

Numerical study of the dispersion relation for e^- -H scattering

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Abstract. Numerical studies of the dispersion relation for forward scattering are reported for electrons scattered by atomic hydrogen. As has previously been shown for electron-helium scattering, the relation of Gerjuoy and Krall has to be modified. The extra term to be included, the so-called discrepancy function $\Delta(E)$, is related to the non-analyticity of the exchange part of the scattering amplitude for negative energies. This function, which corresponds to an integral over the left-hand cut discontinuity, is evaluated.

1. Introduction

Recently a number of papers have appeared on the analytic structure of the elastic forward electron-atom scattering amplitude (see de Heer *et al* 1976 and references therein). It has become clear that the forward dispersion relation for electron-atom scattering, as formulated by Gerjuoy and Krall (1960, 1962) is not satisfied by current experimental and theoretical data. This may be either because there are unsuspected and substantial errors in these data, or because the dispersion relation is false, or both. A number of authors (see e.g. Byron *et al* 1976, Burke and Blum 1977) have noted that the first Born approximation to the elastic exchange amplitude contains a singularity at minus the binding energy, $E = -E_b$, and for atoms other than hydrogen perhaps other singularities to the left of this on the real axis in the complex energy plane. In fact it can be demonstrated for an arbitrary electron-atom system that the direct amplitude is analytic apart from the spectrum of the full Hamiltonian, whereas the Born contribution to the exchange amplitude is analytic except on the negative energy axis to the left of $-E_b$. In general the possibility cannot be excluded that the remaining part of the exchange amplitude is non-analytic on the whole negative real energy axis (Tip 1977). If the contribution from the latter does not compensate that of the exchange Born part, the Gerjuoy-Krall dispersion relation is invalidated. This leads to an extra term, the discrepancy function $\Delta(E)$, on the right-hand side of this dispersion relation.

The purpose of this paper is to extend the work of de Heer *et al* (1976)—to estimate the discrepancy function for the electron-hydrogen-atom system. We rely heavily on the study of Hutt *et al* (1976), but modify their approach in a number of ways and extend it to a wider range of energies.

2. The Gerjuoy-Krall dispersion relation

The dispersion relation of Gerjuoy and Krall (1960) for e^- -H scattering is given by

$$\begin{aligned} \operatorname{Re}[f^D(E, 0) - \tfrac{1}{2}f^E(E, 0)] \\ = f_B^D(E, 0) - \tfrac{1}{2}f_B^E(E, 0) + \frac{P}{\pi} \int_0^\infty \frac{\operatorname{Im}[f^D(E', 0) - \tfrac{1}{2}f^E(E', 0)]}{E' - E} dE' - \tfrac{1}{2}\tilde{R}(E) \end{aligned} \quad (1)$$

where $f^D(E, 0)$ and $f^E(E, 0)$ are, respectively, the exact forward direct and exchange elastic scattering amplitudes at impact energy E and $f_B^D(E, 0)$ and $f_B^E(E, 0)$ are the first Born approximations to them. P indicates the principal value and $\tilde{R}(E)$ is the residue at energy E of $[f(E, 0) - f_B(E, 0)]/[\epsilon(H^-) - E]$ where

$$f(E, 0) = f^D(E, 0) + f^E(E, 0) \quad (2)$$

is the amplitude corresponding to singlet scattering ($S = 0$); $\epsilon(H^-)$ is the binding energy of the singlet bound state $H^-(1s)^2\ ^1S_0$. It appears from the work of de Heer *et al* (1976) for electrons on He that equation (1) must be supplemented on the right-hand side with an additional term $\Delta(E)$, the discrepancy function, which is related to the left-hand cut singularity in the exchange amplitude. The residue $\tilde{R}(E)$ can be represented by

$$\tilde{R}(E) = \frac{R}{k^2 + |\epsilon(H^-)|} \quad (3)$$

where k^2 corresponds to the energy E in rydbergs, and the expression and evaluation of R has been discussed extensively by Hutt *et al* (1976). We shall use the same numerical values for R and $\epsilon(H^-)$ in this paper, respectively equal to 0.6271 and 0.055495 Ryd.

