



ESCL8R and LEVIT8R: Software for Interactive Graphical Analysis of HPGe Coincidence Data Sets

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Abstract: Programs for analysis of γ - γ matrices and γ - γ - γ cubes from HPGe coincidence experiments are described. The programs are intended primarily for high-spin spectroscopy studies. Users are able to inspect background-subtracted gated spectra, or combinations of such spectra, quickly and easily. The programs also make use of a proposed level scheme, provided by the user, to calculate an expected spectrum for comparison with the observed spectrum. Electron conversion coefficients, detection efficiency and γ -ray energy calibrations are included in the calculation. A graphics-based editor is included to allow fast and easy modification of the proposed level scheme, and least-squares fits to the matrix or cube can be performed to extract optimum values for the energies and intensities of the level scheme transitions.

1. Introduction

Modern HPGe detector arrays have revolutionized in-beam γ -ray studies, especially for high-spin nuclear structure physics with heavy-ion fusion-evaporation reactions. The analysis of data from such arrays often begins with the creation of two-dimensional histograms from double-coincidence data, or three-dimensional histograms from triple-coincidence data. These histograms can then be examined and by setting "gates", *i.e.* specifying energies for all but one of the axes and inspecting the projection onto the remaining axis. Making sense of the resulting spectra and distilling the information from them into a deduced level scheme can be a tedious and time-consuming process, especially for complicated level schemes with many observed transitions.

New large γ -ray detector arrays such as EUROGAM, GAMMASPHERE and GA.SP are beginning to generate three-, four-, and even five-fold HPGe coincidence data in useful quantities. The unsurpassed sensitivity of these arrays will allow observation of nuclear levels that are well beyond the current detection limits, not only to higher spins but also to higher excitation energies above the yrast line, so that many new weakly-populated bands should be resolvable. But if the information contained in these high-fold data sets is overwhelming, so too can be the size of the data sets and the difficulty of extracting all of the detailed information contained in them. The analysis of specific experiments, such as the study of known superdeformed bands, should pose few technical problems; more general analysis, however, may require substantial enhancements to our present techniques. It may be anticipated that lack of methods of analysing such data sets in general, powerful ways will form a major obstacle to extracting all of the interesting physics in an expeditious and reliable fashion.

General analysis of high-fold coincidence data to construct complete and consistent nuclear level schemes will require sophisticated computer programs to extract the physically interesting numbers from the raw data and present them to the physicist in an easily assimilated manner, to keep track of all γ -ray assignments and expected coincidence intensities, and to quickly find and report major discrepancies between a proposed level scheme and the data so that they can be understood and corrected.

This paper reports on interactive graphical analysis programs which meet many of the above criteria. These programs allow fast and easy inspection of two- and three-dimensional data. Their main advantage, however, is that they provide the user not only with the observed coincidence results, but also with expectations calculated on the basis of a proposed level scheme. In this way, it is easy for the user to find discrepancies between the proposed level scheme and the observed results and to modify the scheme accordingly. In addition, the book-keeping of the analysis is simplified. The level scheme is displayed on the same screen as the observed and expected spectra, and can easily be modified by the user. Least-squares fits directly to the 2D and/or 3D data, with the intensities and energies of the level scheme transitions as parameters, allow fast and accurate extraction of the important quantities from the data. This approach considerably facilitates detailed analysis, especially of higher-fold

data sets.

2. Two-dimensional Data: Program ESCL8R

ESCL8R is an interactive program for graphics-based analysis of γ - γ data for the deduction of level schemes. It allows fast and easy inspection of the γ - γ matrix, making use of parameterized values of the peak shapes, peak widths, detector efficiency and energy calibrations. It uses the two-dimensional background-subtraction algorithm of ref. [1]. It also displays a proposed level scheme which is modified continually as the analysis proceeds. This level scheme is used to calculate expected results for comparison with the observed experimental data. Least-squares fits to the matrix may be performed to extract the optimum energies and intensities of transitions in the level scheme, with up to 500 parameters fitted simultaneously.

