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A PROGRAM FEDEF FOR THE PARAMETRIZATION OF EXPERIMENTAL DATA

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FEDEF is a Fortran program written to perform the data parametrization with theoretical functions. Experimental data are fitted using the least-squares method (LSQ) /1/. The program FEDEF can be adapted for use to any Fortran program where parameter values may be changed to improve an agreement between calculated predictions and experimental data. The program automatically finds out the set of parameters which yields the best least-squares calculated fit to the data.

Method of solution

In the least-squares fitting procedure the quantity

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{D_i - F_i}{\varepsilon_i}\right]^2 \qquad (1)$$

is minimized; i=1,2,...,N is the number of measured experimental points, D_i is the set of experimental values (composed of N numbers) with corresponding errors ε_i and F_i is the calculation result corresponding to D_i. The theoretical function F and hence χ^2 is dependent on the set of parameters p_k, k=1,2,...,M. From this follows that the derivative of χ^2 with respect to the p_k will be zero whenever χ^2 has a maximum. Therefore, for all M values of p_k we have at a minimum

$$\frac{d(\chi^2)}{dp_k} = \frac{1}{N}\sum_{i=1}^{N}\frac{2}{\varepsilon_i^2}(D_i - F_i)\frac{dF_i}{dp_k} = 0 \quad . \qquad (2)$$

Thus, the minimization of Eq.(1) leads to the system of linearly independent equations to be solved for unknown parameters.

Restrictions

A maximum of 10 fitting parameters and 100 data points can be simultaneously treated. It should be noted that these numbers can be arbitrarily increased (or decreased) by changihg the dimensions of variables.

Program structure

The program FEDEF requires subroutines OHIO, AV, TRANS, DER and FCT:

- OHIO - inversion of LSQ-matrix elements within a double precision;
- AV - calculation of the centre-data set;
- TRANS - data transformation into the log scale and vice versa;
- DER - calculation of derivative values of the function F;
- FCT - calculation of parametrized values.

Program input and output

The input read by FEDEF is:

1.line: N, M, IX, IY, KX, KY

with
N the integer number of data points;
M the integer number of fitting parameters;
IX (IY) the integer input number: if negative, then data on x (y)-coordinates are transformed into the log scale before the fitting procedure;
KX (KY) the integer input number: if negative, then the origin of coordinates x_o (y_o) is transformed into the centre-of-data set.

2. to (N+1). line: X(I), Y(I), DY(I)

X(I), Y(I) (I=1,...,N) is the set of experimental data points with corresponding errors DY(I). The format of these lines is (3E15.8). The maximum number of data points in X, Y and of errors in DY is 100.

The output of FEDEF is

a) table of input values;
b) centre-of-data set XØ = , YØ = (if(KX,KY < 0));
c) derivative values of the theoretical function F at all treated points;
d) values of LSQ-matrix elements;
e) table of result values:
X(I), Y(I), DY(I), DIF(I),

where X, Y and DY are input data, F is the result of calculation at a given experimental point and DIF(I)=(F(I)-Y(I)/DY(I);
f) values of fitting parameters with corresponding errors;
g) χ^2 value (see Eq.(1)) CHISQ = , and
h) correlation values of fitting parameters.

Installation

EC-1055 M computer at the Computing Centre of the Laboratory of High Energies, Joint Institute for Nuclear Research, Dubna.

Applications

Two special examples are presented for the FEDEF program applications:

1. The angular dependences of differential polarization $\sigma_o P^{y'}$ from the $^2H(d,\vec{p})^3H$ and $^2H(d,\vec{n})^3He$ mirror reactions at 0.975 MeV were fitted by the expansion in a series of associated Legendre polynomials[2] $P^1_L(\cos\theta)$, L being even:

$$\sigma_o P^{y'}(E,\theta) = \sum_L B_{L1}(E)\, P^1_L(\cos\theta) . \qquad (3)$$

The best least-squares fit of Eq.(3) yielded parameters B_{L1} at $\chi^2 = 1.386$ and $\chi^2 = 1.524$ for the $^2H(d,\vec{p})^3H$ [3] and $^2H(d,\vec{n})^3He$ [4] experimental data, respectively. The results are displayed in fig.1.