For the principal-value integral, the imaginary part of the scattering amplitude is given by

$$\operatorname{Im}[f^D(E', 0) - \tfrac{1}{2}f^E(E', 0)] = (k'/4\pi)\sigma_t(E') \quad (4)$$

where k' is the wavenumber of the incident electrons and $\sigma_t(E')$ is the cross section for total scattering of electrons at the corresponding energy E' . In order to test the dispersion relation numerically, Hutt *et al* (1976) have taken both theoretical and experimental data to construct $\sigma_t(E)$ over the entire energy range. In general we shall follow their procedure, with small modifications as discussed below. On the right-hand side of equation (1) $f_B^D(E, 0)$ is equal to a_0 and $f_B^E(E, 0)$ is given by

$$f_B^E(E, 0) = \frac{2}{(1 + k^2)^3} (3 - \tfrac{10}{3}k^2 - k^4)a_0. \quad (5)$$

Substituting the calculated values for the quantities on the right-hand side of equation (1), it is possible to evaluate $\operatorname{Re}[f^D(E, 0) - \tfrac{1}{2}f^E(E, 0)]$ at every energy E .

We determine $\Delta(E)$, introduced before, by taking the difference between these values from the dispersion relation and the values obtained from *a priori* theoretical calculations at low and high energies, and corresponding estimates, which are further discussed below, at intermediate energies.

In previous work the so-called subtracted dispersion relation has often been used for the analysis, where (1) is written in a form obtained by taking the difference

of $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$ at energy E and energy zero. It has been remarked, however, that both the subtracted and unsubtracted dispersion relations lead to the same 'dispersion value' of $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$ if (1) is valid at zero energy (see, for instance, Bransden and McDowell 1969, Bransden and Hutt 1975). In our case we evaluate a discrepancy function at zero energy, with which (1) is supplemented to be valid. So our forms of subtracted and unsubtracted dispersion relations will lead to the same results in the evaluation of $\Delta(E)$ at any energy. This can be proved analytically and has been confirmed numerically by us. Therefore, we shall confine ourselves to the evaluation of $\Delta(E)$ from (1).

3. Total cross sections

For the estimation or calculation of the total cross sections we have modified the procedure used by Hutt *et al* (1976). Below the inelastic threshold ($k^2 = 0.75$) we took their total cross sections calculated using the variational s-, p- and d-wave phaseshifts of Schwartz (1961), Armstead (1968) and Gailitis (1965) (see also Drachman and Temkin 1972), allowing for higher partial-wave phaseshifts by the expression

$$\delta_l \simeq \frac{\pi P k^2}{(2l-1)(2l+1)(2l+3)} \quad (6)$$

where P is the dipole polarizability of atomic hydrogen and k is the momentum. These theoretical cross sections are given in table 1 up to $k = 0.8 a_0^{-1}$.

Above the inelastic threshold we evaluated the total cross sections by adding total cross sections for ionization, excitation and elastic scattering, taken partly from experiment and partly from theory.

Let us first consider the total elastic cross sections above the inelastic threshold. Between 10 and 50 eV we obtained our σ_{el} data in tables 1 and 2 by interpolation between the theoretical values given by Callaway and Williams (1975) between 10 and 30 eV and those given by J Callaway (1976 private communication) at 54.4 eV. Between 50 and 400 eV we have used the differential elastic scattering data of Lloyd

Table 1. Cross sections for total (σ_t) and total elastic (σ_{el}) scattering between 0 and 20 eV in units of πa_0^2 . Below the inelastic threshold, $\sigma_t = \sigma_{el}$.

$k(a_0^{-1})$	$E(\text{eV})$	σ_{el} theory	σ_t adopted
0.1	0.136	43.13	42.90
0.2	0.544	32.54	32.30
0.3	1.22	24.06	23.95
0.4	2.18	18.65	18.65
0.5	3.40	15.03	14.95
0.6	4.90	12.27	12.22
0.7	6.66	10.01	10.03
0.8	8.70	8.205	8.173
0.9	11.0		6.625
1.0	13.6		5.506
1.1	16.5	4.16	4.845
1.2	19.6	3.41	4.582

Table 2. Different total cross sections between 20 and 400 eV in units of πa_0^2 .

