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ANALYSIS AND DEVELOPMENT OF THE SERIES EXPANSION METHODS IN THRESHOLD DETECTOR ACTIVATION DATA HANDLING

by

G. DI COLA and A. ROTA

1964

Joint Nuclear Research Center
Ispra Establishment - Italy
Scientific Data Processing Center - CETIS

Paper presented at the Symposium on Fast and Epithermal Neutron Spectra in Reactors
Harwell, Didcot (Great Britain) - December 11-13, 1963

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CONTENTS

1. Introduction

The activation measurements of the threshold detectors are frequently used for the in-pile neutron spectra determination; this technique has the following advantages:

- The threshold detectors are not sensible to the high gamma fluxes of the reactors
- The small volume of the detectors prevent any neutron flux deformation
- No connection with the outside of the reactor is required
- The activation measurements are easy and not very expensive.

The experimental measurements may be expressed as A_i numbers: they indicate the reaction probability per second for one nucleus of the i-th isotope, when immersed into the unknown neutron flux. It follows that:

$$(1) \qquad A_i = \int_0^\infty \varphi(E)\,\sigma_i(E)\,dE = \int_{E_i}^\infty \varphi(E)\,\sigma_i(E)\,dE$$

where $\sigma_i(E)$ is the differential neutron cross-section of the i-th isotope for the reaction in question, and $\varphi(E)$ is the fast neutron differential flux (n/cm^2 . sec . Mev). The integration range may be reduced from $(0,\infty)$ to (E_i,∞) as

$$\sigma_i(E) \equiv 0 \qquad \text{for} \qquad E < E_i$$

When the A_i are known, a procedure has to be established for solving the system of equations (1). Many methods have been proposed to attain this solution [1], [2]. This work is a study of the group of methods known as "polynomial" and "orthonormal" methods. This set has been chosen for the following reasons:

1) It seems to be the more suitable for the neutron spectra description, even if it is not reactor generated.

2) A development is possible which allows the activation data interpretation, even if the detectors have not completely linear independent cross-sections.

Generally this second fact prevented the use of these methods with any set of threshold detectors.

2. The Polynomial and Orthonormal Methods

In the polynomial method, introduced by Uthe [3] , the spectral shape is assumed to be a polynomial in energy, with as many terms as detectors used, multiplied by a chosen weighting function. This method is an extension of the simple polynomial method, in which

$$(2) \qquad \varphi(E) = \sum_{0}^{n} a_i E^i \qquad (n = \text{number of detectors})$$

in fact the suggested form is:

$$(3) \qquad \varphi(E) = W(E) \sum_{0}^{n} a_i E^i$$

where W(E) is a suitable weighting function. Originally the actual meaning of (3) was a deformation of the fission spectrum W(E) by a polynomial.

The method using a series expansion of orthonormal functions has been suggested independently by Trice [4] and Hartman et al. [5] . Here $\varphi(E)$ is given by:

$$(4) \qquad \varphi(E) = \sum_{1}^{n} a_i \varphi_i(E)$$

The system of orthonormal functions is obtained using the Schmit's orthogonalization method, beginning from the cross section functions $\sigma_i(E)$.

Brownell et al. [6] proposed the following variation of the above mentioned method:

- $\varphi(E)$ is assumed to be described by

$$(5) \qquad \varphi(E) = W(E) \sum_{1}^{n} b_i \psi_i(E)$$

where W(E) has the usual meaning and the set of ψ_i functions is obtained by the same procedure used by Hartman and Trice.

- Many different solutions $\varphi'(E)$ are obtained by random deviation of the input activation data.
- The resulting curves are then linearly averaged, neglecting the occasional negative values.

The last considered method, due to Laming and Brown [7], has been reconsidered in [6]. $\varphi(E)$ is assumed to be described by:

$$\varphi(E) = W(E) \cdot \sum_{1}^{n} a_i \chi_i(E) \tag{6}$$

where the χ_i, i-degree polynomial, are an orthonormal set of functions, orthogonal, in the $(0, E_{max})$ range to W(E).

3. Series Expansion Methods Generalization

From the above, it is easy to see that all the described methods may be unified in one class where $\varphi(E)$ is expanded in the following series of linearly independent functions:

$$\varphi(E) = W(E) \sum_{1}^{n} a_i \psi_i(E) \tag{7}$$

By a suitable interpretation of the weighting function W(E) and of the system of functions $\psi_i(E)$, the expressions (2), (3), (4), (5), (6) may be obtained.

