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NUMERICAL SOLUTION OF A MINIMUM PROBLEM

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PHYSICS

ABSTRACT

A particular non-linear function of six independent variables is minimized, using the Los Alamos electronic computer. The values of the variables at the minimum correspond to the phase shift angles in the scattering of pions by hydrogen.

The Los Alamos Maniac has been used in solving a numerical problem that is of importance in the interpretation of the scattering of pions by hydrogen. Mathematically, this problem consists of searching for the minimum of a rather complicated function of six angles. The procedure followed in solving this problem and the experience on the performance of the computer will be described. In the last section some general remarks on the use of similar methods in solving complicated systems of ordinary equations with many unknowns will be described.

The Physical Problem.

During the last year a series of experiments have been performed with the synchrocyclotron at the University of Chicago on the scattering of pions with energies of the order of 100 Mev by protons. The experimental results have been in part published.[1]

At each energy three different types of processes are investigated experimentally. They are the elastic scattering of positive and negative pions and the exchange scattering of the negative pions in which a negative pion incident on a proton loses its negative charge to the proton in the scattering process. The pion becomes thereby neutral and the proton is changed into a neutron. For each of these processes a complete angular distribution should be investigated. In the actual experiments data have been taken at three angles only, namely 45°, 90°, and 135° in the laboratory frame of reference. At each energy therefore

(1) Anderson, Fermi, Nagle and Yodh, Phys. Rev., 86, 793 (1952).

nine cross sections are measured. Three of them, σ_-^1, σ_-^2, σ_-^3, are the elastic scattering cross sections of the negative pions for the three above angles converted to the center of mass reference. Similarly, the three cross sections, σ_+^1, σ_+^2, σ_+^3, for the elastic scattering of positive pions are measured. The exchange scattering cross sections cannot be measured directly because of the extremely short lifetime of the neutral pion. One can observe, however, the gamma rays that result from its disintegration. Three gamma ray cross sections, σ_γ^1, σ_γ^2, σ_γ^3, are measured in this case. In what follows, the nine cross sections will be referred to as $\sigma_1, \sigma_2, \ldots, \sigma_9$.

Attempts have been made to express all these cross sections in terms of phase shift angles. On the assumptions discussed in Reference (1) all the cross sections at a given energy can be expressed in terms of six angles which will be here indicated by $\alpha_1, \alpha_2, \ldots, \alpha_6$. The first two angles are the phase shifts of the s-waves of isotopic spin 3/2 and 1/2, respectively, the angles α_3 and α_5 are the phase shifts of the p-waves of angular momentum 3/2 and isotopic spins 3/2 and 1/2, and the angles α_4 and α_6 are the phase shifts of the p-waves of angular momentum 1/2 and isotopic spins 3/2 and 1/2.

The Mathematical Problem.

The nine experimental cross sections $\sigma_1, \sigma_2, \ldots, \sigma_9$, are expressed in terms of the six angles α_1 to α_6 by formulas of the type

$$\sigma_1 = f_1(\alpha_1,\alpha_2,\ldots,\alpha_6)$$

$$\sigma_2 = f_2(\alpha_1;\alpha_2,\ldots,\alpha_6)$$

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(1) $$\sigma_9 = f_9(\alpha_1,\alpha_2,\ldots,\alpha_6)$$

The actual form of the functions f_1 to f_9 will be given later. Because of the experimental error in the measured quantities σ_i the equations (1) will not be exactly verified and one tries to determine the best set of angles α by a least squares procedure. One searches for the set of angles that minimizes the following expression,

(2) $$M(\alpha_1,\alpha_2,\ldots,\alpha_6) = \sum_{1}^{9}\left(\frac{\sigma_n - f_n(\alpha_1,\ldots,\alpha_6)}{\epsilon_n}\right)^2 = \text{minimum}$$

in which ϵ_n is the experimental error of the quantity σ_n.

