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Optical potential approach to electron and positron scattering from noble gases: II. Neon

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Abstract. We have extended our previous work on an optical potential method to electron and positron scattering from neon. In addition, we have modified the approach to include the diagonal potentials previously neglected. This required the use of a numerical form of the Green function. Comparison with recent experimental measurements with positrons indicates the necessity of including absorption effects at higher energies, although these effects appear to be smaller for neon than they were for argon. At energies just above the inelastic excitation thresholds, however, the picture is not so clear at the moment.

1. Introduction

In a previous paper (Bartschat *et al* 1988, hereafter referred to as I) we applied an optical potential method to the scattering of electrons and positrons from argon. This approach takes into account the effects of open inelastic channels on the elastic scattering process. In the case of positron scattering, at energies above the inelastic thresholds, it also removes the minimum in the elastic differential cross section which we had previously predicted (McEachran and Stauffer 1986). It has been demonstrated experimentally that the minimum in the differential cross section for argon becomes progressively shallower as the energy of the incident positron is increased through the inelastic region and disappears entirely somewhere between 20 and 30 eV (Hyder *et al* 1986, Floeder *et al* 1988, Smith *et al* 1990).

In the present work we have extended our calculations to electron and positron scattering from neon. In addition, we have included the diagonal potentials, which were neglected in I, in the formulation of the optical potential. This required the use of numerical Green functions in lieu of the analytic ones used before. This change has a small effect on the results.

The present results for neon are very similar to those we obtained earlier for argon. Thus, the inclusion of the inelastic channels via the optical potentials produced differential cross sections for positron scattering which lacked the minimum obtained with a polarised orbital calculation (McEachran and Stauffer 1986). In the case of

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electron scattering, the differential cross sections for neon do not exhibit the marked structure which occurs in argon. Furthermore, there are some differences between the present calculations and our previous polarised orbital results, especially for small scattering angles.

2. Theory

The theory has been given in detail in I. The only addition that we have to make is to calculate an alternative optical potential by including the diagonal matrix elements in the Q space equations. Specifically, equation (7) of I is replaced by

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l_i(l_i+1)}{r^2} + 2V_{ii}(r) + k_i^2\right) F_{l_i}(r) = 2V_{i0}(r)\, F_0(r). \tag{1}$$

As a consequence, the standard Riccati–Bessel functions f_{l_i} and g_{l_i} in equation (8) of I have to be replaced by the regular and irregular solutions u_{l_i} and v_{l_i} of equation (1) with the right-hand side put to zero. Since the diagonal potentials V_{ii} were obtained in numerical form, these functions must be determined numerically. The remainder of the theory is unaltered.

In order to obtain these numerical solutions we first recast the homogeneous equation corresponding to equation (1) into an integral form. The regular solution is determined by integrating the equation

$$\begin{aligned}\tilde{u}_{l_i}(k_ir) = f_{l_i}(k_ir) &+ \frac{f_{l_i}(k_ir)}{k_i}\int_0^r \mathrm{d}r'\, g_{l_i}(k_ir')\, 2V_{ii}(r')\, \tilde{u}_{l_i}(k_ir') \\ &- \frac{g_{l_i}(k_ir)}{k_i}\int_0^r \mathrm{d}r'\, f_{l_i}(k_ir')\, 2V_{ii}(r')\, \tilde{u}_{l_i}(k_ir')\end{aligned} \tag{2}$$

outward from the origin to a value of r, say r_N, where the potentials V_{ii} are zero. Asymptotically, this function behaves like

$$\begin{aligned}\tilde{u}_{l_i}(k_ir) &= A_{l_i}\, \sin(k_ir - l_i\pi/2) + B_{l_i}\, \cos(k_ir - l_i\pi/2) \\ &= C_{l_i}\, \sin(k_ir - l_i\pi/2 + \eta_{l_i})\end{aligned} \tag{3}$$

where

$$A_{l_i} = 1 + \frac{1}{k_i}\int_0^{r_N} \mathrm{d}r'\, g_{l_i}(k_ir')\, 2V_{ii}(r')\, \tilde{u}_{l_i}(k_ir') \tag{4}$$