This generalization appears trivial, however it is possible to state only one procedure for the solution of the system of equation (1). The appropriate W function and the system $\psi_i(E)$ may be selected on the basis of parameters. In fact, by introducing the expression (7) in the equations (1), one obtains:

$$A_i = \int_{E_i}^{\infty} \sigma_i(E) \left[W(E) \sum_{1}^{n} a_j \psi_j(E) \right] dE = \sum_{1}^{n} a_j S_{ij} \tag{8}$$

where

$$S_{ij} = \int_{E_i}^{\infty} \sigma_i(E) W(E) \psi_j(E) \, dE \tag{9}$$

The solution of the linear equation system (8) gives univocally the coefficents of the expansion (7).

3.1. Input Data for numerical tests

The orthonormal methods have been tested by the following reaction data:

1) Np - 237 (n, f)
2) U - 238 (n, f)
3) Th - 232 (n, f)
4) S - 32 (n, p) P - 32
5) Ni - 58 (n, p) Co - 58
6) Al - 27 (n, p) Mg - 27
7) Fe - 56 (n, p) Mn - 56
8) Al - 27 (n, α) Na - 24

The cross section was taken from literature [8].
Two sets of activation data Ai have been tested:

- a "test" set, derived from the assumed σ_i by a "test" neutron spectrum: $\varphi(E) = \left[e^{-2.3E} + 0.03\, e^{-0.75E}\right] \cdot e^{-\frac{1}{0.5+E}}$
- an "experimental" set obtained from Ispra 1 Reactor in the PH3 position [8].

3.2. The Weighting function

A series of numerical tests have been performed in order to determine the influence of the weighting function when using the orthonormal methods.

The test results show clearly that a good choice of the W(E) function is very important. The fig. 1 shows the results obtained from a set of 6 threshold detector "test" activation data by three different weighting functions:

e^{-E} ; e^{-2E} ; $e^{-E} \operatorname{senh} \sqrt{2E}$ (Watt fission spectrum)

Other similar results have been obtained from experimental data. For neutron thermal pile spectra the more suitable weighting function seems to be e^{-E} (see also [7]).

In all the tests performed with W(E) = 1 no good results have been obtained: for this reason expansions of φ (E) according to (2) and (4) can not be used.

3.3. General Remarks

The use of the above methods suggest the following observations:

1 - The expansion term number is conditioned by the number of the detectors used and vice-versa.

2 - The cross-sections $\sigma_i(E)$ must be linearly independent functions: if this condition is not satisfied the matrix of the system coefficients is singular. The system becomes ill conditioned if the σ_i functions are quasi-linearly dependent.

In the considered sample the couples Th, U and Si, Ni appear to have similarly shaped cross-sections. It follows that the use of the whole set is not always possible (fig. 2); this is true particularly when real problems are considered, because the Ai and $\sigma_i(E)$ values are affected by experimental errors, both absolute and relative to one another. This difficulty appears more evident in the methods where the orthonormal functions are generated starting from the cross-sections (see expansions (4) and (5)).

Many numerical tests have been performed on "test" and "experimental" values (8 detectors), using the above mendioned method with $W(E) = e^{-E}$ and the following type of polynomials:

a) Simple polynomial.
b) Orthonormal polynomials over $(0, E_{MAX})$ range, relative to the specified W(E).
c) Orthonormal polynomials generated by the σ_i functions
d) Laguerre polynomials.

The fig. 2 and 3 show the results respectively obtained with the "test" and "experimental" data. They are completely different from one another and general conclusions are not possible. The most of them are not good: the only reliable results appear to be the ones obtained by simple and Laguerre polynomials from "test" data, despite the fact that they show some deviations above 8 MeV from the "test" spectrum.

The evidenciated troubles could be overcome by the choice of a suitably reduced number of detectors. Numerical tests of this type have been performed:

By using suitable sets of six detectors chosen from the eight available, as suggested by the previous considerations, all the methods have given reliable results. Unfortunately the spectrum shapes are not the same for different choices of detectors sets as shown in fig. 4. The pronounced differences observed are a consequence of the experimental errors of the Ai and σ_i (E) values. There is no significant difference in the results obtained from the test problem using different detectors sets, when the Ai and σ_i(E) are error free . Since for different sets of experimental data (relative to the same experience) different neutron shape spectra are obtained, the problem arises of selecting a representative spectrum.

The above reported remarks suggested a more general formulation of the problem by taking into account the following statements:

1) All the available activation data, independently from the cross-section shape, must have the possibility to be used.
2) The solution must approximate the Ai values in the best possible way.
3) The results are desired to be independent from the particular choice of the ψ functions.

