HPGe measurements software manual

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1 Introduction

The whole tree of necessary python scripts is uploaded to some folder. Your unix shell PATH variable should contain this location (e. g. /home/ems/bin). This folder listing will give something like:

```
bepc  hpge.py  LICENSE  scale  vepp2k
```

From your unix shell you can type now:

```
bash> hpge.py --help
```

and you will see the list of code options:

```
Python script to process HPGe spectra. © 2005-2017 N.Yu.Muchnoi
Usage:      hpge.py [options]              | Last update: February 8, 2017 |

List of options:
-h,           --help                : print this help message and exit.
-i,           --interactive         : if set, script will prompt to proceed.
-k,           --keV                 : use channels not keV.
-l,           --list                : just show the list of files.
-f expr,      --file    = expr      : file name(s) under specified folder(s).
-n N,         --nf      = N         : put several files into one spectrum.
-d YYYYMMDD,  --folder  = YYYYMMDD  : date to start from (year, month, day).
-e YYYYMMDD,  --efolder = YYYYMMDD  : date to  end  with (year, month, day).
-t HHMMSS,    --time    = HHMMSS    : time from which to start (hour, min, sec).
-c filename,  --cfg     = filename  : file to read various parameters,
                                      otherwise "default.cfg" is used.
-s filename,  --scale   = filename  : file to store/get calibration results,
                                      otherwise "escale.root" is used.
-v energy,    --verify  = energy    : calibration results for an energy [keV].
              --edge                : try to measure beam energy by Compton edge.
              --escan               : deal with beam energy scan experiment.
```

2 Configurable program options

2.1 Global parameters

In order to start any kind of analysis one should create one or more "working folders", e. g. /home/ems/test, assuming you will run the analysis from this folder. In this folder there should be the file

globals.cfg

with the following structure:

```
[globals]
data_folder : /home/muchnoi/DATA/BEPC/SPECTRA/ ; data folder
data_origin : BEPC                             ; data origin
# This is how to arrange the full line comments
```

The data folder variable shows the location of the tree of data files. The data origin variable shows where this data files were obtained. Now there are only two possible options for that: BEPC and VEPP2K.

2.2 Specific parameters

The lists of specific parameters for data processing are located in the configuration file(s). According to the code options listed on page. 1, there is a special filename, "default.cfg", which will be used if you don't specify another one.

Any configuration file consists of up to four sections. These sections are:

[scale] – parameters required to perform energy scale calibration by nuclear γ-lines.

[pulser] – parameters needed for application of a pulser.

[edge] – parameters required for the laser - Compton edge measurements.

[scan] – parameters needed to perform analysis of the scan experiment at BEPC-II.

In order to quickly investigate the usage and capabilities of the analysis code, let us show the example of such a configuration file. We don't comment on the file content in the text, cause every parameter is described inside. This particular file was created in order to study the J/Ψ scan experiment performed at BEPC-II in December, 2011. This manual will use this experiment as an example for the analysis. Here it is, the "JPsi_2011.cfg", located in our "working folder":

```
# This is the BEMS configuration for the December 2011 J/Psi scan at BEPC-II with BES-III
[scale]
zero   : 1.5             ; energy of the first histogram channel [keV]
gain   : 0.4585          ; MCA gain [keV/Ch] (E = zero + gain*Ch)
amin   : 0.001           ; min amplitude of peak (relative to max amplitude) for peaks finding procedure
emin   : 250.00          ; energy range: minimum [keV]
emax   : 8500.0          ; energy range: maximum [keV]
erec   : 5.0             ; max recognition difference between line observation and reference energy [keV]
fitL   : 5.0             ; peak fit range in units of sigma ( e_from = mean - fitL*sigma ) [a. u.]
fitR   : 6.0             ; peak fit range in units of sigma ( e_upto = mean + fitR*sigma ) [a. u.]
nitr   : 3               ; number of iterations in the 'scale determination procedure'
cdif   : 0.02            ; differential nonlinearity in spectrum (MCA) channel [a. u.]
tbpa   : 0.050           ; 'The Best Possible Accuracy' one can believe from HPGe measurement [keV]
file   : JPsi_2011.root  ; where to store calibration results
```

```
name0  : Cs137(   0)     ; name of the calibration line to be shown in the 1-st pad
name1  : Co60 (   0)     ; name of the calibration line to be shown in the 2-nd pad
name2  : Co60 (   1)     ; name of the calibration line to be shown in the 3-rd pad
name3  : Tl208(  23)     ; name of the calibration line to be shown in the 4-th pad

[pulser]
zero_p : 0.717           ; pb-5 energy of the first histogram channel [keV]
gain_p : 738.8           ; pb-5 Volts to keV conversion [keV/V] (E = zero_p + gain_p*V)
peer_p : 0.025           ; energy error assigned to pulser calibration peak, keV

[edge]
WaveLength: 10.835231e-6 ; laser wavelength [m] (CO-2 laser 10P42 line)
MinAmpEdge: 30.0         ; minimal succesive edge amplitude [a. u.]
BinsMerger: 4            ; number of histogram bins merged in one for the edge fitting
EdgeRanger: 0.65         ; lower edge fit range will be Wmax*(1 - EdgeRanger/(1+2*Wmax/me)) [keV]
EbepcTuner: -3.0         ; E_true is approximately E_bepc + EbepcTuner [MeV]
Asymmetry:  1.25         ; HPGe response asymmetry, sigma_L = A*sigma_R (if A < 1 sigma_L is set by calibration)

[scan]
bdate    : 20111222      ; scan begin date
edate    : 20111223      ; scan  end  date
efrom    : 1540.0        ; BEPC DB beam energy from, MeV
eupto    : 1555.0        ; BEPC DB beam energy upto, MeV
```

