MISTRAL DATA ANALYSIS

C. THIBAULT
CSNSM-IN2P3-CNRS, Bât. 108, F-91405 Orsay-Campus

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Contents

1 Introduction

This note describes the data analysis which has been developed in order to analyse the data from MISTRAL. Its very starting point was the ''RFDAP" code [1] written for PS189 experiment.
The goal of MISTRAL is to perform mass–ratio determinations through frequency–ratio measurements [2]. Very shortly, when different ions A and B (A=reference and B= unknown mass) are rotating in the same magnetic field, the product of their mass m by their cyclotron frequency f_c is constant :

$$m_A \times f_{cA} = m_B \times f_{cB} \tag{1}$$

MISTRAL is built in such a way that the ions may only reach its final detector when the radio-frequency f injected in its modulator is related to f_c by :

$$f = (n + 1/2) f_c \tag{2}$$

where n "harmonic number", is an integer. In the following, $n + 1/2$, the ''harmonic ratio" will be denoted by $\mathcal{H}$.
The mass ratio of the 2 ions is indeed given by :

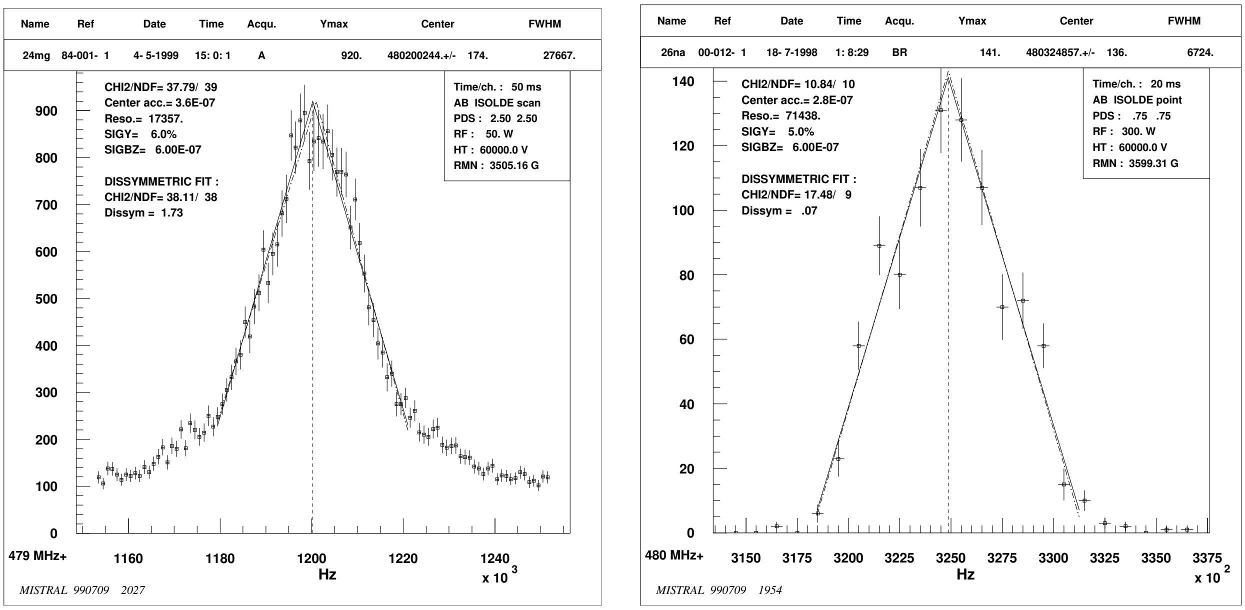
$$R = \frac{m_{A+}}{m_{B+}} = \frac{f_B}{f_A} \times \frac{\mathcal{H_A}}{\mathcal{H_B}} = R_{freq} \times \frac{\mathcal{H_A}}{\mathcal{H_B}} \tag{3}$$