Because of the rather complicated structure of the functions f, a conventional numerical solution of the minimum problem (2) is very laborious and requires one or two weeks of fairly steady computation for solving one single problem. An approximate solution obtained by this method is quoted in Reference (1). Machine computation presents great advantages in handling this problem. One problem can be solved by the Maniac in approximately five minutes.

In order to define completely our problem, the form of the functions f must be given. These functions are best expressed using complex notations. For each of the six angles α_n one defines a corresponding quantity.

(3) $$e_n = \exp(2\,i\,\alpha_n) - 1$$

From these quantities the following nine coefficients are computed.

$$b_p = \frac{e_1+2e_2}{3};\quad a_{\beta p} = \frac{\sqrt{2}}{9}(e_3-e_4+2e_5-2e_6);\quad a_{\alpha p} = \frac{2e_3+e_4+4e_5+2e_6}{9}$$

(4) $$b_N = \frac{\sqrt{2}}{3}(e_1-e_2);\quad a_{\beta N} = \frac{2}{9}(e_3-e_4-e_5+e_6);\quad a_{\alpha N} = \frac{\sqrt{2}}{9}(2e_3+e_4-2e_5-e_6)$$

$$b = e_1;\quad a_\beta = \frac{\sqrt{2}}{3}(e_3-e_4);\quad a_\alpha = \frac{2e_3+e_4}{3}$$

These nine coefficients represent physically the amplitudes of the scattered waves of different spin, angular momentum and electric charge for the three processes. These quantities are used for the computation of nine more quantities as follows:

$$A_- = \frac{2|b_p|^2+9|a_{\beta p}|^2}{8};\quad B_- = \frac{3}{2}\mathcal{R}(b_p a^*_{\alpha p});\quad C_- = \frac{18|a_{\alpha p}|^2-9|a_{\beta p}|^2}{8}$$

(5) $$A_o = \frac{2|b_N|^2+9|a_{\beta N}|^2}{8};\quad B_o = \frac{3}{2}\mathcal{R}(b_N a^*_{\alpha N});\quad C_o = \frac{18|a_{\alpha N}|^2-9|a_{\beta N}|^2}{8}$$

$$A_+ = \frac{2|b|^2+9|a_\beta|^2}{8};\quad B_+ = \frac{3}{2}\mathcal{R}(b a^*_\alpha);\quad C_+ = \frac{18|a_\alpha|^2-9|a_\beta|^2}{8}$$

The symbol $\mathcal{R}$ means "real part of". An asterisk means the complex conjugate. The cross sections are expressed in terms of these nine quantities by the following formulas

$$
\begin{aligned}
\sigma_1 &= A_- + B_- \cos \chi_1 + C_- \cos^2 \chi_1 \\
\sigma_2 &= A_- + B_- \cos \chi_2 + C_- \cos^2 \chi_2 \\
\sigma_3 &= A_- + B_- \cos \chi_3 + C_- \cos^2 \chi_3 \\
\sigma_4 &= A_+ + B_+ \cos \chi_1 + C_+ \cos^2 \chi_1 \\
\sigma_5 &= A_+ + B_+ \cos \chi_2 + C_+ \cos^2 \chi_2 \\
\sigma_6 &= A_+ + B_+ \cos \chi_3 + C_+ \cos^2 \chi_3 \\
\sigma_7 &= 2A_o + \frac{2-q}{3} C_o + pB_o \cos \chi_1' + qC_o \cos^2 \chi_1' \\
\sigma_8 &= 2A_o + \frac{2-q}{3} C_o + pB_o \cos \chi_2' + qC_o \cos^2 \chi_2' \\
\sigma_9 &= 2A_o + \frac{2-q}{3} C_o + pB_o \cos \chi_3' + qC_o \cos^2 \chi_3'
\end{aligned} \tag{6}
$$

In these formulas the cross sections on the left hand side are expressed in units of $\lambda\!\!\!^{-2}$ where $\lambda\!\!\!^{-}$ is the de Broglie wave length in the center of mass system. They are, therefore, pure numbers. The quantities p and q are known constants for each energy and are given by the following formulas.