3 Analysis example

3.1 Scale calibration

The following command:

```
bash> hpge.py -c JPsi_2011.cfg -s Dec2011.root -e 20111230 -n 20 -i
```

will use the "JPsi_2011.cfg" file for configuration parameters and will record the calibration results into "Dec2011.root" file. If the latter is not specified in the command line, the results will be saved to "JPsi_2011.root" as it is specified in "JPsi_2011.cfg". It will start with the date 2011.12.22, as it is specified in "JPsi_2011.cfg", but it will end at 2011.12.30 as it is specified in a command line, again: command line parameter has more priority. It will sum consequently every 20 files from your data and perform the scale calibration. It will wait for pressing Enter button after each 20 files are processed due to "-i" option in the command line.

The last (before the program stop) calibration result is presented in Figure 1. The calibration spikes are fitted by bifurcated Gaussians with the Compton step in the center. The bottom-right plot on the canvas shows the energy resolution vs energy. Right-sigmas of bifurcated Gaussians lie to the right from zero energy. Left-sigmas of bifurcated Gaussians lie to the left from zero energy just for the simplicity of the fitting procedure. The red line is the result of four-parameters combined fit according to the following expression:

$$\sigma_E = \begin{cases} \sqrt{p_0^2 + p_1 \mathrm{g} |E_\gamma|} & \text{if } E_\gamma > 0; \\ \sqrt{p_0^2 + p_1 \mathrm{g} |E_\gamma| + p_2 (p_3 - |E_\gamma|)^2} & \text{if } E_\gamma < 0. \end{cases} \quad (1)$$

Here g = 2.96 eV is the electron-hole pair creation energy in Ge, p_0 and p_3 are in energy units while p_1 and p_2 are dimensionless parameters. At certain energy E_γ the right sigma will be $\sigma_R = \sigma_E(E_\gamma)$, while the left sigma will be $\sigma_L = \sigma_E(-E_\gamma)$.

