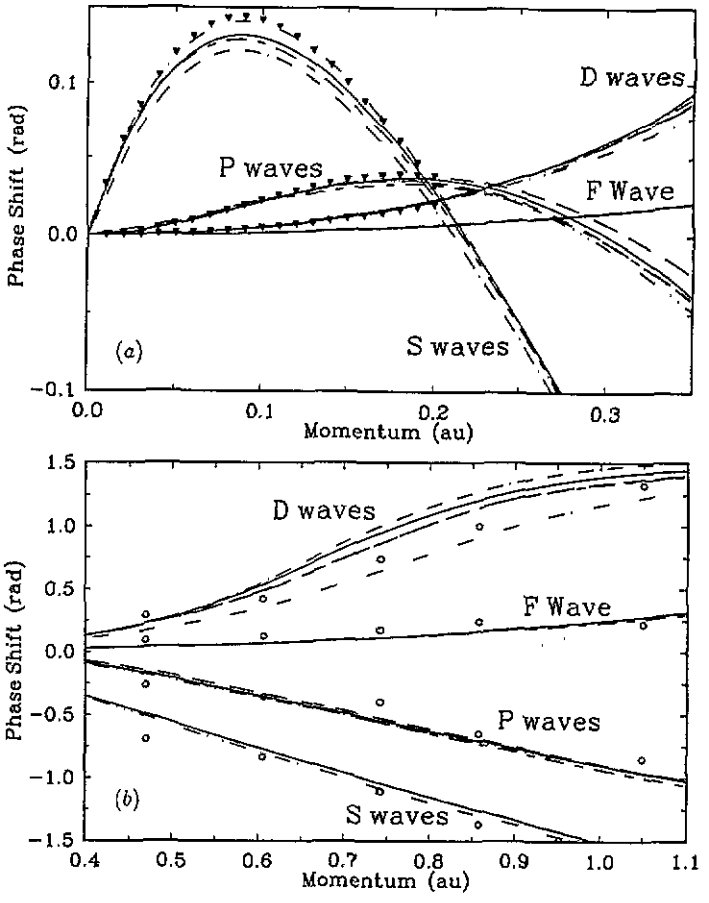

Figure 6. Phaseshifts for elastic scattering from krypton: (*a*) incident momentum from 0 to 0.35; (*b*) incident momentum from 0.4 to 1.1. Theoretical results: ——, DD; — · —, AE; — — —, Sin Fai Lam (1982), spin down; — - —, Sin Fai Lam (1982), spin up; — ··· —, Bell *et al* (1988). Experimental results: ○, Srivastava *et al* (1981); ▼, Weyhreter *et al* (1988).

values especially when it is noted that the experimental measurements include inelastic effects above their respective thresholds. The calculations of Sin Fai Lam (1982) (not shown) are very close to ours while those of Bell *et al* (1988) are in closest agreement with experimental values for energies above the Ramsauer minimum. Similar comments hold for the momentum transfer cross section shown in figure 10. Our DD results are in good agreement with the measurements of Koizumi *et al* (1986) at almost every point and we are in particularly good agreement with Brennan and Ness (1993) for the position of the minimum. Numerical values for the integral and momentum transfer cross sections for krypton are presented in table 2.

2.3. Neon

In our previous AE calculations for neon (McEachran and Stauffer 1983, 1985) we found that it was necessary to scale our dipole polarization potential so that it yielded the correct asymptotic form in order to get satisfactory agreement with experiment. Scaling was not necessary for the other noble gases since our values for the dipole polarizabilities were much more accurate (McEachran *et al* 1979). We cannot carry out a similar scaling for the

