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THE CORRECTION OF RESOLUTION DISTORTION IN CONTINUOUS PULSE-HEIGHT SPECTRA*

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A method has been devised for the correction of distortion effects arising from finite detector resolution in the measurement of continuous beta spectra. The correction procedure can, in principle, be used to correct distortions of any continuous spectrum measured with any spectrometer having a line-shape of fair resolution which can be measured or calculated. The method was applied to beta spectra measured with a 4π scintillation spectrometer. Internal conversion lines were used to determine the basic line-shape of the instrument, which was found to be Gaussian to a very good approximation. The beta spectra of two elements, Tl^{204} and Y^{91}, which have *unique* forbidden shapes were measured and corrected assuming the basic line-shape to be Gaussian. The correction procedure yields results compatible with the Fermi theory, and the experimental shape factor plots for these continuous beta ray spectra are in very good agreement with theoretical *unique* shape factors.

1. Introduction

A recurring problem in nuclear spectroscopy has been the correction in measured distributions for distortion effects arising from finite detector resolution. Since there is no exact general solution to the resolution equation (see eq. (2)) which describes the resolution distortion process, various approximate methods have been proposed for dealing with the problem. When the corrected distribution is composed of discrete spikes, the techniques of spectrum stripping and least-squares fitting of line-shape distributions[1,2]) have had considerable success. Unfortunately, neither of these methods is particularly successful when applied to continuous spectra. For correction of continuous spectra other methods have been proposed[3–5]) which lead to approximate solutions of the integral resolution equation (2). They include Taylor-series expansion of the resolution equation, which leads to the derivative correction rule[3]); matrix equation approximation of the resolution equation for which a solution can be obtained by matrix inversion[4]); and direct iterative solution of the resolution equation by numerical methods[5]). While each of these methods has some merit, none has been truly satisfactory for correcting continuous spectra.

Various causes may be cited for failure of these methods to yield a satisfactory approximate solution of eq. (2). The derivative rule[3]) requires a detailed knowledge of the second derivative of the measured distribution and employs approximations that are only valid in regions of the distribution where the distortion is small. In particular, this type of correction breaks down when applied to seriously distorted portions of the distribution, e.g., the "tail" of a continuous distribution. The other techniques mentioned, matrix inversion[4]) and iterative numerical solution[5]), both suffer from a common fault. When either method is applied to a continuous distribution having a mesh or distance between points which is small compared to the resolution-width of the characteristic line-shape (the response to monoenergetic electrons), any small statistical fluctuations in the measured distribution will be blown up in the corrected distribution into large, wildly fluctuating high frequency variations. This effect can be understood by recalling that the finite resolution of the detector will smooth the observed distribution by averaging over any fluctuations which are rapid compared to the resolution width. Thus a rapid variation in the smoothed distribution would correspond to a very large variation indeed in the original unsmoothed distribution. Otherwise it would have been averaged out altogether. Since the correction process effectively reverses this smoothing and, since it does not distinguish between true and statistical fluctuations, the slightest statistical fluctuation will be magnified out of all proportion in the corrected distribution.

The correction technique which is presented in this paper makes use of the iterative solution technique, but avoids the magnification of statistical fluctuations by performing the correction on an nth-order polynomial which is fitted to the experimental data. The deviations of the corrected polynomial from the original polynomial fit are used to correct the experimental data in a

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4) J. H. Hubbell and N. E. Scofield, IRE Trans. Nucl. Sci. NS-5 (1958) 156,
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way which will be described below. In this way the magnification of statistical fluctuations is avoided without loss of resolution in the corrected distribution. The technique of iterative numerical solution has been used in preference to matrix inversion because it allows the restriction of the solution to a positive definite function and avoids the round-off error problems to which the latter method is subject.

2. Discussion of Technique

The correction procedure which will be described is generally applicable, but it was developed specifically for application to pulse-height distributions which were measured with a 4π beta scintillation spectrometer[6]). In any correction of this type an accurate knowledge of the line-shape of the instrument is required over the energy range of interest. It is well established[7,8]) that in organic scintillators at energies below about 3 MeV, negative beta rays have linear response and a very nearly Gaussian line-shape, the half-width of which varies inversely as the square-root of the energy. This was verified in the present investigation by a study of monoenergetic internal conversion electrons from Sn^{119}, Am^{141}, Eu^{152}, Cs^{137} and Bi^{207}. The sources had about the same intensity and thickness as those used in the continuous spectrum measurements in order that anomolous instrumental distortion of the data would be avoided.

