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Electron and positron scattering by helium and neon

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Abstract. New measurements of the total cross sections for positron scattering by helium and by neon are tested for consistency with a sum rule based on forward dispersion relations. The real parts of the forward scattering amplitudes are calculated and compared with recent theoretical predictions. Revised values of the real part of the forward scattering amplitude for electron scattering by helium are presented.

1. Introduction

Forward dispersion relations (Gerjuoy and Kroll 1960) can be used in the phenomenological analysis of electron–atom collisions in two ways. First, by connecting an integral over the total cross section with the scattering length, the consistency and accuracy of total cross section measurements can be assessed. Once this consistency has been established, the real parts of the forward scattering amplitude can be calculated from the dispersion relation and these values can be used to control a phase shift analysis of differential scattering data, or to discriminate between theoretical models which predict these quantities. (Recent reviews of the application of phase shift analysis to electron–atom scattering and related topics have been given by Bransden 1975 and McDowell 1974.)

The most extensive application so far, of the dispersion relations has been to the electron–helium system by Bransden and McDowell (1969, 1970, hereafter referred to as papers I and II, respectively) following earlier work of Lawson *et al* (1966). In this paper, the conclusions of that work are re-examined in the light of new measurements of the total cross section for electron–helium scattering by Jansen *et al* (1974). The parallel case of positron scattering by helium has been examined by Bransden *et al* (1974) who were able to demonstrate that the measurements of the total cross section were inconsistent with the dispersion relation. Since then, new measurements of the cross section have been published (Jaduszliwer *et al* 1974, Coleman *et al* 1974) which are analysed in this paper, together with similar data for the scattering of positrons by neon.

2. Electron scattering by helium

The basic dispersion relation for electron–helium scattering is (see paper I, equation 24)

$$\mathrm{Re}\, f(k) = f_{\mathrm{B}}^{\mathrm{D}} - f_{\mathrm{B}}^{\mathrm{E}}(k) + \frac{P}{2\pi}\int_0^\infty \frac{k'^2 Q_{\mathrm{tot}}(k')}{k'^2 - k^2}\,\mathrm{d}k' \tag{1}$$

where $f(k)$ is the scattering amplitude in the forward direction and $Q_{tot}(k)$ the total cross section at the momentum k, where k is in atomic units and Q_{tot} is in units of πa_0^2. Appearing on the right hand side of (1) is the first Born approximation to $f(k)$, $(f_B^D - f_B^E(k))$, which is composed of two parts, f_B^D the energy-independent direct term and $f_B^E(k)$ the exchange term. Both f_B^F and $f_B^E(k)$ must be calculated using accurate wavefunctions for helium, but since $f_B^E(k)$ is a rapidly decreasing function of momentum, it is of importance at energies below about 50 eV only.

Less sensistive to the total cross section at very high energies is the subtracted dispersion relation (paper I, equation 29)

$$\mathrm{Re}[f(k)-f(0)] = [f_B^E(k)-f_B^E(0)]+\frac{k^2}{2\pi}P\int_0^\infty \frac{Q_{tot}(k')}{(k'^2-k^2)}\,dk'. \tag{2}$$

If the cross section satisfies the sum rule

$$-A-f_B^D+f_B^E(0) = \frac{1}{2\pi}P\int_0^\infty Q_{tot}(k)\,dk \tag{3}$$

where A is the scattering length†, then the values of Re $f(k)$ obtained from both (1) and (2) are identical.

In paper I, the fit to measurements of the total cross sections given by Golden and Bandel (1965) was adopted for the energy region below 20 eV. This fit is consistent with a scattering length of $A = 1{\cdot}15a_0$. In the higher energy range from 20 to 100 eV the measurements of Normand (1930) were employed. At high energies, the Born approximation is believed to provide accurate values of the total cross section and these were adopted for $E > 273$ eV ($k^2 = 20$). The cross section between 100 and 273 eV was then obtained from a smooth interpolation. New estimates of the total cross section by de Heer *et al* (1974), based on experimental measurements, have been made in the energy range 100 to 1000 eV (see also Jansen *et al* 1974). The measurements of Normand (1930) in the energy interval 100 to 400 eV (which were not employed in paper I) fall progressively below the new estimates, until at 400 eV, the new estimate exceeds the value of Normand by 50% (see table 1). For this reason, we have recalculated Re $f(k)$, making slightly different assumptions about the cross section at the higher energies, to examine the sensitivity of the results to this region. Below 100 eV, the cross sections used in paper I were employed, and from 100 to 1000 eV the values given by de Heer *et al* (1974) were used (see table I).

