Validity of dispersion relations for electron-atom scattering

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This paper summarizes the usual assumptions made in applying dispersion relations to electron-atom scattering. It is shown that in the static exchange approximation, electron exchange gives rise to a third-order pole, and the position and strength of this pole are calculated. It is then argued that this singularity is a feature of the exact scattering amplitude. Finally a numerical study is carried out which confirms the existence of additional left-hand singularities.

I. INTRODUCTION

Dispersion relations are of fundamental importance in elementary particle physics. In atomic physics they have been used to analyze experimental data,[1] in particular for forward scattering of electrons on hydrogen and rare-gas atoms. In this paper we discuss the dispersion relation suggested by Gerjuoy and Krall[2] for forward electron-hydrogen-atom scattering:

$$\mathrm{Re}f^{\pm}(k^2,0) = f_B(k^2,0) \pm g_B(k^2,0)$$

$$+ \frac{P}{\pi} \int_0^\infty dk'^2 \frac{\mathrm{Im}f^{\pm}(k'^2,0)}{k'^2 - k^2} + \frac{r}{k^2 - k_b^2}.$$

$$(1)$$

Here f^+ and f^- are the singlet and triplet scattering amplitudes, f_B and g_B are the first Born direct and exchange amplitudes, given by

$$f_B = 1 \quad \text{and} \quad g_B = 2(3 - \tfrac{10}{3}k^2 - k^4)/(k^2 + 1)^3,$$

and the pole term corresponds to the bound state of the negative hydrogen ion which occurs in the singlet state.

The basic assumption from which this dispersion relation follows is that the amplitudes $f^{\pm}(k^2,0)$ $- f_B(k^2,0) \mp g_B(k^2,0)$ are analytic functions in the complex energy plane with the properties (i) both have a branch point at $k^2 = 0$ with the branch cut taken along the positive real energy axis, (ii) the only singularities on the negative real energy axis are poles corresponding to bound states, and (iii) the contour integral over the circle at infinity vanishes. Application of Cauchy's integral formula then leads immediately to Eq. (1).

These assumptions have never been rigorously proved for electron-atom scattering although they are in accord with the analytic behavior of the forward scattering amplitude proved in potential scattering.[3] However, in electron-atom scattering the basic problem stems from the composite nature of the target and the allowance which must be made for electron exchange. That these effects

influence the singularity structure of the scattering amplitude has been shown by Rubin et al.[4] for the case of Yukawa potentials. For electron-atom scattering the validity of dispersion relations have been discussed recently by various authors.[5] Using a combination of experimental data and numerical calculations, they conclude that the dispersion relations used so far are not fulfilled. These results indicate the existence of further singularities, in addition to (i) and (ii) above.

So far, no attempt has been made in atomic physics to determine the nature and the position of these additional singularities. In this paper we make a first step into this direction. Using the static exchange approximation as a model we consider the effect of exchange on the analytic behavior of the amplitude for electron-hydrogen scattering. We show that the electron exchange leads to a third-order pole at $k^2 = -1$, and we evaluate the strength of this pole. This result is related to the modification of Levinson's theorem,[6] proposed by Swan,[7] and we show that it can be expected to be a feature of the exact scattering amplitude. We discuss these topics in Sec. II of this paper. In Sec. III we give results of a numerical study. We first show that the effective range extrapolation is consistent with a higher-order pole in the amplitude, and we test the dispersion relation (1) and the corresponding zero-energy relation in the static exchange approximation. The results show that both relations are only fulfilled if exchange is neglected. Of particular importance in the numerical study is the calculation of the position and the residue of the H⁻ pole term, and we discuss this in some detail.

II. ANALYTIC SOLUTION OF EXCHANGE EQUATIONS

In this section we discuss the singularity structure of the amplitudes $f^{\pm}$. We concentrate on a discussion of the triplet amplitude f^- in the static exchange approximation. At the end of this section we discuss briefly how our results can be general-

ized to the exact amplitude.