4. Relative Deviation Minimization Method R D M M

Suppose the searched flux may be expanded in the series:

$$(10) \qquad \varphi(E) = W(E) \cdot \sum_i^{\infty} a_i \psi_i(E)$$

the best aproximation $\overline{\varphi}_m(E)$ to $\varphi(E)$ is assumed to be the one minimizing the quadratic form:

$$(11) \qquad Q(m, a_1, a_2, \ldots a_m) = \sum_1^m i \left[\frac{A_i - \int \sigma_i(E)\, \overline{\varphi}_m(E)\, dE}{A_i} \right]^2$$

where:

$$(12)\quad \bar{\varphi}_m(E) = W(E) \sum_1^m a_i \psi_i(E)$$

($m \leq n$ = number of detectors)

The quadratic form (11) represents the sum of the squares of the relative deviation of the A_i and, according to the Legendre least square postulate, the obtained solution gives, in the sense of least square, the best aproximation to the exponential data. The search of the minimum of Q, once m is fixed, is performed by the Gauss Method.

The requirement of the minimum of Q imposes the conditions:

$$(13)\quad \frac{\partial Q}{\partial a_k} = 0 \qquad k = 1, \ldots, m$$

and hence leads to the linear system in the m unknowns a_1, a_2, ... a_m :

$$(14)\quad S^T S\, a = S^T e$$

where:

$$a \equiv (a_1, a_2, \ldots a_m)$$

$$e \equiv (1, 1, \ldots 1)$$

$$S \equiv \{S_{ij}\} \qquad (i = 1, \ldots n\,;\ j = 1, \ldots m)$$

$$S_{ij} = \frac{1}{A_i} \int_0^\infty \sigma_i(E)\, W(E)\, \psi_j(E)\, dE$$

S^T indicates the transpose of the matrix S. Among the solutions $\bar{\varphi}_1, \bar{\varphi}_2, \ldots \bar{\varphi}_m$, the one that gives the minimum value of Q is chosen.

When m = n, this method is actually equivalent to the collocation method [9], where the simple system S a = e is solved. The last one is the method used in all the procedures described in sect. 3, that may be regarded as particular cases of rhe RDMM, once imposed m = n.

5. R D M M Results and Discussion

In order to carry out the data processing by the RDMM a FORTRAN code for the standard IBM-7090 has been prepared. This code has been used to process the "experimental" and "test" data with different choices of polynomial expansions. In all the tests performed the weighting function $W(E) = e^{-E}$ was used.

The more significant results are shown in fig.s 4 to 6.

The spectra obtained by using the reduced sets of detectors (with the collocation method: see 3.3), as well as a spectrum obtained by the complete set of detectors are shown in fig. 4. The comparison of these curvs indicates that the spectrum obtained by the RDMM may be regarded as an average between the ones obtained by the collocation method.

The fig. 5 shows the results obtained from "experimental" data (complete set of 8 detectors) by the RDMM using the polynomials a), b), d) of sect. 3.3 and the Chebyshev polynomials. Significant differences exist for experimental data only at high energy values of spectrum. These differences do not appear when "test" data are used. This fact indicates that the RDMM results may be considered indipendent from the particular choice of the ψ functions.

In the test performed with 8 detectors the values fo the quadratic form Q (11) were not very different from each other when m = 5,6,7. This fact results in very similar spectrum shapes, as may be seen in fig. 6. This figure shows the curves $\bar{\varphi}_5$, $\bar{\varphi}_6$, $\bar{\varphi}_7$ obtained by using the Laguerre polynomials.