The line-shape of the instrument can be written as

$$G(E,E') = (\pi kE)^{-\frac{1}{2}} \exp -(E'-E)^2/kE\,, \qquad (1)$$

where E' is the energy of the incident beta particle and E is the pulse-height expressed in energy units. This function is normalized to have unit area, which corresponds to a probability of one that an incident beta will produce some pulse-height in the spectrometer. An experimentally observed spectrum, $Q(E)$, will be related to the true spectrum, $P(E')$, by the resolution equation

$$Q(E) = \int_0^{E_{max}} G(E,E')P(E')\,dE'\,. \qquad (2)$$

This equation must be solved for $P(E')$ to give the desired correction, and to do this an iterative numerical technique is used. Each iteration generates an approximate solution $P^n(E')$, where n is the iteration number. This approximate solution is obtained from that of the preceeding iteration by the relation

$$P_n(E) = P^{n-1}(E) + \alpha\left[Q(E) - \int_0^{E_{max}} P^{n-1}(E')G(E,E')\,dE'\right] \qquad (3)$$

where α is a convergence constant between one and zero. For the 0th approximation, i.e., the initial estimate of P, we will use $P^0(E) = Q(E)$. The iteration is continued until some arbitrary degree of convergence is attained i.e., $P^n \approx P^{n+1}$. Usually this occurs within a few iterations.

As mentioned above, this method alone is not sufficient to correct satisfactorily a continuous distribution, for it cannot distinguish between true fast variations in the measured distribution and purely statistical fluctuations, and the latter will be grossly magnified in the corrected distribution. Clearly, the statistical variations must be removed from the experimental distribution before it is corrected to avoid this problem. To accomplish this the experimental spectrum is least-squares fitted[9]) with an nth order polynomial, thus effectively smoothing the distribution to an extent determined by the degree of the polynomial. The polynomial fit is then corrected by the iterative procedure outlined above. A set of deviations of the corrected polynomial from the uncorrected polynomial are then calculated, and these are applied as corrections to the original experimental distribution, i.e.,

$$P(E) = Q(E) - [\bar{Q}(E) - \bar{P}(E)] \qquad (4)$$

where $\bar{P}$ and $\bar{Q}$ are the corrected and uncorrected polynomial fits, respectively. This represents the final corrected distribution.

In a beta spectrum to which this technique was applied, the spectrum was usually separated into two parts which were overlapped to assure that the data was fitted with a smooth curve. This allowed a good fit to the data to be obtained using a lower order polynomial than would otherwise have been necessary. The iterative correction was applied to a composite of the fits from the two parts of the experimental distribution.

3. Discussion of Computer Program

From the discussion above it should be apparent that the numerical corrections described are more suited to computer evaluation than to hand calculation. The corrections which will be presented below were performed using a FORTRAN program which was written for use with the IBM 709 computer of the Indiana University Research Computing Center.

The flow diagram shown in fig.1 shows, in somewhat

6) D. A. Howe and L. M. Langer, Phys. Rev. **124** (1961) 519.
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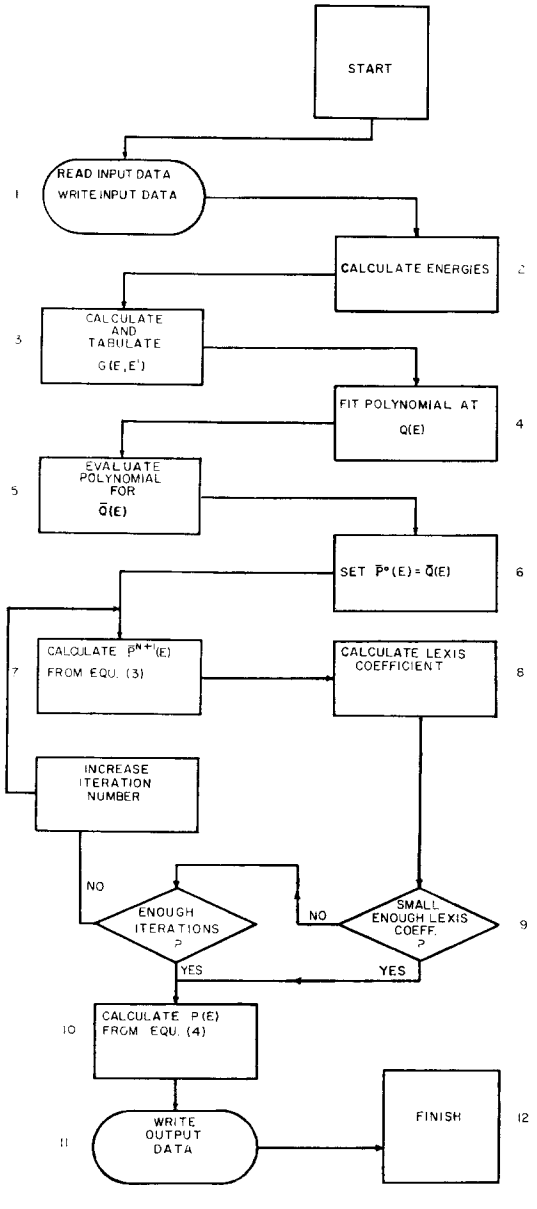