$E(\text{eV})$	σ_{exc}^a	σ_{exc}^b	σ_{ion}^a	σ_{ion}^b	σ_{inel}^a	σ_{inel}^b	σ_{el}^a	σ_{el}^c	σ_{t}^a	σ_{t}^c	σ_{t}^d	σ_{t}^e
20	1.17		0.311		1.48		3.35		4.83		4.57	
25	1.30		0.49		1.79		2.57		4.36		4.32	
30	1.37		0.61		1.98		2.01		3.99		4.05	
35			0.68								3.83	
40	1.36		0.75		2.11		1.40		3.51		3.62	
50	1.32	1.61	0.77	0.991	2.09	2.60	1.00	0.560	3.09	3.06	3.28	3.88
60		1.46	0.785	0.980		2.44					3.00	
70	1.20	1.34	0.775	0.940	1.98	2.28				2.77	2.77	
80		1.24	0.760	0.892		2.14				2.50	2.50	
90	1.10	1.16	0.74	0.843	1.84	2.00				2.33	2.33	
100	1.04	1.08	0.715	0.796	1.76	1.88	0.60	0.299	2.36	2.18	2.18	2.39
150	0.832	0.829	0.580	0.616	1.41	1.45				1.65	1.65	
200	0.700	0.679		0.500	1.20	1.18	0.22	0.154	1.42	1.33	1.33	1.40
300		0.505		0.365		0.871				0.975	0.975	1.00
400		0.408		0.289		0.697	0.065	0.0781	0.762	0.775	0.775	0.797

^a See text.^b Kim and Inokuti (1971) Bethe approximation.^c Born approximation.^d Adopted.^e Byron and Joachain (1975) eikonal-Born series approximation.

et al (1974) and Williams (1975). We have calculated σ_{el} from these data by integration:

$$\sigma_{\text{el}} = 2\pi \int_0^\pi \sigma_{\text{el}}(\Theta) \sin \Theta \, d\Theta. \quad (7)$$

Because data were only available between a lower angular limit $\Theta_m \neq 0$ and an upper angular limit $\Theta_M \neq \pi$, we had to split up the integral into three parts as done by de Heer and Jansen (1975) and extrapolate the data in the angular intervals $(0, \Theta_m)$ and (Θ_M, π) . The experimental data used extended between $\Theta = 15^\circ$ or 20° and $\Theta = 140^\circ$. The angles Θ_m and Θ_M were taken as 10° and 140° respectively. The missing data below 15° and 20° were obtained by using theoretical cross sections of Byron and Joachain (1975) in the eikonal-Born series (EBS) approximation. The theoretical data were normalized to experiment at the smallest angle where measurements had been taken.

The splitting of the integral leads to

$$\sigma_{\text{el}} = 2\pi[I(0, \Theta_m) + I(\Theta_m, \Theta_M) + I(\Theta_M, \pi)] \quad (8)$$

where

$$I(x, y) = \int_x^y \sigma_{\text{el}}(\Theta) \sin \Theta \, d\Theta \quad 0 < \Theta_m < \Theta_M < \pi. \quad (9)$$

$I(\Theta_m, \Theta_M)$ was calculated by numerical integration; $I(0, \Theta_m)$ and $I(\Theta_M, \pi)$ were obtained by extrapolation of the integrand $\sigma_{\text{el}}(\Theta) \sin \Theta$ by a parabolic function for $0 \leq \Theta \leq \Theta_m$ and a linear function for $\Theta_M < \Theta < \pi$. The results of this procedure are given in table 3. We take the average of the experimental values and compare them with EBS (Byron and Joachain 1975), Born (Byron and Joachain 1975, Inokuti and McDowell 1974) and pseudo-state close-coupling distorted-wave calculations of J Callaway (1976 private communication) at 54.4 eV. The point at 50 eV of Callaway was obtained by interpolation.