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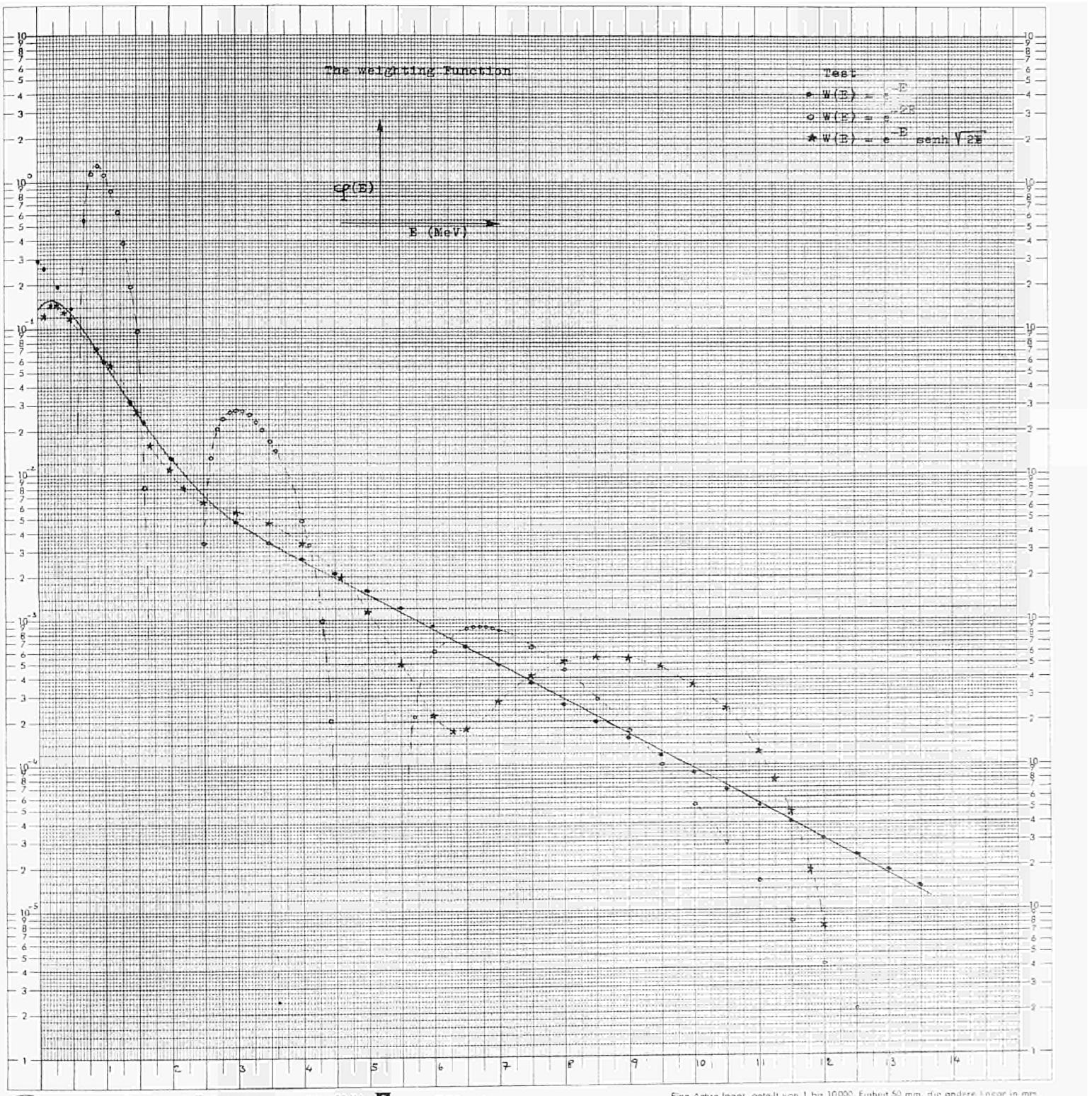

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FIG. 1

Eine Achse logar. geteilt von 1 bis 10000, Einheit 50 mm, die andere linear in mm

