REMOVAL OF AMBIGUITIES IN PHASE-SHIFT ANALYSIS

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We show that the set of n equations obtained from a phase shift analysis of scattered spin-0 and spin-$\frac{1}{2}$ particles with unknown polarization has (in a certain generalized sense) 2^n solutions including some that are nonunitary; furthermore, it is shown that this statement is true also for every subset of n equations of the set of $2n-1$ equations obtained from a phase-shift analysis of scattered spin-zero particles. In both cases the "complete experiment" involving $2n-1$ measurements can be replaced by a "necessary experiment" of just $n+1$ measurements.

1. MULTIPLICITY OF PHASE-SHIFT ANALYSIS

A phase-shift analysis is a method of deriving a matrix from experimental data, such that exact unitarity is obtained by introducing phase shifts. The number of measurements needed at different angles and for a given energy is found to be finite if one restricts the number of states in which one wishes to determine the interaction. In other words, finite accuracy can be obtained for the elements of the scattering matrix as functions of the scattering angle only if one makes use of a finite parametrization.

It is known[1] that the results of a "complete experiment" are sufficient for a phase-shift analysis. Many of the experiments, however, which enter into such a complete set are difficult to perform. It is therefore of some importance to determine the minimum set of measurements necessary for a phase-shift analysis at a given energy, with the subsidiary condition that only the first n phases be considered nonvanishing.

If the measurements are taken over a sufficiently wide energy range, the number of measurements at each energy may be decreased by making use of the causality condition. Additional information is obtained by studying the interference between the interaction being measured and the Coulomb interaction or some other interaction, as calculated theoretically for a number of states. Although in principle interference will give any number of equations for the unique determination of the required phase shifts, experimental accuracy will not often allow the use of all or even nearly all of them.

Thus in a phase-shift analysis one is not dealing with the complete problem of establishing the entire scattering matrix, but the problem of finding for the first n phase shifts values that give the best fit to the experimental data, if one assumes all the other phase shifts negligibly small or given a priori.

In order to obtain a finite number of sets of n phase shifts satisfying the experimental data equally well, one must have at least n independent equations. Such equations are obtained if one expands the experimental angular distributions in a series of Legendre polynomials and then equates coefficients of this expansion with the corresponding expression in terms of the phase shifts.

In studying elastic scattering of spinless particles, a complete experiment requires a measurement of the angular distribution of the scattering. In scattering of spin-$\frac{1}{2}$ particles by spin-0 particles, this experiment requires measurements of the differential cross section and the polarization of the recoil particles as a function of angle. In both cases the Legendre polynomial expansion of the theoretical and experimental angular distributions will lead to a set of equations of the form

$$\sum_{k,l=1}^{n} C_{kl}^{(i)} \sin\delta_k \sin\delta_l \cos(\delta_k - \delta_l) = A_i, \qquad (1)$$

where the $C_{kl}^{(i)}$ are constants, the δ_k are the phase shifts for the different states, the A_i are the expansion coefficients of the experimentally observed differential scattering cross section (divided by $\lambda\!\!\!^{-2}$) for an expansion in linearly independent functions of the scattering angle; in the first case $i = 1, \ldots, 2n-1$, while in the second $i = 1, \ldots, n$. For nonzero phase shifts we take here the states in the order S, P, D, ... in the first case, and in the order $S_{1/2}$, $P_{1/2}$, $P_{3/2}$, $D_{3/2}$, ... in the second case.

Before proceeding we must determine the number of solutions of a set of n such equations. It is shown in the Appendix that every set of n equations of the form of (1) has exactly

$$N = 2^n \tag{2}$$

solutions such that $-\pi/2 \le \operatorname{Re} \delta_k \le \pi/2$. In special cases, when (1) is degenerate and may have an infinite number of solutions, as well as when one of the phase shifts passes through resonance, the number of solutions is defined as the number of solutions at almost all points of a certain region of the n-dimensional complex-valued space of the A_i. Then $N = 2^n$ everywhere.