In the static exchange approximation the wave function is given by the expression

$$\psi^{\pm}(\vec{r}_1, \vec{r}_2) = \phi(\vec{r}_1)u^{\pm}(\vec{r}_2) \pm \phi(\vec{r}_2)u^{\pm}(\vec{r}_1), \tag{2}$$

where $\phi(\vec{r})$ is the hydrogen ground-state wave function and $u^{\pm}(\vec{r})$ describes the motion of the scattered electron. The upper and lower signs refer to singlet and triplet scattering, respectively.

We start with the observation that the s-wave static Schrödinger equation for triplet scattering is satisfied identically by $u_0(r) = r\phi(r)$ (where u_0 denotes the s-wave function). Therefore each function of the form

$$u_0(r, a) = \overline{u}_0(r) + ar\phi(r) \tag{3}$$

is a solution if $\overline{u}_0$ is a solution (a is an arbitrary parameter). This degeneracy can be removed without modifying the asymptotic form of the wave function for $k^2 > -1$, by requiring that

$$\int_0^{\infty} u_0(r, a)r\phi(r)dr = 0. \tag{4}$$

This orthogonality condition modifies the s-wave Schrödinger equation. It can then be verified that $u_0 = r\phi(r)$ is an eigenfunction of the modified equation belonging to the eigenvalue $k^2 = -1$.[8]

This eigenfunction is clearly connected with the antisymmetry of the wave function (2), that is, with electron exchange. The effect of eigenfunctions of this type on the low-energy behavior of the scattering phases (Levinson's theorem[6]) has been considered by Swan.[7]

We now show that the existence of this eigenfunction leads to a third-order pole in the amplitude at $k^2 = -1$. We transform the s-wave Schrödinger equation (which is an integro-differential equation) into two coupled differential equations:

$$\frac{d^2u_0}{dr^2} + k^2u_0(r) = 2U(r)u_0(r) - 2\phi(r)v(r), \tag{5}$$

$$\frac{d^2v}{dr^2} = -\phi(r)u_0(r). \tag{6}$$

The function $v(r)$ is defined by

$$v(r) = \int_0^r u_0(r)r\phi(r)dr + r\int_r^{\infty} u_0(r)\phi(r)dr, \tag{7}$$

and the local potential is given by

$$U(r) = -(1 + 1/r)e^{-2r}. \tag{8}$$

We are interested in a solution satisfying the boundary conditions ($k^2 > -1$):

$$u_0(0) = v(0) = 0,$$

$$u_0(r) \rightarrow A(k^2)e^{-ikr} + B(k^2)e^{ikr}, \quad r \rightarrow \infty \tag{9}$$

$$v(r) \rightarrow 0, \quad r \rightarrow \infty.$$

The last condition follows from the orthogonality condition (4). The function $A(k^2)$ and $B(k^2)$ determine the s-wave amplitude f_0^- through

$$f_0^- = -\frac{1}{2ik}\left(\frac{B(k^2)}{A(k^2)} + 1\right). \tag{10}$$

We have determined the "Jost functions" $A(k^2)$ and $B(k^2)$ near $k^2 = -1$ by iteration, starting with Eq. (9). We obtained (writing $k = iK$)

$$u_0(r) = Ae^{Kr} + e^{-r}\left[\frac{A}{2(K-1)}\left(1 - \frac{4}{(K-1)^2}\right)e^{(K-1)r} \right.$$
$$\left. + Be^{-(K-1)r}\right] + \cdots, \tag{11a}$$

$$v(r) = -\frac{2A}{(K-1)^2}e^{(K-1)r}$$
$$+ e^{-2r}\left[-\frac{A}{(K-1)(K-3)^2}\left(1 - \frac{4}{(K-1)^2}\right)e^{(K-1)r}\right.$$
$$\left. - \frac{2B}{(K+1)^2}e^{-(K-1)r}\right] + \cdots. \tag{11b}$$

We know that the system has the solution $u_0 = r\phi$ for $k^2 \rightarrow -1$. We therefore require

$$u_0(r) \rightarrow r\phi(r) = 2re^{-r},$$
$$v(r) \rightarrow 1 - (1 + 1/r)e^{-2r}, \tag{12}$$

as $k^2 \rightarrow -1$. The terms neglected in Eq. (11) cannot easily be determined. However, they vanish asymptotically more rapidly than e^{-r} and e^{-2r}, respectively and do not contribute at $k^2 = -1$ in accordance with condition (12).