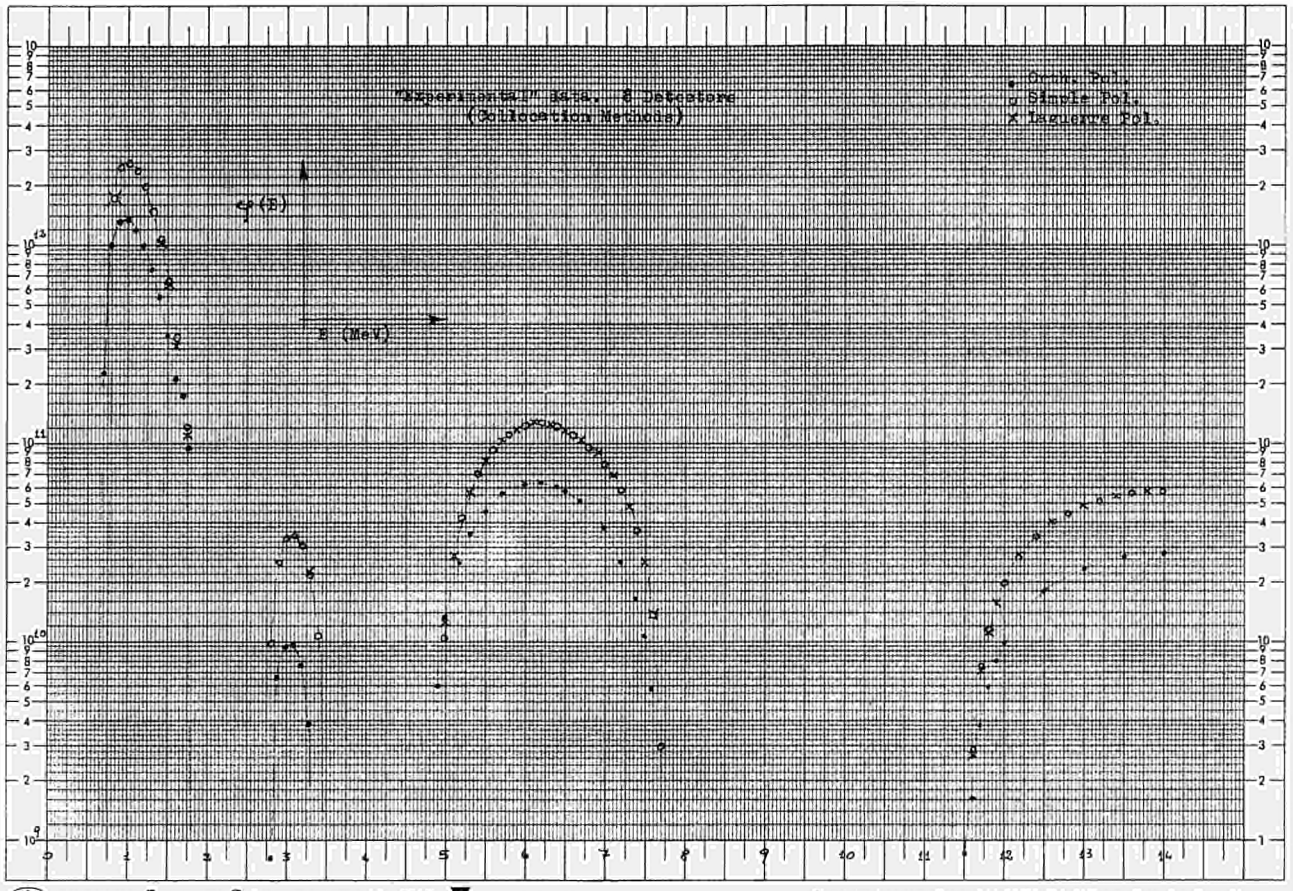

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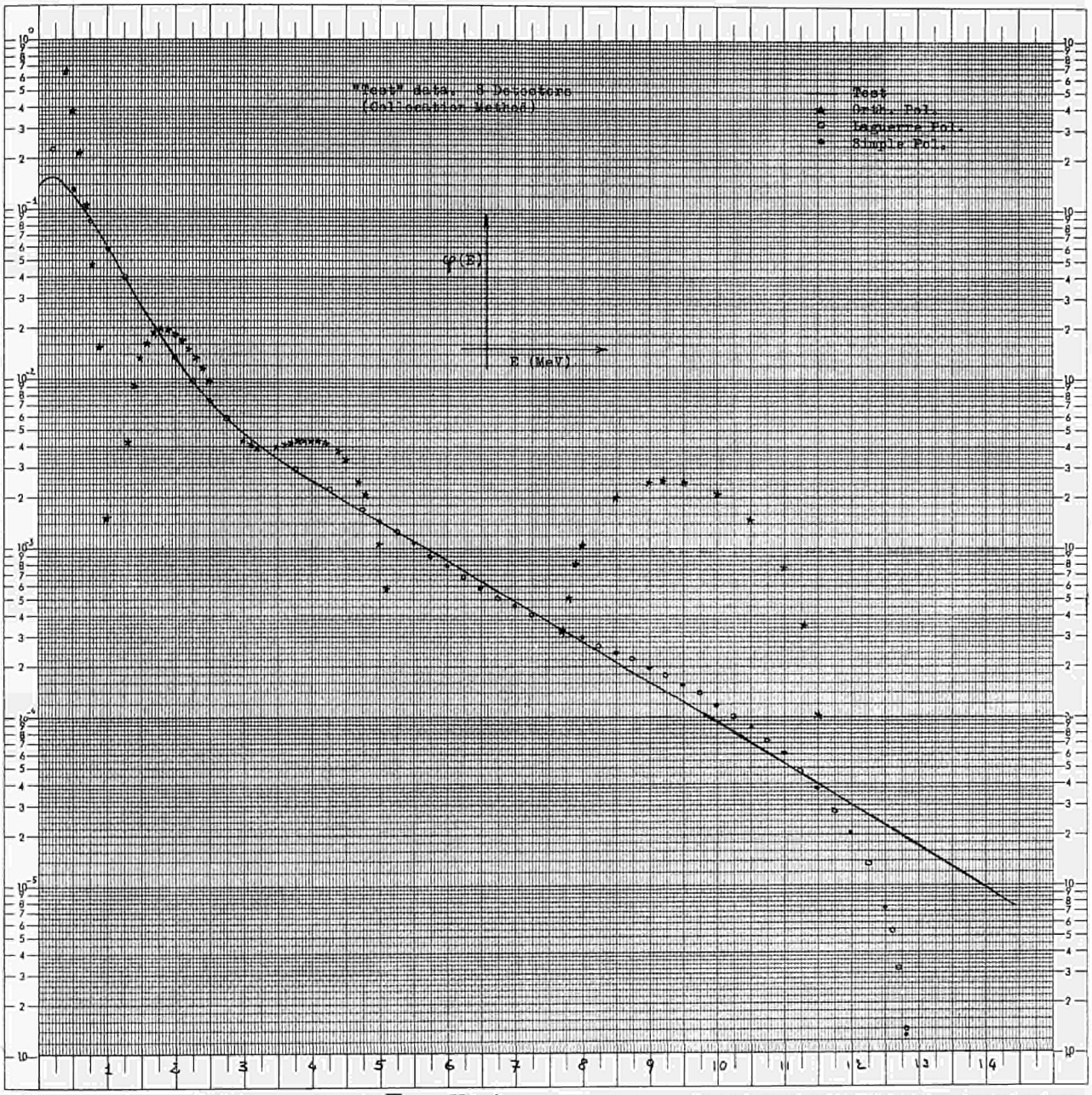
FIG. 2