Thus the experimental data on just the angular distribution of scattering of spin-0 and spin-½ particles will lead, if the polarization is unknown, to 2^n different solutions. Among these are both unitary (real δ_k) and nonunitary solutions. This result is equally valid for the phase-shift analysis of elastic scattering of spinless particles if one wishes to find the n phase shifts by using only n of all the $2n-1$ expansion coefficients of the angular distribution.

If some of the phase shifts are given and one wishes, as before, to determine only the first n, the number of solutions remains that given in (2). For in this case the left sides of Eq. (1) will contain an additional finite or infinite number of terms of this form in which one of the phase shifts is given. Since the given phase shifts must vanish for zero energy, the result following from (A7) will not change.

We remark that the number of solutions of the set of n equations with n unknowns is independent of the experimental accuracy with which the A_i are determined. On the other hand, the number of solutions admissible (with a given probability) for an overdetermined system depends strongly on this accuracy.

2. EXAMPLES OF AMBIGUITY IN A PHASE SHIFT ANALYSIS

We note first that all the solutions of (1) can be divided into two groups one of which is obtained from the other by the replacement $\delta_k \to -\delta_k$. Further, as has been shown by Minami,[2] if one wants to obtain an even number of phase shifts for a spin 0–spin ½ scattering problem, one finds that the $C_{kl}^{(i)}$ do not change when one interchanges states with the same total angular momentum but with opposite parity. Therefore the associated interchange of these phase shifts will not change the differential cross section, and this fact thus separates all the solutions for this case into two additional classes.

In spin-0–spin-½ scattering, the equation for a single phase shift

$$\sin^2 \alpha = \sin^2 \alpha_0 \tag{3}$$

has only the two solutions

$$\alpha_1 = \alpha_0; \qquad \alpha_2 = -\alpha_0.$$

The set of equations for two phase shifts, namely

$$\begin{gathered} \sin^2 \alpha + \sin^2 \beta = \sin^2 \alpha_0 + \sin^2 \beta_0, \\ \sin \alpha \sin \beta \cos (\alpha - \beta) = \sin \alpha_0 \sin \beta_0 \cos (\alpha_0 - \beta_0) \end{gathered} \tag{4}$$

has the four solutions

$$\begin{aligned} &\alpha_1 = \alpha_0, \quad \beta_1 = \beta_0; \quad \alpha_2 = -\alpha_0, \quad \beta_2 = -\beta_0; \\ &\alpha_3 = \beta_0, \quad \beta_3 = \alpha_0; \quad \alpha_4 = -\beta_0, \quad \beta_4 = -\alpha_0. \end{aligned}$$

For this case the Minami transformation and the change of sign exhaust all possibilities.

The set of equations for three phase shifts, namely

$$\begin{aligned} &\sin^2 \alpha + \sin^2 \beta + 2 \sin^2 \gamma = \sin^2 \alpha_0 + \sin^2 \beta_0 + 2 \sin^2 \gamma_0, \\ &\sin \alpha \sin \beta \cos (\alpha - \beta) + 2 \sin \alpha \sin \gamma \cos (\alpha - \gamma) \\ &\quad = \sin \alpha_0 \sin \beta_0 \cos (\alpha_0 - \beta_0) \\ &\quad + 2 \sin \alpha_0 \sin \gamma_0 \cos (\alpha_0 - \gamma_0), \\ &\sin^2 \gamma + 2 \sin \beta \sin \gamma \cos (\beta - \gamma) \\ &\quad = \sin^2 \gamma_0 + 2 \sin \beta_0 \sin \gamma_0 \cos (\beta_0 - \gamma_0) \end{aligned} \tag{5}$$

should, according to the above, have eight solutions.