Comparing Eqs. (11) and (12), we see that A must have a double zero at $k^2 = -1$ and B a simple pole. We normalize to

$$A(K) = a_0(K - 1)^2, \tag{13}$$

where a_0 is a constant. We expand B into a power series

$$B(K) = b_0/(K-1) + b_1 + b_2(K-1) + \cdots. \tag{14}$$

The coefficients a_0, b_0, and b_1 are determined by substituting Eqs. (13) and (14) into Eqs. (11) and equating powers of $(K-1)$. This gives

$$a_0 = -\tfrac{1}{2}, \quad b_0 = -1, \quad b_1 = 0. \tag{15}$$

From this and Eqs. (10) follow

$$f_0^- = -\frac{8}{(k^2+1)^3} + \frac{2}{(k^2+1)^2} + \cdots. \tag{16}$$

Equation (16) shows that f_0^- has a third-order pole at $k^2 = -1$ but with a different coefficient than g_B. Although the total wave function (2) vanishes identically in the limit $k^2 \rightarrow -1$, we see from Eqs. (16) that the pole affects the s-wave amplitude for ener-

gies removed from $k^2 = -1$. Since the pole occurs only in the s wave [because it is associated with the bound state $\phi(r)$], it is unlikely to be cancelled in the full amplitude and will contribute to the dispersion integral.

We now consider briefly how the arguments leading to Eq. (16) may be generalized. We write the exact wave function in the form

$$\psi^{\pm}(\vec{r}_1, \vec{r}_2) = \sum_n [\phi_n(\vec{r}_1) u_n^{(\pm)}(\vec{r}_2) \pm \phi_n(\vec{r}_2) u_n^{(\pm)}(\vec{r}_1)], \quad (17)$$

where the sum includes the integral over all continuum states of the hydrogen atom. We note that the function $\psi^{\pm}$ is invariant under the transformation

$$u_i^{(\pm)} \rightarrow u_i^{(\pm)} + \sum_j a_{ij}^{(\pm)} \phi_j, \quad (18)$$

where the arbitrary parameter $a_{ij}^{(+)}$ $(a_{ij}^{(-)})$ is symmetric (antisymmetric) in the indices i and j for the triplet (singlet) case. As discussed for the static solution, this can be used to ensure that

$$\langle u_i^{(-)} | \phi_j \rangle = 0 \quad \text{for } i \geq j \quad (19)$$

for triplet scattering and

$$\langle u_i^{(+)} | \phi_j \rangle = 0 \quad \text{for } i > j \quad (20)$$

for singlet scattering. The coupled integro-differential equations for $u_i^{(\pm)}$ have bound-state solutions of the type, for the triplet case,

$$\begin{bmatrix} u_1^{(-)} \\ u_2^{(-)} \\ u_3^{(-)} \\ \vdots \end{bmatrix} = \begin{bmatrix} \phi_1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \begin{bmatrix} 0 \\ \phi_2 \\ 0 \\ \vdots \end{bmatrix}, \cdots \begin{bmatrix} \phi_2 \\ \phi_1 \\ 0 \\ \vdots \end{bmatrix}, \begin{bmatrix} \phi_3 \\ 0 \\ \phi_1 \\ \vdots \end{bmatrix}, \cdots \quad (21)$$

and for the singlet case

$$\begin{bmatrix} u_1^{(+)} \\ u_2^{(+)} \\ u_3^{(+)} \\ \vdots \end{bmatrix} = \begin{bmatrix} \phi_2 \\ -\phi_1 \\ 0 \\ \vdots \end{bmatrix}, \begin{bmatrix} \phi_3 \\ 0 \\ -\phi_1 \\ \vdots \end{bmatrix}, \begin{bmatrix} 0 \\ \phi_3 \\ -\phi_2 \\ \vdots \end{bmatrix}, \cdots \quad (22)$$

It is clear that these "bound-state" solutions will give rise to singularities in the full amplitude $f^{\pm}$ in a similar way to those discussed in the static exchange case.

