j1PAC: a code for 1-PAC measurements

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Introduction: The j1PAC code was developed for automatic In-111 γ-spectrum processing in one-detector perturbed angular correlation (1-PAC) experiments [1]. This code includes automatic energy calibration procedure, determination of γ-peak areas and calculation of R-values for each spectrum, and statistical analysis of R-values for several measurements of the sample.

j1PAC algorithms: The major j1PAC algorithm is the determination of the peak areas in the γ-spectra of ^{111}In. This algorithm was developed using the specifics of all peaks involved:

1. The statistics of peaks is high ($>10^6$ counts)
2. The shape of all peaks is distorted due to high count rate (8000 counts/s)
3. X-ray peaks show complex structures *ab initio* (as a first approximation – doublets).
4. Coincidence summing peaks have low-energy tails, which depend on the conditions of measurement.

These factors make standard algorithms of determination of peak areas inconvenient in our case. The procedure developed therefore includes several steps:

- non-linear fitting of the peaks in the spectra by Gaussian function. The results are the FWHM and centroid of the peaks or doublet components;
- selection of background regions around the peaks;
- calculation of the net area of the peaks.

In a first step, singlet lines (171, 245, 171+245 keV) are approximated by gauss function with background:

$$F(x) = a + bx + I \exp\left(\frac{(x-x^0)^2}{0.5\sigma^2}\right)$$

and doublet lines ($K_{\alpha\beta}$, 171+$K_{\alpha\beta}$, 245+$K_{\alpha\beta}$) by the sum of two gauss functions:

$$F(x) = a + bx + I \sum_{i=1}^{2} \delta_i \cdot \exp\left(\frac{(x-x_i^0)^2}{0.5\sigma_i}\right)$$

with I – amplitude of peak, x^0- centroid, δ-relative intensity of doublet components, *a* and *b* – parameters of background.

The background regions on both sides of the peak are selected independently. The centre of the background region is selected when the area of the half of the peak changes insignificantly (for less than 0.5σ) when moving from the centroid channel of the peak (fig.1):

$$\left| A_i - A_{i+1} \right| \leq 0.5\sqrt{A_i}$$

with

$$A_i = \sum_{j=i}^{m} c_j - B_i\left(\left|m-i\right|+1\right) \text{ and } B_i = \frac{1}{2nb+1}\sum_{j=i-nb}^{i+nb} c_j$$

[c_j - number of counts in *j* - channel, *m* - channel of centroid of the peak, B_i - background calculated over (2*nb+1) channels]. The number of channels for
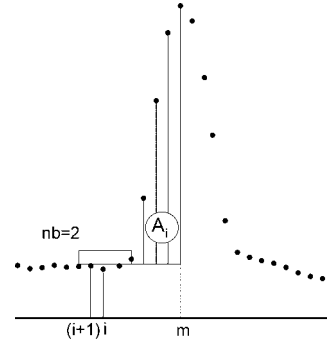

Fig.1. Search for the background region

background calculation are 9 (nb = 4) for 8192 channel spectra and 5 (nb = 2) for 4096 channel spectra.
The areas of the peaks for singlets:

$$S = \sum_{i=l}^{r} c_i - B_l(m-l+1) - B_r(r-m)$$

and for doublets:

$$S = \sum_{i=l}^{r} c_i - B_l(m_1-l+1) - (\delta_1 B_l + \delta_2 B_r)(m_2-m_1+1) - B_r(r-m_2)$$

with m_i – centroid channels, $B_{r,l}$ – background from the right and left side, 1 and r-centres of background regions.

The R-values are calculated as described in [1]:

$$R_{\gamma_1+\gamma_2} = N_{K_{\alpha,\beta}+\gamma_1} \cdot \frac{S_{\gamma_1+\gamma_2} \cdot S_{K_{\alpha,\beta}}}{S_{\gamma_2} \cdot S_{\gamma_1+K_{\alpha,\beta}}}$$

$$R_{\gamma_1+\gamma_2} = N_{K_{\alpha,\beta}+\gamma_2} \cdot \frac{S_{\gamma_1+\gamma_2} \cdot S_{K_{\alpha,\beta}}}{S_{\gamma_1} \cdot S_{\gamma_2+K_{\alpha,\beta}}}$$

with $N_{K_{\alpha,\beta}+\gamma_1} = 0.9176(10)$, $N_{K_{\alpha,\beta}+\gamma_2} = 0.9507(10)$.

If the sample was measured several times, the R-values from these measurements are averaged using a maximum-like hood method.

j1PAC operation: The j1PAC program is a client-server application. The server-side code is written using JAVA. The client is a standard internet browser. The program was successfully used to process spectra of more than 200 samples measured on three different HPGe detectors (with efficiencies ranging from 9-64%). In all cases the algorithm has demonstrated good stability and almost no dependence on parameters of the detector.

References:
[1] D.V. Filossofov et al., Appl. Rad. and Isot. **57**, 437 (2002)