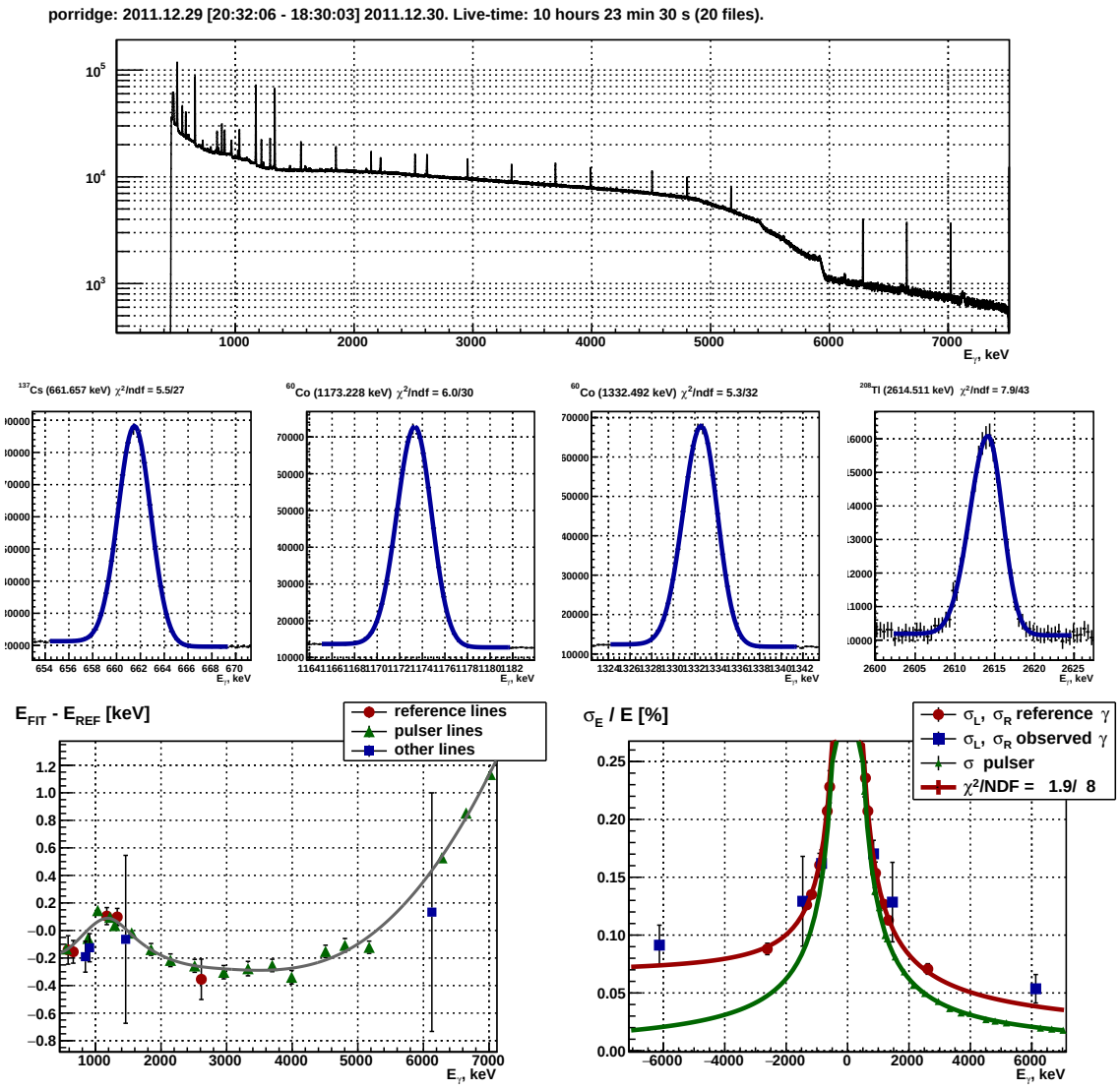

Figure 1: Energy scale calibration canvas

Absolute scale calibration relies on the following lines, as it follows from the terminal output:

Calibration Isotopes:

Line Name	Height	Ey,keV	sR,keV	sL,keV	Compton	Backgr	x2/NDF
Tl208(7)	59984	583.05	1.3749	01.331	0.03839	22933	2.8/ 26
Cs137(0)	235659	661.50	1.3710	01.371	0.02484	19627	5.5/ 27
Co60 (0)	231389	1173.33	1.4869	01.585	0.01535	12748	6.0/ 30
Co60 (1)	223695	1332.59	1.5028	01.680	0.01060	11836	5.3/ 32
Tl208(23)	30901	2614.16	1.8487	02.302	0.00789	10143	7.9/ 43

Other lines observed but not taken into calibration:

Other Isotopes:

Line Name	Height	Ey,keV	sR,keV	sL,keV	Compton	Backgr	x2/NDF
Mn55 (0)	34881	846.56	1.4415	01.371	0.05522	16735	5.3/ 28
Ac228(0)	40065	911.16	1.3992	01.462	0.01852	16298	3.0/ 28
K40 (0)	5363	1460.69	1.8773	01.888	0.00000	11502	8.5/ 40
O16 (0)	1978	6129.40	3.2858	05.597	0.10000	1027	63.3/ 99

3.2 Verification of Scale Calibration

After the scale calibration is performed, one may check its results by issuing the command:

```
bash> hpge.py -v 4000 -s Dec2011.root
```

It will apply the calibration results from Dec2011.root file for a fixed energy $E_\gamma = 4000$ keV (see Figure 2). Top-left plot shows the stability and accuracy of a certain MCA channel conversion to absolute energy values with isotope lines. Top-right plot shows the energy correction due to MCA nonlinearity, obtained by pulser. Bottom plots show in-time behavior of the HPGe detector resolution (σ_R and σ_L).