III. NUMERICAL TESTS

A. Effective range expansion

The general arguments given in the Introduction suggest strongly that the relation (1) is not ful-

filled. The discussion in Sec. II shows that indeed "left-hand" singularities, neglected so far in atomic physics, exist. In this section we discuss some numerical tests which support our theoretical arguments.

We start with an investigation of the triplet amplitude f_0^- in the effective range approximation. The s-wave amplitude can be written in the form

$$f_0^- = 1/(k \cot \delta_0^- - ik), \quad (23)$$

where δ_0^- denotes the triplet phase. The usual effective range expansion gives

$$k \cot \delta_0^- = -1/a + \tfrac{1}{2} r_0 k^2 + O(k^4), \quad (24)$$

where a is the scattering length and r_0 the effective range. In this approximation the amplitude has, in general, two poles in k. Under certain circumstances one of the poles represents a bound state (negative ion). The other pole has to do with the potential; it approximates the "left-hand" cut of the partial-wave amplitude.

Plotting $k \cot \delta_0^-$ against k^2 one obtains a straight line within the limits of the approximation (24). The position of the poles is given by the crossing point of this line extrapolated to negative energies with the curve $-(-k^2)^{1/2}$.

We calculated the s-wave phases for triplet scattering numerically using the R-matrix method,[9] and plotted $k \cot \delta_0^-$ against k^2. Figure 1 shows that for triplet scattering the extrapolated line is within numerical error a tangent to this curve close to $k^2 = -1$, consistent with the existence of a higher-order pole in f_0^- in accordance with Eq. (16). The deviation of the contact point from our theoretical value $k^2 = -1$ is connected with the relative large distance between the pole and the physical region, whereas the extrapolation (24) is expected to be good only for small k^2.

B. Test of the zero-energy dispersion relation

Further information on whether the relation (1) is correct can be obtained from a numerical investigation of the dispersion relation itself. Using the R-matrix method we calculated the phase shifts for the first seven partial waves for singlet and triplet scattering in the static exchange approximation and, in addition, in the static approximation neglecting exchange. From these, the real and imaginary parts of the scattering amplitudes can be obtained. The effect of the neglected higher partial waves is taken into account by writing

$$\text{Re} f = \frac{1}{2k} \sum_{l=0}^{6} (2l+1)(\sin 2\delta_l - 2\delta_{l,B}) + f_B,$$

$$(25)$$

$$\text{Im} f = \frac{1}{k} \sum_{l=0}^{6} (2l+1)(\sin^2 \delta_l - \delta_{l,B}^2) + \tfrac{1}{4} k \sigma_{\text{tot}, B}.$$
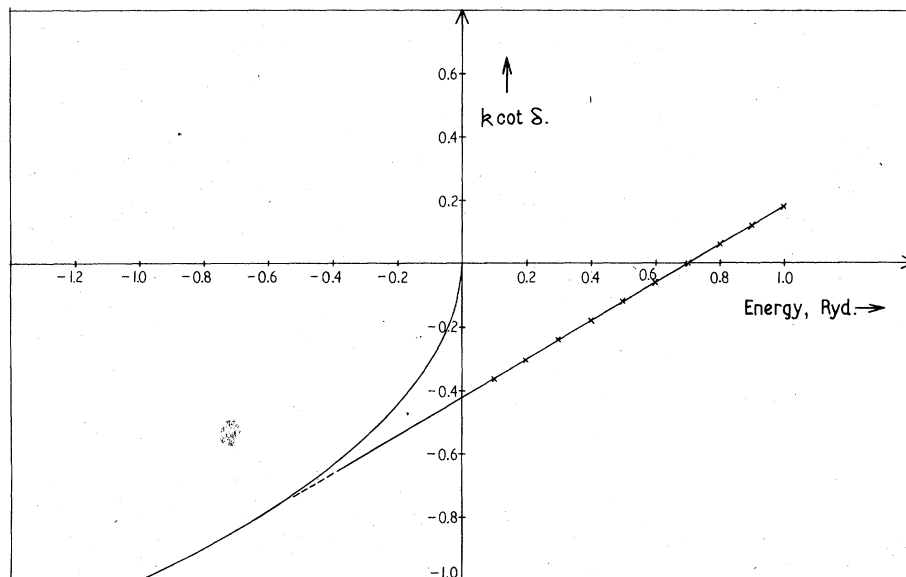
FIG. 1. Effective-range expansion for the triplet amplitude.