Table 3. σ_{el} in units of πa_0^2 between 50 and 400 eV.

$E(\text{eV})$	Experiment			Theory		
	Lloyd <i>et al</i> (1974)	Williams (1975)	Average	EBS	Born	Callaway
50	1.19	1.24	1.22	1.37	0.560	1.00
100	0.605	0.588	0.597	0.496	0.299	
200	0.231	0.204	0.217	0.200	0.154	
400		0.0653	0.0653	0.0881	0.0781	

The ionization cross sections in table 2 were evaluated by taking the average values of the experimental data of Boyd and Boksenberg (1959) and of Fite and Brackman (1958). The difference between the two sets of data is generally small ($\lesssim 5\%$). Above 150 eV the theoretical (three-term) Bethe data of Kim and Inokuti (1971, equations (47a), (47c)) have been used and almost coincide with the experimental data.

The excitation cross sections were calculated in the following way. From threshold to 200 eV we adopted the hybrid (pseudo-state close-coupling distorted-wave) 2s and 2p calculated cross sections of Callaway *et al* (1975) and McDowell *et al* (1975) just as done by Hutt *et al* (1976). These are within $\pm 10\%$ of the experimental values (normalized to the Williams and Willis (1974) value for σ_{2p} at 11.02 eV) of Long *et al* (1968) and Kauppila *et al* (1970). Similarly for $n = 3$ we adopted the values of Syms *et al* (1975), which are in close agreement with the experimental values of Mahan (1974). The higher excited levels have been accounted for by assuming that the cross sections for excitation of level n is proportional to n^{-3} , so that

$$\sigma_{\text{exc}} = \sigma(n = 2) + 2.08 \sigma(n = 3). \quad (10)$$

In table 2 we see that the σ_{exc} cross sections thus obtained are consistent with the Bethe excitation cross sections of Kim and Inokuti (1971, equation (46)) for $m/M = 1$ above about 100 eV.

We obtain σ_{inel} by adding σ_{ion} and σ_{exc} and compare it again with the 'sum-rule' data of Kim and Inokuti (1971, equations (45a), (45c)).

The total cross section σ_{t} is then obtained by adding σ_{el} and σ_{inel} and compared to the Born value and that of the eikonal-Born series (see Byron and Joachain 1975). Again, as we have found before for He (see de Heer and Jansen 1975) at energies where σ_{el} and σ_{inel} deviate strongly from the Born approximation, their sum σ_{t} is well approximated by it. The Born approximation used for σ_{t} is the sum of the (three-term) Bethe cross section of Kim and Inokuti (1971) and the Born cross section of Inokuti and McDowell (1974):

$$\sigma_{\text{inel}} = 4 \frac{R}{E} \left(\ln \frac{E}{R} + 1.836 - \frac{11}{4} \frac{R}{E} \right) \pi a_0^2 \quad (11)$$

where R is the Rydberg energy and

$$\sigma_{\text{el}} = (2.333 k^{-2} - 1.0 k^{-4}) \pi a_0^2 \quad (12)$$

where k^2 is the energy in rydbergs.

Both the calculated and Born values for σ_{t} approach the eikonal-Born series cross sections at higher energies. For use in (1) and (4), the calculated and theoretical

total cross sections presented in tables 1 and 2 were approximated by the following expressions in units of πa_0^2 :

$$\begin{aligned}
 E = 0-0.544 \text{ eV} & \quad \sigma_t = 44.79 + 126.37k - 254.37k^2 + 4479.43k^4 + 269.94k^2 \ln k^2 \\
 E = 0.544-3.40 \text{ eV} & \quad \sigma_t = 43.6405 - 338.307k^2 + 1572.09k^4 - 2711.64k^6 \\
 E = 3.40-8.70 \text{ eV} & \quad \sigma_t = 26.7644 - 66.3173k^2 + 89.5618k^4 - 48.8123k^6 \quad (13) \\
 E = 8.70-20 \text{ eV} & \quad \sigma_t = 20.5258 - 29.2481k^2 + 17.8783k^4 - 3.6501k^6 \\
 E = 20-70 \text{ eV} & \quad \sigma_t = 8.1265539 + 0.64400942k^2 - 0.04242931k^3 \\
 E = 70 \text{ eV}-\infty & \quad \sigma_t = 9.677k^{-2} - 12k^{-4} + 4k^{-2} \ln k^2.
 \end{aligned}$$