Table 1. Total cross sections for e^-–He scattering from 100 to 1000 eV in units of πa_0^2.

E (eV)	A	B	C
100	1·28	1·21	1·59
200	0·80	0·76	0·95
300	0·60	0·54	0·70
400	0·50	0·32	0·55
500	0·42	—	0·46
1000	0·24	—	0·26

A de Heer *et al* (1974).
B Normand (1930).
C Born approximation from equation (4).

† $A = -\mathrm{Re}\,F(k=0)$.

Asymptotically, it is again assumed that the total cross sections given by the Born approximation are accurate. The expression† for this, given in paper I,

$$Q(k) = \frac{1}{k^2}\left(6{\cdot}18 + 3{\cdot}011 \ln k^2 - \frac{4{\cdot}06}{k^2} + \frac{2{\cdot}23}{k^4}\right) \tag{4}$$

has recently been confirmed by Inokuti and McDowell (1974). To join the measured region to the asymptotic region two methods were used: (a) a quadratic interpolation was made linking the data at the two highest energies given by de Heer *et al* with the Born cross section at 1500 eV; (b) the measured cross section was fitted to the form

$$\frac{1}{k^2}\left(6{\cdot}18 + 3{\cdot}011 \ln k^2 + \frac{A}{k^2} + \frac{B}{k^4}\right) \tag{5}$$

which has the same leading terms as (4). The values of A and B were found to be

$$A = -178{\cdot}4 \qquad \text{and} \qquad B = 4875{\cdot}4.$$

It was found that the results of using methods (a) and (b) differed only by a few per cent and as (b) seems preferable on physical grounds, numerical results are given for this case.

The values of the scattering length and the low energy Born amplitudes were those used in paper I ($A = 1{\cdot}15, f_B^D(0) = 0{\cdot}791, f_B^E(0) = 3{\cdot}833$). The value of $f_B^E(0)$ was corrected as before by the sum rule (3), (for details see paper I) and the corrected value is $f_D^E(0) = 4{\cdot}309$.

The revised values of Re $f(k)$ and the forward scattered intensity $I(k)$ for elastic scattering are given in table 3 for a number of energies. Comparison with the results of papers I and II shows a small increase in $I(k)$ at energies below 100 eV and a small decrease above this energy. The differences are generally less than 15%, so that the main conclusions of papers I and II are confirmed. Naccache and McDowell (1974) have made a new phase shift analysis of the low energy data, using a more recent and more accurate data set than that of paper I. From the new phase shifts, Re $f(k)$ can be calculated and some values are included in table 2. The error in these values of Re $f(k)$ is considered to be of the order of 12%. The errors in the values arising from the dispersion relations are not possible to estimate very closely, because the errors in the cross sections of Normand in the energy region 20–100 eV are not known. In the region less than 10–15 eV, the dispersion relation integrand will be influenced largely by the data of Golden and Bandel and in this region the errors are of the order of 10 to 15%, so that agreement between the phase shift analysis and the dispersion relation result is within the combined errors. In the energy region 10–20 eV, Re $f(k)$ from the dispersion relation is up to 20% larger than that predicted by the phase shift analysis, which may indicate that the Normand cross sections are a little large.

At higher energies from 100 to 500 eV, the new predictions of $I(k)$ are now in close agreement with the values obtained by extrapolating experimental differential scattering data to zero angle given in paper II. New absolute measurements of the elastic scattering differential cross section have been published by Bromberg (1974).

Near the forward direction, the measurements extend to 2° and cover the energy range 200–700 eV. We have extrapolated these results to the forward direction using the two methods (known as methods I and III) found to be the most satisfactory in paper II. Details of the parametric forms are given in paper II and will not be repeated here. The fits were made over the angular range 2–20° (2–10° for $E = 200$ eV), assuming a statistical

† Here and elsewhere, total cross sections are in units of πa_0^2.

Table 2. The real part of the forward elastic scattering amplitude and the forward intensity for electron–helium collisions. $I(k) = |\mathrm{Re}\, f(k)|^2 + (k^2/16)[Q_{\mathrm{tot}}(k)]^2$ is the forward elastic scattered intensity in units of a_0^2, with $\mathrm{Re}\, f(k)$ from the dispersion relation.