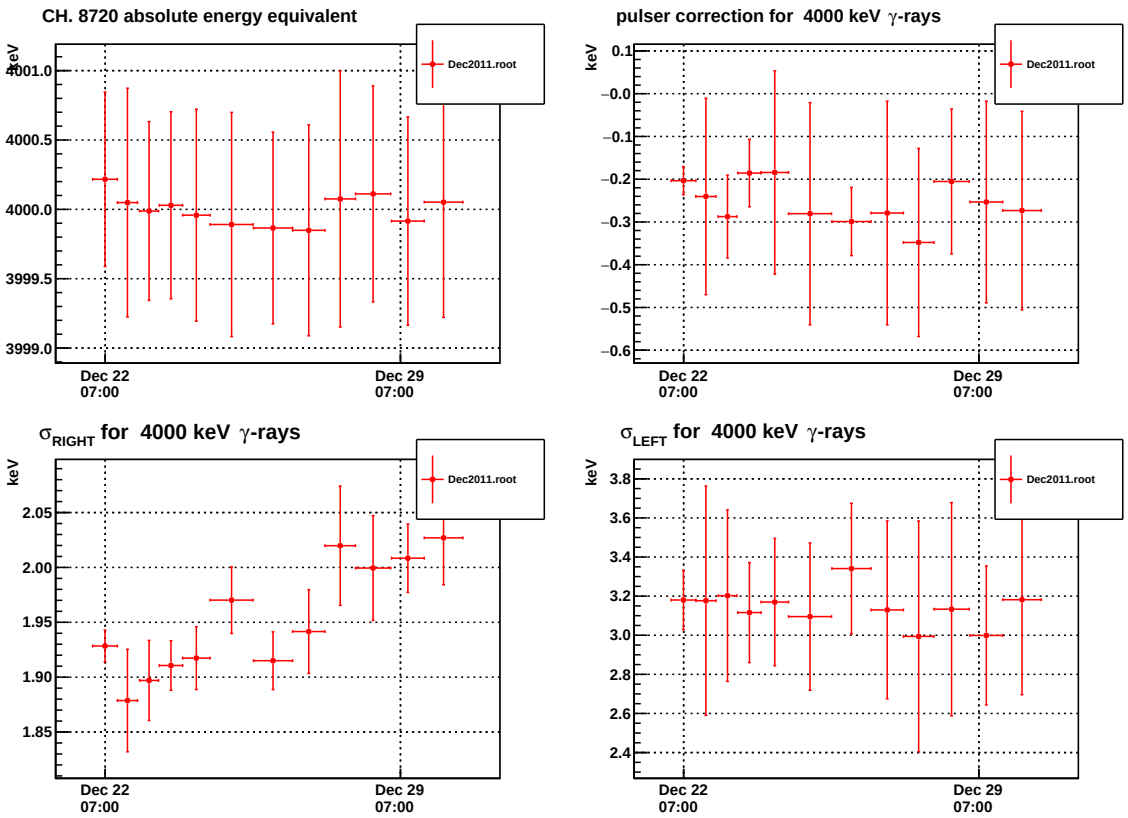

Figure 2: Verification of the energy scale calibration at certain energy

3.3 Single beam energy measurement by laser backscattering

The following command:

```
bash> hpge.py -c JPsi_2011.cfg -s Dec2011.root --edge -i -f elec -n 2
```

will use existing scale calibration for the measurement of the energy of the Compton edge in the HPGe spectrum. It will take two consequent files for electron beam (-f elec -n 2) starting from the date specified in "JPsi_2011.cfg". The calibration curves will be taken from "Dec2011.root". Among many records in calibration file one is chosen according to the coincidence between the time of calibration and the time of measurement. If it is impossible, the code stops.