2.1. User interface and display

The most recent version of ESCL8R (called XmESC) makes use of X Windows and the Motif graphical user interface. An earlier version (ESCL8R_GLS) had only a command-line user interface, but still used X Windows for the graphics display. Two graphics windows are created by the program, one for the level scheme and one for gated spectra. For users without access to X Windows, the first version of ESCL8R displayed only the spectra and not the level scheme, and used a more primitive level scheme file format that included no graphical information.

Figure 1 shows an X-Windows/Motif display running XmESC. A terminal-emulator window is on the top right; this is the window that was used to launch the application and which is used to display and ask for textual information. The window on the top left is for the level scheme, but also includes pull-down menus and a command widget. The bottom window displays the gated spectra. It should be emphasized that the level-scheme and spectrum displays are for more than just informational purposes; they are used to select or specify transitions, bands, levels and γ -ray energies, and thus form an important part of the user interface.

There are several ways in which the user is able to specify gates on the two-dimensional data, as described below. As each gate is taken, the program automatically displays the observed and calculated spectra, the difference between them, and the residual spectrum (i.e., the difference spectrum divided by the experimental uncertainty). In this way, it is easy for the user to find places where the proposed level scheme fails to reproduce the observed results. A graphics-based editor is incorporated to make it easy for the user to modify or add to the level scheme.

2.2. Experimental data

In addition to the coincidence matrix, the program requires a two-dimensional (2D) background, and knowledge of the efficiency and energy calibrations and the peak shapes and widths as a function of γ -ray energy.

The coincidence data set used by ESCL8R is stored as a $2k \times 2k$ -channel or $4k \times 4k$ -channel γ - γ "matrix", or 2D histogram of counts vs. energy vs. energy. This matrix is symmetrised, so that the two energy axes are equivalent.

The program uses the background-subtraction algorithms of ref. [1], where the 2D background is defined as the sum of one-dimensional spectrum cross-products. Rather than using a matrix with the background already removed, it subtracts the background from each gate. This is done to allow the program to keep track of the raw counts, and hence the uncertainties on the counts-per-channel, in the gated spectrum.

The energy calibrations used by ESCL8R (and LEVIT8R) are simply polynomial expressions of the γ -ray energy as a function of channel number, usually derived from least-squares fits to the centroids of peaks in calibration source spectra. The program accepts polynomials of order four or less.

The parameterization of the photopeak efficiency of the detector array is more complicated. A typical logarithmic plot of efficiency vs. γ -ray energy is shown in figure 2. It has the approximate appearance of two straight lines joined by a smooth turnover. We generalize the straight lines to quadratic functions and use the parameterization

$$ln(\varepsilon) = \{ (A + Bx + Cx^2)^{-G} + (D + Ey + Fy^2)^{-G} \}^{-\frac{1}{G}},$$
 (1)

where

$$x = ln\left(\frac{E_{\gamma}}{100}\right) , \qquad (2)$$

$$y = ln\left(\frac{E_{\gamma}}{1000}\right) , \qquad (3)$$

 ε is the efficiency, and the γ -ray energy E_{γ} is in keV. The parameter G determines the shape of the turn-over region between the high and low energy efficiency curves; the larger the value of G, the sharper the turn over at the maximum in the efficiency. The parameter C is not usually required and is often fixed to zero.

The program EFFIT can be used to perform least-squares fits of the above parameterization to measured efficiency calibrations. The solid line of figure 2 results from such a fit. The values of the parameters A through G in this example are 6.95(13), 0.62(17), 0, 5.287(5), -0.855(13), -0.066(3) and 15(5), respectively. Since the matrix used by ESCL8R is symmetric, all detectors are treated equivalently by the program and the efficiency parameters used should, of course, correspond to those of the full detector array.