	$\mathrm{Re}\, f(k)$		$I(k)$		
E (eV)	A	B	C	D	E
3·1	−0·18	—	0·58	—	—
5·1	0·20	0·21	0·79	—	—
7·1	0·49	0·47	1·10	—	—
9·1	0·72	0·67	1·41	—	—
13·1	1·08	0·96	2·01	—	—
17·1	1·35	1·15	2·62	—	—
50·0	1·93	—	4·31	—	—
100	1·91	—	4·27	—	—
200	1·61	—	3·27	2·89	2·73
300	1·42	—	2·57	2·51	2·46
400	1·33	—	2·20	2·22	2·20
500	1·29	—	2·04	1·88	1·91
700	1·25	—	1·93	1·43	1·47

A Re $f(k)$ from the dispersion relation.
B Re $f(k)$ from the phase shifts of Naccache and McDowell (1974).
C The value of $I(k)$ found from the dispersion relation.
D The value of $I(k)$ obtained by extrapolating the data of Bromberg (1974) to the forward direction, using method I.
E The same, using method III.

Table 3. Total cross sections for positron–neon scattering in units of πa_0^2.

E (eV)	A	B
100	2·44	9·38
200	1·80	5·35
300	1·25	3·79
400	0·95	2·95
600	0·92†	2·06
800	0·88†	1·59
1000	0·81†	1·30
1500	0·67†	0·90
2000	0·49†	0·69
3000	0·41†	0·48
5000	0·27†	0·30

A Measured cross section to 400 eV. Above 400 eV the values with daggers attached are from the extrapolation (7).
B The Born approximation values from (6).

error of 1 %, except that where the quoted errors were larger these were employed. The values obtained are subject to an overall normalization error of ±2·5 %. The results are shown in table 2, compared with the value of $I(k)$ obtained from the dispersion relation. From 300–500 eV, the agreement is close, but at the highest energy (700 eV) the extrapolated value from the data of Bromberg falls nearly 30 % below the value from the dispersion relation. This is rather difficult to understand unless either the differential

cross section or the total cross section estimates are badly in error at this energy. At the lowest energy where comparison is possible (200 eV) the dispersion relation result is again rather high compared with that from the extrapolation. In contrast to the fits for 300 to 700 eV, neither form I nor III provided a good fit at 200 eV, suggesting that the random errors at this energy are larger than those assumed. Any increase in these errors makes the extrapolation more uncertain but the disparity in the two values may be connected with the suspicion that the total cross section measurements in the 20–100 eV region are somewhat too large.

The general consistency of experiment with the dispersion relations is clearly satisfactory, but more closely determined total cross sections with fully analysed errors are still required in the region from 20 to 500 eV for results of greater precision to be obtained.

3. Positron scattering by helium

For scattering by positrons, the basic relations (1), (2) and (3) apply, provided the exchange amplitude $f_B^E(k)$ is set to zero. To apply the dispersion relations, only the energy-independent parameters f_B^D and the scattering length are required. For positron–helium scattering, the direct Born amplitude has the same magnitude, but is of opposite sign to the case of electron–helium scattering, so we have $f_B^D = -0{\cdot}791$. The momentum transfer cross section at thermal energies has been measured by Leung and Paul (1969) to be $1{\cdot}05\pi a_0^2$ which corresponds to a scattering length of $|A| = 0{\cdot}5$. This is consistent with a theoretical evaluation by Humberston (1973) who obtained the value $-0{\cdot}472$†. Taking the theoretical value for A, the left hand side of the sum rule (3) has the value 1·26, with an error probably not exceeding 5%.

To calculate the right hand side of the sum rule, one of two independent sets of measurements can be used: those of Jaduszliwer and Paul (1973) and Jaduszliwer *et al* (1974) covering the ranges 4 to 16 eV and 16 to 270 eV respectively and those of Coleman *et al* (1974) from 2·0 to 400 eV. Jaduszliwer *et al* (1974) have calculated the integral on the right hand side of the sum rule from their data. They find the value of the right hand side of the sum rule is in the range 1·39 to 1·42 depending on the details of the extrapolation to the high energy region‡. The sum rule is thus satisfied to within about 10%, the indications being that the measured total cross section is a little large.

We have repeated the sum rule test using the alternative data of Coleman *et al* (1974). Their cross sections are everywhere smaller than those of Jaduszliwer *et al* (1974), the maximum difference being of the order of 20% near 20 eV. The cross sections of Coleman *et al* extrapolate very smoothly to the total cross section for the Born approximation, with the result that the right hand side of the sum rule has the value $1{\cdot}24 \pm 0{\cdot}05$, for both extrapolation methods (a) and (b). For this case, the coefficient appearing in the extrapolation (b), equation (5), are $A = -83{\cdot}56$ and $B = -16{\cdot}36$. We conclude that the data of Coleman *et al* fits the sum rule significantly better than those of Jaduszliwer *et al*.