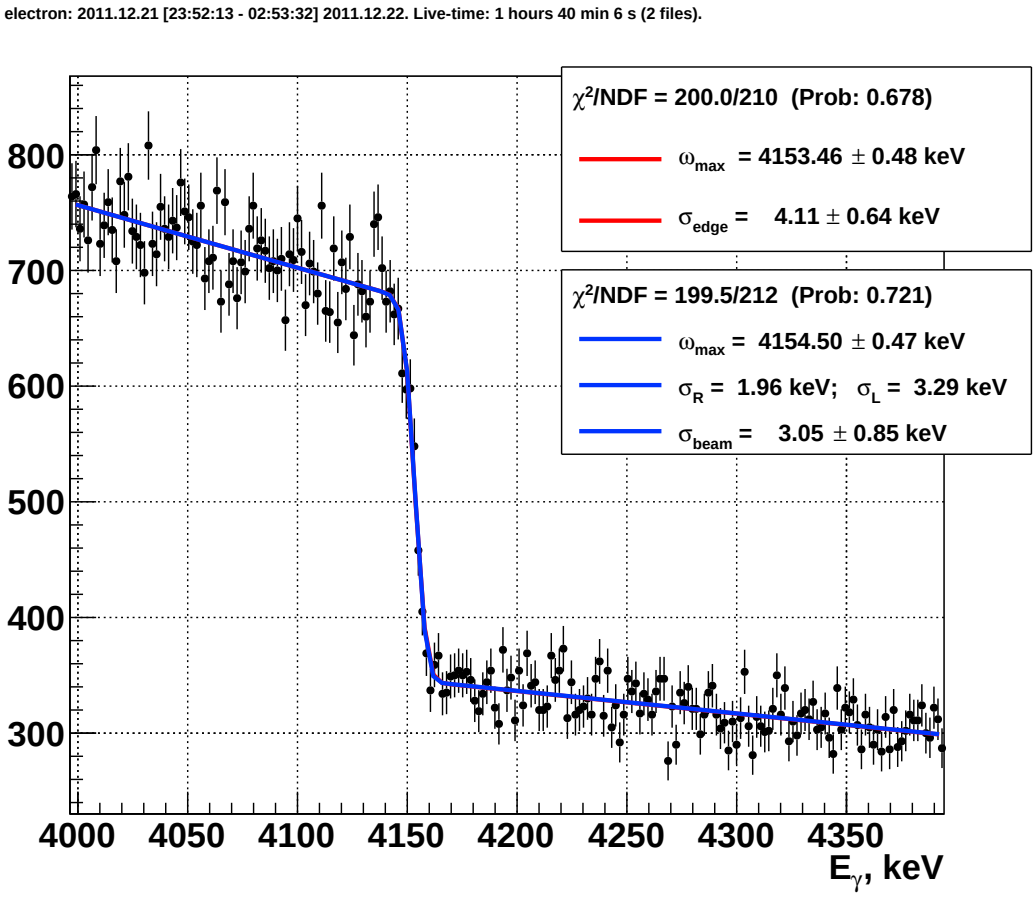

Figure 3: The Compton edge fitting example

The result is presented in Figure 3. Note there is ∼1 keV difference in ω_{max} between the first (symmetric) and the second (asymmetric) fits. After two fits, the ω_{max} is corrected by pulser correction (see Figure. 2).

```
Wmax: 4153.46 +- 0.48 keV (symmetric fit)
Wmax: 4154.50 +- 0.47 keV (asymmetric fit)
Wmax: 4154.69 +- 0.47 keV (spline correction )
```

The electron beam energy is calculated from measured value of ω_{max} according to

$$E_{beam} = \frac{\omega_{max}}{2}\left(1 + \sqrt{1 + m^2/\omega_0\omega_{max}}\right), \tag{2}$$

where ω_0 is the laser photon energy, taken from the [edge] section in "JPsi_2011.cfg". Then the beam energy is scaled from North IP to South IP due to synchrotron radiation losses.

```
electron Beam Energy Determination:
           BEPC beam energy = 1544.223 +- 0.096 MeV was taken from database
           Measurement time from 2011.12.21 23:52:13 to 2011.12.22 02:53:32.

BEMS beam energy = 1541.661 +- 0.087 MeV (SR correction to IP +0.027 MeV was added)
BEMS beam spread =      565 +-   157 keV
```

3.4 The energy scan experiments at BEPC-II

In order to accelerate the analysis of the scan experiments with BEMS at BEPC-II, additional option was implemented. The following command:

```
bash> hpge.py -c JPsi_2011.cfg -s Dec2011.root --escan
```

will perform the energy calibration separately for each "scan point" and save (add) the results of calibration to existing "Dec2011.root" file. First you will see how the code recognize the "scan points" by reading of the beam set energy values from our database (*.sta files):

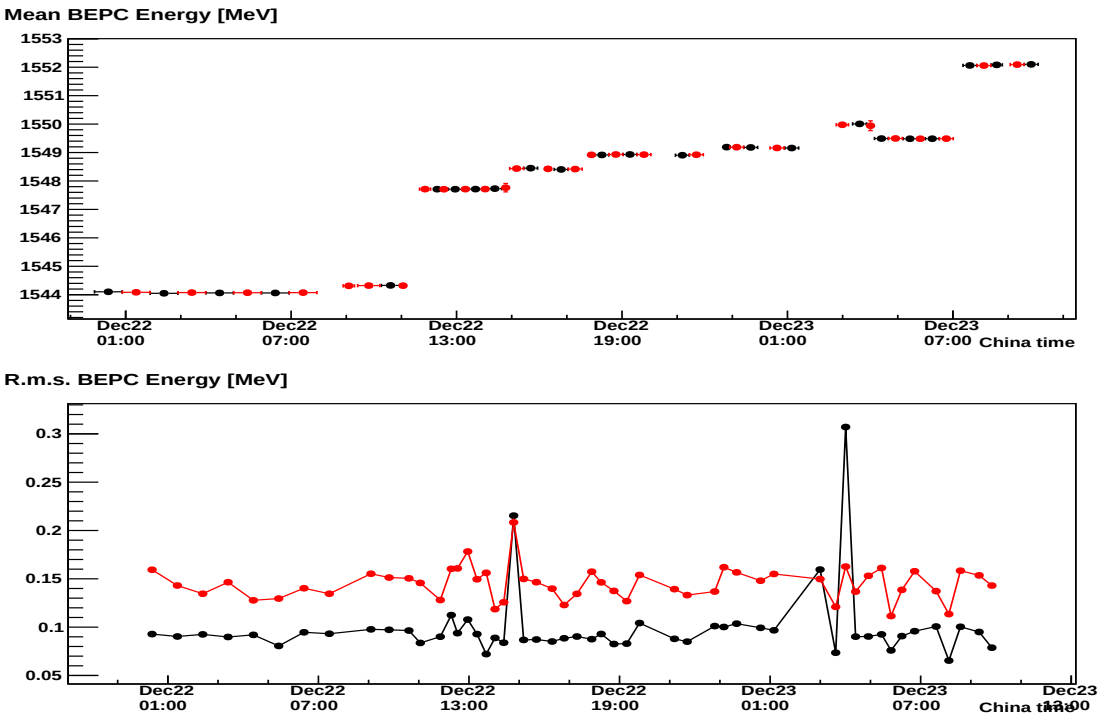

Figure 4: Scan points are recognized by reading the history of BEPC-II beam energy changes.

