Phaseshift analysis in single-channel reactions

Phaseshift Analysis in Single-channel Reactions *)

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1. Introduction

A general method for phaseshift analysis of single channel reactions is outlined. The purpose of this paper is to give a complete survey of this subject[1]...[6], in order to relate the phaseshift ambiguities closely to the mathematical structure of the cross section and to allow the quick numerical calculation of all mathematical phase shifts compatible with input data. The method is outlined for the general case of arbitrary maximum orbital angular momentum, and discussed in detail for S, P and D wave analyses.

2. Outline of the Method

The differential cross section for the scattering of neutrons by zero spin nuclei is given by

$$
k^2\, \sigma(\theta) = \left| \sum_L (\boldsymbol{a}_L/2\,i)\, P_L(\cos\theta) \right|^2,
$$
$$
+ \left| \sum_L (\boldsymbol{b}_L/2\,i)\, P_L'(\cos\theta) \right|^2, \tag{1}
$$

where

$$
\boldsymbol{a}_0 = (\cos 2\,\delta_1^0 - 1) + i \sin 2\,\delta_1^0, \tag{2a}
$$

$$
\boldsymbol{a}_L\,(L > 0) = u_L - (2\,L + 1) + i\,v_L, \tag{2b}
$$

$$
\boldsymbol{b}_L = \exp(2\,i\,\delta_{2L+1}^L) - \exp(2\,i\,\delta_{2L-1}^L), \tag{2c}
$$

and

$$
u_L = \alpha_L \cos 2\,\delta_{2L+1}^L + \beta_L \cos 2\,\delta_{2L-1}^L, \tag{3a}
$$

$$
v_L = \alpha_L \sin 2\,\delta_{2L+1}^L + \beta_L \sin 2\,\delta_{2L-1}^L. \tag{3b}
$$

δ_{2J}^L is the phaseshift for the interaction in the state of orbital angular momentum L and total angular momentum $J = L \pm 1/2$; and $\alpha_L = L + 1$, $\beta_L = L$. Let L_{max} be the

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maximum orbital angular momentum involved at the considered scattering energy. Equation (1) can be written as

$$k^2 \, \sigma(\theta) \; = \; \sum_{N=0}^{2\,L_{max}} A_N \cos^N \theta \, , \tag{4}$$

where the coefficients A_N, expressed in terms of the real and imaginary part of $\boldsymbol{a}_L$ and $\boldsymbol{b}_L$, are determined by the least square fit of the measured angular distribution. Using the optical theorem $\mathrm{Im} \, \boldsymbol{f}(0^0) = (k^2/4\,\pi) \, \sigma(k)$, where $\boldsymbol{f}(0^0) = \sum_L (\boldsymbol{a}_L/2\,i)$, and the relation $k^2 \, \sigma(0^0) = [\mathrm{Re} \, \boldsymbol{f}(0^0)]^2 + [\mathrm{Im} \, \boldsymbol{f}(0^0)]^2$, one obtains

$$\cos 2 \, \delta_1^0 + \sum_L u_L = U_L \, , \tag{5a}$$

$$\sin 2 \, \delta_1^0 + \sum_L v_L = V_L \, , \tag{5b}$$

where in the case of $L = L_{max}$

$$U_{L_{max}} = \sum_{N=0}^{L_{max}} [(2\,N+1) - 2\,A_{2N}/(2N+1)] \, , \tag{6a}$$

$$V_{L_{max}} = 2\,\Omega_V \left[\sum_{N=0}^{2\,L_{max}} A_N - \left(\sum_{N=0}^{L_{max}} A_{2\,N} \Big/ \{2\,N+1\} \right)^2 \right]^{1/2} , \tag{6b}$$

Ω_V being the signum function*)

$$\Omega_V = \pm 1 \, . \tag{7}$$

Since $V_{L_{max}}$ is a real quantity, the angular distribution coefficients must obey the condition

$$\sum_{N=0}^{2\,L_{max}} A_N - \left(\sum_{N=0}^{L_{max}} A_{2\,N} \Big/ \{2\,N+1\} \right)^2 \geqslant 0 \, . \tag{8}$$