Fig. 1. Flow diagram of resolution correction program. These major steps of the program illustrate the resolution correction technique.

abbreviated form, the major steps in the operation of the program.

Step 1. Input data is read into the computer memory, including

1. the number of the data points in the pulse-height distribution,
2. the pulse-height distribution to be corrected,
3. pulse-height-to-energy calibration parameters,
4. spectrometer resolution at 1 MeV resolution energy dependence,
5. order of polynomial fit and convergence coefficient,
6. maximum number of iterations and/or minimum Lexis coefficient.

The calculation terminates when either the maximum number of iterations is reached or the correction has converged to the degree of goodness of fit specified by the Lexis coefficient[10]). The latter is used rather than a χ-squared test for describing the goodness of fit because the value of the Lexis coefficient is relatively independent of the number of data points or degrees of freedom in specifying a given goodness of fit. A listing of the input data (excluding item 2) is included in the printed output of the program.

Step 2. Energies corresponding to channel numbers are calculated and tabulated from the calibration parameters which were read in, using the function $E(I) = aI + b$, where I is the channel number and a and b are the calibration parameters.

Step 3. The spectrometer line-shape function $G(E, E')$, in this case a Gaussian distribution, is calculated and tabulated for all values of E and E' in the region of interest.

Step 4. The uncorrected pulse-height distribution is fitted by least-square methods, as described in reference 10, to an nth order polynomial in E, where n is an input parameter. The least-squares normal equations are solved for the fitting parameters using the high speed matrix inversion routine[11]), SIMPLE.

Step 5. The fitted polynomial is evaluated and tabulated over the same energy range as the input data, generating the function $Q(E)$.

Step 6. As an initial estimate, the undistorted distribution $P(E)$ is approximated by $Q(E)$. Such an initial estimate, chosen because the correction to the data is small, is required by the iterative solution technique employed.

Step 7. $P^n(E)$ is calculated in accordance with eq. (3).

Step 8. A Lexis coefficient[9]) is defined by

[10]) R. D. Evans, *The Atomic Nucleus* (McGraw-Hill, New York, 1955) p. 774.

[11]) J. G. Cramer Jr., *Subroutine for inverting matrices and processing linear equations*, Indiana University Physics Dept. (1962) (unpublished).

$$C_n = \sum_{i=1}^{n} \left\{ \left[\bar{Q}(E_i) - \int_0^{E_{max}} P^{n-1}(E') G(E_i, E')\, dE' \right]^2 \Big/ n\bar{Q}(E_i) \right\} .$$

The Lexis coefficient is just the χ-squared parameter divided by the number of data points. In this case it characterizes the goodness of fit between the polynomial fit to the uncorrected pulse height distribution and the corrected distribution after deliberate resolution distortion.

Step 9. The Lexis coefficient and the number of iterations are examined to determine if either or both satisfy the conditions for termination of the iteration cycle, as set by the input data. If the termination conditions are not met, the program increases the iteration number by one and teruns to Step 7 above. Otherwise the program proceeds to Step 10.

Step 10. The final result of the iteration process is set equal to $P(E)$, the corrected equivalent of the polynomial fit $\bar{Q}(E)$. It is now assumed that the same deviation will be found between the corrected and uncorrected polynomial as between the corrected and uncorrected data, and equation (4) is used to calculate the corrected pulse-height distribution $P(E)$.

Step 11. The results of the calculation are listed in the output. This tabulation consists of the following:

1. number of iterations and Lexis coefficient,
2. channel number,
3. energy,
4. original experimental spectrum, $Q(E)$,
5. corrected experimental spectrum, $P(E)$,
6. fit to $Q(E)$ by polynomial, $\bar{Q}(E)$,
7. corrected polynomial, $P(E)$,
8. deviation $\bar{Q}(E) - P(E)$.

Step 12. *Finish.* In practice, control is transferred to a beta spectrum analysis program[12]) which acts on the corrected distribution, $P(E)$, to calculate electron momentum distributions and Fermi-Kurie plots and to perform shape factor analysis.