Besides the plots in Figure 4 you will see the terminal output:

```
Point  0 energy: 1544.103 MeV. Number of files: 8
Point  1 energy: 1544.313 MeV. Number of files: 4
Point  2 energy: 1547.713 MeV. Number of files: 9
Point  3 energy: 1548.437 MeV. Number of files: 5
Point  4 energy: 1548.919 MeV. Number of files: 7
Point  5 energy: 1549.190 MeV. Number of files: 5
Point  6 energy: 1549.976 MeV. Number of files: 3
Point  7 energy: 1549.492 MeV. Number of files: 6
Point  8 energy: 1552.063 MeV. Number of files: 5
```

If you proceed by pressing the Enter button, the code will put together the HPGe spectra for each energy point and perform an energy scale calibration with them. The results of this calibration will be recorded to the calibration file "Dec2011.root". If now we repeat the command

```
bash> hpge.py -v 4000 -s Dec2011.root
```

we will see the following figure:

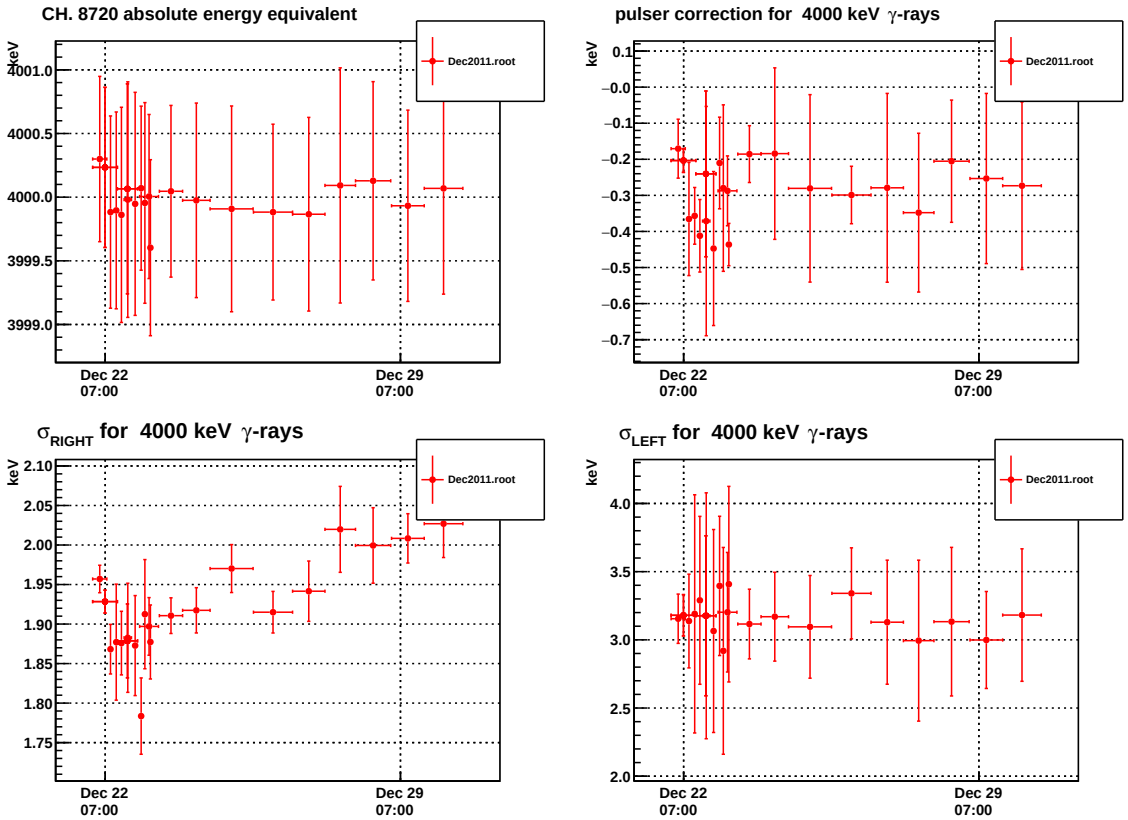

Figure 5: Verification of the energy scale calibration at certain energy

If we compare Figure 5 and Figure 2, at the beginning of the plots we see more calibration results then there were before, with less statistical accuracy. However now I have no good idea about how to choose between several appropriate calibrations contained in a single file, so further here we'll use the original "Dec2011.root" file, without the points appeared in Figure 5.

While using the software, it is a user worry how to supply appropriate calibration, but it's better to work with the calibration files without mixed results.

So now we can obtain a table of c.m.s. energies for the J/Ψ scan by the following command:

```
bash> hpge.py -c JPsi_2011.cfg -s Dec2011.root --escan --edge
```