The following procedure will be entirely based on Equations (3); the importance of these equations arises from the fact that they allow the determination of the two phaseshifts corresponding to a given $L > 0$, provided all other phaseshifts are known. The solution of Equations (3) in compact form may be written as

$$\cos 2 \, \delta_{2L+1}^L = F_+(\Omega_L, u_L, v_L)/\alpha_L \, , \tag{9a}$$

$$\sin 2 \, \delta_{2L+1}^L = F_+(\Omega_L, v_L, -u_L)/\alpha_L \, , \tag{9b}$$

$$\cos 2 \, \delta_{2L-1}^L = F_-(\Omega_L, u_L, v_L)/\beta_L \, , \tag{9c}$$

$$\sin 2 \, \delta_{2L-1}^L = F_-(\Omega_L, v_L, -u_L)/\beta_L \, , \tag{9d}$$

where

$$\left. \begin{aligned} F_{\pm}(\Omega_L, p, q) = \{ &p \, [(p^2 + q^2) \pm (\alpha_L^2 - \beta_L^2)] \\ &\pm \Omega_L \, q \, [(2\,\alpha_L\,\beta_L)^2 - (p^2 + q^2 - \alpha_L^2 - \beta_L^2)^2]^{1/2} \} \, \{2\,(p^2+q^2)\}^{-1} \, . \end{aligned} \right\} \tag{10}$$

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*) Unless otherwise stated the symbol Ω will always be referred to a sgn function.

Equations (9) show that the evident ambiguity implied by Equations (3) is described by the sgn function Ω_L. (In the particular case of $L = 1$, this ambiguity corresponds, in the neutron-He⁴ scattering, to the normal or inverted doublet, which is known as the FERMI-YANG ambiguity in the π^+-proton case).

Since we consider elastic scattering only, the following inequality must be satisfied, in order to ensure that the L phaseshifts be real

$$| u_L^2 + v_L^2 - \alpha_L^2 - \beta_L^2 | \leqslant 2\,\alpha_L\,\beta_L\,. \tag{11}$$

A geometrical representation of Equations (5) is shown in Figure 1, which visually demonstrates the two doublets.
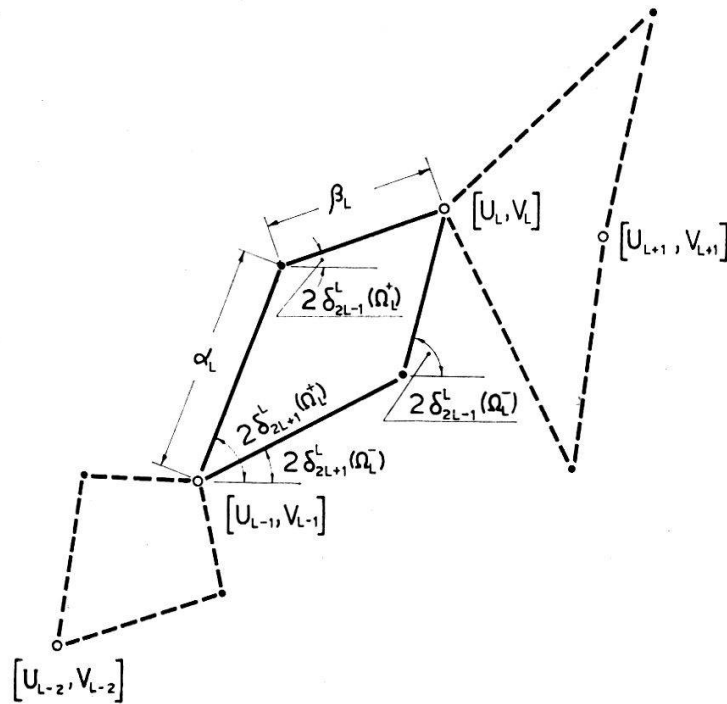

Fig. 1

Linkage system allowing the calculation of the δ^L doublet, if all other phaseshifts are known. The Ω_L ambiguity is evident.