Two-dimensional coincident peaks are simply taken as the cross-product of one-dimensional peaks, which in turn are usually assumed to have a purely Gaussian shape. Non-Gaussian peaks with a low-energy tail can be included, but experience indicates that this is not usually necessary for analysis of in-beam experiments unless the peak-to-background ratio is exceptionally good.

The widths of the peaks (FWHM) are used by the program not only in the calculation of the expected spectrum, but also for the setting of gates. A default gate width of one FWHM is used so that the user is able to specify a gate by its energy alone. This considerably simplifies the inspection of the γ - γ matrix; for example, gates can be set by using the mouse to select transitions in the displayed level scheme.

The FWHM of the peaks (in channels) is parameterized as

$$FWHM(x) = f + g\sqrt{\frac{x}{1000}} + h\frac{x}{1000}$$
, (4)

where x is the channel number. The first (constant) term arises from noise in the detector and amplifier, the second term arises from the statistics of the charge collection process, and the third (linear) term is due to Doppler-broadening of the peaks from emission of the γ rays from recoiling residual nuclei. If a thick target is used, so that the recoils are stopped, then this last term should be set to zero. Typical values of the above parameters are approximately f=3, g=1 and h=4 for an energy dispersion of 0.5 keV per channel and a recoil velocity of approximately 2.5% of the speed of light. These parameters also depend on the detector array, electronics, energy dispersion, etc. Their values may be modified within the program, or fitted by least-squares regression to a selected gated spectrum, in order to optimize the agreement between the level-scheme predictions and the observed data.

2.3. Level scheme

In order to enable a program to keep track of γ -ray assignments and compare the observed results with those expected from a proposed level scheme, routines were developed to read and display level schemes stored in disk files. These also included modified subroutines supplied by the National Nuclear Data Center that calculate internal conversion coefficients from the Hager-Seltzer tables [2]. Additional code was written to allow graphical editing of the files, to generate postscript files of level scheme figures, and to check intensity balances and energy sums. The files include data on level energies, spins and parities, and transition energies, intensities, multipolarities, mixing ratios and conversion coefficients, as well as on the graphical layout for display purposes. An example of an expanded level scheme display is reproduced in figure 3.

Editing routines allow the user to easily add, delete, modify or move bands, levels and transitions in the level scheme. For example, a new transition between levels that already exist in the scheme can be added simply by indicating the initial and final levels with the mouse. The energy and multipolarity of the transition will be taken from the differences in level energy, spin and parity of the two levels. If one of the two levels does not yet exist, the energy of a new γ ray can be given by using the mouse to select the energy of a peak in the gated spectrum, or by typing the value in keV; the program then asks for the multipolarity, and calculates the energy, spin and parity of the new level from the energy and multipolarity of the transition. Both the new level and the new transition are then added to the scheme. Simplified commands to add series of E2 or M1 transitions to the top of a band allow very fast and easy entry of new band structures; in this case all that the user needs to supply is the γ -ray energies, which is usually done with the mouse on the gated spectrum.

By incorporating these level-scheme routines, ESCL8R can calculate predicted gated spectra to be compared with the observed spectra. That is, the program can work backwards from the proposed level scheme, and attempt to reproduce the observed γ - γ matrix on the basis of the proposed intensities, branching ratios and conversion coefficients. It can also modify the level scheme file, and fit the γ -ray energies and intensities directly to the 2D data, to improve the agreement with the observed results. Consistency checks such as the testing of energy sums and intensity balances can also be readily performed.

An additional advantage of this approach is that it allows level scheme figures and tables of the level and transition data to be generated quickly and easily. This also helps to document an ongoing analysis. More complicated manipulations of the level scheme data, such as a calculation of the total population of bands as a function of spin, etc., are also greatly facilitated.

Since least-squares fits can be performed to the full coincidence data set, it is important to reproduce all coincidences as correctly as possible. For example, coincident peaks arising from the reaction channel of primary interest may be contaminated by coincidences from other residual nuclei. Therefore a level-scheme file to be used with an analysis program should include all bands or transitions observed with significant intensity in the data, whether or not they are assigned to the principal isotope being studied.