f_A and f_B are the "resonance" values of the radio-frequency for which the transmission, *i.e.* the number of counts reaching the final detector of MISTRAL, is maximum.
While measuring the transmission versus the frequency in the neighbouring of the resonance, the obtained "mass peak" is theoretically symmetric and assimilated to a triangle [2]. According to the Phase Defining Slit (PDS) aperture, the tails which are normally present between the peaks (Fig. 1-*a*) may be eliminated (Fig. 1-*b*) or not. Sometimes an unexpected flattening of the top has been observed. Nevertheless a triangular function may be fitted on selected parts which still provide an accurate determination of the center of symmetry of the triangle (Fig. 1).
Since the ions have a charge $q = +1$, and are accelerated by potentials V_A and V_B ($m_A \times V_A = m_B \times V_B$), the at rest atomic mass of B is given by :

$$m_B = \frac{m_A - m_e + V_A}{R} + m_e - V_B \tag{4}$$

2 Reading data from acquisition

For A measurements, the RF frequency is incremented step-by-step, synchroneously with the MCS scan in order to cover the selected range. This mode is the so-called "sweeping mode".
For B measurements,
• when a steady beam (stable isotopes) is available, the RF frequency dependance may be obtained using the same sweeping mode as for A.
• when the radioactive beam from ISOLDE is used, as its intensity is time dependant, a "point-by-point mode" has to be used : for each proton pulse from the PS booster, a MCS scan is performed with the same RF frequency value for all its channels. The RF frequency is then incremented from one proton pulse to the next one.
Taking into account the new acquisition scheme, it is useful to define some terms in order to try to make everything clear :



(a) (b)

Figure 1: Examples of fits : (a) when the PDS is widely opened ; (b) when the PDS cuts the tails

Scan Recording of a series of channels corresponding to a single triggering of the MCS.

Sweeping Exploration of all the required frequency steps in a single scan.

Nota in point-by-point mode, a B "scan" may have several channels in order to give a time information on the behaviour of the B intensity, but there is no frequency "sweeping".

Pass
- In sweeping mode, A-B, or A_1-B-A_2 frequency sweepings.
- In point-by-point mode, either A frequency sweeping + B scan, or only one B scan.

Cycle
- In sweeping mode, a cycle contains only 1 pass.
- In point-by-point mode, a cycle is obtained when the number of passes (*i.e.* the number of B scans) is such that all frequency steps have been explored. It is worth noting that they are explored randomly.

Measure Series of identical cycles launched by the acquisition. Each measure corresponds to a specific data file.

Run Series of measurements recorded with the same parameters.

Manip Series of runs recorded with different parameters. Each manip corresponds to a specific directory.

The *Read_file* command allows to read the data corresponding to a specific measure. All provided parameters are stored, and the main ones are printed.

In point-by-point mode, the mass peak is built using the random RF frequency values provided by the acquisition (Fig. 1). If intensities have been recorded without RF power, a normalization may be performed if required by the user. The time-dependance recorded by the B scans is also built (Fig. 2).