In analyzing the scattering of π mesons by protons, only four solutions have been used heretofore; these are

$$\begin{gathered} \alpha_1 = \alpha_0, \qquad \beta_1 = \beta_0, \qquad \gamma_1 = \gamma_0; \\ \alpha_2 = -\alpha_0, \qquad \beta_2 = -\beta_0, \qquad \gamma_2 = -\gamma_0; \\ \alpha_3 = \alpha_0, \qquad \beta_3 = \Theta - \beta_0, \qquad \gamma_3 = \Theta - \gamma_0, \\ \Theta = \operatorname{arctg} \frac{\sin 2\beta_0 + 2 \sin 2\gamma_0}{\cos 2\beta_0 + 2 \cos 2\gamma_0} \end{gathered} \tag{6*}$$

(the Fermi-Yang transformation);

$$\alpha_4 = -\alpha_0, \qquad \beta_4 = -\beta_3, \qquad \gamma_4 = -\gamma_3.$$

There exist, however, four other solutions which have real phase shifts for sufficiently small β_0 and γ_0 [if $\alpha_0 \ll 1$, $\beta_0 \ll 1$, $\gamma_0 \ll 1$ and if $\alpha_0^2 \gg 3\gamma_0(\gamma_0 + 2\beta_0)$] and

*arctg = $\tan^{-1}$.

$$\alpha_{5,6} = \operatorname{arctg} \frac{\sin 2\alpha_0 + \sin 2\beta_0 + 2 \sin 2\gamma_0}{\cos 2\alpha_0 + \cos 2\beta_0 + 2\cos 2\gamma_0 - 2} - \alpha_0,$$

$$\alpha_{7,8} = -\alpha_{5,6}. \qquad (7)$$

The corresponding values of β and γ are given by expressions which are too complicated to be presented here, although they are easily obtained graphically.

For larger β_0 and γ_0 the last four solutions become nonunitary, i.e., the corresponding phase shifts become complex. At certain energies the complex values for these phase shifts may cross the real axis, and this leads to the additional ambiguities in the phase-shift analysis for real phase shifts, as found by Igushkin.[3]

To find the operator group of order 2^n whose elements will transform a solution of a set of equations such as (1) into another is a problem which has not yet been solved in general. In the examples presented above the groups are Abelian, and are the direct product of n groups of two elements; this would seem to be true for the general case.

3. "NECESSARY EXPERIMENT"

We have seen that among the 2^n solutions of the phase-shift analysis there are both unitary and nonunitary ones. The unitarity condition, written as a reality condition on the phase shifts, is not analytic and can therefore not be included in the integral treated in the Appendix in attempting to reduce the number of solutions. In order to choose a single physically admissible solution from among the 2^n, one must use additional information; nevertheless, it is desirable to find the minimum amount of information necessary. It is then found that the number of measurements necessary to establish the scattering amplitudes is less than the number of measurements in the "complete experiment."

The phase-shift analysis of spin-zero scattering can be carried through in two ways. In the first an electronic computer is used to minimize the sum of the weighted square deviations of the experimental differential cross sections at certain definite angles from the expressions for these cross sections in terms of the phase shifts. In this way one obtains many minima for the sums of the squares, some of which correspond to solutions of the problem, while others arise from different sources entirely. To find the physical solution among them is often quite difficult even if the different minima have different depths.

In the second method one starts by looking for the coefficients of the expansion in Legendre polynomials (or some other linearly independent functions of the cosine of the angle) of the differential cross section. This expansion is unique, and it is rapidly calculated since the problem is linear and its solution does not require successive approximations. One then finds that set of phase shifts which exactly solves the equations obtained by equating the above coefficients to their expressions in terms of the phase shifts.

But the greater the number of A_i coefficients, the lower as a rule the accuracy with which they can be found from given data. Therefore knowledge of the higher $n-1$ among the $2n-1$ quantities A_i determined by the n phase shifts, may be of no help whatsoever, since they are highly inaccurate. In other words, when the experimental errors are large some of Eqs. (1) are "almost missing." Such elimination of some of the conditions may cause ambiguity in the analysis even if there is none in principle (in an "overcomplete experiment").

Instead of this it is best to find just the first (or largest) n coefficients, from which, as has been shown above, one can obtain 2^n solutions for the phase shifts. One can then plot all the curves that remain when one discards the solutions eliminated by the unitarity condition.

