A SECOND-ORDER POLES OF THE S MATRIX AND RESONANCE SCATTERING

Yu. N. DEMKOV and G. F. DRUKAREV

Leningrad State University

Submitted to JETP editor March 16, 1965

J. Exptl. Theoret. Phys. (U.S.S.R.) **49**, 691-698 (August, 1965)

The general pattern of the motion of the poles of the S matrix on the unphysical sheet of the complex plane of the energy E as the potential is varied is investigated. Conditions for the appearance of a second-order pole are found. For a potential well with a barrier this pole can lie near E = 0. Resonance scattering is considered in the case in which two simple poles coincide or are close to each other.

1. INTRODUCTION

THE question of higher-order poles of the S matrix has recently been attracting much attention both in connection with the general structure of the S matrix[1] and in connection with the law of decay of unstable particles.[2] The existence of higher-order poles is also closely connected with features of the resonance scattering of particles. A simple comparison of well known formulas for resonance scattering already leads, as we shall soon see, to the conclusion that there is a second-order pole of the S matrix.

Let us consider the scattering of particles of energy E by a central force field V(r) with a finite range [V(r) = 0 for $r \geq R$]. We shall assume that the particles are slow, so that $kR \ll 1$, where $k = (2mE/\hbar)^{1/2}$, and accordingly shall take into account only the partial wave with zero angular momentum ($l = 0$). Two types of resonance scattering are usually distinguished[3]: 1) scattering by a potential well when there is a level close to the limit of the continuous spectrum (or when there is a so-called virtual level); 2) scattering when there is a quasistationary state, for example in the case of a potential well surrounded by a barrier.

There are two corresponding expressions used for the S matrix, which is connected with the phase δ of the wave function by the relation $S = e^{2i\delta}$.

In case 1) (cf., e.g., [4])

$$S = e^{2i\varphi(k)} \frac{(1 + k/k_1)}{(1 - k/k_1)}, \qquad (1)$$

here $k_1 = i\kappa_1$ is a pure imaginary number. When there is a bound state $\kappa_1 > 0$; $\varphi(k)$ is the phase of the nonresonance part of the scattering—the so-called potential scattering. In the low-energy case in which we are interested we can take

$$\varphi = kr_0. \qquad (2)$$

For $|\kappa_1| r_0 \ll 1$ we get from (1) and (2) the well known formula

$$k \operatorname{ctg} \delta = -a^{-1} + {}^1/_2 \rho k^2, \qquad (3)^*$$

where the scattering length a and the effective range ρ can be expressed in terms of κ and r_0:

$$a = \varkappa^{-1}, \qquad \rho = 2r_0. \qquad (4)$$

In case 2) the expression used for the S matrix is[4]

$$S = e^{2i\varphi} \frac{(1 + k/k_1)(1 - k/k_1^*)}{(1 - k/k_1)(1 + k/k_1^*)}, \qquad (5)$$

where k_1 and $-k_1^*$ are complex numbers which lie in the lower half of the k plane and are located symmetrically relative to the imaginary axis.

The position of the poles of the S matrix is determined by the form of the potential energy V. If we change V, for example by slowly decreasing the depth of the potential well, then it would be natural to expect that we could trace the transition from resonance scattering of type 1) to resonance scattering of type 2). It is easy to see, however, that such a transition cannot be traced by means of the formula (1). Indeed, as is well known, the S matrix can be represented in the form

$$S = f(-k) / f(k),$$

where f(k) is the so-called Jost function, which is an analytic function in the entire k plane in the case in which V is zero for $r \geq R$ (see Sec. 2). Consequently, the poles of the S matrix are zeroes of the Jost function. The formula (5) is written in

*ctg ≡ cot.

the approximation in which two zeroes of f(k) are taken into account. Since the number of zeroes of an analytic function cannot change as it is continuously varied, it is clear that no motion of the zeroes of f(k) can take us from Eq. (5) to Eq. (1).