$$p = \frac{2\gamma}{\eta} - \frac{1}{\eta^2} \ln \frac{\gamma+\eta}{\gamma-\eta} \tag{7}$$

$$q = 2 + \frac{6}{\eta^2} - \frac{3\gamma}{\eta^3} \ln \frac{\gamma+\eta}{\gamma-\eta} \tag{8}$$

in which γ and η are the total energy and the momentum of the pion in the center of mass system expressed in units μc^2 and μc, respectively, (μ = pion mass; c = velocity of light). The quantities X_1, X_2, and X_3 are the angles at which the cross sections are measured (45°, 90°, 135°), converted to the center of mass system. X_1', X_2', X_3' are the angles converted to the center of mass system for the case that the particle observed is a gamma ray. Both sets of angles are computed easily for each energy with the transformation formulas of relativity.

The Coding of the Problem.

In order to solve numerically the minimum problem (2) the Maniac must be instructed first to compute the quantity M for six given phase shift angles. These angles will then be changed by small steps according to a pattern to be described, searching for lower and lower values of M until a minimum is found. The coding consists therefore of a first part that contains the instructions for the computation of the function M and a second part with the instructions for the search of the minimum.

The first part is rather lengthy but logically quite straightforward. The machine computes in succession the real and imaginary parts of the quantities (4) and then combines them to compute the quantities (5) and the cross sections (6). Then it forms the sum of squares that appear in (2). For this computation the sines and cosines of the six angles are needed. For the initial values of the six angles the sines and cosines are given as part of the input of the problem. In the successive computation as the angles are changed, a simple routine is used that gives the new values of the trigonometric functions by using the old values and the addition theorem. The coding of this part of the problem requires approximately 150 memory positions. In spite of the complication of the function M, the machine computes its value in approximately 4/10 of a second, whereas a hand computation of the same function takes about 20 minutes.

The search for the minimum involves a sequence of successive computations of M for different values of the angles. Each time that new angles yield a value of M smaller than any of the preceding ones, this value is stored as a temporary minimum. The procedure stops when a set of angles, $\alpha_1, \alpha_2, \ldots, \alpha_6$, is found such that the values of M for this set are smaller than the 12 values of M obtained when one of the six angles is either increased or decreased by a specified small step. The smaller is the step, the higher is the accuracy of the minimum values found.

For a coarse search of the minimum, steps of $1/2^\circ$ were chosen. After computing the value for M for the initial angles, the computer is instructed to seek a new value of M obtained by increasing α_1 by $1/2^\circ$. If this value is smaller than the original, the computer keeps on calculating values of M, adding each time $1/2^\circ$ to α_1 until the value of α_1 is reached such that adding $1/2^\circ$ to it increases M instead of decreasing it. If the first addition of $1/2^\circ$ to α_1 produces an increase in M, the computer is instructed to subtract from α_1 a half degree at a time until M stops decreasing. After this operation is completed, the computer repeats the same operation on α_2, and then on α_3, etc., up to α_6. This cycle is repeated until two successive cycles do not produce a further decrease of the value of M. After this coarse search for the minimum is completed the computer is instructed to go through a similar operation using this time a step of $1/16^{\circ}$. After this second search is completed optimum angles and the values of the cross sections at the minimum are printed.

If the function M had one single minimum, one would expect that no matter what is the set of angles from which one starts, the procedure should always end very close to the same minimum position. Errors up to about $1/2^{\circ}$ are possible because of the finite step of $1/16^{\circ}$ used. For the practical problem errors of this magnitude are quite irrelevant. If the function M has several minima, one might expect that, depending on the set of angles from which one starts, the computer may end up at a different relative minimum.