Eine Achse logar. geteilt von 1 bis 10000, Einheit 50 mm, die andere linear in mm.



 Nr. 396½ FIG. 3

Eine Achse logar. geteilt von 1 bis 10000, Einheit 50 mm, die andere linear in mm.

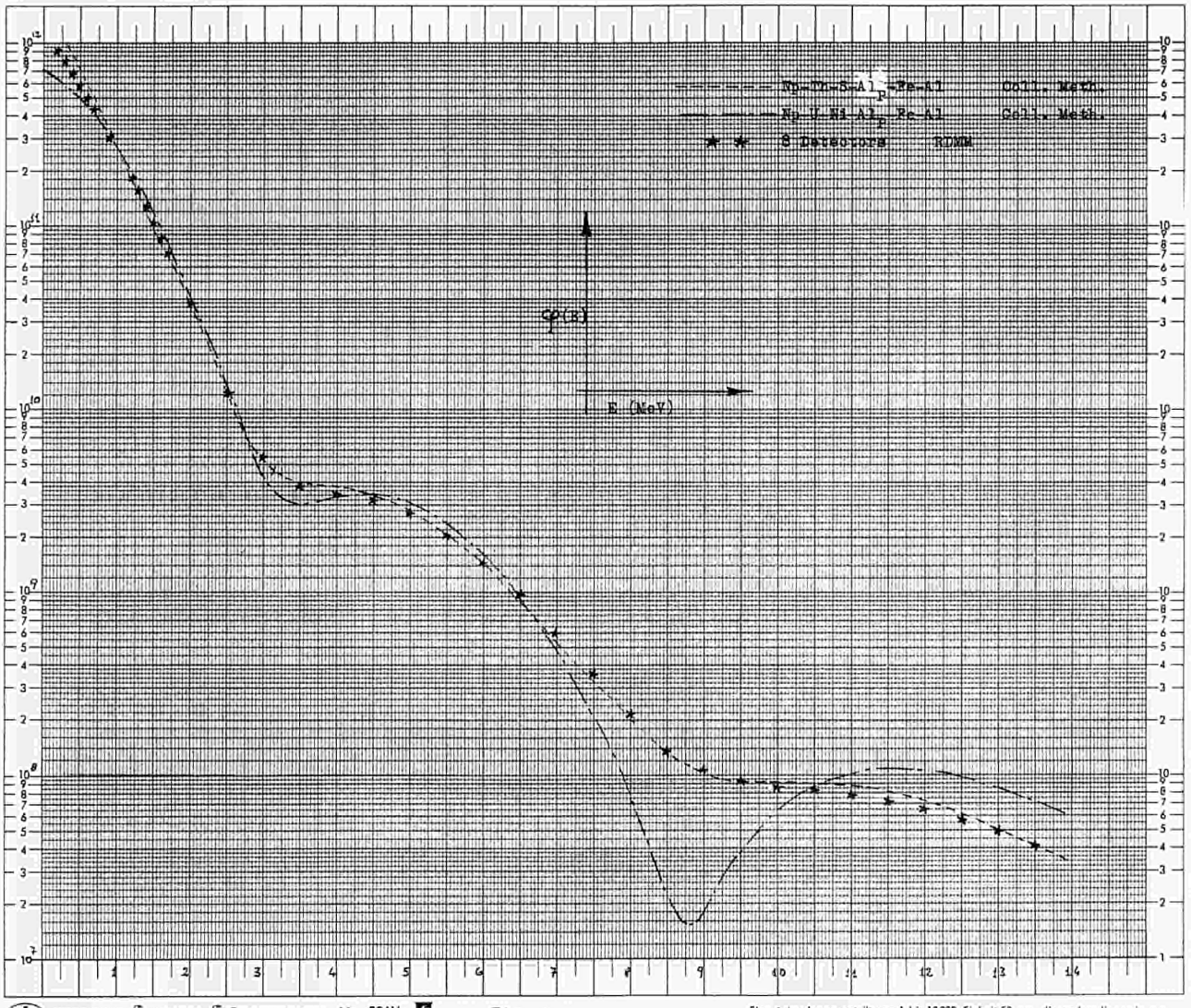


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Fig. 4