In order to trace the connection between different cases of resonance scattering it is necessary to have a formula which includes two zeroes of the Jost function both in the case in which they are placed symmetrically relative to the imaginary axis and also in the case in which they lie on the imaginary axis. It seems obvious that in the transition from one case to the other we must inevitably pass through a case in which the two zeroes of the function f(k) coincide on the imaginary axis. Corresponding to this the S matrix must have a second-order pole.

In the present paper a general investigation is made of the motion of the zeroes of the Jost function as the potential V is varied, and the conditions are found under which merging of two zeroes occurs. An example is given in which the double zero lies close to the point k = 0. A formula is obtained for the S matrix, in the approximation of two zeroes of the Jost function, when these zeroes are either complex or pure imaginary. The latter case is a generalization of Eq. (1), which enables us to trace the transition between the different types of resonance scattering.

In the two-zero approximation one also gets a formula of the type of (3) for k cot δ, and in the case in which the point where the point of confluence lies close to k = 0 the effective range ρ is negative and large in absolute value.

2. THE JOST FUNCTION

The Jost function f(k) is defined as the value at r = 0 of the solution of the equation

$$\frac{d^2f(k,r)}{dr^2}+(k^2-V)f(k,r)=0, \tag{6}$$

which has for $r \to \infty$ the asymptotic form

$$f(k,r)=e^{ikr}. \tag{7}$$

(The properties of the function f(k) are treated in detail in [5,6], for example.) In our case the form (7) is exact everywhere for $r \geq R$. Then f(k) is analytic in the entire complex plane of k. Moreover, the function f(k) has the symmetry property

$$f(k^*)=f^*(-k).$$

In the upper half-plane f(k) can have zeroes only on the imaginary axis. These zeroes correspond to bound states of the particle in the field V. In the lower half-plane f can have zeroes both on and off the imaginary axis. In the latter case it follows from the symmetry property that the zeroes occur in pairs symmetrical relative to the imaginary axis. Zeroes which lie on the imaginary axis near the point k = 0 correspond to virtual states. Pairs of zeroes located close to the imaginary axis (and symmetrically relative to it) correspond to quasistationary states.

We now proceed to study the zeroes of f(k) on the imaginary axis. We set $k = i\kappa$ and write

$$f(i\varkappa)=g(\varkappa). \tag{8}$$

$g(\kappa)$ is the value at r = 0 of the function $f(\kappa, r)$ that satisfies the equation

$$d^2g/dr^2-(\varkappa^2+V)g=0 \tag{9}$$

and has the form

$$g(\varkappa,r)=e^{-\varkappa r} \tag{10}$$

for $r \geq R$. We denote the zeroes of the function $g(\kappa)$ by κ_n:

$$g(\varkappa_n)=0. \tag{11}$$

For real κ, r the functions $g(\kappa, r)$, $g(\kappa)$ are real.

We use a formula given in a paper by one of the writers [7] for the derivative of the Jost function at a point where the function itself is equal to zero. In the notation of the present paper this formula can be written in the form

$$-2\varkappa_n\frac{1}{g(-\varkappa_n)}\left(\frac{dg}{d\varkappa}\right)_{\varkappa=\varkappa_n}=e^{-2\varkappa_nR}+2\varkappa_n\int_0^R g^2(\varkappa_n,r)\,dr. \tag{12}$$

If $\kappa_n > 0$, i.e., if the zero corresponds to a bound state, then Eq. (12) can be simplified and takes the form

$$\frac{g'(\varkappa_n)}{g(-\varkappa_n)}=-\int_0^\infty g^2(\varkappa_n,r)\,dr<0. \tag{13}$$

Let $\kappa_n > \kappa_{n+1} > 0$ be two adjacent zeroes; then $g'(\kappa_n)$ and $g'(\kappa_{n+1})$ have opposite signs. Consequently, the quantities $g(-\kappa_n)$, $g(-\kappa_{n+1})$ also have opposite signs, and accordingly there is at least one zero of the function $g(\kappa)$ between the points $-\kappa_n$ and $-\kappa_{n+1}$. It follows, in particular, that in the upper half-plane there can be no multiple zeroes of the Jost function f(k), because the result just proved means that f(-k) would then also be zero, which is in contradiction with the uniqueness theorem.