If the electronic computer is programmed to choose the best real phase shifts, it is easy to differentiate between the unitary solutions and the nonunitary ones. Indeed, a real solution for the phase shifts has the property that the sum of the square deviations of the A_i from their expressions in terms of the phase shifts vanishes, while nonunitary solutions give more shallow minima. The real parts of solutions with small imaginary parts will in this sense be "almost solutions." The problem of finding all the solutions is simplified by the fact that their total number is known. If the cross section is measured at n points, the first type of analysis will lead to a minimum sum of squares equal to zero for unitary solutions, but to a nonzero value for sets of real phase shifts close to nonunitary solutions. The depth of the minimum may serve as an indication of how close the solution is to unitarity.

It turns out in practice that there are half as many different angular distribution curves as there are sets of phase shifts, since a simultaneous change of sign of all the phase shifts will not change the cross section. Then one can find an angle θ_0 where no pair of the 2^{n-1} curves intersects, and where in fact they are most separated. A sufficiently accurate measurement of the cross-section at this angle will eliminate all solutions except two, one of which is causal, while the other is not. In order to identify the correct one, one must make use of interference, for instance with Coulomb scattering. If, further, one has information on the energy dependence of the solutions, one of the solutions, the noncausal one, can be eliminated with the aid of dispersion relations.

In some special cases it may turn out that for a given energy region it is easier to distinguish between the 2^{n-1} curves by measurements not at a single point, but at two or more points.

The question of the number of solutions remaining after the "complete experiment" has been performed will be treated separately.

In order to find all the parameters of an n-parameter curve, one need measure it only at n points. It is assumed, of course, that n has already been chosen from considerations of the nature of the interaction, from analogy, or on the basis of previous experiments. Klepikov and Sokolov[4] (Chapter V) have shown that when a curve with n degrees of freedom is measured at exactly n points, the standard deviations of the coefficients are lower than if the measurements had been performed at more points, but with the same total effort devoted to the measurement. They also show how to find the best measurement points and how most efficiently to distribute the time devoted to measurements at these points for every specific case. It follows from such considerations that the phase-shift analysis of spinless particle scattering is best performed on the basis of cross-section measurements at exactly n points. Subsequently one can eliminate the resulting ambiguity by a single added measurement at the best possible angle θ_0. If the measurements are performed at more than n points, each additional point can be used to reduce the ambiguity, but the effort devoted to the measurements at these points may turn out to be quite inefficiently expended. As for the work involved in finding the best angle θ_0, it is usually considerably less than would be needed for additional measurements.

The phase-shift analysis of scattering of spin-$\frac{1}{2}$ particles by spin-zero particles (or vice versa) can also be performed by the two methods discussed. In this case, however, the differential cross section at any angle is a linear function of the n coefficients A_i. It follows then that there is no additional point at which knowledge of the cross section will decrease the ambiguity of the phase-shift analysis, whose multiplicity, as described above, is 2^n. But the same phase shifts determine the angular dependence of the polarization of the scattered spin-$\frac{1}{2}$ particles. Therefore a polarization measurement at a single successfully chosen angle θ_0 can remove the ambiguity of the analysis. In general (when all the solutions are unitary) one obtains 2^{n-1} different polarization curves, since the polarization is not changed by simultaneously changing the signs of all the phase shifts and interchanging the even-state phase shifts with the odd-state ones of the same total angular momentum (an interchange of the causal and noncausal solutions). If the polarization measurements are impossible, it is impossible to distinguish between four possible sets of phase shifts.

Interference with the Coulomb interaction is an aid in distinguishing the solutions. If the energy dependence of the phase shifts is known, the dispersion relations and the low-energy dependence of the phase shifts can also be used. Indeed, for sufficiently low energies, the momentum dependence of the phase shift is determined entirely by the orbital rather than the total angular momentum; then $\delta_l \sim k^{2l+1}$.

As in the previous case, we can conclude that it is most useful to measure the differential cross section at n points and the polarization at one point. In principle we can choose any n of the $2n-1$ equations for the expansion coefficients of the cross section and the polarization. However, the polarization measurements are usually much more laborious. Furthermore, one must bear in mind the fact that for the polarization these equations are of a different form. Instead of (1), one obtains

$$\sum_{k,\, l=1}^{n} D_{kl}^{(i)} \sin\delta_k \sin\delta_l \sin(\delta_k - \delta_l) = B_i. \tag{8}$$

Therefore the number of solutions of the mixed system can be either more or less than 2^n (but not more than $2 \times 3^{n-1}$).