2.4. Setting gates

The user is able to take and view gates on the matrix in a variety of simple ways, for example by typing a desired energy, or by using the mouse to select transitions in the level scheme or peaks in the spectrum. Since these specify only a mean energy for the gate, a width is also required; by default, this is taken as one FWHM, calculated according to equation 4 in subsection 2.2 above. Alternatively, limiting channels for gates can be placed by the use of the graphics cursor or entered with the keyboard. Logical and arithmetic combinations of gates can also be taken just as easily. Lists of gates can be created, or read from a file, and the sum of gated spectra from such gate lists can be calculated with a single command.

As each gate is taken, all transitions with energies that lie within the gate limits are highlighted in the level scheme display and listed on the text window. The program then displays the observed and calculated spectra (overlaid in different colors), the difference between them, and the residual spectrum (i.e., the difference spectrum divided by the experimental uncertainty); see figure 1 for an example. In this way, it is easy for the user to find places where the proposed level scheme fails to reproduce the observed data, and to modify it accordingly.

If the user wishes to see where a transition in the level scheme should appear in the spectrum, selection of that transition with the mouse in the level-scheme display can be used to show the limits of the corresponding gate in the spectrum window. Similarly, using the mouse to specify the energy of a peak in the gated spectrum can highlight and list all

transitions in the level scheme that have energies within one half-width of the peak energy. A peak search routine can be used to automatically label strong peaks in the spectrum by their energy.

As mentioned above, the matrix used by ESCL8R does not have the background already removed; rather, the background is subtracted from each gate as it is read from the matrix. In this way, the program is able to keep track of the uncertainties on the counts-per-channel in the gated spectrum.

2.5. Calculation of expected γ - γ matrix from level scheme

In order to calculate the expected coincidence matrix (or gated spectrum), the program first calculates the intensities of all γ - γ coincidences. This coincidence intensity depends on

- 1. the γ -ray intensity of the higher (feeding) transition,
- 2. the branching ratio from the final state of the higher transition through to the lower (fed) transition, and
- 3. the conversion coefficient of the lower transition.

Thus the program also calculates branching ratios for the transitions deexciting each level, taking into account the electron conversion coefficients. All γ -ray flux entering a level is assumed to be divided according to these branching ratios.

Once the coincident intensities have been evaluated, they can be multiplied by the two detector efficiencies to obtain an expected coincident yield. The γ -ray intensities in the level scheme are in arbitrary units, so a normalization factor is required to relate the expected yield to the observed peak areas. This normalization coefficient is initially chosen by the program to give the strongest observed coincidence an intensity value of about 100 units, but can be modified by the user.

The peak shapes and widths are calculated according to the paramerizations of subsection 2.2, and the expected yield distributed accordingly. Finally, the 2D background is added if comparison with the original matrix is required.

2.6. Least-squares fits

ESCL8R provides the user with the capability to perform least-squares fits to the observed data to extract optimum values for the γ -ray energies and intensities of transitions in the proposed level scheme. It is possible to fit the energies or intensities separately, or both simultaneously. The current version allows up to a maximum of 500 parameters to be fitted at one time, but this limit could easily be increased. The fits are performed directly to the full 2D coincidence matrix; any displayed gate has no effect on the results of the fit. An extensive fit will typically have hundreds of thousands of degrees of freedom.

The transitions to be fitted are selected by clicking with the mouse on the level scheme display; one can choose individual transitions or all transitions depopulating levels or bands.

Choosing transitions that have already been selected will deselect them, i.e. remove them from the list of transitions to be fitted.

All coincidence relationships that contain information on the intensity of a fitted transition are included in the least-squares analysis, such as coincidences between the fitted γ ray and the γ rays which it feeds. If the fitted transition is not the only one depopulating its initial level, the program also includes coincidences between higher γ rays and all transitions populated from the initial state, *i.e.* coincidences which yield information on the branching ratio for the fitted transition.