Here $\delta_{l,B}$ and $\sigma_{\text{tot},B}$ denote the phase and total cross section in the Born approximation. We note that $\sigma_{\text{tot},B}$ can be calculated analytically.

We used the numerical values of the amplitudes for a test of the zero-energy dispersion relation, obtained from Eq. (1) by putting $k^2 = 0$:

$$-a^{\pm} = f_B(0, 0) \pm g_B(0, 0)$$

$$+ \frac{1}{\pi} \int_0^{\infty} \frac{\text{Im} f^{\pm}(k'^2, 0)}{k'^2} dk'^2 - \frac{r}{k_b^2} . \qquad (26)$$

It follows from the low-energy behavior of the phases that $\text{Im} f \sim \sqrt{k^2}$ for $k^2 \to 0$. The integrand in Eq. (26) (but not the integral itself) has therefore a singularity at zero energy, and, thus, a large contribution to the integral comes from the region with small k^2. The calculation of the low-energy part of the integral must therefore be done with care.

We found that the position k_b and the residue r of the singlet bound state affects the numerical results considerably. It is necessary to have accurate values for both k_b and r. We obtained these using analytical expressions in terms of the Wigner R matrix. The details are given in the Appendix. We obtained -0.0266 Ry for the position and -0.627 for the residue of the pole.

The results for our three cases of interest are shown in Table I. Table I shows that Eq. (26) is satisfied only if exchange is neglected. We also considered a modified dispersion relation where the nuclear term $16/(k^2 + 1)^3$ is omitted from g_B. This is consistent with the orthogonality condition

(4). As can easily be seen this modified equation is not fulfilled as well.

C. Nonzero-energy dispersion relation

Finally we inserted our numerical values for Ref and Imf into relation (1). The singularity at $k^2 = k'^2$ in the integrand was taken into account by expanding the numerator of the integrand in a Taylor series. We note that the bound state in the singlet case and the existence of a virtual state in the no-exchange amplitude gives rise to a rapid variation of the s-wave phase shift at very small energies. The calculation of the low-energy part of the integral must therefore be done carefully.

The results given in Table II show that the dispersion relation (1) is only fulfilled if exchange is neglected. L and R denote the left-hand and right-hand side of Eq. (1). The numbers show that the difference between L and R decreases for higher energies where the influence of exchange effects becomes less important.

TABLE I. Contributions to the zero-energy dispersion relation (26).