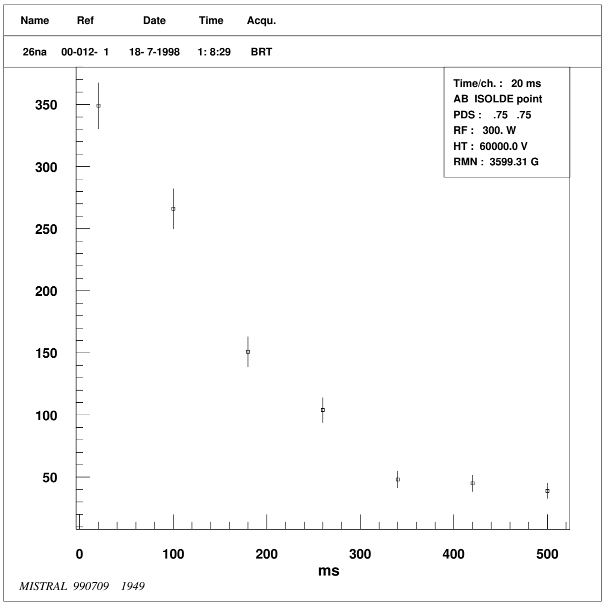


Figure 2: Time dependance of ^{26}Na after a proton pulse

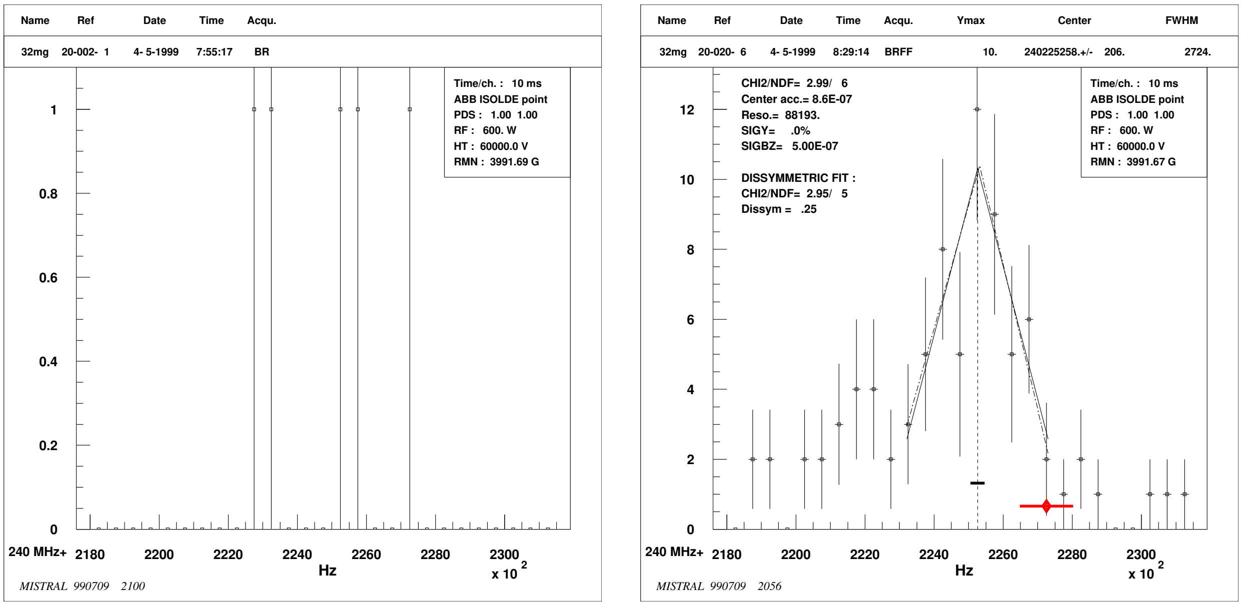
3 General Scheme of the Analysis.

3.1 Sweeping mode :

For every pass (or cycle), *i.e.* every A–B couple, the following steps are performed :
• The A and B mass peaks are fitted using a least squares method. For each peak, the center of symmetry, the FWHM and the height of the fitted symmetric triangle are determined as well as their uncertainties.
• A fit with a dissymmetric triangle is also performed to check that the dissymmetry is negligible.
• R is then determined using equation 3 and the B mass is deduced for every A–B couple, using equation 4.
• All data resulting from peaks analysis are stored. Their uncertainties are also stored when necessary.

3.2 Point-by-point mode :

• For every pass where A was recorded, the A mass peak is fitted, and the result is stored.
• For every cycle, the B mass peak is built. The counting rates may be normalized if data have been taken with and without RF power.
– Using *FIT BRFF*, R_{freq} is determined by comparison of f_B with the averaged value of f_A. The B mass is deduced and stored.
– Using *FIT BRFN*, the frequency of each B scan is normalized relative to f_A. This procedure allows to get free from long term magnetic field drifts. In that case, R_{freq} is directly obtained by fitting the mass peak. The B mass is deduced, and stored.
In case of very low statistics, it is also possible to cumulate several cycles or measures before fitting the B mass peak (Fig. 3).



(a) (b)

Figure 3: ^{32}Mg : an example of low statistics. (a) 1 cycle ; (b) 20 cumulated cycles

4 Data Input for the fitting procedure

Direct data from the experiment are the frequencies f_i and the counting rates y_i recorded with RF power on. From these, we derive input data and their uncertainties for the fitting procedure : $X_i \pm \sigma X_i$ and $Y_i \pm \sigma Y_i$.