From the above list of quantities that determine coincidence intensities, it is evident that any γ ray that does not feed other γ rays, and that is the only transition from its initial level (so that it has a branching ratio of unity independent of its intensity), has no coincidences that depend on its intensity. Thus, for example, in an even-even nucleus the intensity of the $2^+ \to 0^+$ transition in the ground-state band cannot be fitted by ESCL8R, and must instead be deduced from intensity balances. If there are two or more transitions at the bottom of a band, but none of these feed lower transitions, then it is possible to fit all but one of them by means of their branching ratios; however, the absolute magnitudes must then again be taken from the intensity balance.

If a proposed level scheme is incomplete, or contains incorrectly ordered or erroneous transitions, then the results of the least-squares fit will be compromised. The 2D background and efficiency calibration must also be accurate in order to obtain good results. Since the the energies of the transitions also affect their fitted intensities, it is prudent to fit both energies and intensities simultaneously once they are both reasonably close to their correct values.

ESCL8R and LEVIT8R assume that the detection probability of γ rays does not depend on the multipolarity and/or mixing ratio of the transition. In many cases, this is true to within a good approximation, since many detector arrays (such as the 8π spectrometer [4]) have nearly isotropic distributions of the HPGe detectors, and the γ - γ matrix results from the sum of all combinations of detectors. However, some detector systems are significantly anisotropic. For data taken with such arrays, neither the fitted intensities nor the calculated expected spectra will be accurate.

3. Three-dimensional Data: Program LEVIT8R

LEVIT8R is a program for graphical analysis of γ - γ - γ data; essentially, it is a three-dimensional version of ESCL8R. It uses the same type of parameterized peak shape, peak width, detector efficiency and energy calibrations. It uses an equivalent algorithm for background subtraction, extended to three dimensions [1]. It also reads, displays and edits the same type of level scheme file. The user interface is the same as for ESCL8R, except for extensions to allow additional commands for gating and fitting the cube.

By incorporating the level-scheme routines, LEVIT8R calculates predicted gate spectra to be compared with the observed spectra. That is, the program works backwards from

the proposed level scheme, and attempts to reproduce the observed γ - γ - γ cube on the basis of the proposed intensities, branching ratios and conversion coefficients. As with ESCL8R, least-squares fits to the data set may be performed to extract the optimum energies and/or intensities of transitions in the level scheme, with up to 500 parameters being fitted simultaneously. By default, the fitting is done to the two-dimensional projection, but separate commands allow fitting of the full three-dimensional data set. Fits to the cube consume great amounts of CPU time; they typically have tens of millions of degrees of freedom.

One major difference from ESCL8R is that LEVIT8R allows a non-linear gain (i.e. an energy-dependent dispersion) for storage of the experimental data. This is usually used in such a way as to yield an approximately constant FWHM (in channels) of the peaks, independent of energy. This approach produces a considerable saving in disk storage required for the data, especially for high-fold data, without sacrificing usable resolution at low energies. When such non-linear spectra are displayed, the counts-per-keV (rather than the more conventional counts-per-channel) are shown, as a function of energy (rather than channel number); that is, the spectra are displayed linearly with energy, so that the displayed bin width is energy-dependent.

The use of such an energy-dependent dispersion is illustrated in figure 4, for a typical heavy-ion fusion-evaporation reaction with a detector array such as the 8π spectrometer 5]. In this example, a FWHM of two cube channels is used, and the non-linear gain saves a factor of 1.9 for each dimension, over the range 100 to 2000 keV. For the triples data, this amounts to a reduction in the required storage space by a factor of 6.4. Even greater savings are realized when higher energies are required; for example, if the cube covered the range 100 to 3000 keV, using nonlinear gain saves a factor of 13 in disk space.

A program called LUFWHM is used to generate a lookup-table, or array of integers L(i), to map (linear) ADC channels in event-by-event data to (nonlinear) cube channel numbers; that is, the cube channel is L(ADC channel). LUFWHM uses equation 4 to obtain the FWHM as a function of ADC channel, and creates bins of increasing width by rounding the FWHM to the nearest whole number of ADC channels.