For potentials of rather general form (well, barrier, well surrounded by a barrier) it can be shown that the right member of (12)

$$\xi(\varkappa)=e^{-2\varkappa R}+2\varkappa\int_0^R g^2(\varkappa,r)\,dr \tag{14}$$

is zero for only one value $\kappa = \bar{\kappa} < 0$, and that $\xi(\kappa) > 0$ for $\kappa > \bar{\kappa}$ and $\xi(\kappa) < 0$ for $\kappa < \bar{\kappa}$. Then by using (12) we can easily show that all real zeroes of the function $g(\kappa)$ [imaginary zeroes of the function $f(k)$] can be divided into two groups:

$$\text{a)}\quad \varkappa_1 > \varkappa_2 > \ldots > \varkappa_N > \bar{\varkappa},$$

where the last zero κ_N can be either positive or negative, and all the others are positive, and

$$\text{b)}\quad \varkappa_2' < \varkappa_3' < \ldots < \varkappa_N' < \bar{\varkappa},$$

which values lie in the intervals

$$-\varkappa_1 < \varkappa_2' < -\varkappa_2, \quad -\varkappa_2 < \varkappa_3' < -\varkappa_3, \ \ldots,$$

$$-\varkappa_{N-1} < \varkappa_N' < \bar{\varkappa}.$$

Since the function $g(\kappa)$ approaches unity for $\kappa \to +\infty$, we have $g'(\kappa_1) > 0$, $g(-\kappa_1) < 0$, and the question of whether or not there is a zero in the interval $-\infty < \kappa < -\kappa_1$ depends on the sign of the function $g(\kappa)$ for $\kappa \to -\infty$. Using the equation for $g(\kappa)$

$$g(\varkappa) = 1 - \int_0^R V(r)\, g(\varkappa, r)\, dr,$$

we easily show that if as r increases the potential $V(r)$ is positive just before becoming zero (well surrounded by a barrier), then $g(\kappa) > 0$ for $\kappa \to -\infty$, and there is one further zero $\kappa_1' < -\kappa_1$, so that the total number of zeroes is even. If, on the other hand, the potential $V(r)$ was negative before it became zero, then $g(\kappa) < 0$ for $\kappa \to -\infty$, there is no zero κ_1', and the total number of zeroes is odd. It is particularly clear from this result that arbitrarily small changes of the potential $V(r)$ at the limit of the range of action of the forces change the number of zeroes of the function $g(\kappa)$ for large negative κ, so that these zeroes have little physical meaning.

It must be pointed out that for more complicated, for example oscillating, potentials the function $\xi(\kappa)$ can be zero several times, and then the simple picture of the distribution of the zeroes which we have described becomes more complicated. Such potentials are of no particular interest, however, and we shall not consider them.

Let us find out how the zeroes κ_n and κ_n' move as the potential V is varied. Using Eq. (9), in which we now set $\kappa = \kappa_n$, and taking (10) and (11) into account, we can easily show that the shift $\delta\kappa_n$ which corresponds to a small variation δV is given in first approximation by

$$\delta\varkappa_n = -\frac{1}{\xi(\varkappa_n)} \int_0^R g^2(\varkappa_n, r)\, \delta V\, dr, \tag{15}$$

where $\xi(\kappa)$ is given by the expression (14).[1)] Let us consider a variation δV such that

$$\int_0^R g^2\, \delta V\, dr > 0 \tag{16}$$

for real κ. A particular example of a variation δV which satisfies this condition is a decrease of the depth of a potential well. Then, when we use the properties of $\xi(\kappa)$ which we have established, we get

$$\text{a)}\ \delta\varkappa_n < 0 \text{ for } \varkappa_n > \bar{\varkappa}, \qquad \text{b)}\ \delta\varkappa_{n'} > 0 \text{ for } \varkappa_{n'} < \varkappa. \tag{17}$$

This means that the zeroes of each group move toward those of the other. (The point $\bar{\kappa}$ itself obviously also moves when there is a change of V.)