We see that in both of the above cases, the "complete experiment" consisting of $2n-1$ measurements can be replaced by a "necessary experiment" of only $n+1$ measurements. As has been stated, the $n+1$ measurements can be chosen so that the information obtained on the phase shifts is greater than in the "complete experiment" involving the same effort.

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APPENDIX

NUMBER OF SOLUTIONS OF A PHASE-SHIFT ANALYSIS

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Equations (1), for which we want to know the number of solutions, can be written in the form

$$f_i(x, a) = \sum_{k,l=1}^{n} C_{kl}^{(i)} \left\{\frac{x_k x_l (1 + x_k x_l)}{(1 + x_k^2)(1 + x_l^2)} - \frac{a_k a_l (1 + a_k a_l)}{(1 + a_k^2)(1 + a_l^2)}\right\} = 0, \quad \text{(A1)}$$

where $x_k = \tan \delta_k$, $i = 1, \ldots, n$. Equation (A1) contains the experimentally determined values of the A_i in terms of one of the solutions $x_k^{(1)} = a_k$. It is clear that $x_k^{(2)} = -a_k$ is also a solution. However Eqs. (1) or (A1) have also other solutions.

When dealing with elastic scattering, only the real phase-shift (unitary) solutions of these equations are used. Nevertheless we find it convenient to consider the variables x_k and parameters a_k complex. Consider $C^n(x)$, the space of the complex variables $x = (x_1, \ldots, x_n)$, and $C^n(a)$, the space of the complex variables $a = (a_1, \ldots, a_n)$. Reducing the terms of each of the equations of (A1) to their common denominator, we obtain the set of equations

$$F_i(x, a) = 0, \quad \text{(A2)}$$

$(i = 1, \ldots, n)$ involving polynomials of degree 2^n of n variables. Clearly the number of solutions N_2 (counting multiplicities) of (A2) is no less than the number of solutions N_1 of (A1). From elimination theory (see, for instance, van der Waerden,[5] Secs. 77 and 78) it follows that $N_1 \le N_2 \le 2^{n^2}$, unless there exists a variable x_i such that

$$D_j(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n; a_1, \ldots, a_n) = 0$$

$$(j = 1, \ldots, h, h \geqslant 1) \quad \text{(A3)}$$

is an identity in $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n$. Here the D_j are the resultants of Eq. (A2) with respect to the x_i. Therefore N_2 is always a finite number unless conditions (A3) are fulfilled.

It is possible that these conditions are fulfilled for some a in $C^n(a)$. Let us denote the set of such a by P. In particular, $a = (a_1, \ldots, a_n)$ is in P for spin-0-spin-$\frac{1}{2}$ scattering, with n even, if $a_1 a_2 = -1$, $a_3 a_4 = -1, \ldots, a_{n-1} a_n = -1$. This is easily verified if (1) is written in the form

$$\frac{1}{4} \sum_{k,l=1}^{n} C_{kl}^{(i)} [1 + \cos 2(\delta_k - \delta_l) - \cos 2\delta_k - \cos 2\delta_l] = A_i. \quad \text{(A4)}$$

Under this condition $|\delta_1 - \delta_2| = \pi/2, \ldots, |\delta_{n-1} - \delta_n| = \pi/2$, and all terms of the form $\cos 2\delta_1 + \cos 2\delta_2, \ldots, \cos 2\delta_{n-1} + \cos 2\delta_n$ vanish. According to Minami's theorem[2] this exhausts all combinations of terms that do not contain phase differences. Equations (A4) still contain terms with all possible phase differences. We can therefore introduce only a single continuous parameter. According to the mechanism described elsewhere[6] this case can occur if the vertex H is made coincident with the origin O, after which the mechanism can be rotated through any angle about the origin, so that the vanishing of all terms with cosines of double phase shifts indicates that there is no relation of the mechanism to the coordinate system, or that only internal relations exist. Points in $C^n(a)$ at which $a_k = \pm i$ for at least one value of k also present some difficulties on going from (A1) to (A2); in applications, however, these points are never needed.