A cube replay program, called INCUB8R, can then use this lookup-table mapping to generate a cube. By ordering the three energies, the program needs to store and increment only one-sixth of the whole cube. Two bytes of storage are allocated to each cube channel. Such a cube typically has about 900 channels in each dimension and requires about 240 Mbytes of disk space.

Storing only one-sixth of the cube is efficient for the replay, but has the drawback that, in order to obtain a double-gated spectrum, a great number of records need to be read from the cube file. In order to speed up the extraction of gates, a second cube file format can be used, which stores one-half of the full cube. In this second format, one byte of storage is allocated to each cube channel, but tables of overflows (i.e., channels that require more than one byte since they contain more than 255 counts) are included. Such files typically

require about 370 Mbytes, and can be generated from the INCUB8R files using a program called FOLDOUT.

Both cube formats can be read by LEVIT8R, although taking double-gates with the second (one-half cube) format is an order of magnitude faster than with the first format; it typically requires about 0.1s per double-gate on a modern workstation. The user is able to take and view a gate on the two-dimensional projection simply by, for example, typing the energy of the required gate or clicking on transitions in the level scheme. A double-gate on the triples set requires pairs of energies to be specified; this can again be done either with the mouse or the keyboard. Combinations of gates can also be taken just as easily, especially through the use of lists of gates. For example, the sum of all pairs of gates taken from two gate lists can be generated with a single command. The background is subtracted from each gate as it is read from the cube, allowing the program to keep track of the uncertainties on the counts-per-channel in the gate spectrum.

An example of a LEVIT8R display is reproduced in figure 5.

4. Conclusion

The unsurpassed sensitivity of large γ -ray detector arrays such as EUROGAM, GAM-MASPHERE and GA.SP will allow spectroscopic studies that go well beyond the present frontiers of high-spin γ -ray spectroscopy. Unfortunately, the size of the high-fold data sets from these spectrometers, and the difficulty of extracting all of the detailed information contained in them, can be overwhelming.

Programs ESCL8R and LEVIT8R, for interactive graphical analysis of two-fold and three-fold data respectively, allow fast and easy inspection of the data. They present the user not only with the observed coincidence results, but also with expectations calculated on the basis of a proposed level scheme. In this way, it is easy for the user to find places where the proposed level scheme fails to reproduce the observed results. The book-keeping of the analysis is also simplified.

Least-squares fits directly to the 2D and/or 3D data, with the intensities and energies of the level scheme transitions as parameters, allow expeditious extraction of the observable quantities from the data. The level scheme can be easily modified, and printed in the form of a postscript figure. Tables of the level and transition data, including tests of energy sums and intensity balances, can be generated quickly and easily. This approach considerably improves the ease, speed and reliability of detailed data analysis, especially in extracting "complete" level schemes from higher-fold data sets.

ESCL8R, LEVIT8R and associated programs run on both VMS and unix platforms. Copies of the code are available by anonymous ftp from cul.crl.aecl.ca.

The assistance of R.W. MacLeod in porting software described here from VMS to unix is gratefully acknowledged. This work has benefited greatly from helpful discussions with