In order to evaluate the S phaseshift, it has been found convenient to start from the coefficient A_0, the general expression for which is found from Equations (1), (2), (3)

$$4\,A_0 = |\lambda|^2 + |\mu|^2 + 2\,(\cos 2\,\delta_1^0 - 1)\,(\operatorname{Re}\lambda - 1) + 2\,\sin 2\,\delta_1^0\,\operatorname{Im}\lambda\,, \tag{12}$$

where

$$\lambda = \sum_{N=1}^{\infty} (-1)^N\,2^{-2N}\,\frac{(2N)!}{(N!)^2}\,a_{2N}\,, \tag{13a}$$

$$\mu = \sum_{N=0}^{\infty} (-1)^N\,2^{-2N}\,\frac{(2N+1)!}{(N!)^2}\,b_{2N+1}\,. \tag{13b}$$

After some lengthy manipulations, using Equations (5) with $L = 1$, and (12), the S phaseshift is still found to obey Equations (9a), (9b), where now

$$u_0 = (U_1 - 2)/2 + \mathrm{Re}\,\lambda\,, \tag{14a}$$

$$v_0 = V_1/2 + \mathrm{Im}\,\lambda\,, \tag{14b}$$

$$\alpha_0 = 1\,, \tag{14c}$$

$$\left.\begin{array}{l} \beta_0 = [2\,|\,\lambda\,|^2 + |\,\mu\,|^2 - |\,b_1\,|^2 + (U_1 - 4)\,\mathrm{Re}\,\lambda + V_1\,\mathrm{Im}\,\lambda \\ \qquad\qquad - U_1 - (U_1^2 + V_1^2)/4 - 4\,A_0 + 8]^{1/2}\,. \end{array}\right\} \tag{14d}$$

It may be remarked that the sgn function Ω_0 introduces an ambiguity even for the S phaseshift, as does Ω_L for higher partial waves.

3. S and P Wave Approximation

In the $L_{max} = 1$ approximation, $U_1 \equiv U_{L_{max}}$ and $V_1 \equiv V_{L_{max}}$ are determined from Equations (6), so that Equations (14) become

$$u_0 = (U_1 - 2)/2\,, \tag{15a}$$

$$v_0 = V_1/2\,, \tag{15b}$$

$$\alpha_0 = 1\,, \tag{15c}$$

$$\beta_0 = \left[\sum_{N=0}^{2} (-1)^N A_N\right]^{1/2}\,. \tag{15d}$$

A straightforward calculation gives then δ_1^0, by means of Equations (9a), (9b), (10), provided condition (11) is satisfied, which in this case becomes

$$|A_0 - A_1 + A_2/3| \leqslant \left[\sum_{N=0}^{2} (-1)^N A_N\right]^{1/2}\,. \tag{16}$$

The P doublet is now immediately found by means of Equations (9), (10), since $u_1 = U_1 - \cos 2\,\delta_1^0$ and $v_1 = V_1 - \sin 2\,\delta_1^0$, are known quantities. The inequality (11) now reads

$$|(U_1 - \cos 2\,\delta_1^0)^2 + (V_1 - \sin 2\,\delta_1^0)^2 - 5| \leqslant 4\,. \tag{17}$$

Since the inequality (17) is a condition imposed on the S phaseshift, a preliminary resolution of the Ω_0 ambiguity turns out to be possible in particular cases. The problem is now completely solved, i.e. $2^3 = 8$ mathematical solutions are compatible with the input experimental data (3 = number of independent sgn functions). The choice of the physical solutions cannot obviously be made simply on mathematical grounds and additional physical information [polarization, continuity prescriptions versus energy, effective range approach[7]) etc.] is required for this purpose.