In the present problem it was known that the function M had at least four minima, two of them corresponding to entirely different sets of angles, and two more obtained from them by changing the signs of all angles. In order to investigate whether there are any additional minima, it would be necessary to have a rather complete mapping of the function, a very staggering task for a function of six independent variables. This point was investigated partially as follows: A search of the minimum with the same experimental data was repeated some 30 times, starting each time with a different set of initial angles chosen at random. The minima obtained were recorded and classified. Three essentially different minima were found; for each of them sometimes one sign of the variables and sometimes the opposite is found. Two of the minima are in the vicinity of the positions that were already known, and the third is at quite different values of the angles. This last minimum, however, is irrelevant from the practical point of view, because it is only a relative minimum with a rather high value of M and would give therefore a very poor least square solution of the problem. While this procedure does not guarantee that no further minima exist, we feel that it is not very probable that any should have escaped this type of search.

Results.

Tables I and II summarize the results obtained for 113 and 135 Mev pions. In each table, Column 1 indicates the quantity represented in the corresponding line. Column 2 gives the measured cross sections with experimental error expressed in mb/sterad. The third and fourth columns, labeled "First Minimum" and "Second Minimum", give the results of the two solutions of the problem corresponding to the two lowest minima of M. In computing the fifth column the same code was used but the input was changed because the three errors of σ_-^1, σ_-^2, σ_-^3 were increased by about a factor 1000. It is clear from (2) that if this is done the first three of the nine terms of M become negligibly small. The minimum value of M will then be very close to 0 because, at least in general, it will be possible to find a set of six angles that represent exactly the remaining six cross sections. In the actual case the solution is not quite exact because of the finite step adopted in search for the minimum of M. One will notice that the cross sections for which the error has not been changed (lines 4 - 9 of the tables) are quite close to the measured values. The first three cross sections, for which the errors have been made practically infinite, are represented, instead, rather poorly.

A similar procedure was repeated by increasing once the errors of the three cross sections σ_+ (column 6) and once the errors of the cross sections σ_γ (column 7). In all of these three cases three of the cross sections were computed from the measured values of the remaining six, without any use of their experimental values being made in the computation. Inspection of the table shows that although the computed cross sections do not come very close to the measured values, they still have values somewhat similar to them.

Solutions of Minimum Problems by Electronic Computers.

The problem that has been here discussed is an example of a minimum problem for a function of many variables. In principle, problems of this type could be handled in two ways. One involves standard mathematical procedure of equating to 0 all the partial derivatives of the function and obtaining thereby a system of n equations with n unknowns (n number of variables). The second procedure is the one chosen in the present example: to search for the minimum value by computing the function at very many points until the minimum is attained.

There are, of course, no general criteria for preferring one method to the other and the choice may be different for different problems. The present procedure was chosen in our example because to solve the six equations with six unknowns obtained by equating to 0 the partial derivatives would have been probably a more complicated task than to compute directly the values of the function.

The following experience was gathered: If one searches for a minimum without any previous knowledge of its location, one will start from an arbitrary set of initial angles. It usually takes a relatively long time before the first cycle of variation of the six variables has taken place. In the average, this may be approximately two minutes, corresponding to computing the function 400 times. The next cycle of variation of the six variables is usually much shorter, and may last on the average perhaps 30 seconds. In most cases the coarse minimum, corresponding to a step of $1/2^{\circ}$, is reached in about a dozen cycles, totaling three or four minutes.

The fine search of the minimum with steps of $1/16^{\circ}$ takes on the average between one and two minutes. Only exceptionally it has happened that the coarse minimum was actually rather far from the true minimum position and in this case the further approach to the minimum with the fine step is more lengthy.

A Method for Solving Systems of Equations with Many Variables.

The same general procedure followed in the present problem for obtaining a minimum may be applied to the problem of solving a complicated system of n equations with n unknowns. Let the equations be of the form

$$(9)\qquad \begin{aligned} f_1(x_1x_2\ldots x_n) &= a_1 \\ f_2(x_1x_2\ldots x_n) &= a_2 \\ &\text{- - - - - -} \\ f_n(x_1x_2\ldots x_n) &= a_n \end{aligned}$$

Consider the expression:

$$(10)\qquad M = \sum_{1}^{n} f_i(x_1\ldots x_n) - a_i^{\;\;2}$$

M vanishes for a solution of (9) and is greater than 0 otherwise. A solution corresponds therefore to a minimum of M which can be found by a searching procedure of the same type used for our problem. Of course, only minima where $M = 0$ will correspond to actual solutions of the system nine and there might be other relative minima that would have to be discarded.