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Figure Captions

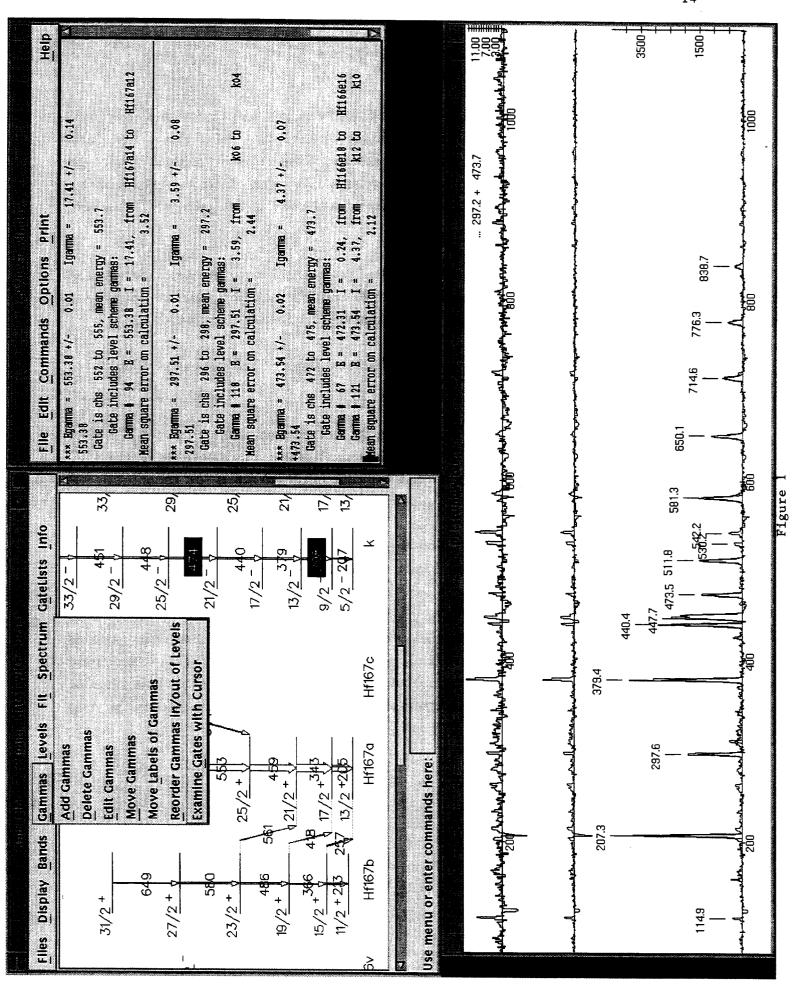
Figure 1. Screen dump of an ESCL8R session (Motif version). The window on the top right is a terminal-emulator window. The window on the top left is the level scheme and graphical user interface. The bottom window displays spectra. Observed and predicted spectra are overlaid in the bottom of the spectrum window; on a color screen, these are distinguishable by their colors. The experimental spectrum shown is the sum of two gates, at 298 and 474 keV.

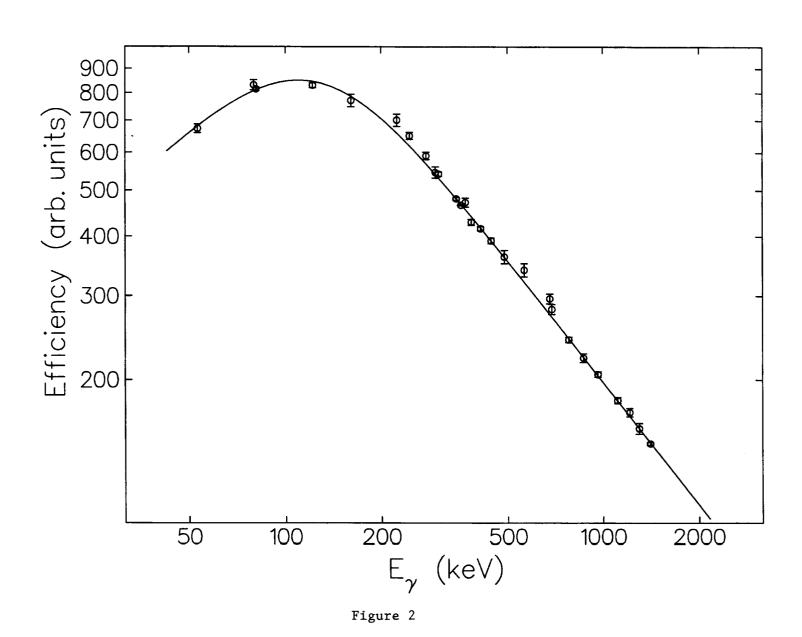
Figure 2. An example of a logarithmic plot of detector efficiency vs. γ -ray energy. The circles represent data points measured with ¹³³Ba and ¹⁵²Eu sources, while the solid line is the result of a least-squares fit using the program EFFIT. See text for details.