At the point $\bar{\kappa}$ the relation (15) cannot be applied, since the denominator is zero. To study the motion of the zeroes near the point $\bar{\kappa}$, we must make the formula (15) more precise. It suffices to include the correction to $\xi(\kappa)$ near the point $\bar{\kappa}$ which is of first order in $\delta\kappa_n$, i.e., to set

$$\xi(\varkappa_n) = \delta\varkappa_n (d\xi/d\varkappa)_{\bar{\varkappa}}. \tag{18}$$

Then we get instead of (15)

$$(\delta\varkappa_n)^2 = -\frac{1}{(d\xi/d\varkappa)_{\bar{\varkappa}}} \int_0^R g^2 \delta V\, dr. \tag{19}$$

It follows from the properties of the quantity $\xi(\kappa)$ that at the point $\bar{\kappa}$ we have $(d\xi/d\kappa)_{\bar{\kappa}} > 0$. Consequently, for variations satisfying (16) the quantity $(\delta\kappa_n)^2$ is negative, so that $\delta\kappa_n$ is imaginary.

Recalling that we had previously set $k = i\kappa$, we see that an imaginary variation $\delta\kappa_n$ corresponds to a real variation of k, so that the zeroes move off the imaginary axis. Thus we arrive at the conclusion that for a potential variation satisfying (16) the zeroes for which $\kappa_n > \bar{\kappa}$ move toward those for which $\kappa_n < \bar{\kappa}$. Each pair merges at the point $i\bar{\kappa}$, and then separate and move to the right and the left from the imaginary axis. The trajectory of the zeroes is shown in Fig. 1. An unpaired zero, if there is one, moves down along the imaginary axis, always remaining above the point $i\bar{\kappa}$. This general picture of the motion of the zeroes has been confirmed by Nussenzveig[9] by numerical calculation for the special case of a rectangular well.

[1)] We note that (15) is analogous to Zel'dovich's formula[8] for the change δE of the energy of a quasistationary state when there is a small change δV of the potential.

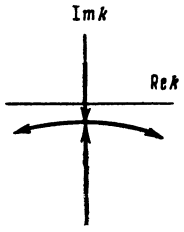

FIG. 1

Let us now consider the condition for merging of zeroes. It follows from (12) that this condition is

$$e^{-2\bar{\varkappa}R} + 2\bar{\varkappa}\int_0^R g^2(\bar{\varkappa}, r)\,dr = 0.$$

It can be rewritten in the form

$$\int_0^R (e^{-2\bar{\varkappa}r} - g^2)\,dr = \frac{1}{2\bar{\varkappa}}.$$

A case of particular interest is that in which the point of merging lies close to the origin, so that $|\kappa|R \ll 1$; then the integral

$$\frac{1}{2}\int_0^R [e^{-2\bar{\varkappa}r} - g^2(\bar{\varkappa}, r)]\,dr \approx \frac{1}{2}\int_0^R [1 - g^2(0, r)]\,dr$$

is practically equal to the effective range ρ (cf., e.g., [4]), so that

$$\rho = 1/\bar{\varkappa}.$$

It follows from this that ρ is negative and that $|\rho| \gg R$.

This situation occurs in the case of a potential well surrounded by a potential barrier. Figure 2 shows the general behavior of the function g for this case, and makes it quite clear that $\rho < 0$, and also that $|\rho| \gg R$. The order of magnitude of $\bar{\kappa}$ is determined by the penetrability of the barrier; that is, it is exponentially small, and consequently ρ is exponentially large. A direct calculation, which can easily be carried through completely

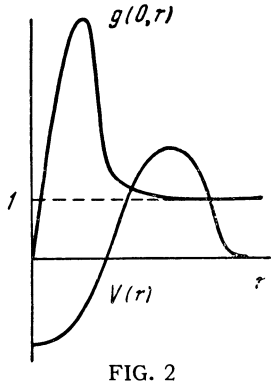

FIG. 2

for a well with a rectangular barrier, confirms the correctness of the picture shown in Fig. 2.