$$B_{l_i} = -\frac{1}{k_i}\int_0^{r_N} \mathrm{d}r'\, f_{l_i}(k_ir')\, 2V_{ii}(r')\, \tilde{u}_{l_i}(k_ir') \tag{5}$$

$$C_{l_i} = (A_{l_i}^2 + B_{l_i}^2)^{1/2} \tag{6}$$

and

$$\eta_{l_i} = \tan^{-1} B_{l_i}/A_{l_i}. \tag{7}$$

The properly normalised regular solution is then given by

$$u_{l_i}(k_ir) = \tilde{u}_{l_i}(k_ir)/C_{l_i}. \tag{8}$$

Finally, the irregular solution can be determined by integrating the equation

$$v_{l_i}(k_i r) = a_{l_i} f_{l_i}(k_i r) + b_{l_i} g_{l_i}(k_i r) + \frac{f_{l_i}(k_i r)}{k_i} \int_{r_N}^{r} \mathrm{d}r' \, g_{l_i}(k_i r') \, 2V_{ii}(r') \, v_{l_i}(k_i r') - \frac{g_{l_i}(k_i r)}{k_i} \int_{r_N}^{r} \mathrm{d}r' \, f_{l_i}(k_i r') \, 2V_{ii}(r') \, v_{l_i}(k_i r') \tag{9}$$

inward from r_N. Asymptotically, this function will behave like

$$v_{l_i}(k_i r)_{r \to \infty} = \cos(k_i r - l_i \pi/2 + \eta_{l_i}) \tag{10}$$

provided

$$a_{l_i} = -\sin \eta_{l_i} \qquad b_{l_i} = \cos \eta_{l_i}. \tag{11}$$

Hence, $v_{l_i}(k_i r)$ will be the required irregular solution. It should be noted that if the branch used by the arctangent subroutine to determine η_{l_i} lies in the range $-\pi/2$ to $+\pi/2$ then it is necessary to add π to η_{l_i} whenever $A_{l_i} < 0$ in order to obtain a consistent value for the phaseshift. This will also ensure that the Wronskian of the functions $u_{l_i}(k_i r)$ and $v_{l_i}(k_i r)$ will always be of the same sign.

3. Results

We have repeated our calculations for argon using the numerical Green function described in section 2. We found remarkably little change when using this new Green function in lieu of the analytic one. The largest differences between the values for the differential cross section calculated with these two different forms are of the order of 3%. The same is true in the case of neon, as we will illustrate in the figures below.

In our calculation of the optical potential for neon we have used the following 13 bound states in the Q space:

$(2p^5 3s)\,{}^1P^o$	$(2p^5 4s)\,{}^1P^o$	$(2p^5 5s)\,{}^1P^o$
$(2p^5 3p)\,{}^1S, {}^1D$	$(2p^5 4p)\,{}^1S, {}^1D$	$(2p^5 5p)\,{}^1S, {}^1D$
$(2p^5 3d)\,{}^1P^o, {}^1F^o$	$(2p^5 4d)\,{}^1P^o, {}^1F^o$.	

(12)

In figure 1 we show our results for positron scattering from neon at 20 eV. The general behaviour is the same as that in argon, i.e. the polarised orbital approximation predicts a minimum in the elastic differential cross section at small scattering angles while the optical potential results show a maximum at roughly the same angle. We show optical potential results using both forms of the Green function, demonstrating the small difference due to these two forms. We also display the results of adding the imaginary (absorption) part of the optical potential to our polarised orbital potential. We see that this has very little effect on the cross section as was the case in argon. In these calculations the polarised orbital potential is the scaled potential used by McEachran and Stauffer (1985). The normalised experimental results of Kauppila *et al* (1990) exhibit a minimum and are in good agreement with our polarised orbital calculations (with or without the inclusion of the absorption potential). We note that this energy of 20 eV is just below the ionisation threshold for neon. Furthermore, the shape of