For every energy point it will sum separately electrons and positrons spectra, determine the edge parameters, beam energies and energy spreads. Finally it calculates the mean c.m.s. energies with an account for BES-III 22 mrad collisions and the widths of the c.m.s energy distribution σ_W. The results will appear in the text file "SCAN.results" in your working folder:

```
# t           dt   E c.m.s.  dE      S_W    dS_W
1324500850  14517  3082.664  0.088   0.943  0.099 # point  0 (1544.103 MeV)
1324522885   4086  3088.794  0.175   1.002  0.192 # point  1 (1544.313 MeV)
1324534640   5871  3095.249  0.137   1.162  0.148 # point  2 (1547.713 MeV)
1324545266   4727  3096.648  0.116   0.805  0.130 # point  3 (1548.437 MeV)
1324558292   7518  3097.611  0.119   1.180  0.108 # point  4 (1548.919 MeV)
1324573360   4898  3098.132  0.137   1.263  0.136 # point  5 (1549.190 MeV)
1324593302   5139  3098.924  0.112   1.050  0.115 # point  7 (1549.492 MeV)
1324604617   4903  3104.126  0.133   1.543  0.130 # point  8 (1552.063 MeV)
```

4 System requirements and software installation

The tool was developed and tested on the host with the following configuration:

- Linux Mint 18.1 64-bit
- Linux kernel 4.4.0-62-generic
- ROOT 6.08/00 with PyROOT (https://root.cern.ch)

It has not been checked to run on other/older versions, but I hope it can do so.

The following additional packages are required:

- python-scipy
- python-numpy
- python-configglue

The software can be downloaded from github with the following command:

```
bash> git clone https://github.com/muchnoi/HPGe.git
```

5 Algorithms, functions, etc.

5.1 ω_{max} and its derivative

In Compton scattering

$$\omega_{max} = E_0 \frac{\kappa}{1+\kappa}, \text{ where } \kappa = \frac{4\omega_0 E_0}{m^2}\cos^2(\alpha/2), \tag{3}$$

ω_0 is the laser photon energy. Hence

$$\frac{\partial \omega_{max}}{\partial E_0} = \frac{(2+\kappa)\kappa}{(1+\kappa)^2}, \quad \sigma_{\omega_{max}} = \frac{(2+\kappa)\kappa}{(1+\kappa)^2}\sigma_{E_0}, \quad \Delta_{E_0} = \frac{(1+\kappa)^2}{(2+\kappa)\kappa}\Delta_{\omega_{max}}. \tag{4}$$

5.2 Corrected Zhukovsky formula

The influence of constant EM field on the cross section of Compton scattering was studied in [**?**] [1]. The energy spectrum of scattered photons was obtained from the solution of the Dirac equation. The result may be expressed as follows:

$$\mathfrak{F}(\omega, E) \equiv \frac{d\dot{N}_\gamma}{d\hbar\omega} \propto \nu_1 \int_z^\infty \mathrm{Ai}(z')dz' - \nu_2 \,\mathrm{Ai}'(z) + \nu_3 \,\mathrm{Ai}(z), \tag{5}$$

where

$$\begin{aligned}
z &= \xi^{\frac{2}{3}}\left(\left[\frac{u}{\kappa}\right]^{\frac{2}{3}} - \left[\frac{\kappa}{u}\right]^{\frac{1}{3}}\right), \\
u &= \frac{\omega}{E-\omega}, \quad \kappa = \frac{4E\omega_0}{m^2}, \quad \xi = 4\cdot\frac{\omega_0}{m}\cdot\frac{B_0}{B}, \\
\nu_1 &= \frac{1}{8}\left\{2 + \frac{u^2}{1+u} - 4\frac{u}{\kappa} + 4\left[\frac{u}{\kappa}\right]^2 - 16\left[\frac{u}{\kappa}\right]^2\xi^2\right\}, \\
\nu_2 &= \left[\frac{u}{\kappa}\right]^{\frac{4}{3}}\xi^{\frac{2}{3}}\left\{4\xi^2 + \frac{u^2(1+4\xi^2)}{2(1+u)}\right\}, \\
\nu_3 &= \left[\frac{u}{\kappa}\right]^{\frac{2}{3}}\xi^{\frac{4}{3}}\left\{2(1-\frac{u}{\kappa}) + \frac{u^2}{(1+u)}\left(1-2\frac{u}{\kappa}\right)\right\}.
\end{aligned} \tag{6}$$

Further we consider the initial photon energy ω_0 and the magnetic filed in the interaction area B as constants. While $\xi \ll 1$ only the first term in (5) is important and though the change in $\mathfrak{F}$ is coupled with the change in z as:

$$\Delta\mathfrak{F}(\Delta z) \equiv \mathfrak{F}(z+\Delta z) - \mathfrak{F}(z) \simeq -\Delta z\,\mathrm{Ai}(z), \tag{7}$$

In case when an electron has certain energy E the spectrum derivative is:

$$\begin{aligned}
\Delta\mathfrak{F}(\omega, \Delta\omega) &= (\partial z/\partial\omega)\cdot\Delta\omega\cdot\mathrm{Ai}(z), \text{ where} \\
\frac{\partial z}{\partial\omega} &= \xi^{\frac{2}{3}}\left(\frac{2}{3}\left[\frac{u}{\kappa}\right]^{\frac{2}{3}} + \frac{1}{3}\left[\frac{\kappa}{u}\right]^{\frac{1}{3}}\right)\left(\frac{1}{w} + \frac{1}{E-\omega}\right).
\end{aligned} \tag{8}$$

[1] misprint corrections for the term ν_3 were published in [2].

