Theremino MCA Deconvolution Algorithm

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The crystals of sodium iodide doped with thallium are used for decades as radiation detectors, because of some interesting characteristics such as high stopping power, good energy resolution, the relatively low cost.
The scintillation detectors are undoubtedly among the most prevalent particle detectors used today in nuclear physics.
They include a scintillating material optically coupled to a photomultiplier.
When the radiation interacts with the scintillator a spark of light is emitted. The light is transmitted through the scintillator crystal to the photomultiplier (PMT) where it is converted into a weak current of photoelectrons which is then further amplified. The so produced current signal is then analyzed by the electronics of the acquisition.

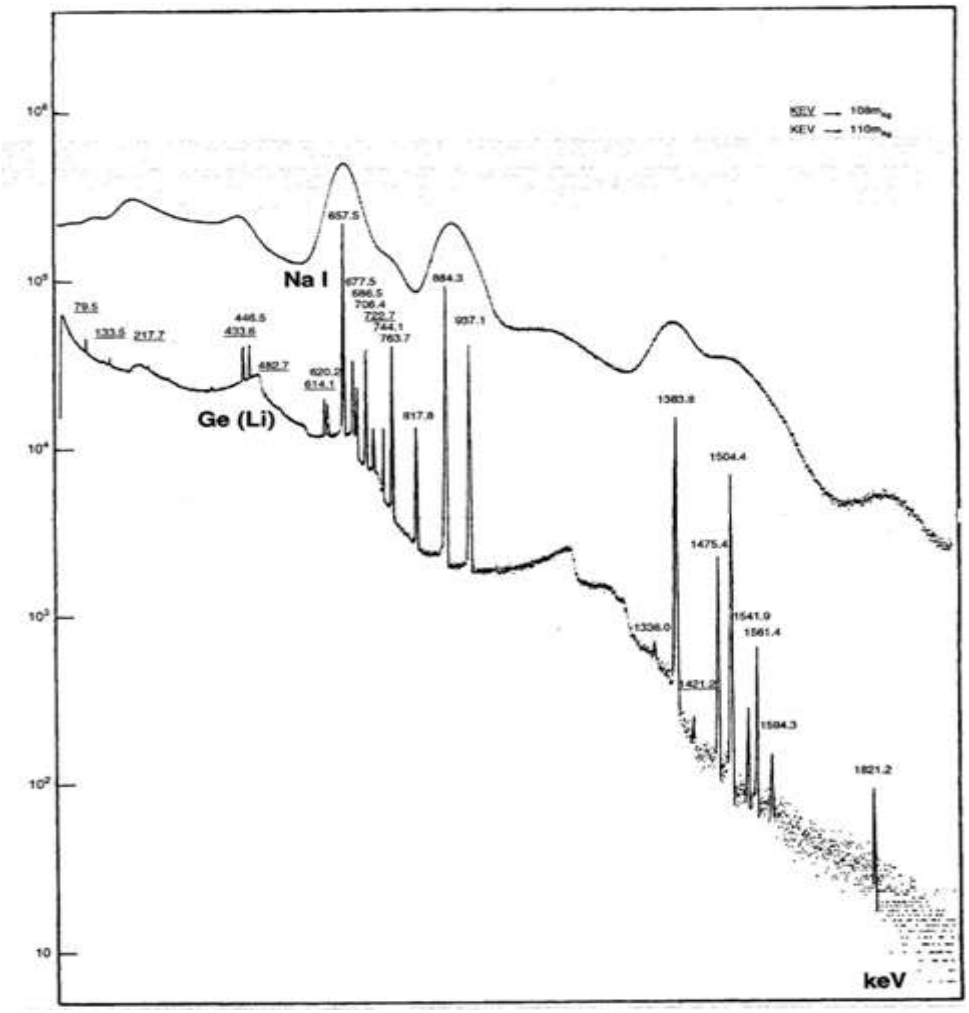
Among the main characteristics of a detector are its detection efficiency and energy resolution.
The first defines the ratio between the number of incident particles on the detector with respect to the number of measurable generated signals and depends on various factors (nature of the detector, the geometry, the type of the incident radiation, etc.).
The energy resolution of a detector represents the ability of the detector to distinguish between energy values next to each other.
Actually, the interaction of radiation with matter, at the microscopic level, is a stochastic phenomenon therefore a dispersion of excitations and ionizations is unavoidable: consequently the response of a detector to a monochromatic radiation, rather than corresponding to a narrow peak or more correctly to a Dirac delta function, assumes a Poisson or Gaussian shape, with a width dependent on the type of detector.