Let Q denote the set of those a in $C^n(a)$ at which (A2) has at least one solution with at least one infinite coordinate. For real phase shifts this means that at least one of them is equal to $\pi/2$ (resonance). We shall call the points in $C^n(a) - (P + Q)$ ordinary. It is clear that the set of ordinary points is connected; in other words any two ordinary points can be connected by a continuous curve L consisting entirely of ordinary points (see, for instance, Fuks,[7] Sec. 12).

Further, let R(a) be a bounded closed set of ordinary points, and let R(x) be the set of all solutions of (A1) corresponding to points in R(a). Then R(x) is also bounded. Indeed, if this were not the case, there would exist a sequence $x^{(l)}$ in R(x) converging to a point with at least one infinite coordinate. Let x be a solution of (A1) for $a = a^{(l)}$. Since R(a) has no intersection with P, the number of $a^{(l)}$ points is infinite. From the sequence $a^{(l)}$ we can choose a subsequence $a^{(l_m)}$ converging to a point $a^{(0)}$ in R(a). Then going to the limit in m in the equations

$$f_i(x^{(l_m)}, a^{(l_m)}) = 0, \qquad i = 1, \ldots, n \quad \text{(A5)}$$

we would obtain a contradiction with the requirement that $a^{(0)}$ is not in Q.

Levine[8] (see also Cherne[9]) has obtained an integral representation for the number of solutions of the equations

$$\varphi_i(x) = A_i, \quad \text{(A6)}$$

in a bounded region D under the following conditions: (1) the $\varphi_i(x)$ are meromorphic functions, (2) the number of solutions is finite, (3) there are no solutions on the boundary of D.

Let $a^{(1)}$ and $a^{(2)}$ be two ordinary points in $C^n(a)$, and let L be a continuous curve connecting them. As has been shown above, the set of all solutions of (A1) with a in L is bounded in $C^n(x)$. There therefore exists a region D such that all these solutions are in its interior. Using Levine's integral representation, it is easily shown that the number of solutions of (A1) depends continuously on a in L.* It therefore follows that the number of such solutions is the same for all ordinary points.

In order to include also points that are not ordinary, we make the following definition: the system (A1) with $a = a^{(0)}$ in $C^n(a)$ has N solutions in the generalized sense if there exists a neighborhood S of $a^{(0)}$ such that for almost all points in S Eqs. (A2) have exactly N solutions in the usual sense. It is then clear that the number of solutions in the generalized sense is the same for all points in $C^n(a)$.

In order to find this number N, we need only count the number of solutions of (A1) at any ordinary point of $C^n(a)$. We choose the point $a = (0, \ldots, 0)$, and we show that for this point (A1) has only vanishing solutions. It will then follow that $(0, \ldots, 0)$ is an ordinary point of $C^n(a)$. Indeed, for $a_1 = \ldots = a_n = 0$ (zero energy) all the A_i of (1) vanish. This means that the product of the scattering cross section by the square of the wave number also vanishes in the limit. Then the product of the wave number and the scattering amplitude also vanishes. Since it is expanded in orthogonal functions of the angle, $e^{2i\delta k} - 1$ must also vanish for all k. It follows then that for zero energy the only solutions are $x_1 = \tan \delta_1 = 0, \ldots, x_n = \tan \delta_n = 0$.

All that remains is to count the number of solutions of (A1) for $a = (0, \ldots, 0)$. As is well known, this number can be found in the following way. Let ν_i be the smallest number for which at least one of the partial derivatives of order ν_i of the function $f_i(x, 0)$ does not vanish for $x = (0, \ldots, 0)$. Then

$$N = \prod_{i=1}^{n} \nu_i. \tag{A.7}$$

It is easily verified that for (A1) $\nu_i = 2$ for all i and therefore

$$N = 2^n. \tag{A8}$$

We note that this number is considerably below its upper bound $N \leq 2^n$ obtained by elimination theory.

We have thus shown that each of our phase-shift analysis problems has exactly 2^n solutions including, of course, the nonunitary ones.

*It is possible that this continuity can also be proved in a more elementary way.

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