3. THE S MATRIX IN THE TWO-POLE APPROXIMATION

Let $k_1, k_2, \ldots$ be the zeroes of the Jost function. If the zeroes are distributed in such a way that the series Σk_n^{-1} converges, the Jost function can be represented in the form of an infinite product

$$f = e^{-i\varphi(k)}\prod_n\left(1 - \frac{k}{k_n}\right)$$
$$= e^{-i\varphi(k)}\left[1 - k\sum_n\frac{1}{k_n} + k^2\sum_{n,m}\frac{1}{k_n k_m} + \ldots\right].$$

Let us consider the case in which two zeroes k_1 and k_2 are close to their merging point and this point itself is close to $k = 0$. Then only these zeroes are important for the scattering of slow particles. Accordingly, in the sums $\Sigma_n k_n^{-1}$ and $\Sigma_{n,m} k_n^{-1}k_m^{-1}$ we can neglect all of the terms except $k_1^{-1} + k_2^{-1}$ and $k_1^{-1}k_2^{-1}$. This gives us $f(k)$ in the two-zero approximation. When we further use the approximation (2) for $\varphi(k)$, we get

$$f(k) = e^{-ikr_0}[1 - k(k_1^{-1} + k_2^{-1}) + k^2(k_1k_2)^{-1}].$$

From this we have for the S matrix

$$S = e^{2ikr_0}\frac{(1 + k/k_1)(1 + k/k_2)}{(1 - k/k_1)(1 - k/k_2)}. \qquad (20)$$

For $k_2 = -k_1^*$ the formula (20) agrees with Eq. (5). In the case when k_1 and k_2 lie on the imaginary axis, (20) is a generalization of (1) to the case of two zeroes. We represent k_1 and k_2 in the form

$$k_1 = \sqrt{\Delta} - i\alpha, \qquad k_2 = -\sqrt{\Delta} - i\alpha. \qquad (21)$$

The quantity $\alpha = \frac{1}{2}i(k_1 + k_2)$ gives the position of the "center of gravity" of the zeroes on the imaginary axis, with the signs chosen so that $\alpha > 0$ when the center of gravity lies in the lower half-plane; the quantity $2\Delta^{1/2}$ gives the distance between the zeroes. Case 1) of Sec. 1 corresponds to $\Delta < 0$, and case 2) to $\Delta > 0$; the transition between them goes through the point $\Delta = 0$.

We note that it follows from the results of Sec. 2 that it is impossible for α to be zero. The quantity α is always positive (in the two-zero approximation).

Using the relation $S = e^{2i\delta}$, the formula (20), and the notations (21), we get for the scattering length the expression

$$a \equiv -\lim_{k\to 0}[k\operatorname{ctg}\delta]^{-1} = -(2\alpha/(\alpha^2 + \Delta) + r_0). \qquad (22)$$

In cases with $r_0 \ll |a|$, a formula of the type of (3) can be obtained from (20)

$$k \operatorname{ctg} \delta = -1/a + 1/2 (2r_0 - 1/\alpha) k^2. \quad (23)$$

Thus the quantity that now appears as the effective range is

$$\rho = 2r_0 - 1/\alpha. \quad (24)$$

As can be seen, for sufficiently small α the quantity ρ becomes negative and large in absolute value. We note that the condition $r_0 \ll 1/\alpha$, which is necessary for this, can be satisfied simultaneously with the condition $r_0 \ll \alpha/(\alpha^2 + \Delta)$, which is necessary for the applicability of Eq. (23).

In conclusion we give the formula for the effective scattering cross section in the case $\Delta = 0$ (or $|\Delta| \ll \alpha^2$ together with $r_0 \ll \alpha^{-1}$). In this case the cross section is determined by the single parameter α:

$$\sigma = 16\pi\alpha^2/(k^2 + \alpha^2)^2. \quad (25)$$

States which correspond to this (or a closely similar) distribution of the zeroes will be long-lived and also will decay not according to an exponential, but according to a power law.[7] The longer the lifetime considered, however, the smaller is the range of the parameters occurring in the potential for which such states exist, so that finding them experimentally, for example in nuclei, is very difficult.