An example of this procedure for solving a system of six equations with six unknowns is given in the previous calculations in columns 5, 6, and 7 of the two tables. In fact the procedure followed would correspond exactly to the one described in this section if three of the errors had been made infinite instead of being only very large. The reason why the errors were made large but not infinite was merely a practical one, because by so doing one does not have to re-code the problem at all, but merely to change some of the input data.

Naturally, if one wanted to obtain more accurate solutions of the equation, one would have to use a smaller step. Probably it would save computing time to search for the solution to start with a coarse step and to reduce the step successively as closer and closer solutions are found.

It is questionable whether a procedure of this type would be practical in solving a system of linear equations. Probably in this case a method of successive elimination would be faster than the search for a minimum. On the other hand, it is likely that the search for a minimum may be a very practical approach for the case of complicated equations where the elimination procedure would not be easily feasible.

We wish to acknowledge the assistance of Mr. John B. Jackson during the course of computer operation.

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Table I

113 Mev

	Measured	First Minimum	Second Minimum	ε_- increased	ε_+ increased	ε_γ increased
σ_-^1	0.55 ± 0.23	0.707	0.702	1.362	0.603	0.672
σ_-^2	0.48 ± 0.22	0.382	0.372	0.605	0.436	0.419
σ_-^3	0.73 ± 0.19	0.698	0.705	0.931	0.740	0.711
σ_+^1	3.61 ± 0.65	3.913	3.946	3.618	4.231	3.672
σ_+^2	5.29 ± 0.62	5.034	5.041	5.258	4.383	5.207
σ_+^3	13.46 ± 0.96	13.397	13.429	13.479	21.281	13.382
σ_γ^1	4.34 ± 0.65	3.967	3.941	4.337	4.324	3.544
σ_γ^2	5.17 ± 0.64	5.419	5.410	5.316	5.113	6.146
σ_γ^3	10.45 ± 0.99	10.340	10.333	10.294	10.453	11.661
α_1		13.4°	13.3°	15.5°	16.8°	15.0°
α_2		- 6.8	- 6.9	- 2.1	- 1.9	-13.2
α_3		-27.1	-10.3	-26.4	-27.6	-26.5
α_4		- 1.1	-35.8	- .8	-18.0	- 0.8
α_5		11.8	13.7	12.1	5.0	11.7
α_6		14.0	10.4	20.3	15.6	12.0
M		1.584	1.786			

Table II

135 Mev

	Measured	First Minimum	Second Minimum	ε_- increased	ε_+ increased	ε_γ increased
σ_-^1	0.87 ± 0.37	1.074	1.070	2.336	1.157	0.893
σ_-^2	0.65 ± 0.35	0.400	0.370	0.732	0.481	0.618
σ_-^3	0.87 ± 0.20	0.926	0.926	1.234	0.904	0.873
σ_+^1	5.66 ± 2.18	6.399	6.688	5.818	9.423	5.723
σ_+^2	6.75 ± 2.14	6.490	6.507	6.652	8.666	6.723
σ_+^3	21.64 ± 3.55	22.100	22.344	21.610	26.834	21.497
σ_γ^1	6.50 ± 1.00	5.581	5.606	6.486	5.881	4.137
σ_γ^2	6.70 ± 0.90	6.676	6.462	6.687	6.826	5.310
σ_γ^3	12.80 ± 0.90	12.683	12.762	12.806	12.766	10.461
α_1		21.2°	20.3°	24.2°	40.9°	25.2°
α_2		- 2.7	- 2.4	5.4	- 1.7	- 2.4
α_3		-37.9	-21.2	-35.6	-34.4	-35.2
α_4		-11.5	-48.7	-11.8	-20.9	-11.6
α_5		16.8	15.1	46.0	18.8	4.9
α_6		3.8	9.0	5.9	6.6	14.4
M		1.90	2.16			

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