4.1 A mass and B mass without normalization

X_i and Y_i are directly the measured values :

- $X_i = f_i$

- $\dfrac{\sigma X_i}{X_i} = SIGB$

where $SIGB$ is the relative fluctuation of the magnetic field B.
$SIGB$ is fixed by the user. A good estimation is provided by the variance of the resonance frequencies in series of identical measurements. Typically, $SIGB \simeq 4\ 10^{-7}$

- $Y_i = y_i$

- $\dfrac{\sigma Y_i}{Y_i} = \sqrt{\dfrac{1}{y_i} + SIGY^2}$

where $\sqrt{y_i}$ is the statistical uncertainty on y_i, and $SIGY$ is the relative uncertainty which corresponds to unstatistical fluctuations such as given by a 50 Hz ripple. $SIGY$ may be evaluated from the variance of the intensity without RF power. If not, it is adjusted by the user in order to get a χ^2 value around 1. $SIGY$ is generally found to be in the range 0–5%

4.2 Normalized B frequencies

- $X_i = \dfrac{f_i}{f_{Ai}}$ In case of $A_1{-}B{-}A_2$ mode, $f_{Ai} = (f_{A1i} + f_{A2i})/2$

- $\dfrac{\sigma X_i}{X_i} = \sqrt{\left(\dfrac{\sigma f_{Ai}}{f_{Ai}}\right)^2 + SIGB^{\,2}}$

4.3 Normalized B counting rates

If counting rates have been alternately recorded with RF and without RF, it is possible to normalize the B counting rates :

- $Y_i = \overline{ynor_i}\dfrac{y_i}{ynor_i}$

where $ynor_i$ is the counting rate without RF power, and $\overline{ynor_i}$ is the mean value of $ynor_i$ so that one has $Y_i \simeq y_i$.
The relative uncertainty on Y_i is the quadratic sum of the statistical uncertainties on y_i and on $ynor_i$, and of the $SIGY$ fluctuations.

- $\dfrac{\sigma Y_i}{Y_i} = \sqrt{\dfrac{1}{y_i} + \dfrac{1}{ynor_i} + SIGY^2}$

5 Fitting Procedure

As already mentioned, a symmetric triangular shape is assumed, which implies 3 parameters in order to be defined. These 3 parameters have been chosen to be closely related to the experimental data (Fig. 4) :
• cm : center of symmetry
• dm : FWHM (resolving power $= f/dm$)
• ym : height
The function to adjust is given by $Y_i \pm \sigma Y_i = f(X_i \pm \sigma X_i)$, *i.e.* :

- for $\begin{cases} & X_i \le cm - dm \\ \text{or} & X_i \ge cm + dm \end{cases}$ $$Y_i \pm \sigma Y_i = 0 \qquad (5)$$

- for $cm - dm \le X_i \le cm + dm$ $$Y_i \pm \sigma Y_i = ym\left(1 - \frac{|X_i \pm \sigma X_i - cm|}{dm}\right) \qquad (6)$$

  which may be written $$Y_i \pm \sigma Y_i \pm \frac{ym}{dm}\sigma X_i = ym\left(1 - \frac{|X_i - cm|}{dm}\right) \qquad (7)$$

The weights w_i are taken as

$$w_i = \frac{1}{\sigma Y_i^2 + (\sigma X_i \times ym/dm)^2}$$

5.1 Initial Estimates of the parameters ym, dm, cm

Initial estimates of parameters to be fitted are:
$ym = Ymax$
$dm = (Xmax - Xmin)/2$
$cm = (Xmax + Xmin)/2$
where $Ymax$, $Xmax$ and $Xmin$, are the maximum and minimum values of Y_i or X_i.