The above formulas can be geometri-
cally represented by the linkage system
shown in Figure 2 where all possible
configurations allowed in S and P wave
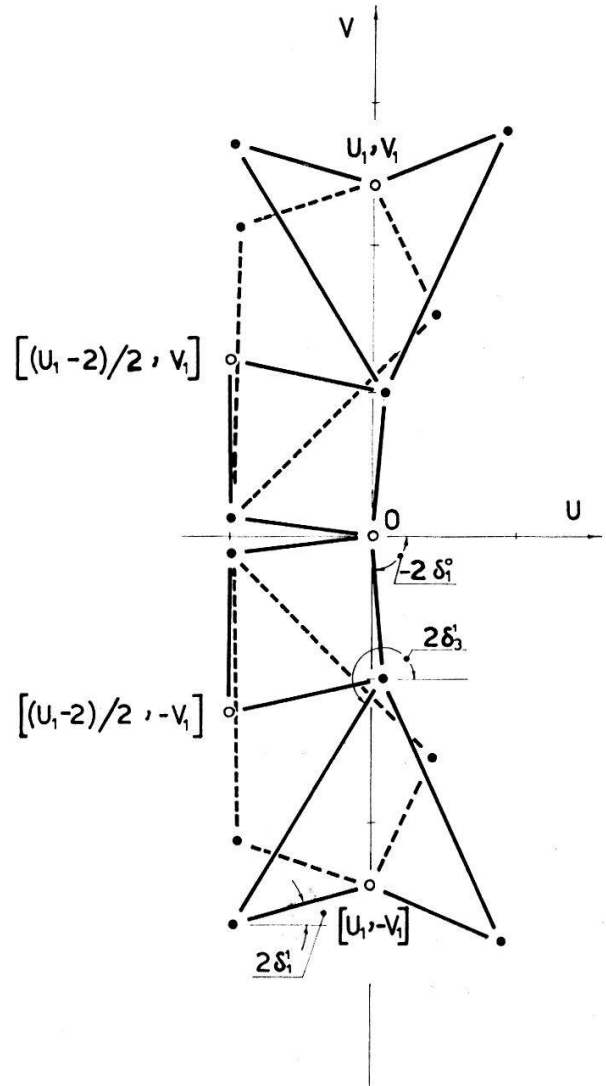approximation are drawn.

Fig. 2

Linkage system for phaseshift calculation in
the $L_{max} = 1$ approximation. The configu-
ration refers to neutron-He^4 elastic scattering
at the neutron energy of 2.87 MeV[8]), where
the D waves contribution has been found
negligible. The system, completely «frozen»,
shows that all mathematical ambiguities,
including the S wave one, are allowed here,
because condition (17) is satisfied. 'Physical'
phaseshifts are explicitely shown.

4. S, P and D Wave Approximation

In the $L_{max} = 2$ approximation*), $U_2 \equiv U_{L_{max}}$ and $V_2 \equiv V_{L_{max}}$ are known, whereas
the unknown quantities U_1 and V_1 are connected by the following relation

$$(U_1 - U_2 + 3)^2 + (V_1 - V_2)^2 = 4\left(1 + (4/15)\,A_4\right). \qquad (18)$$

The geometrical meaning of Equation (18) is evident: the point (U_1, V_1), lies on a
circle of center $(U_2 - 3, V_2)$, and radius $R = 2\sqrt{1 + (4/15)\,A_4} = \sqrt{x^2 + y^2}$. Equation

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*) For easy reference, the angular distribution coefficients in the $L_{max} = 2$ approximation are
listed below

$$4\,A_0 = |a_0|^2 + |b_1|^2 + (1/4)\,|a_2|^2 - \mathrm{Re}(a_0\,a_2^*),$$

$$4\,A_1 = 2\,\mathrm{Re}(a_0\,a_1^*) - \mathrm{Re}(a_1\,a_2^*) + 6\,\mathrm{Re}(b_1\,b_2^*),$$

$$4\,A_2 = |a_1|^2 - |b_1|^2 - (3/2)\,|a_2|^2 + 9\,|b_2|^2 + 3\,\mathrm{Re}(a_0\,a_2^*),$$

$$4\,A_3 = 3\,\mathrm{Re}(a_1\,a_2^*) - 6\,\mathrm{Re}(b_1\,b_2^*),$$

$$4\,A_4 = (9/4)\,|a_2|^2 - 9\,|b_2|^2.$$

(18) reduces the mobility of the linkage system to one degree of freedom only. It follows that all phaseshifts can be parametrized as functions of one variable parameter only. An additional condition between *all* phaseshifts, and input coefficients is then required in order to 'freeze' the system.

Choosing as variable parameter the abscissa $x = U_1 - U_2 + 3$ of the point (U_1, V_1), relative to the center of the circle, it is immediately found that $y = \Omega_y \sqrt{R^2 - x^2}$.

