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Analysis of Double Decay Spectra by the SIMPLEX Stepping Method*

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Abstract. The principle of a computer programme for the analysis of multiple decay spectra, as obtained in positron lifetime measurements, is described. It is based on the SIMPLEX algorithm. The performance of the analysis method is discussed.

Index Headings: Numerical analysis (curve fitting and parametrization) – Positron annihilation (lifetimes)

The use of the SIMPLEX algorithm for non-linearizeable curve fitting has repeatedly been suggested [1, 2], because by virtue of its construction it could never be diverging and relatively insensitive to spurious solutions.

The basic idea is to construct a set of $(N+1)$ points (called the SIMPLEX) in the N-dimensional space of the fitting parameters (Fig. 1). Each point is identified by its coordinates and by the value of its optimizing function which may be either the chi-square or the likelihood function. From comparison of the value of this optimizing function in the different vertices, information is obtained about the approximate position of the optimum, and the SIMPLEX is gradually deformed until it encloses the convergence point. Finally the dimensions of the SIMPLEX are decreased and the solution obtained.

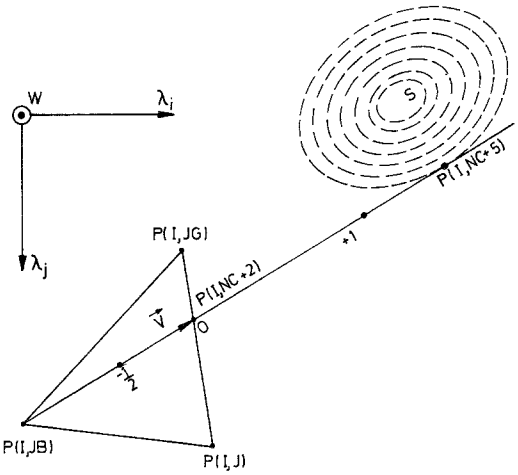

Fig. 1. Illustration of the SIMPLEX principle in the two-dimensional λ_i, λ_j space. The point $P(I, JB)$ (which has the "worst" chi-square value) is replaced by $P(I, NC+5)$ (which is the point with the best chi-square along the vector $\bar{V}$

Application of the Method

We have developed a set of computer programmes for a diskoperated PDP 15/20, (16K memory) for the treatment of multi-component exponential decay spectra, as obtained in positron lifetime studies. The exact analytical form of the spectrum was described before [3].

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First the programme DECNOR takes the raw data from the multichannel analyzer (as punched out on paper-tape) in order to perform all necessary corrections and catalogue the spectrum on magdisk or magtape. Additional data as time calibration, position of zero-time and name of the file to be formed are entered through teletype. The contribution from random coincidences is calculated and subtracted. Subsequently the total number of counts in the whole spectrum is calculated. Then any number of correction spectra (e.g. the spectrum due to annihilation in the foil covering the source) [4] can be subtracted.

A choice of correction spectra with the proper calibration is available on magdisk. The corrected spectrum, together with the square roots of the original spectrum, to be used as variances in the analysis, and with the relevant other data such as calibration, zero time etc., is then catalogued under the chosen name.

The actual analysis is done by a set of programs and subroutines. DECAN is the main programme and provides a series of input and output statements. The real SIMPLEX process is performed by the subroutine LINEX; return to DECAN takes place only after the solution for decay constants and intensities is reached. DECAN then iterates for the real zero time and writes out the results. Then the variations $(X_i - Y_i)/S_i$ are represented on the screen of a storage oscilloscope by the subroutine ERPLOT (X_i: experimental values to be fitted, Y_i: values of the fitted curve, S_i: variances on X_i).

In LINEX the SIMPLEX is formed for the non-linear parameters only. Each point of the SIMPLEX is characterized by its position vector $P(I, J) = \lambda_i(j)$ (i or I is the indicator of the component and ranges from 1 to NC, and j or J is the indicator of the vertex of the SIMPLEX and ranges from 1 to $NC+1$) and by the corresponding value of the chi-square QUI(J). The SIMPLEX process is realized only in the λ-space; the chi-square is calculated through CALL CHI(J, N) (N: number of channels used in the fit) and in this subroutine the intensities are fitted using a Gauss-Seidel elimination method in the form of the standard IBM subroutine SIMQ. In this way QUI(J) stands for the best obtainable chi-square with the particular $\lambda_i(j)$ coordinates. The "worst" point in the SIMPLEX is identified and given the index JB. The weighted mean of the remaining "best" points is $P(I, NC+2)$; QUI($NC+2$). The vector $\bar{V} = [\bar{P}(I, NC+2) - \bar{P}(I, JB)]$ is supposed to be pointing from the worst point towards the convergence region. Each point lying along $\bar{V}$ can be represented as $\bar{P}(I, NC+2) + k\bar{V}$. The value of chi-square is calculated in two more points on this line, i.e. for $k = -1/2$ and for $k = 1$.

The chi-square is supposedly a quadratic function of k along this line. The minimum of the parabola through the points with $k = 0$, 1 and $-1/2$ is sought. In most cases this point has a substantially better chi-square than any of the other SIMPLEX points. If this is the case it replaces the "worst" point of the SIMPLEX and the whole process is repeated. If such a point is not found, the whole SIMPLEX is redefined by replacing $\bar{P}(I, J)$ by $\bar{P}(I, JG) + \alpha[\bar{P}(I, JG) - \bar{P}(I, J)]$. This means an inversion arround the best point (identified by JG) with eventually a contraction if $\alpha < 1$. In practical cases we will alternatively invert and invert-contract with $\alpha = 0.3$.

Either by direct improvements or by contractions and inversions the SIMPLEX method will finally centre around a convergence point and then decrease. When it has become so small that the differences in chi-square between the individual points are less than 0.1%, the process is ended, and control is returned to the main program DECAN.

Performance

Approximately 100 lifetime spectra have been analysed by DECAN. Most of them were two component analysises as in the case of defect metals and in some glasses [4, 5]. Also some 3 component analysises have been done, but computer time increases very strongly for an additional component.

Table 1. General performance of DECAN for a two component analysis of a positron lifetime spectrum in a deformed copper sample (thickness reduction: 7.3%). Source correction was 7% polyester foil and 1.5% P-bronze (source supporting ring). Columns 1 and 2: Starting values for the iteration in ps. Columns 3–5: Obtained fitted parameters in ps resp.-%. Column 6: Chi-square reduced by the number of degrees of freedom. Column 7: total running time on a PDP 15/20 in sec

τ_1 1	τ_2 2	τ_1 3	τ_2 4	I_2 5	χ^2/ν 6	T[s] 7
120	220	142.2	300.7	23.4	0.8902	185
170	240	142.5	301.1	24.5	0.8902	296
125	350	142.8	301.9	24.3	0.8902	150

Computer time and goodness of fit depend strongly on the accuracy of the subtraction of random coincidences and of the sources foil spectra [4]. We have observed that a shift of 0.5 channels of the simulated source spectrum with respect to the experimental spectrum is likely to induce strange behaviour of the chi-square and slower convergence. The main features of the performance of the method are shown in Table 1.

The main advantage of this programme is that it can be run on a fairly small computer, and in single precision (i.e. 6 digits). A listing of the programme is available from the authors, either in PDP or IBM version.

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