Having checked the consistency of the total cross section with the dispersion relations, the subtracted dispersion relation (2) was employed to predict Re $f(k)$ from both the data of Coleman *et al* and of Jaduszliwer *et al*. The results at the lower energies are displayed in figure 1 for energies up to 12 eV. In this energy region, the differences

† Earlier work by Drachman (1968) and Houston and Drachman (1971) suggests slightly more negative values for A, $-0{\cdot}511$, $-0{\cdot}524$ respectively.

‡ We have also obtained the value of 1·39 using the data of Jaduszliwer *et al* with our extrapolation method (a).

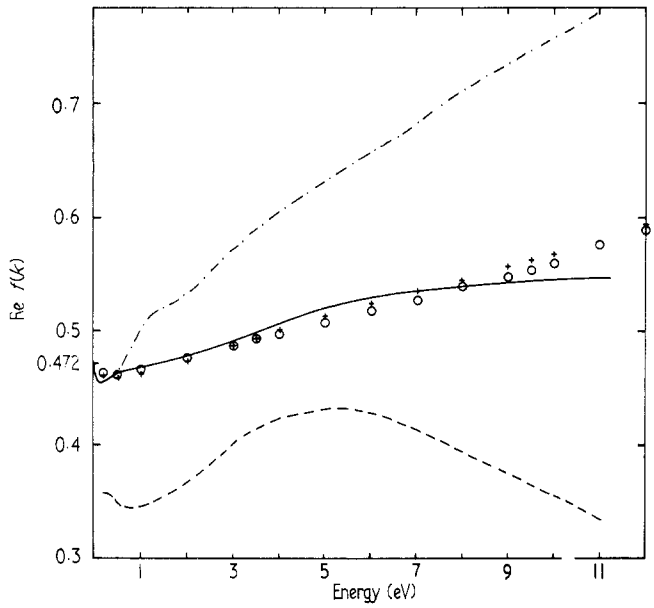

Figure 1. The real part of the elastic forward scattering amplitude for positron scattering by helium. +, calculated from the forward dispersion relation using the data of Jaduszliwer *et al* (1974); ○, calculated from the forward dispersion relation using the data of Coleman *et al* (1974); ——, calculated from the s-wave phase shift of Humberston (1973) and the lowest of the p- and d-wave phase shifts given by Drachman (1966)†; · – · – ·, calculated from the s-wave phase shift of Humberston (1973) and the p- and d-wave phase shifts of Drachman (1971)†; – – – –, calculated from the $l = 0, 1, 2, 3$ phases of Aulenkamp *et al* (1974)†.

†Allowance is made for higher order phase shifts—see text.

between Re $f(k)$ predicted from the two data sets are quite small, not exceeding 1 %, and Re $f(k)$ is well determined. There are several sets of low-energy partial wave calculations: Drachman (1966, 1968, 1971), Houston and Drachman (1970), Humberston (1973), Wardle (1973) and Aulenkamp *et al* (1974). Although there is some measure of agreement between the calculated s-waves there is none between the sets of calculated p- and d-wave phases. In figure 1, we show Re $f(k)$ determined from the theoretical phase shifts in three ways. For the first, we have taken the s-wave of Humberston together with the lowest of the four sets of p- and d-phase shifts given by Drachman (1966). For the second, we have again taken the s-wave of Humberston but with the p- and d-phase shifts of Drachman (1971) and for the third we have used the s-, p-, d- and f-phase shifts calculated by Aulenkamp *et al*. It is essential in calculating Re $f(k)$ to allow for the effect of higher phase shifts and in each case, these were calculated from the expression

$$\delta_L \simeq \frac{\pi P k^2}{(2L-1)(2L+1)(2L+3)}$$

where P is the dipole polarizability of helium. It can be seen that there is considerable disagreement between the three curves which can be ascribed to the difference between the phases for $l > 0$. Only the lowest p- and d-waves of Drachman (1966) when combined with the s-wave of Humberston give good agreement up to about 8 eV with the

values derived from both experiments and we can conclude that these p- and d-waves are likely to be the most accurate. However the total cross section calculated from this set of phases is in significantly better agreement at these energies with the data of Coleman *et al* than that of Jaduszliwer and Paul (Humberston 1974).

4. Positron scattering by neon

Coleman *et al* (1974) have also measured† the total cross section for positron scattering by neon from 2 to 400 eV. For this case Bransden *et al* (1973) have obtained the value $f_B^D = 3{\cdot}12$ using Hartree–Fock wavefunctions, while Inokuti and McDowell (1974) using the configuration interaction results of Peixoto *et al* (1969) obtained $f_B^D = -3{\cdot}32$, the value that we use in this paper. No direct measurement of the thermal cross section has been reported, but Montgomery and LaBahn (1970) have calculated the scattering length from a polarized orbital model and find the value $A = -0{\cdot}6$. This value is consistent with the low-energy scattering data, but we adopt it here, giving the left hand side of the sum rule the value 3·93.