All phaseshifts are now obtainable as functions of x. The D doublet is determined by taking into account that $u_2 = 3 - x$ and $v_2 = -y$. The determination of δ_1^0 is carried out by means of Equations (14), which, by means of (18), can now be written as*)

$$u_0 = (U_2 - 3)/2 + x, \tag{19a}$$

$$v_0 = V_2/2 + y, \tag{19b}$$

$$\alpha_0 = 1, \tag{19c}$$

$$\beta_0 = \left[\sum_{N=0}^{4} (-1)^N A_N \right]^{1/2}. \tag{19d}$$

Finally the P doublet is calculated using the relations

$$u_1 = (U_2 - 3) + x - \cos 2\delta_1^0, \quad v_1 = V_2 + y - \sin 2\delta_1^0.$$

Inequality (11) becomes

$$\left| (U_2 - 3 + x - \cos 2\delta_1^0)^2 + (V_2 + y - \sin 2\delta_1^0)^2 - 5 \right| \leqslant 4. \tag{20}$$

This inequality would allow a preliminary elimination of the Ω_0 ambiguity as in the S and P wave. The linkage system for the determination of the phaseshifts as functions of x, is shown in Figure 3.

The 'freezing' condition is now provided by either of the two odd angular distribution coefficients, for instance by solving the equation

$$W(x) = -(4/3) A_3, \tag{21}$$

with

$$
\left.
\begin{aligned}
W(x) = {} & (x + 2)(U_2 - 6 + x - \cos 2\delta_1^0) + y(V_2 + y - \sin 2\delta_1^0) \\
& + 2(\cos 2\delta_3^1 - \cos 2\delta_1^1)(\cos 2\delta_5^2 - \cos 2\delta_3^2) \\
& + 2(\sin 2\delta_3^1 - \sin 2\delta_1^1)(\sin 2\delta_5^2 - \sin 2\delta_3^2).
\end{aligned}
\right\} \tag{22}
$$

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*) It must be stressed that the determination of the interval in which the parameter x is to be varied, involves timeconsuming procedures which are more cumbersome than may first appear. The following restrictive conditions, derived from (11), define, together with the obvious $|x| \leqslant R$, the 'accessible' intervals of x:

$$\left| x - (8/45) A_4 \right| \leqslant 2, \quad \left| \Omega_v \Omega_y |V_2| \sqrt{R^2 - x^2} - (1 + \beta_0^2) + (R^2 + S^2) - (U_2 - 3) x \right| \leqslant 2\beta_0,$$

where

$$4 S^2 = (U_2 - 3)^2 + V_2^2.$$

Inspection of the last inequality shows that the domains of existence of phaseshifts solutions, depend on the twofold ambiguity of the product sgn function $\Omega_v \Omega_y$.

For each value of x, one has in general $2^5 = 32$ sets of phaseshifts, corresponding to 5 sgn functions; furthermore the effective number of solutions might be different in each case, depending on the possible manifold of solutions of Equation (21). It must be said however that in practical cases the various restrictive conditions required by the procedure outlined in Section (3) and (4) drastically reduce the number of solutions mathematically compatible with the input data.