The energy resolution is conventionally defined as the ratio between the peak FWHM (Full Width at Half Maximum), that is, the width of the spectral distribution at half the maximum height, and the energy value of the centroid, E_m. So the resolution is given as a dimensionless quantity, usually expressed in percentage, that is :

$$R = \frac{FWHM}{E_m} \cdot 100 = \frac{235 \cdot \sigma}{E_m}$$

From which we see the relationship between FWHM and the standard deviation (σ) of the Gaussian distribution.
The high purity Germanium detectors can reach a resolution lower than 1%, while scintillators used for γ spectrometry normally have a resolution of 7 to 20 %.
Among the most widely used scintillators there are NaI(Tl), CsI(Tl), KI(Tl), LiI(Eu) and CsF_2. Among the not alkaline materials there are mainly $Bi_4Ge_3O_{12}$ (Bismuth Germanate, aka BGO), the BaF_2 and the ZnS(Ag). In these crystals the passage of a ionizing radiation can result in the transition of an electron from the valence band to the conduction band and then back in the valence band with light emission. Because PMT respond best to radiation in the visible region (and much less in the UV) and being crystals transparent in this range of spectrum, to increase the probability of emission of optical photons during the mechanism of de-excitation, the structure of the bands is modified by means of introduction of appropriate impurities, atoms of appropriate substances, called dopants and indicated in parenthesis next to the formula of the scintillating material.
The inorganic scintillators, compared to those organic, for the same energy deposited by the incident radiation emit much more light (almost an order of magnitude) furthermore their relatively high atomic number makes them much more efficient.

As described, each measure is the result of scintillator pulse dispersion plus other statistical and systematic errors such as fluctuations due to electronics noise or due to the intrinsic noise of the detector.
All these elements cause a broadening of peaks that assume a shape of Gaussian type.
The broadening of the peaks makes it more likely the overlapping with consequent difficulty of recognition of gamma energies which are close to each other and also with the complication arising from having to discriminate the counts associated with decays that interferes to each other.
For this reason , for analytical purposes , it is better the use of semiconductor detectors such as GeHP operated at liquid nitrogen temperature that guarantee narrow peaks (FWHM of about 1%) compared to the much cheaper and easier to handle (not requiring liquid nitrogen) scintillation detector.
Below the two types of detector are compared :



As we see the analysis of a gamma spectrum obtained with a scintillator may be difficult or even impossible to interpret. Here below we describe a method of deconvolution of the experimental data that can reconstruct the Gaussian shape of the photo peaks of a spectrum, making it suitable for a qualitative and quantitative analysis.

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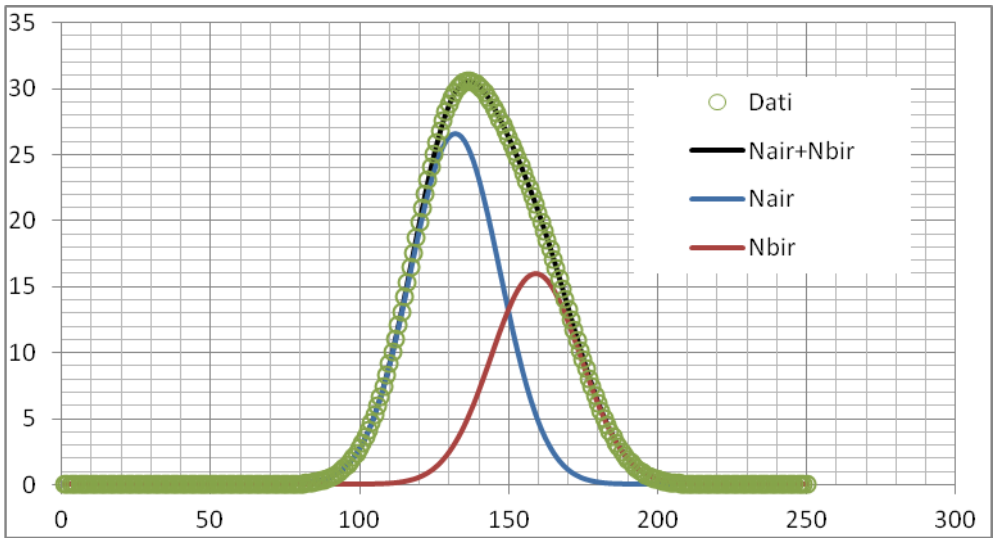
Sometimes it is said that the techniques of deconvolution cannot add anything to the raw data and "what has been subtracted is finally lost and you cannot recreate it". But when you know some of the characteristics of the system being studied like the observed radioisotopes sources emission spectrum and the energy width associated to each photopeak you can "re-create" the missing parts "adding" this knowledge, in order to achieve effective and real improvement of data quality.