2. Following the R-matrix approach[5], the energy dependences of expansion coefficient $B_{21}(E)$ from the $^2H(d,\vec{n})^3He$ and $^2H(d,\vec{p})^3H$ reactions at low energies were fitted by the relation

$$B_{21}(E) = b_1\Omega_1(E) + b_2\Omega_2(E) + b_{02}\sqrt{\Omega_0(E)\Omega_2(E)} , \qquad (4)$$

where Ω are the barrier penetration factors[6] defined on the sphere of interaction radius r. They are expressed by means of regular and irregular Coulomb functions $F_\ell(kr)$ and $G_\ell(kr)$[2], respectively. In this case, the program FEDEF was used along with the well-known subroutine RCWFN[7] for the Coulomb function calculations. The best least-squares fit gives parameters b_1, b_2, b_{02} and interaction radius r as well with $\chi^2 = 0.416$ and $\chi^2 = 1.605$ for the $^2H(d,\vec{p})^3H$ and $^2H(d,\vec{n})^3He$ experimental data, respectively. The results of these fits are displayed in fig.2. The B_{21} values were fitted to log scale.

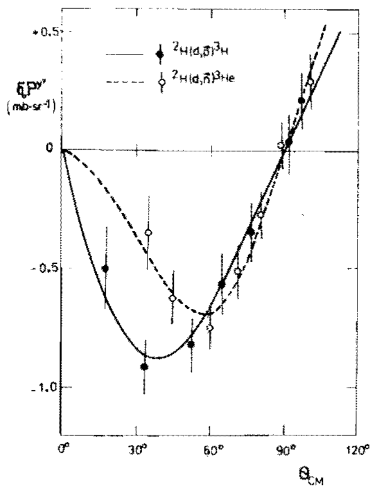

Fig.1. The least-squares fit of the experimental angular distribution of nucleon polarization from the $^2H(d,\vec{p})^3H$ and $^2H(d,\vec{n})^3He$ mirror reactions at about 1 MeV.

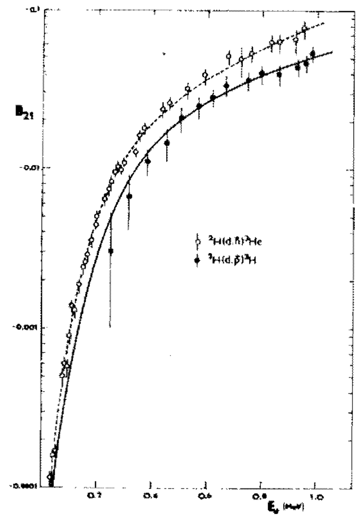

Fig.2. The least-squares fit of the experimental energy dependence of nucleon polarization from the $^2H(d,\vec{p})^3H$ and $^2H(d,\vec{n})^3He$ reactions in the theoretical framework of R-matrix approximation[5,6].

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Программа FEDEF для параметризации экспериментальных данных

Программа FEDEF проводит подготовку экспериментальных данных с помощью параметрических функций методом наименьших квадратов. Набор сотни экспериментальных данных и десяти параметров подгонки можно совместно проанализировать. Программа FEDEF может быть использована вместе с другими програмами, требующими согласия между теоретическими предсказаниями и значениями экспериментальных данных.

Работа выполнена в Лаборатории высоких энергий ОИЯИ.

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Перевод Л.Н.Барабаш

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A Program FEDEF for the Parametrization of Experimental Data

A program FEDEF provides the parametrization of experimental data with theoretical functions by the least-squares method. A set of about 100 data points and 10 fitting parameters can be simultaneously treated. The program FEDEF can be adapted for use to programs where parameters may be changed to improve an agreement between calculated predictions and experimental data.

The investigation has been performed at the Laboratory of High Energies, JINR.

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