5. Numerical Calculation

A straightforward analogic determination of the phaseshifts is made possible using the linkage system described in Figures 2 and 3. A program for this kind of calculations, using digital computers, can be readily written, by following previous considerations (Section 3 and 4).
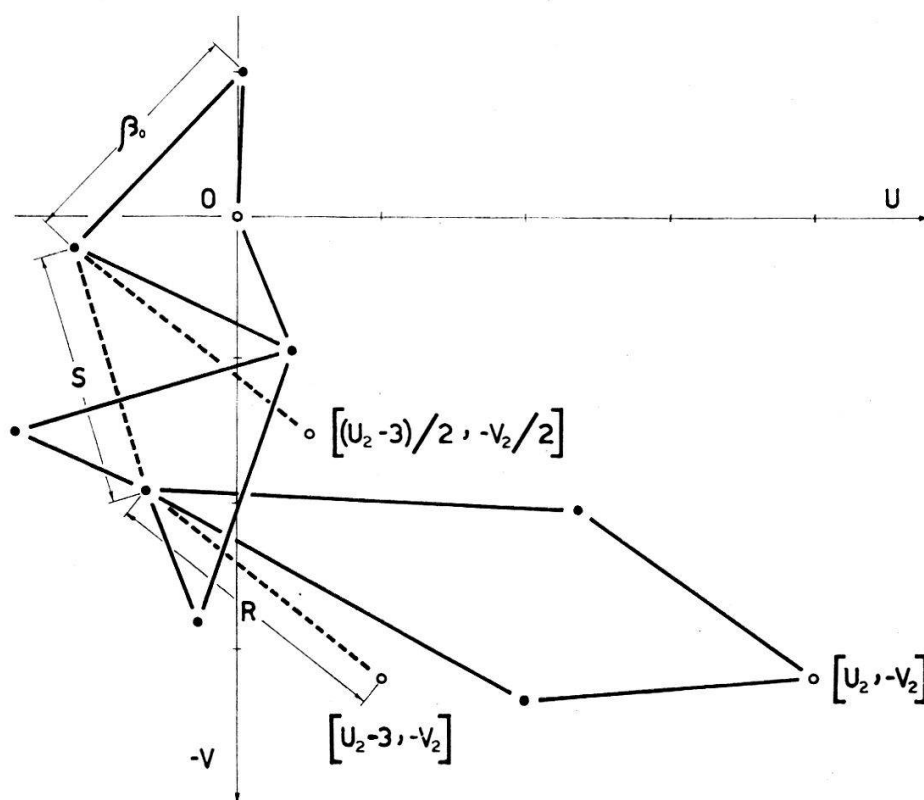

Fig. 3

Linkage system for phaseshift analysis in the $L_{max} = 2$ approximation. Points signed by open circles are fixed, according to the experimental A_N coefficients. The system is seen to have one degree of freedom.

Phaseshift analyses are remarkably simplified, both in the $L_{max} = 1$, and $L_{max} = 2$ approximations, by using the following symmetry properties: the quantities U_1, U_2, x, $W(x)$, $\cos 2\delta_{2J}^L$ are symmetric, and V_1, V_2, y, $\sin 2\delta_{2J}^L$ antisymmetric, against the simultaneous reversal of all sgn functions. Such a specular symmetry reduces by half the number of phaseshift solutions to be calculated. The linkage system, which introduces into the phaseshift analysis the element of continuous movement, is a useful device for preliminary calculation of those single channel reactions for which the energy dependence of phaseshifts is not well known. In fact, the linkage system

realizes the continuity prescriptions on the phaseshifts versus energy, which are concealed by standard electronic programming. In particular, the use of the linkage system, the degrees of freedom of which are established by the mathematical structure of the cross section, might represent in some cases an additional criterion for testing the reliability of the experimental data [see conditions (8) and (11)]. Of course, once the general trend of the phaseshift behaviour is known, the electronic computer can be used for a precise calculation, while the phaseshift stability against variation of the data, within quoted experimental errors, is readily evaluated by small movements of the analogic system.

6. Ambiguities

It may be useful to relate the well-known ambiguities in single channel reactions to the sgn functions Ω.

It is immediately established that the symmetry properties of $\cos \delta_{2J}^L$ and anti-symmetry properties of $\sin \delta_{2J}^L$ with respect to a symultaneous reversal of all sgn functions, is equivalent to the obvious property that the cross section is invariant with respect to the change of sign of all phaseshifts.

The P wave ambiguity, arising when D waves are absent, is brought about by sign reversal of Ω_1 (Ω_0 and Ω_V being fixed). It follows that the well-known relation holds

$$\delta_3^1(\Omega_1^+) - \delta_1^1(\Omega_1^+) = \delta_1^1(\Omega_1^-) - \delta_3^1(\Omega_1^-) . \qquad (23)$$

Equation (23) is no longer valid when D waves are switched on. In the general case, there still exists a D wave ambiguity, the nature of which is somewhat more complicated than the well-known P ambiguity. This fact is brought about by the function $W(x)$, which does not possess definite symmetry properties under the reversal of one sgn function only. It follows that each component of the D doublet is associated with a different S and P wave set of phaseshifts.