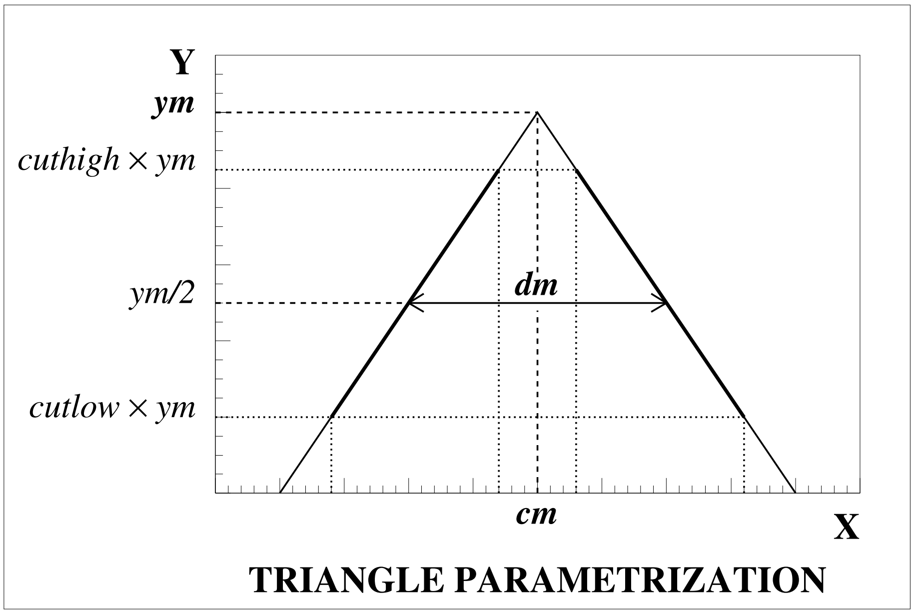


Figure 4: Triangle parametrization used in least squares fit

5.2 Initial Selection of Data

As mentioned in introduction, since some tails are generally present (Fig. 1-a), it is highly desirable to limit the fitting procedure to linear parts of the experimental mass peaks. The initial selection keeps (X_i,Y_i) couples for which

$$X_{mi} \leq X_i \leq X_{ma}$$

where X_{mi}, X_{ma} are the minimum and maximum values of X_i for which : $Y_i \geq$ $cutlow \times ym$ $cutlow$ is fixed by the user in order to ignore the tails (Fig. 1, 4).

5.3 Least Squares Fit

The function to be fitted is linearized in the neighbouring of estimates :

$$Y_i = ym\left(1 - \frac{|X_i - cm|}{dm}\right) + \frac{\partial f}{\partial ym}P(1) + \frac{\partial f}{\partial dm}P(2) + \frac{\partial f}{\partial cm}P(3) \tag{8}$$

Defining :

$$Y_{0i} = Y_i - ym\left(1 - \frac{|X_i - cm|}{dm}\right) \tag{9}$$

one gets $P(1,2,3)$ and their uncertainties $\sigma P(1,2,3)$ by a standard least squares fit :

$$Y_{0i} = \left(1 - \frac{|X_i - cm|}{dm}\right)P(1) + \frac{ym|X_i - cm|}{dm^2}P(2) + \varepsilon\frac{ym}{dm}P(3) \tag{10}$$

with $\varepsilon = \pm 1$, its sign being that of $X_i - cm$.
New estimates are thus obtained :

$$ym = ym + P(1)$$
$$dm = dm + P(2)$$
$$cm = cm + P(3)$$

While performing the least squares fit, various matrix inversion codes were tested either based on i) Cholesky's method, or on ii) triangular factorization with row interchanges. Finally, the "DFINV" CERN Library code using ii) was adopted. The method is powerful and this code has the advantage to give diagnoses in case of problems, without inducing fatal errors.

5.4 Iterating Least Squares Fit

New values of Y_{0i} are deduced fom the new estimates of ym, dm, cm.
$P(1,2,3)$ are recalculated as in § 5.3.
Once the iterative phase is started, σY_i is derived from the calculated value of Y_i rather than from the experimental one :