Eine Achse logar. geteilt von 1 bis 10000, Einheit 50 mm, die andere linear in mm.

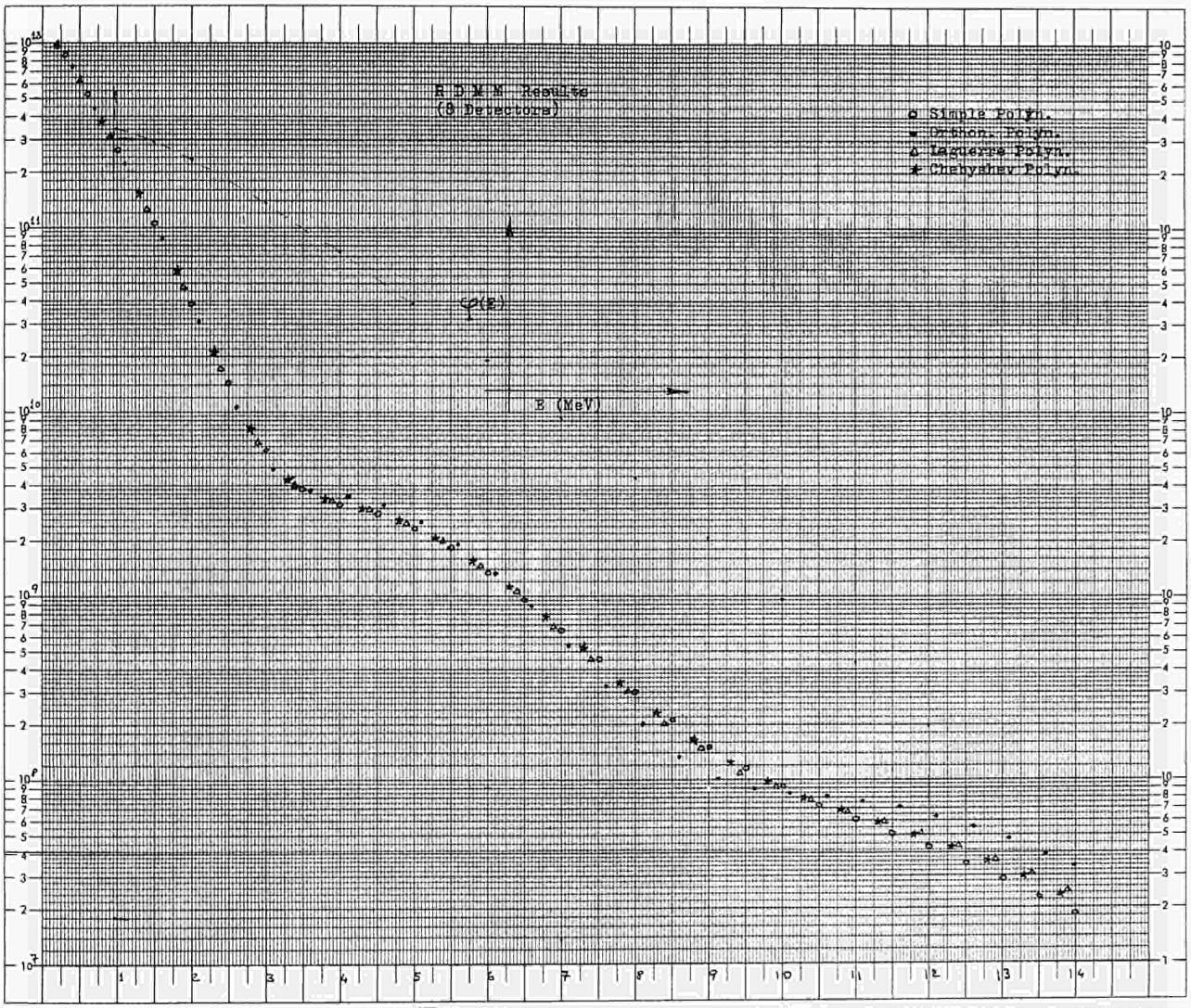

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FIG. 5

Eine Achse logar. geteilt von 1 bis 10000, Einheit 50 mm, die andere linear in mm.