If there is some deviation in E, at certain photon energy ω the spectrum derivative is:

$$\begin{aligned} \Delta\mathfrak{F}(\omega,\Delta E) &= (\partial z/\partial E)\cdot\Delta E\cdot \mathrm{Ai}(z),\ \text{where} \\ \frac{\partial z}{\partial E} &= -\xi^{\frac{2}{3}}\left(\frac{2}{3}\left[\frac{u}{\kappa}\right]^{\frac{2}{3}}+\frac{1}{3}\left[\frac{\kappa}{u}\right]^{\frac{1}{3}}\right)\left(\frac{1}{E}+\frac{1}{E-\omega}\right). \end{aligned} \tag{9}$$

At certain scattered photon energy ω the influence of the beam energy spread will have the equivalent impact to the spectrum shape when $\Delta\mathfrak{F}(\omega,\Delta\omega)=\Delta\mathfrak{F}(\omega,\Delta E)$. Hence:

$$\Delta\omega=\Delta E\frac{\partial z/\partial E}{\partial z/\partial\omega}\quad\text{and}\quad\frac{\sigma_\omega}{\omega}=\frac{\sigma_E}{E}\left(2-\frac{\omega}{E}\right). \tag{10}$$

When $\omega=\omega_{max}$, equation (10) gives exactly the same answer as equation (4). Since we're interested in the beam energy spread influence to the spectrum in a small energy range around ω_{max}, equation (4) is proved to be good for this purpose in case of curved electron trajectory.

5.3 HPGe response function & the beam energy spread impact

HPGe response is described by bifurcated Gaussian:

$$f(x)=\frac{\sqrt{2}}{\sqrt{\pi}(\sigma_R+\sigma_L)}\begin{cases}\exp\left(-\dfrac{x^2}{2\sigma_R^2}\right) & \text{if } x>0;\\[2ex] \exp\left(-\dfrac{x^2}{2\sigma_L^2}\right) & \text{if } x\le 0.\end{cases} \tag{11}$$

Its convolution with symmetric Gaussian (σ), originating from the beam energy spread gives:

$$S(x)=\frac{1}{\pi\sigma(\sigma_R+\sigma_L)}\int dy\begin{cases}[0\div+\infty]: & \exp\left(-\dfrac{y^2}{2\sigma_R^2}-\dfrac{(x-y)^2}{2\sigma^2}\right)\\[2ex] [-\infty\div 0]: & \exp\left(-\dfrac{y^2}{2\sigma_L^2}-\dfrac{(x-y)^2}{2\sigma^2}\right)\end{cases} \tag{12}$$

Rewrite:

$$S(x)=\frac{\exp(-x^2/2\sigma^2)}{\pi\sigma(\sigma_R+\sigma_L)}\int dy\begin{cases}[0\div+\infty]: & \exp\left(-\dfrac{y^2}{2}\left[\dfrac{1}{\sigma_R^2}+\dfrac{1}{\sigma^2}\right]+\dfrac{xy}{\sigma^2}\right)\\[2ex] [-\infty\div 0]: & \exp\left(-\dfrac{y^2}{2}\left[\dfrac{1}{\sigma_L^2}+\dfrac{1}{\sigma^2}\right]+\dfrac{xy}{\sigma^2}\right)\end{cases} \tag{13}$$

As far as

$$\int_0^{+\infty}\exp\bigl(-ax^2+bx\bigr)dx=\frac{1}{2}\sqrt{\frac{\pi}{a}}\exp\Bigl(\frac{b^2}{4a}\Bigr)\mathrm{erfc}\Bigl(\frac{-b}{2\sqrt{a}}\Bigr), \tag{14a}$$

$$\int_{-\infty}^{0}\exp\bigl(-ax^2+bx\bigr)dx=\frac{1}{2}\sqrt{\frac{\pi}{a}}\exp\Bigl(\frac{b^2}{4a}\Bigr)\mathrm{erfc}\Bigl(\frac{b}{2\sqrt{a}}\Bigr), \tag{14b}$$

finally one gets the normalized function:

$$S(x) = \frac{\sigma_R \exp\left[\frac{-x^2/2}{\sigma_R^2+\sigma^2}\right] \mathrm{erfc}\left[\frac{-x\sigma_R/\sigma}{\sqrt{2(\sigma_R^2+\sigma^2)}}\right]}{(\sigma_R+\sigma_L)\sqrt{2\pi(\sigma_R^2+\sigma^2)}} + \frac{\sigma_L \exp\left[\frac{-x^2/2}{\sigma_L^2+\sigma^2}\right] \mathrm{erfc}\left[\frac{x\sigma_L/\sigma}{\sqrt{2(\sigma_L^2+\sigma^2)}}\right]}{(\sigma_R+\sigma_L)\sqrt{2\pi(\sigma_L^2+\sigma^2)}}. \quad (15)$$

Expression (15) should be then convoluted with the Compton cross section near ω_{max} for accurate description of the spectrum edge shape.