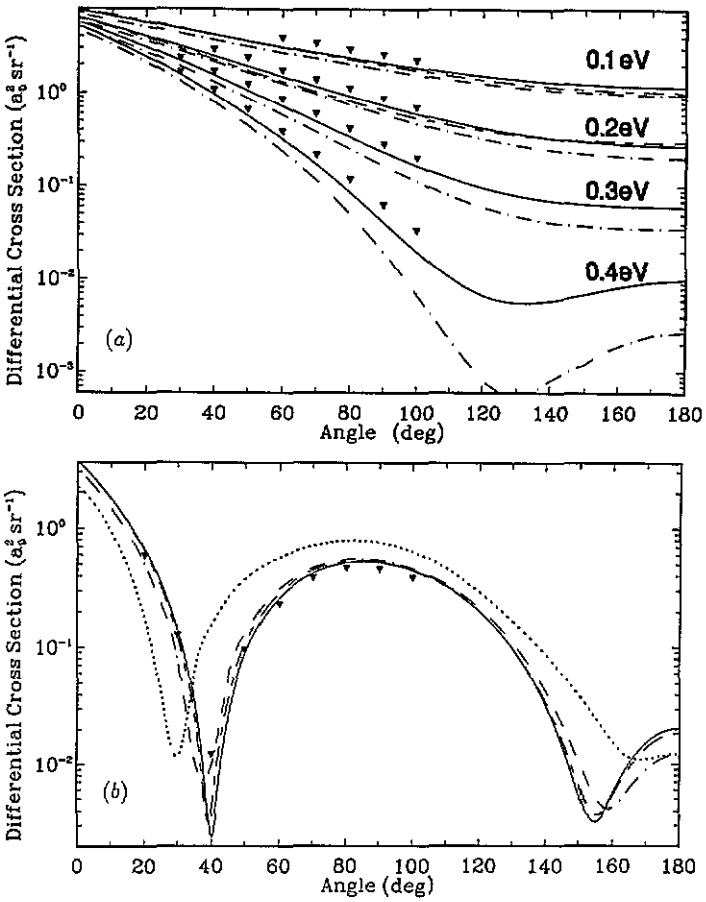

Figure 7. Differential cross sections for elastic scattering from krypton: (*a*) 0.1 eV to 0.4 eV; (*b*) 1 eV. Theoretical results: ——, DD; — · —, AE; · · · · · ·, Sienkiewicz and Baylis (1992); — — —, Sin Fai Lam (1982). Experimental results: ▼, Weyhreter *et al* (1988).

DD calculations since the higher-order multipole polarizabilities are not accurately known. Thus our fully converged neon potential V_{dp}^{34} does not yield accurate results. In fact the V_{dp}^{12} potential gives much superior results. Simply scaling the dipole part of the potential and leaving the higher-order terms unchanged does not improve matters either. Typical results for the differential cross sections at 20 eV are shown in figure 11.

3. Conclusions

We have investigated the effects of including dynamic distortion in the calculation of elastic scattering of electrons from the heavier noble gases. Dynamic distortion has the largest effect at lower energies as would be expected and, in general, its inclusion improved the agreement between the theoretical calculations and the experimentally determined data. This was particularly true for argon. For neon, however, the inclusion of the dynamic distortion terms did not lead to an improvement. In fact, it increased the difference between our previous theoretical work and the experimental values.

The reason for the different behaviour in neon from that in argon and krypton is due, as far as we are able to determine, to the relative accuracy to which we are able to calculate

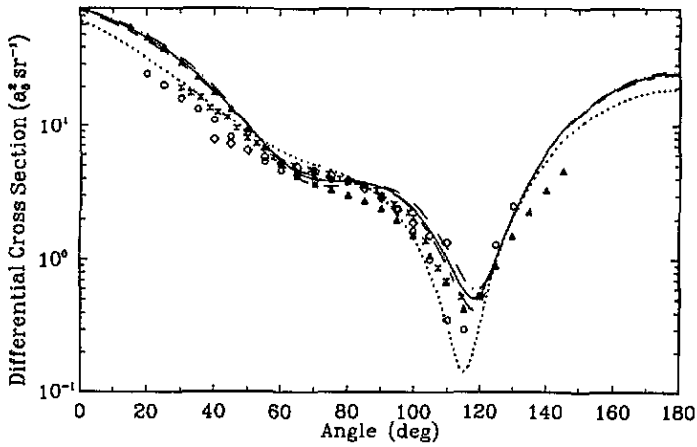

Figure 8. Differential cross sections for elastic scattering from krypton at 10 eV. Theoretical results: the legend is the same as for figure 7. Experimental results: *, Heindorff *et al* (1976); ▲, Jost and Otto (1983); ○, Srivastava *et al* (1981); ◇, Zhou Qing *et al* (1982).

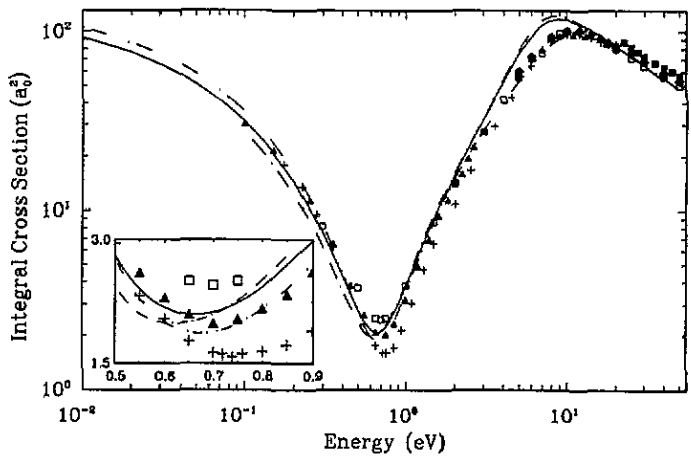

Figure 9. Integral cross sections for elastic scattering from krypton. Theoretical results: ——, DD; — · —, AE; — · · · —, Bell *et al* (1984). Experimental results: +, Buckman and Lohmann (1987); ▲, Ferch (1992); □, Jost and Otto (1983); ♦, Kanik *et al* (1992); ■, Wagenaar and de Heer (1980).

the long-range part of the interaction potentials. This long-range behaviour is reflected in the coefficients given in table 1. The coefficients α_ν, the multipole polarizabilities of the atoms, have been the subject of a good deal of research interest and we can draw some quantitative conclusions by examining the values for these quantities.

