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NASA TECH BRIEF

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Numerical Least-Square Method for Resolving Complex Pulse Height Spectra

With the development of extremely precise multichannel analyzers over the past years, a great interest has developed in the precise determination of differential energy spectra from measurement of the pulse height spectrum. Important applications of this technique can be found in gamma-ray spectroscopy for work in decay scheme determination and activation analysis, in X-ray spectroscopy for work in so-called nondispersive analyses, and in charged-particle spectroscopy for work in alpha-particle scattering and its application to geochemical analysis to name a few applications.

The basic problem involved in the spectroscopic investigations just mentioned is the determination of the "actual" incident differential energy spectrum from a measurement of the pulse height spectrum. The pulse height spectrum is in truth a measurement of the interaction of the incident flux with the detector. The measurement of the incident flux is further degraded by many other factors in the detection system itself. The approach taken in the methods employed in the computer program is to try to infer the actual incident differential energy spectrum by correcting the measured pulse height spectrum for the instrumental smearing and geometric efficiency.

Although an exact solution cannot be obtained, and although the problem is not linear in solution, most probable solutions can be obtained using the linear least-square solution. The solutions obtained by this method agree with the true values in all cases tested (e.g., X-ray and gamma-ray spectroscopy). The technique allows for the calculation of relative intensity, of the statistical variance based on counting statistics of the correlation between library components, and of the goodness-of-fit chi square.

In order to obtain a unique solution and nonoscillating solution, physical constraints are imposed on the solution. In particular, constraints involving the finding of solutions in the positive domain and the use of nuclear decay to eliminate library correlations have been included in the program. These constraints are included as either an iterative search mode for nonnegativity or a component subtraction mode in the computer program.

The problem of nonlinearities in the pulse height scale that can be attributed to gain shift and zero drift has been considered. Both of the search modes to find the proper gain shift and zero drift and the use of constant gain shift and zero drift have been included in the analytic method developed herein. Another mode is available in the program for correcting the pulse height scale of the library function for zero drift and gain shift. In this mode, each component can be separately compensated for so that all the components can be set on a common scale.

A method for background subtraction and the use of the background as a library component in the least-square analysis is considered. There is an option for the use of either method in the computer program developed. Techniques for compensating for background gain shift and zero drift have also been developed and are included in the program. The search mode can be performed in the same range as that for the input of a data spectrum or can be performed in the mode used for correcting the library spectra to a common pulse height scale.

(continued overleaf)

Notes:

1. The present program is written in Fortran II for use with an IBM 7094 computer. The program is adaptable to almost any computer having a memory of 32 thousand, 36-bit words and a Fortran compiler by minor modifications of the formulas and format statements. All data are inputed by magnetic tape which can be fed by a punched card reader. The output is fed to magnetic tape which is then printed out by means of a line printer or punched cards.

2. Inquiries concerning this program may be directed to:

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   Reference: B67-10480

Patent status:

No patent action is contemplated by NASA.

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