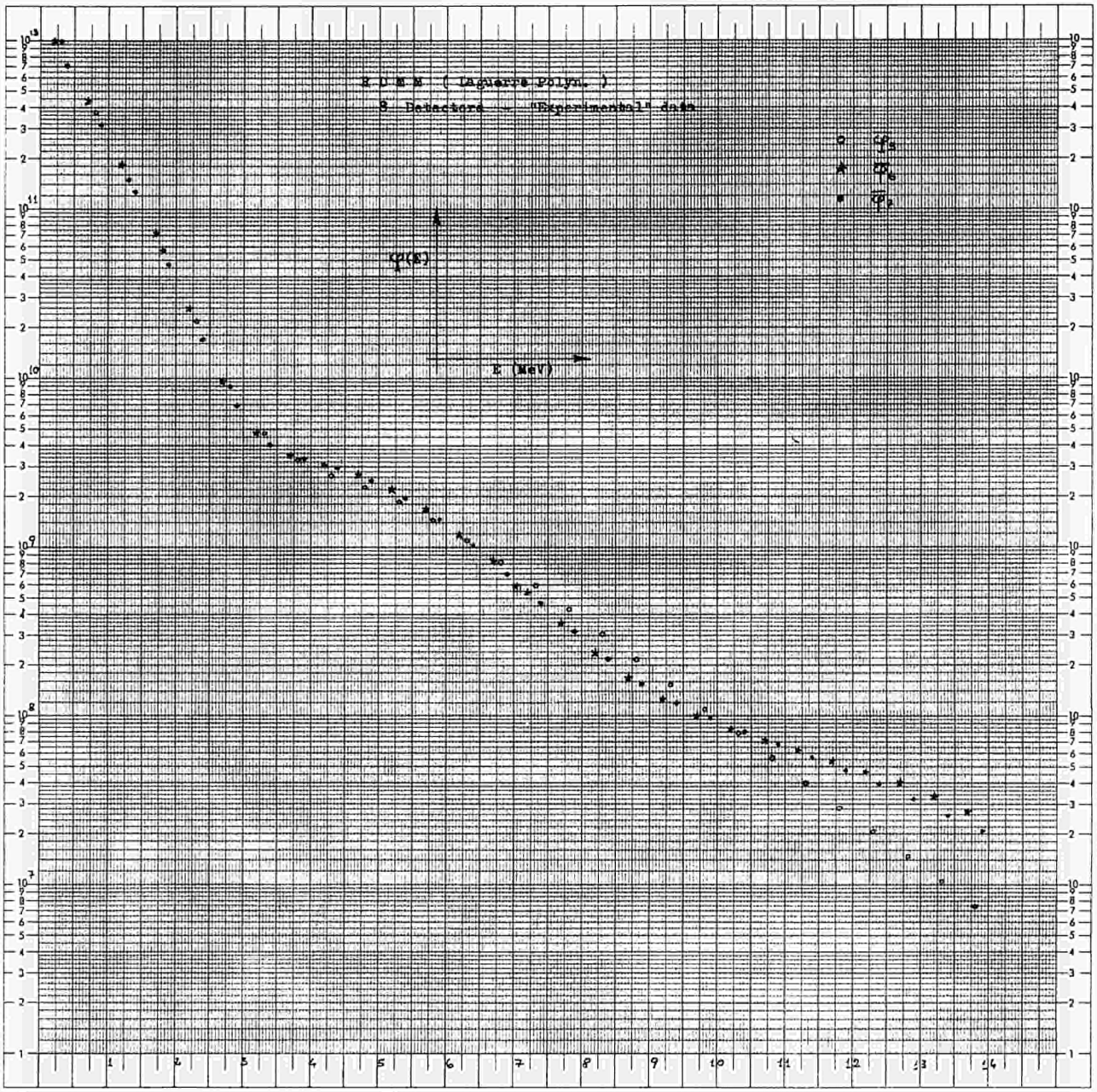

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FIG. 6

Eine Achse logar. geteilt von 1 bis 10000, Einheit 50 mm, die andere linear in mm.