4. Example Corrections

Two negative beta emitters whose spectra have *unique* forbidden shapes, Tl^{204} and Y^{91}, were studied with the 4π scintillation spectrometer[6]) mentioned above. Since the spectra of these isotopes are well known[13]), such measurements put very stringent requirements on both the instrument and the correction procedure; for when the data is subjected to shape factor analysis, the slightest

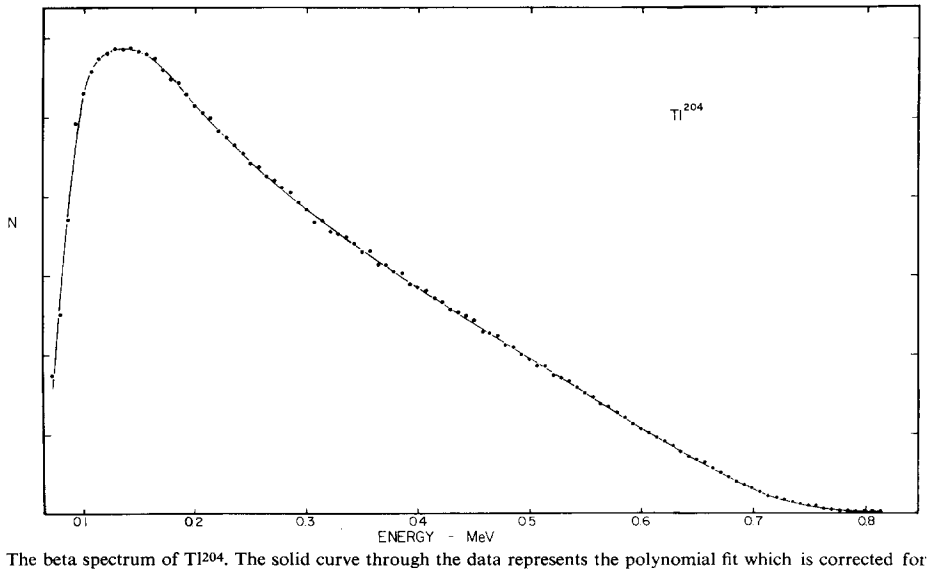

Fig. 2. The beta spectrum of Tl^{204}. The solid curve through the data represents the polynomial fit which is corrected for distortion by the iterative procedure and is then used to correct the data.

[12]) D. E. Wortman, *Beta analysis program*, Indiana University Physics Department (1962) (unpublished).

[13]) Nuclear Data Sheets, compiled by K. Way *et al.* (National Academy of Science – National Research Council, Washington D.C.).

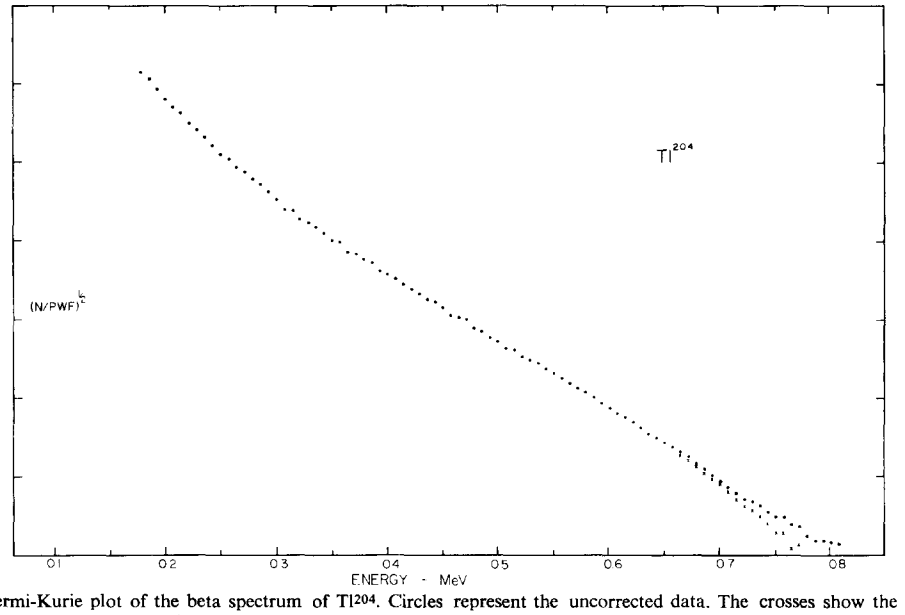

Fig. 3. Fermi-Kurie plot of the beta spectrum of Tl^{204}. Circles represent the uncorrected data. The crosses show the data near the end point after the correction procedure has been applied. It is this region where the correction is most noticeable. Below $E \approx 950$ keV the corrected and uncorrected points are essentially indistinguishable in this representation, and so the former are not shown.