For the sake of completeness, it should be stressed that the sgn function Ω_0 gives rise to an S wave ambiguity. In the examples given below (Figures 2 and 4), this ambiguity turns out to be eliminated, in the π^+-proton scattering, because one of the two solutions is forbidden by condition (20), and in the neutron-He⁴ scattering, because one of the two solutions is physically unacceptable.

The S wave ambiguity is also implied in the Minami ambiguity[9]), according to which the cross section is invariant with respect to the interchange of all phaseshifts belonging to the same J and different parity. In the very special case, where all phaseshifts with $J \geqslant 3/2$ are zero, it can be easily demonstrated that the Minami ambiguity corresponds to changing Ω_0^+ into Ω_0^-, and viceversa.

As an example, Figures 2 and 4 show the properties of the mathematical ambiguities, in a practical case of $L_{max} = 1$ [neutron-He⁴ scattering at 2.87 MeV[8])] and $L_{max} = 2$ analyses [π^+-proton scattering at 310 MeV[10])] respectively. By inspection of Figure 4, the Minami ambiguity is seen to be still connected with an S arm inversion.
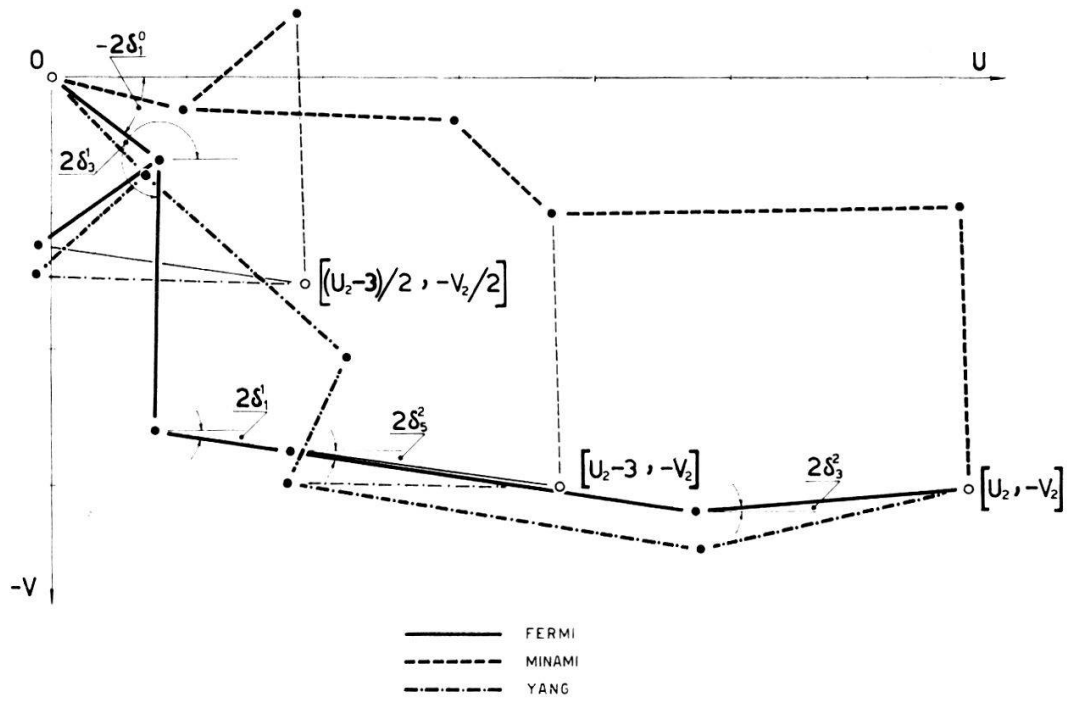
Fig. 4

π-proton scattering at 310 MeV, analized in the $L_{max} = 2$ approximation[10]. a) Only one S wave is allowed for each of the three solutions. b) 'Fermi' and 'Yang' solutions show an inversion in P arms only, and belong to slightly different values, since small D waves contributions are present. c) It has to be stressed that a Minami-like ambiguity is here possible, without resorting to F waves, owing to the smallness of the δ_5^2 phaseshift; of course the correspondence δ_{2L+1}^L (Fermi) = δ_{2L+1}^{L+1} (Minami) is only approximately satisfied. d) The 'Minami' solution, compared to the 'Fermi' one, shows an inversion in the S, P and D arms.

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