All of our arguments can also be carried through for scattering with nonzero angular momentum, i.e., for $l \neq 0$. In this case, because of the centrifugal barrier, which is impenetrable for $k = 0$, the merging of the zeroes occurs at the origin, and they then move away to the right and left along the real axis of k, and bend into the lower half-plane so that $\operatorname{Im} k_n \sim (\operatorname{Re} k_n)^{2l}$. Thus for scattering with $l = 0$, unlike s scattering, quasistationary states appear immediately after the disappearance of a bound state and the merging of two zeroes.

We note that in studying the behavior of the zeroes on the imaginary axis we actually have made no use of such properties of the Jost function as its analyticity in the entire complex plane, and so on. Therefore the results can also be extended to potentials which decrease exponentially, as $e^{-\gamma r}$, of course with the restriction to the region $-\gamma < \kappa < +\infty$.

4. CONCLUSION

Accordingly, for the resonance scattering of low-energy particles it is as a rule necessary to use not the one-pole, but the two-pole approximation for the S matrix. This must always be done for scattering with angular momentum l different from zero (in Sec. 131 of the book by Landau and Lifshitz[3] it is in fact precisely this circumstance which is taken into account). An exception is s scattering by a potential well, for which the two-pole approximation is practically useless, because in this case when the two poles in the lower half of the k plane approach each other their distance from the origin is of the same order as that of the next pole in the upper half-plane. In the case of a well surrounded by a barrier, however, when the penetrability ϵ of the barrier is small ($\epsilon \ll 1$), the two-pole approximation is good down to energies $E < \Delta E$, where ΔE is the distance between levels in the vicinity of $E = 0$. At the same time the one-pole approximation is either not applicable at all, or else applies in a very small region $E < \epsilon \Delta E$, if one of the poles is at a distance from the origin much smaller than $\epsilon \Delta E$.

Any sort of stabilization of an s state going over into the continuous spectrum means that the point of merging of the poles comes close to the origin, so that it is necessary to use the two-pole approximation. In more complicated problems such stabilization can be caused not only by a potential barrier, but also by other circumstances: weakness of the dynamical interaction with the particles of the scatterer, special properties of a system with a large number of particles, and so on.

This kind of behavior of the poles of the S matrix on the "unphysical" sheet of the energy E is also important in the treatment of slow collisions of negative atoms with atoms, when at close approach a bound state of the electron is "pushed out" into the continuous spectrum.[10] Depending on how close to the origin the point of merging is, qualitatively different results can appear as to the probability of stripping off of the electron during the collision. These questions are discussed in more detail in a following paper.[11]

In conclusion we thank V. A. Fock, L. D. Faddeev, and G. V. Dubrovskiĭ for a discussion of the questions considered in this paper.

[1] R. J. Eden and P. V. Landshoff, Phys. Rev. **136**, B1817 (1964).

[2] M. L. Goldberger and K. M. Watson, Phys. Rev. **136**, B1472 (1964).

[3] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Second edition, Fizmatgiz, 1963, Chapter 27.

[4] A. I. Akhiezer and I. Ya. Pomeranchuk, Nekotorye voprosy teorii yadra (Some Problems in the Theory of the Nucleus), Second edition, Gostekhizdat, 1950, Chapter 3, Sec. 23.

[5] R. Newton, J. Math. Phys. **1**, 319 (1963).

[6] L. D. Faddeev, Uspekhi Mat. Nauk **14**, 57 (1959).

[7] G. F. Drukarev, JETP **21**, 59 (1951).

[8] Ya. B. Zel'dovich, JETP **39**, 776 (1960), Soviet Phys. JETP **12**, 542 (1961).

[9] H. M. Nussenzveig, Nuclear Phys. **11**, 499 (1959).

[10] Yu. N. Demkov, JETP **46**, 1126 (1964), Soviet Phys. JETP **19**, 762 (1964).

[11] Yu. N. Demkov, JETP **49**, 885 (1965), Soviet Phys. JETP 22, (1966), in press.

Translated by W. H. Furry
89