	No exchange	Singlet	Triplet
a (scattering length)	−9.45	8.095	2.350
$f_B(0, 0)$	1.0	1.0	1.0
$g_B(0, 0)$	...	6.0	6.0
Integral term	8.45	8.21	2.82
Pole term	...	−23.56	...
Discrepancy	0.0	0.26	−0.17

TABLE II. Contributions to the positive-energy dispersion relation (1).

k^2 (Ry)	No exchange		Singlet		Triplet	
	L	R	L	R	L	R
0.4	0.96	0.96	0.26	0.02	0.87	0.87
0.8	0.93	0.93	0.02	−0.19	1.45	1.38
1.2	0.94	0.94	0.04	−0.15	1.56	1.47
1.6	0.95	0.95	0.16	−0.03	1.56	1.46
2.0	0.96	0.96	0.22	+0.09	1.53	1.41
4.0	0.98	0.98	0.55	0.47	1.36	1.26
6.0	0.99	0.99	0.70	0.65	1.26	1.18

IV. CONCLUSIONS

The future use of dispersion relations in atomic physics depends critically on a better understanding of the nature of the singularities on the left-hand cut. In this paper we have been able to determine the position and strength of one of these singularities in the case of electron–hydrogen-atom scattering in the static exchange approximation. However, a full description of the left-hand singularities is not yet available, and until this is achieved the application of dispersion relations in analyzing experimental data will be seriously restricted. It is our hope that the results presented in this paper will provide a stimulus for continued effort to understand the analytic structure of the scattering amplitude for electron-atom scattering.

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APPENDIX

In this appendix we derive an expression for the residue r of the bound state occurring in Eqs. (1) and (26) for singlet scattering. We use the R-matrix method.[9] Wigner's R matrix is defined for single-channel scattering by

$$R(E) = \frac{1}{2a} \sum_\lambda \frac{w_\lambda^2(a)}{E_\lambda - E} . \tag{A1}$$

Here a is chosen in such a way that the potential $V(r) \simeq 0$ for $r \geq a$. w_λ is a complete set of eigen-

functions satisfying the usual R-matrix boundary conditions. We need to find an energy E such that

$$u_0(a) = R(E)\left(a\frac{du_0}{dr} - bu_0\right)_{r=a}, \tag{A2}$$

where b is the logarithmic derivative satisfied by the R-matrix states. At a bound state we have

$$u_0(r) \rightarrow e^{-Kr} \quad \text{for} \quad r \rightarrow \infty \tag{A3}$$

$(E = -\frac{1}{2}K^2)$. Let us assume that $b = 0$ and $u_0(r)$ satisfies (A3) for all $r \geq a$. This is true in our case of interest (static exchange approximation). It then follows from Eqs. (A2) and (A3) that

$$R(E_b) = -1/Ka . \tag{A4}$$

Writing the wave function in the form

$$u_0(r) = Ae^{ikr} + Be^{-ikr} \quad \text{for} \quad r \geq a, \tag{A5}$$

the S matrix is given by

$$S = -A(E)/B(E). \tag{A6}$$

At the bound-state energy $E = E_b$ the S matrix has a pole with residue

$$r' = -\frac{A(E_b)}{(dB/dE)_{E=E_b}}, \tag{A7}$$

and near the pole we have

$$S(E) \approx r'/(E - E_b).$$

Substituting Eq. (A5) into Eq. (A2) gives ($k = iK$)

$$(Ae^{-Ka} + Be^{Ka}) = R(E)aK(-Ae^{-Ka} + Be^{Ka}).$$

Taking the derivative with respect to E of this equation, evaluating this for $E = E_b (K = K_b)$, and using Eqs. (A4) and $B(E_b) = 0$, we obtain

$$Ae^{-K_b a}\left\{\left(\frac{dR}{dE}\right)_{E_b} aK_b + \frac{1}{K_b^2}\right\} = -2\frac{dB}{dE}e^{K_b a},$$

and thus the residue (A7)

$$r' = \frac{2e^{2K_b a}}{aK_b(dR/dE)_{E_b} + 1/K_b^2} . \tag{A8}$$

Because we have

$$f_0(k^2, 0) = -\frac{1}{2K_b}S(E_b) = -\frac{1}{2K_b}\frac{r'}{E - E_b} = \frac{r}{k^2 - k_b^2},$$

we obtain the expression

$$r = -\frac{2e^{2K_b a}}{aK_b^2(dR/dE)_{E_b} + 1/K_b} \tag{A9}$$

for the residue occurring in Eq. (1).

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