Figure 3. An example of an expanded level scheme display. The nucleus is ¹⁵⁷Ho, taken from ref. [3].

Figure 4. Illustration of the relation between E_{γ} , cube channel number and FWHM when an energy-dependent dispersion is used. In this example, the energy dispersion for the ADC is 0.5 keV/ch, and the energy dispersion in the cube is 1.0 keV/ch at low energies and 4.0 keV/ch at 2 MeV, selected to give an approximately constant FWHM of 2 channels. In the bottom panel, the smooth curve gives the FWHM in keV, while the sawtooth curve shows the FWHM in cube channels. The discrete steps correspond to changes of the contraction factor between the ADC channels and the cube channels.

Figure 5. Screen dump of a LEVIT8R session (Motif version). The window on the top right is a terminal-emulator window. The window on the top left is the level scheme and graphical user interface. The bottom window displays spectra. Observed and predicted spectra are overlaid in the bottom of the spectrum window; on a color screen, these are distinguishable by their colors. The experimental spectrum shown is the sum of 90 double-gates on the yrast superdeformed band of ¹⁴⁹Gd.





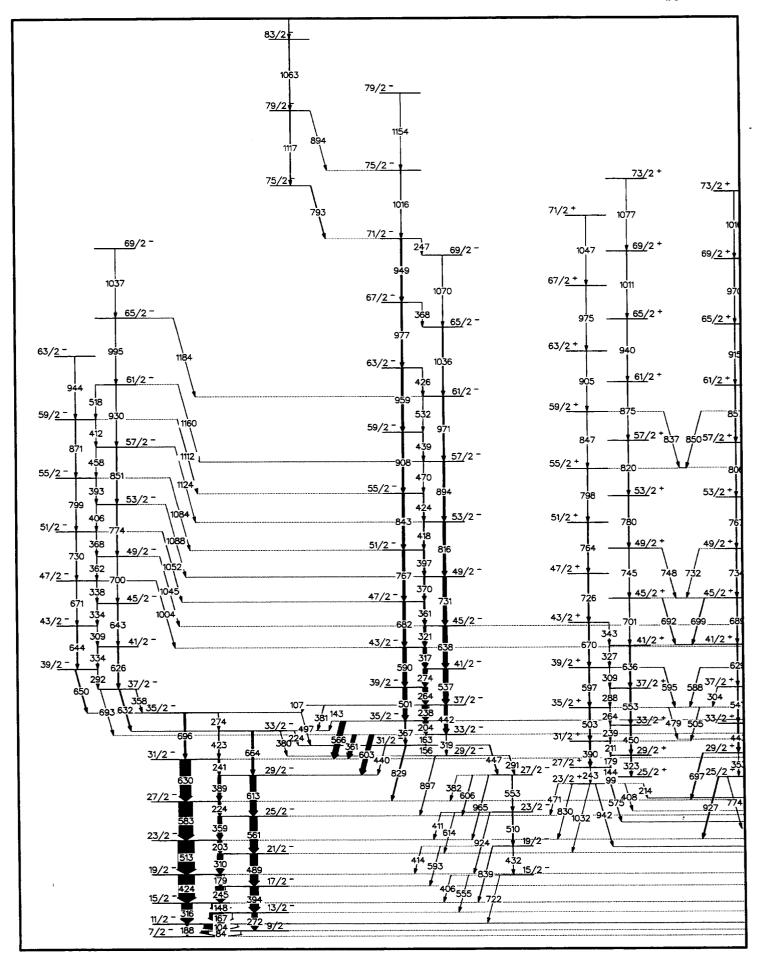


Figure 3