The chart below shows a simple example in which the experimental data hide two gamma lines, where the second (right-most) is masked by the first . The technique of Gaussian deconvolution here proposed allows the resolution of the two peaks whose original sum, as we see, overlaps perfectly to the data .



Let's look at the development using i e j indexes with the following meaning:
i: bin index;
j: energy row index.

In general the number of counts relative to the bin number i is the sum of all contributions of emitting gamma radionuclides, the predominant ones are those having the closest energy, while the ones having energy very different than the bin i are negligible :

$$N_i = \sum_j N_j f_{i,j}$$

where

$$f_{i,j} = \frac{1}{\sqrt{2 \cdot \pi \cdot \sigma^2}} e^{-\frac{(E_i - E_j)^2}{2 \cdot \sigma^2}}$$

with E_i indicates the energy related to the bin number i and E_j the energy of the bin related to the gamma emission number j

The counting number into the bin 1, 2, 3, … etc, chosen for example among those energies related to the rows at the base of the envelope, allow to build the following system of linear equations :

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$$\begin{aligned} N_1 &= \overline{N_1}\cdot f_{1,1} + \overline{N_2}\cdot f_{1,2} + \overline{N_3}\cdot f_{1,3} + \cdots \\ N_2 &= \overline{N_1}\cdot f_{2,1} + \overline{N_2}\cdot f_{2,2} + \overline{N_3}\cdot f_{2,3} + \cdots \\ N_3 &= \overline{N_1}\cdot f_{3,1} + \overline{N_2}\cdot f_{3,2} + \overline{N_3}\cdot f_{3,3} + \cdots \\ &\vdots \end{aligned}$$

Whose solution allows for the retrieval of the $\overline{N_j}$ terms which are expressing the total number of counts of energy E_j, that in the case of a radionuclide with a single line (and probability unitary) of gamma emission corresponds to the concentration (or to the activity) of radionuclide j.
Employing the Cramer method the following solutions are obtained :

$$\overline{N_J} = \frac{\det A_j}{\det A}$$

Where A is the coefficients matrix:

$$A = \begin{Vmatrix} f_{1,1} & f_{1,2} & f_{1,3} & \cdots \\ f_{2,1} & f_{2,2} & f_{2,3} & \cdots \\ f_{3,1} & f_{3,2} & f_{3,3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{Vmatrix}$$

While A_j is the matrix A where the column j has been substituted with the known terms array :
Example.

$$A_1 = \begin{Vmatrix} \overline{N_1} & f_{1,2} & f_{1,3} & \cdots \\ \overline{N_2} & f_{2,2} & f_{2,3} & \cdots \\ \overline{N_3} & f_{3,2} & f_{3,3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{Vmatrix}$$

$$A_2 = \begin{Vmatrix} f_{1,1} & \overline{N_1} & f_{1,3} & \cdots \\ f_{2,1} & \overline{N_2} & f_{2,3} & \cdots \\ f_{3,1} & \overline{N_3} & f_{3,3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{Vmatrix}$$

And so on.
At this point, given the total number of counts for each emission line, you can decide to obtain a more convenient view of the spectrum using peaks as narrow as you want, by redistributing the $\overline{N_j}$ counting over a Gaussian function with a proper chosen sigma parameter. The resultant deconvoluted spectrum will be the sum of the contributions N_i, namely