The expression used between 70 eV– ∞ represents the Born approximation as derived from $\sigma_{el} + \sigma_{inel}$ as given before. The functions for the region below 20 eV are the same as used by Hutt *et al* (1976). The values of σ_t used for the principal-value integral, corresponding with these expressions are listed as ‘adopted’ both in tables 1 and 2. The reliability of the adopted σ_t values is believed to be within the error limit of 10%.

4. Numerical study of the dispersion relation

By means of the expressions just quoted and equation (4) the principal-value integral has been calculated analytically. As we have stated before (de Heer *et al* 1976), this method introduces no significant error provided the energy at which the integral is evaluated does not lie too close to the boundary of an interval where we change from one expression to another. In such cases the boundary between the relevant intervals has been shifted. The coefficients of the expressions have been fitted in such a way that, extending the length of one interval by 15% at the side of the critical boundary, a deviation of at most 3% is introduced in the σ_t value of the new end-point as compared to the σ_t value of the expression used before. Taking the exact theoretical values for $f_B^D(E,0)$, $f_B^E(E,0)$ (see equation (5)) and the approximate $\tilde{R}(E)$, we calculate $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$ by means of equation (1), the result of which is given under the column ‘dispersion’ in table 4. These values of $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$ are compared with those from theory. The theoretical values up to $k = 0.8 a_0^{-1}$ have been obtained by using the variational phaseshifts. The theoretical $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$ at 50, 100, 200, 300 and 400 eV are from the EBS calculations (Byron and Joachain 1975). However, we know that this theory is accurate almost to order $1/k^2$ and may break down at below about 100 eV. In the region 10–150 eV the $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$ values have been estimated in the following way. The differential elastic cross section in the forward direction can be expressed as

$$\sigma_{el}(E,0) = \{\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]\}^2 + \{\text{Im}[f^D(E,0) - \frac{1}{2}f^E(E,0)]\}^2. \quad (14)$$

Here the imaginary part follows via equation (4) from the σ_t values adopted (see tables 1 and 2) corresponding to the expressions quoted before. At $k = 0.95-1.5$ and $k = 2.0 a_0^{-1}$ we take the $\sigma_{el}(E,0)$ values calculated by Callaway and Williams (1975) and J Callaway (1976 private communication) so that by means of equation (14) the real part of $f^D - \frac{1}{2}f^E$ can be calculated. These numbers are quoted under the

Table 4. Real part of the forward elastic scattering amplitude; $\Delta(E)$ is the discrepancy function (both in units a_0).

$k(a_0^{-1})$	$E(\text{eV})$	$\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$			$\Delta(E)$
		Dispersion	Theory	Estimated ^a	
0	0	-2.11	-2.82		0.71
0.1	0.136	-1.48	-2.16		0.68
0.2	0.544	-0.302	-1.02		0.72
0.3	1.22	0.674	0.10		0.57
0.4	2.18	1.50	0.95		0.55
0.5	3.40	1.94	1.56		0.38
0.7	6.66	2.65	2.31		0.34
0.95	12.2	3.02		2.69	0.33
1.1	16.5	3.24		2.65	0.59
1.2	19.6	3.34		2.62	0.72
1.3	23.0	3.32		2.60	0.72
1.4	26.7	3.28		2.54	0.74
1.5	30.6	3.22		2.51	0.71
1.71	40	3.06		2.44	0.62
1.92	50	2.90	3.11	2.38	0.52
2.00	54.4	2.84		2.36	0.48
2.27	70	2.62		2.28	0.34
2.42	80	2.53		2.24	0.29
2.71	100	2.37	2.40	2.17	0.20
3.32	150	2.10		2.04	0.06
3.83	200	1.94	1.94		0
4.70	300	1.75	1.75		0
5.42	400	1.64	1.64		0
6.06	500	1.57			
8.57	1000	1.39			