To calculate the integral over the total cross section we again have to connect the data which is available up to 400 eV with the Born approximation result, which is (Inokuti and McDowell 1974)

$$Q_{\text{tot}} = \frac{1}{k^2}\left(63{\cdot}29 + 7{\cdot}7 \ln k^2 - \frac{90{\cdot}3}{k^2} + \frac{131{\cdot}0}{k^4}\right). \tag{6}$$

Whereas by 200 eV, the total cross section for positron–helium scattering is already within 20 % of the Born value, the position is very different for neon, where the measured cross section is only one third of the Born value‡ at 400 eV. Nevertheless, the smooth behaviour of the total cross section allows an extrapolation by method (b) of the form

$$Q_{\text{tot}} = \frac{1}{k^2}\left(63{\cdot}29 + 7{\cdot}7 \ln k^2 + \frac{A}{k^2} + \frac{B}{k^4}\right) \tag{7}$$

with coefficients $A = -3274, B = 43\,155$. Some cross section values and the extrapolated values are shown in table 3. With this extrapolation, the right hand side of the sum rule becomes $3{\cdot}71 \pm 0{\cdot}18$. The sum rule is well satisfied, if we assume a reasonable error on the calculated scattering length, of the order of 5 %.

As in the case of helium, the subtracted dispersion relation can now be used to predict values of $\text{Re}\, f(k)$. This is shown in figure 2, compared with values from the calculations of Montgomery and LaBahn (1970). These authors calculate the phase shifts in two polarized orbital approximations. In the first, only the 2p orbitals were perturbed by d component and in the second both the 2p → d and the 2s → p components were employed. Figure 2 shows clearly that the first procedure leads to $\text{Re}\, f(k)$ in complete disagreement with the dispersion relation, but where both the 2p and 2s orbitals are polarized, fair agreement is obtained.

† This work corrects the values previously reported in Canter *et al* (1972). In the 4–14 eV region other measurements have been published by Jaduszliwer and Paul (1974).

‡ van Wingerden *et al* (1974) have obtained evidence that for electron–neon scattering the Born approximation is not accurate until the keV region is reached.

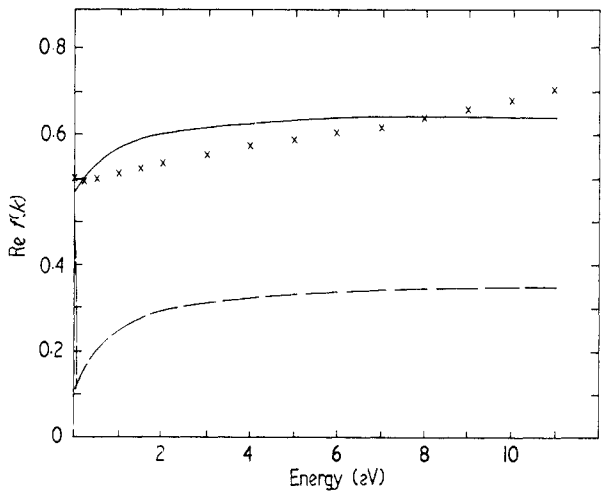

Figure 2. The real part of the elastic forward scattering amplitude for positron scattering by neon. ×, calculated from the forward dispersion relation using the data of Coleman *et al* (1974); ——, curve A from the calculations of Montgomery and LaBahn in the (2s–p and 2p–d) approximation; – – – –, curve B in the (2p–d) approximation.

5. Conclusions

Although the positron–helium and positron–neon cross sections fit the dispersion relation sum rule well and meaningful predictions of Re $f(k)$ can be given, it would be desirable to extend direct measurements to higher energies so that the errors associated with the extrapolation to the high-energy Born approximation could be assessed more accurately. Extension of the work to other systems is quite straight-forward as the constant f_B^D required can be determined accurately. For electron–helium scattering further progress requires more precise measurements of the total cross section about 20 eV, with well-defined errors. Work has been in progress for some time by the Durham and Royal Holloway College groups on the application of the electron scattering dispersion relations to atoms other than helium (see McDowell 1974). The chief difficulty has proved to be the calculation of the exchange Born amplitude $f_B^E(k)$, with sufficient accuracy. It has been established that Hartree–Fock wavefunctions are inadequate for this purpose. For example, in electron–neon scattering the sum rule predicts that $f_B^E(0)$ should be 8·21, which can be compared with the Hartree–Fock value of 5·9 (Bransden *et al* 1973).

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