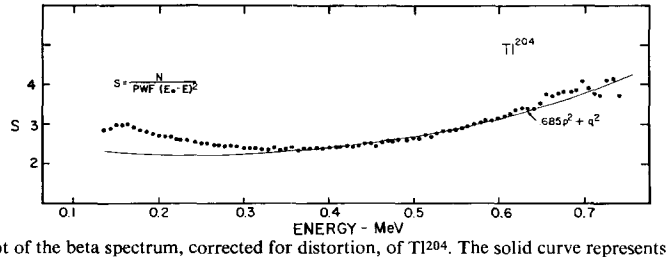

Fig. 4. Shape factor plot of the beta spectrum, corrected for distortion, of Tl^{204}. The solid curve represents the *unique* shape factor of the form $0.685\ p^2+q^2$ as predicted by theory. The end point consistent with the data is 0.771 MeV.

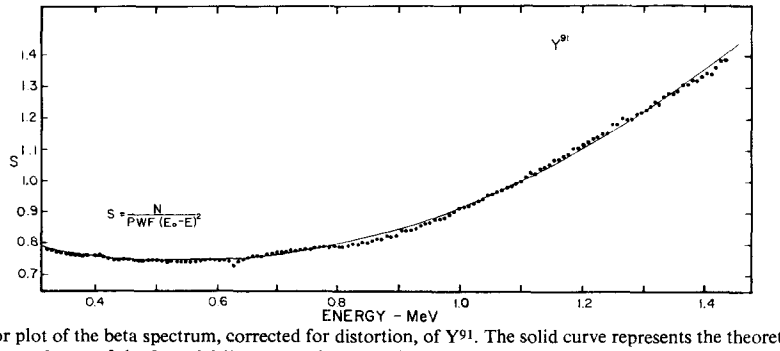

Fig. 5. Shape factor plot of the beta spectrum, corrected for distortion, of Y^{91}. The solid curve represents the theoretical *unique* shape factor of the form $0.965\ p^2+q^2$. The end point consistent with the data is 1.52 MeV.

distortion of the spectrum will be revealed as pronounced deviations from the *unique* forbidden shape. Such analysis provides a much more sensitive way of displaying small deviations from the *unique* shape than does the conventional Fermi-Kurie plot.

Both spectra were measured with the 4π scintillation spectrometer, and the energy calibration and resolution of the instrument were measured with internal conversion electrons both before and after the measurement of the β spectrum. Fig. 2 shows the experimental pulse-height distribution and the polynomial fit to this data, the latter indicated by the solid line, for the Tl^{204} spectrum. Fig. 3 shows a Fermi-Kurie plot of the same data both before and after the correcting procedure has been applied. The difference in the two is particularly noticeable in the region of the end point, as has been noted elsewhere[8]).

Fig. 4 shows a shape-factor plot of the corrected data, taken with the Tl^{204} source, along with a theoretical prediction of this function[14]) given by the relation, $S(W) = 0.685p^2 + q^2$. Previous work[13]) has shown that these should be in good agreement, as indeed they are. Fig. 5 shows a similar shape-factor plot of the corrected data from a measurement of the Y^{91} spectrum, and again it is seen that the shape predicted by theory[14]), $0.965p^2 + q^2$, is in good agreement with the experimental data, as previous work[13]) has shown.

5. Conclusion

The shape factor analysis shown above is a severe test of the resolution distortion correction which has been described in this paper, and represents strong evidence for the accuracy of this procedure. Moreover, the technique is fairly general in its application and is not necessarily limited to situations where the spectrometer has a Gaussian line-shape. In principle, the method can be used to correct distortions in any spectrometer having a line-shape which can be measured or calculated, e.g., in instruments used for measuring continuous gamma ray spectra or high energy beta spectra[8]). It should be noted, however, that the accuracy of any such correction will necessarily be limited by the accuracy with which the line-shape of the instrument is known in the region of interest, and that when the line-shape is broad and poorly resolved, e.g., the proton recoil distribution obtained when measuring a neutron energy spectrum with a plastic scintillator, information and detail will necessarily be lost.

It is hoped that this technique will prove useful in cases such as those mentioned, where line-shape distortion is a problem, making possible more quantitative measurements with scintillation and solid state devices.

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14) T. Kotani and M. Ross, Phys. Rev. **113** (1959) 622.