^a See §4.

column 'estimated' of table 4. The other estimated numbers at $k = 1.5$ – $3.38 a_0^{-1}$ have been derived by graphical interpolation (see figure 1). In this figure we have plotted both the 'dispersion' (right-hand side of equation (1)), theoretical and estimated values of $\text{Re}[f^D(E,0) - \frac{1}{2}f^E(E,0)]$. The difference is equal to the function $\Delta(E)$ (we have omitted the negative sign, see both figure 1 and table 4) missing in equation (1). Just as found before for e^- -He (de Heer *et al* 1976) the behaviour of $\Delta(E)$ is consistent with the existence of a left-hand cut singularity in the exchange amplitude. Thus if the left-hand cut begins at $E = -E_b = -1$ and $\rho(E)$ is the discontinuity across this cut then

$$\Delta(E) = \frac{P}{\pi} \int_{-1}^{+\infty} \frac{\rho(E') dE'}{E + E'} \quad (15)$$

and for reasonably behaved $\rho(E)$ vanishes for sufficiently large E . Work on inverting this expression to obtain the discontinuity function $\rho(E)$ is in hand.

The structure in $\Delta(E)$ is not well understood. However, the peak at higher energies appears to be closely associated with the opening of the first and higher inelastic channels. It might also be due to inaccuracies in our adopted inelastic cross sections at intermediate energies. However, we have checked this by altering these cross sections between 0 and 70 eV by multiplying them with the function $[1 + a(1 - E/70)]$, and

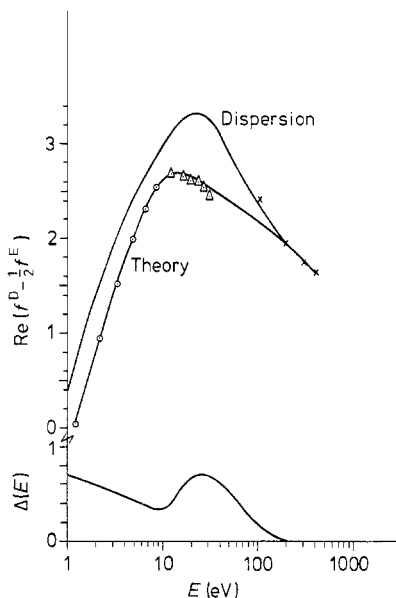


Figure 1. Real part of the forward elastic scattering amplitude $\text{Re}(f^D - \frac{1}{2}f^E)$ and $\Delta(E)$ (see text) as functions of electron impact energy. \circ Schwartz (1961), Armstead (1968) and Gailitis (1965); \triangle Callaway and Williams (1975); \times Byron and Joachain (1975).

using for a the values ± 0.20 and ± 0.10 respectively. Although the $\Delta(E)$ values near $E = 0$ vary substantially as a function of a , near 12 eV the differences reduce to smaller than 9% already and the peak at higher energies does not show any major change. Such an inelastic peak was not found in e^- -He scattering, where the elastic cross section dominates relatively more than in e^- -H scattering near the inelastic thresholds. At the same time we see a similar structure in the imaginary part of $f^D - \frac{1}{2}f^E$ for e^- -H scattering (see figure 2).

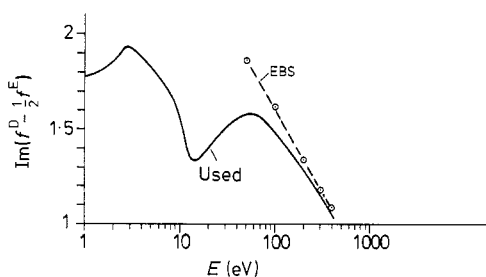


Figure 2. Imaginary part of the forward elastic scattering amplitude $\text{Im}(f^D - \frac{1}{2}f^E)$ as a function of electron impact energy.

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