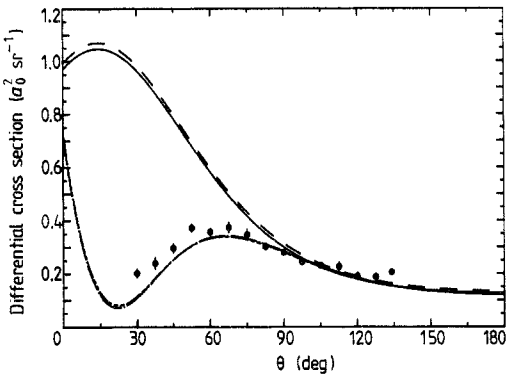

Figure 1. Elastic differential cross section for positrons at 20 eV. Theory: —— · —— ·, polarised orbital approximation; —— --, plus 13-state absorption potential; —— —— ——, optical potential from 13 states with numerical Green function; ——————, optical potential from 13 states with free Green function; •, experimental data of Kauppila *et al* (1990) (normalised to our polarised orbital plus 13-state absorption potential calculation at 90°).

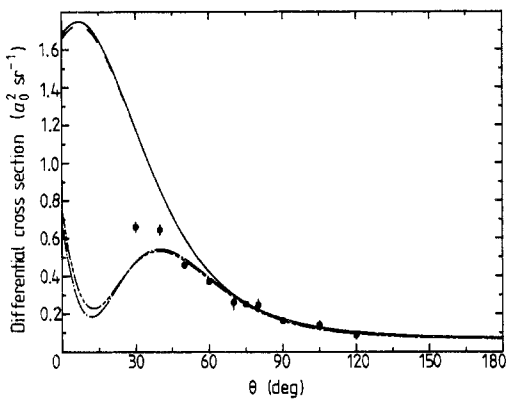

Figure 2. As for figure 1 but at 50 eV; •, experimental data of Smith (1989).

the experimental curve is similar to that for argon at 15 eV which is also just below the corresponding ionisation threshold (Smith *et al* 1990).

Figure 2 shows the results for the scattering of positrons from neon at 50 eV. Note that the experimental data (Smith 1989) at this high energy do not indicate a minimum in the differential cross section at small scattering angles. This is in *qualitative* agreement with the optical potential calculations. For a more *quantitative* test, however, absolute experimental cross sections are required.

For electron scattering from neon we show in figure 3 our differential cross section results at 20 eV along with several sets of experimental data. The optical potential results are similar to those for positrons in that they exhibit a maximum at small scattering angles in lieu of the minimum seen in the polarised orbital calculations (McEachran and Stauffer 1983). At larger angles all the calculations predict similar values, although there are some differences at backward scattering angles. Clearly the polarised orbital calculations agree much better with the experimental results, particularly below 60°. This is similar to positron scattering, where the two forms of the Green function yield almost identical results, as do the polarised orbital calculations

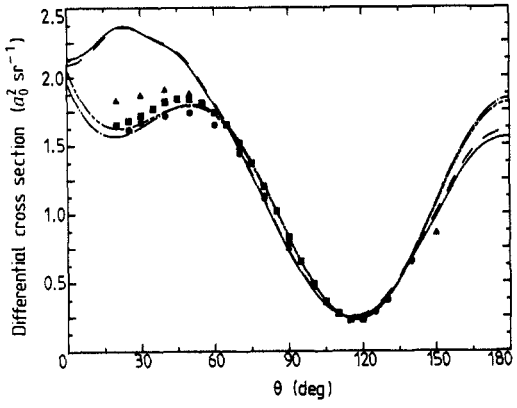

Figure 3. As for figure 1 but for electrons. Experiment: △, Williams and Crowe (1975); ▪, Brewer *et al* (1981); •, Register and Trajmar (1984).

with or without the absorption potential.

Figure 4 shows the corresponding results for 50 eV. There is less difference between the various sets of calculations at this energy; in fact, only one optical potential curve is plotted, since the two calculations are indistinguishable within the resolution of the graph. However, the optical potential results are clearly below the polarised orbital ones and the experiments at small scattering angles. This deficiency in the optical potential method is almost entirely due to the lack of the full dipole polarisation interaction caused by truncating our expansion in Q space.