$$N = \sum_i \sum_j N_{i,j} g_{i,j}$$

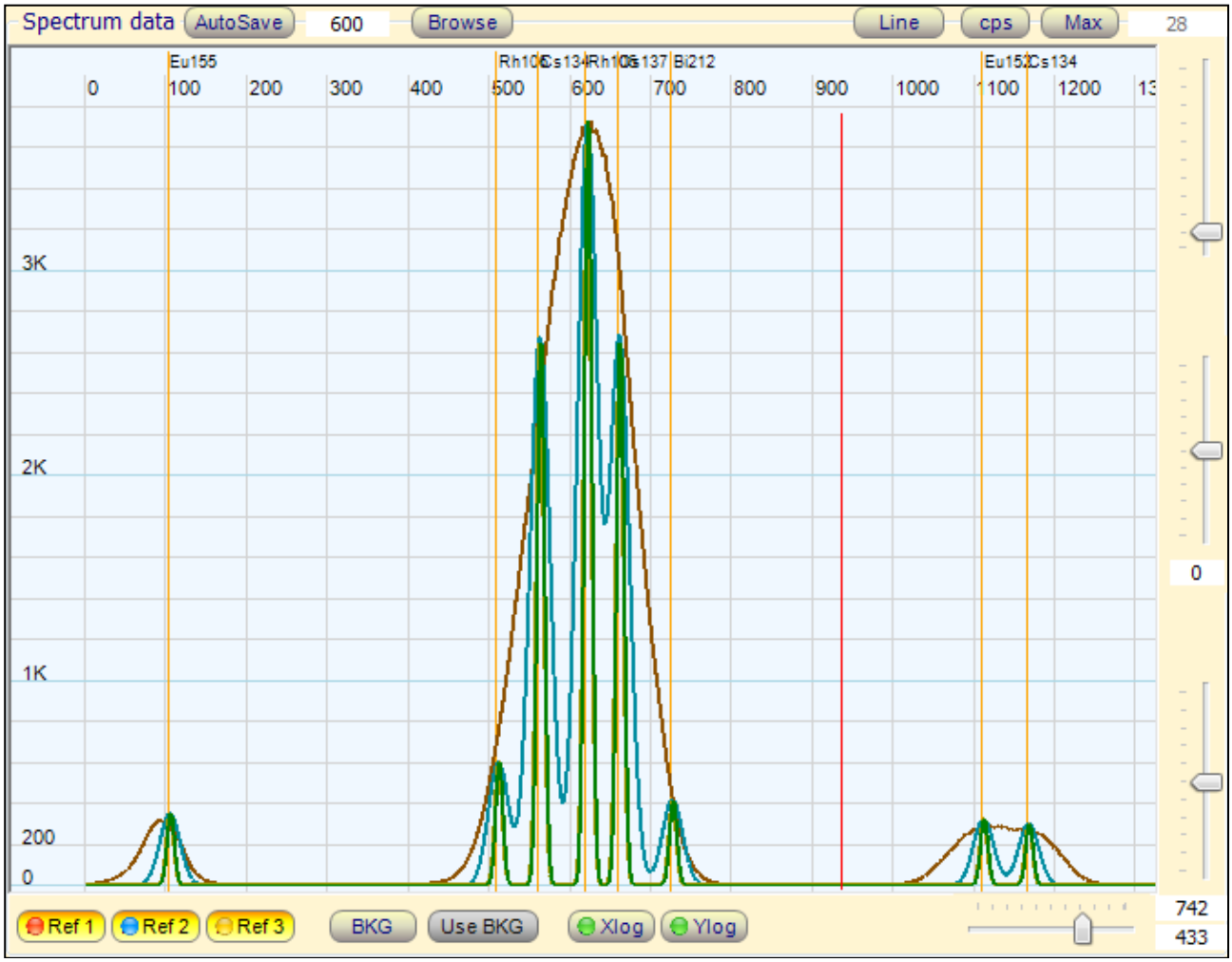
where

$$g_{i,j} = \frac{1}{\sqrt{2\cdot\pi\cdot\sigma_c^2}} e^{-\frac{(E_i - E_j)^2}{2\cdot\sigma_c^2}}$$

where σ_c is the width of the new Gaussian distribution, N is the total counting number over the entire spectrum and $N_{i,j}$ is the counting number inside the bin number i coming from the emission of energy E_j.

It can be noted that the more σ_c is close to the value of σ the more the deconvoluted function resembles the shape of the starting spectrum.

Below it is shown the effect of the algorithm by setting a fixed width of the peaks at the origin of the envelope (σ=20 Kev) and a gradually decreasing reconstructed peak width (σ_c = 25, σ_c = 12, σ_c = 4).



The above described deconvolution method might work even better (given the best approximation associated with the use of the Gaussian function) in those cases in which you must resolve overlapping peaks.