The results we obtained for these coefficients were based upon the coupled Hartree–Fock (CHF) approximation (McEachran *et al* 1977, 1979). Experimental results are available for the dipole polarizabilities α_1. More accurate calculations, which include correlation effects, have been carried out in the coupled-electron pair approximation (CEPA) by Werner and Meyer (1976) and by Reinsch and Meyer (1976, 1978). They obtained very accurate values for α_1 in neon and argon and found that the contribution made by correlation effects (as measured by the difference between the CHF and CEPA results) is 11.6% in neon but only

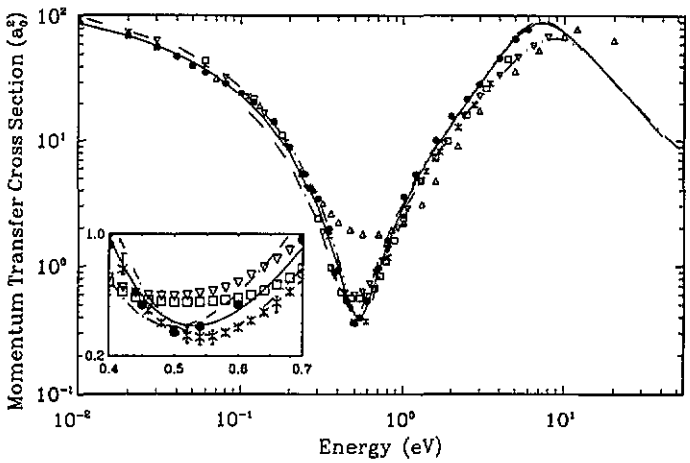

Figure 10. Momentum transfer cross sections for krypton. Theoretical results: the legend is the same as for figure 9. Experimental results: *, Brennan and Ness (1993); □, England and Elford (1988); △, Frost and Phelps (1964); ▽, Hunter *et al* (1988); ●, Koizumi *et al* (1986).

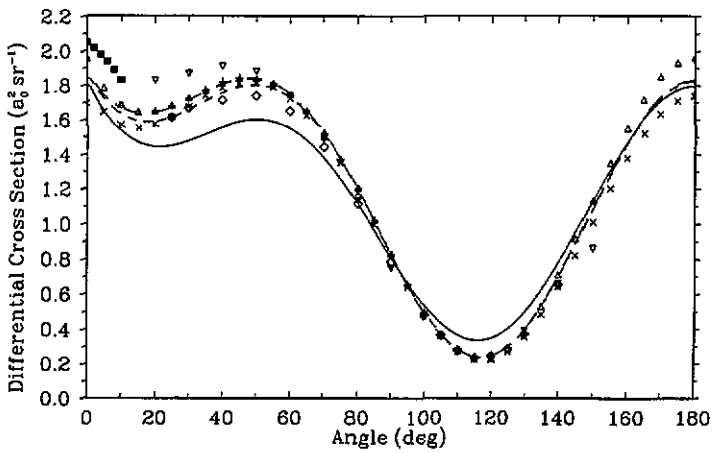

Figure 11. Differential cross sections for elastic scattering from neon. Theoretical results: ——, DD results using V_{dp}^{34}; – – –, DD results using V_{dp}^{12}; — · —, AE. Experimental results: △, Andrick and Bitsch (1983); +, Brewer *et al* (1981); ◇, Register and Trajmar (1984); ■, Wagenaar *et al* (1986); ×, Williams (1979); ▽, Williams and Crowe (1975).

3.6% in argon. For the quadrupole polarizabilities α_2, there are no experimental values with which to compare and little in the way of accurate calculations. However, based on the work of Reinsch and Meyer (1978) correlation effects contribute 16.3% to α_2 in neon. Unfortunately, comparable results are not available for argon.

Based on these limited data, and the good agreement of our CHF values for α_1 for argon, krypton and xenon (McEachran *et al* 1979), with the experimental measurements, we conclude that our CHF calculations for the interaction potentials are quite accurate for the heavier noble gases but much less so for neon and this is reflected in the effects that the inclusion of the dynamic distortion terms have on the scattering data.

In conclusion, we have shown that it is important to include dynamic distortion effects

in scattering calculations in order to achieve accurate results at low energies. However, it is also important, from our neon results, that these dynamic distortion contributions must themselves be highly accurate if they are to produce more accurate scattering data.

Acknowledgments

We are grateful to Drs M J Brennan and J Ferch for providing us with their experimental results in advance of publication. Professor P A Fraser was kind enough to provide us with a working program for his effective range method. This research was supported in part by the Natural Sciences and Engineering Research Council of Canada.

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