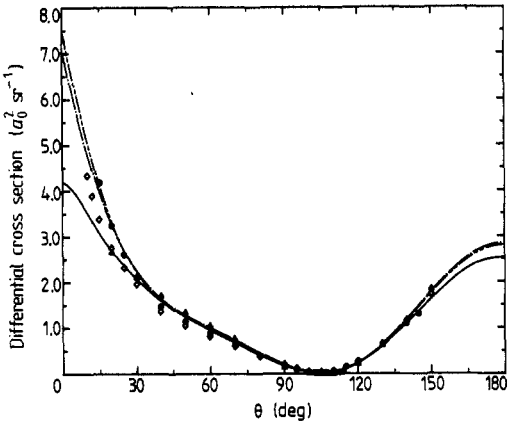

Figure 4. As for figure 3 but at 50 eV; only one optical potential calculation is shown, since the results are indistinguishable within the accuracy of the graph; ◇, DuBois and Rudd (1976).

Finally, we present our integrated elastic, absorption and total cross sections in table 1. (See I for the definition of these quantities.) As in the corresponding argon calculation described in I, the total cross section for electron scattering is dominated by the contribution from the elastic channel. There is good agreement between theory and experiment (cf McEachran and Stauffer (1983) for references to the experimental results), and the effect of the different forms of the Green function is quite small.

For positron scattering, the neglect of the positronium formation and ionisation

Table 1. Integrated cross sections (a_0^2).

	Electrons				Positrons			
Energy (eV)	a	b	c	d	a	b	c	d
Elastic scattering								
20	13.393	13.349	14.264	14.438	2.899	2.889	5.130	5.301
30	13.370	13.296	13.140	13.244	2.945	2.916	4.868	4.915
40	12.912	12.832	12.044	12.130	2.922	2.887	4.633	4.640
50	12.251	12.175	11.090	11.163	2.874	2.838	4.428	4.420
100	9.085	9.030	7.891	7.927	2.596	2.569	3.717	3.700
Absorption								
20	0.000	0.403	0.735	0.376	0.000	0.264	0.572	0.251
30	0.000	0.738	1.011	0.755	0.000	0.496	0.684	0.482
40	0.000	0.822	1.006	0.842	0.000	0.541	0.648	0.532
50	0.000	0.844	0.981	0.863	0.000	0.534	0.599	0.528
100	0.000	0.594	0.631	0.599	0.000	0.351	0.356	0.349
Total								
20	13.393	13.752	14.999	14.814	2.899	3.153	5.702	5.552
30	13.370	14.034	14.151	13.999	2.945	3.412	5.552	5.397
40	12.912	13.654	13.050	12.972	2.922	3.428	5.281	5.172
50	12.251	13.019	12.071	12.026	2.874	3.372	5.027	4.948
100	9.085	9.624	8.522	8.526	2.596	2.920	4.073	4.049

[a] Polarised orbital. [b] Local polarisation plus 13-state absorption potential. [c] 13-state optical potential (free Green function). [d] 13-state optical potential (numerical Green function).

channels is the main reason for the theoretical underestimation of the absorption and total cross sections (cf Kauppila and Stein 1982 and Sinapius *et al* 1980). This result confirms our earlier findings for argon and indicates the necessity of incorporating these channels in future work.

4. Conclusions

In the present work we have demonstrated that the effect produced by using the Green function calculated with or without the diagonal potentials in the Q space is surprisingly somewhat small.

The effect of using the optical potential in the calculation of electron and positron scattering from neon is similar to that found in I for scattering from argon. In particular, the optical potential results for positron scattering do not indicate the minimum predicted by the polarised orbital approach. At higher energies the optical potential method yields reasonable agreement with the shape of the experimental differential cross section for positron scattering and good results for both the shape and magnitude in the case of electron scattering.

In summary, we have shown that the inclusion of the effects of the open inelastic channels via the optical potential method produces the same qualitative behaviour of the cross sections in neon as it did in argon. However, the lack of the positronium formation channel is probably the most important cause of the disagreement with experiment in the case of positron scattering at energies below the first ionisation threshold. At higher energies, the ionisation channels are expected to be quite important for both electron and positron scattering. We hope to include both of these effects in future work on the optical potential method.

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