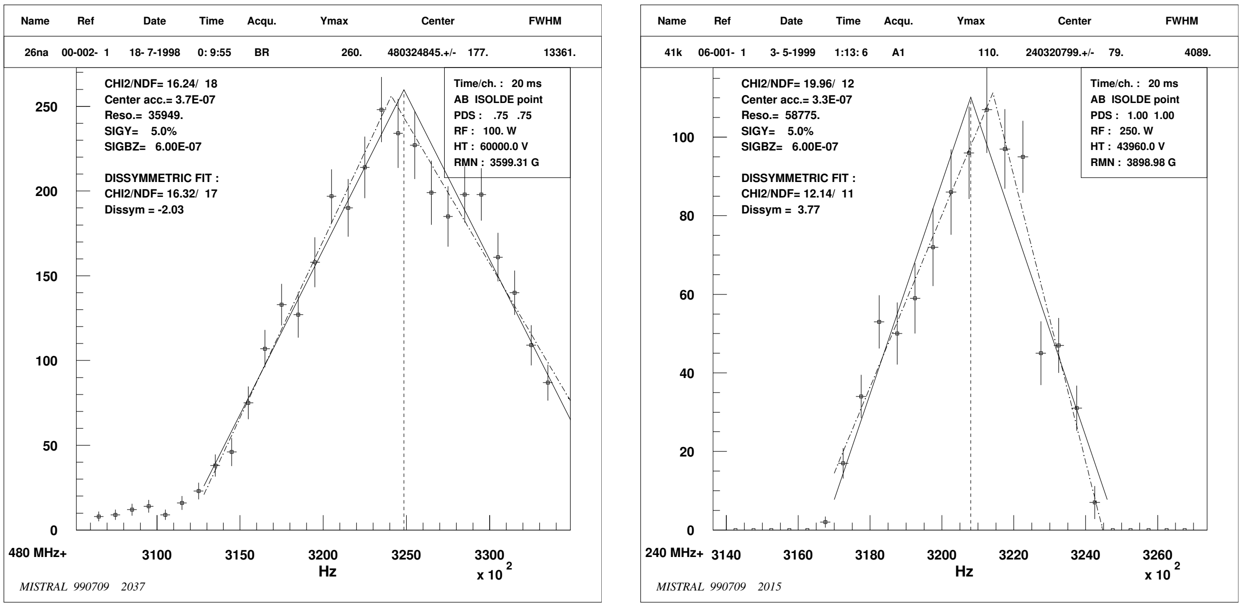
$$\frac{\sigma Y_i}{Y_i} = \sqrt{\frac{1}{Y_i} + SIGY^2}$$

This avoids to attribute excessive weights to anomalously low counting rates. It also avoids systematic underestimations of ym, especially when $SIGY \neq 0$.
Actually, if the new estimate of cm does not affect the initial sharing of X_i values around cm, the fitting procedure is completed : new estimates will stay unchanged. If not, the fitting procedure must be iterated. The decision to continue iterative phase is based on the stability of χ^2. In order to take care of a possible oscillation, the new χ^2 value is compared to the 2 previous ones. If both differences are larger than $\chi^2/1000$, the iteration goes on. The number of iterations is limited to 50, but is usually around 5.

5.5 Iterating Data Selection

When the least squares fit iterative phase is achieved, an improved selection of data is performed, which keeps (X_i,Y_i) couples such that
$cm - dm(1 - cutlow) \leq X_i \leq cm - dm(1 - cuthigh)$
or
$cm + dm(1 - cuthigh) \leq X_i \leq cm + dm(1 - cutlow)$
cuthigh may be fixed by the user in order to eliminate an unwanted flat top (Fig. 1-*a*, 4).
In order to optimize *cutlow* and *cuthigh*, the user has to find the best compromise : on one side, too stringent conditions may heavily affect statistics ; on the other side, too lax ones will produce a large χ^2.
• *cutlow* stands normally below 25%, depending on the PDS aperture (Fig. 1).
• *cuthigh* is only needed in case of a nasty beam trajectory. Even in such a case, it may generally be forgotten because the points very near the center of symmetry have a relatively small weight.
If the new selection is different from the previous one, the fitting procedure is started again. The last fitted values of ym, dm, cm are used as initial estimates and the iterative phase is pursued as described in § 5.3 and 5.4. Usually, only 2 or 3 successive selections are needed.

The fit convergence is obviously faster when the experimental mass peak is well centered. Nevertheless these successive selections allow a good fit, even for peaks where a part is missing (Fig. 5-a). Whereas this process usually converges towards a unique selection, it sometimes oscillates between 2 ones. This is taken into account by limiting at 7 the number of selections and printing both solutions when 7 is reached.



(a) (b)

Figure 5: Examples of fits performed in bad conditions : (a) case of a truncated mass peak ; (b) case of a dissymmetric peak

5.6 Dissymmetric Fit

Once the symmetric fitting procedure is completed, a dissymmetric fit is performed on the last selected data (Fig. 1, 5). Initial estimates are the ym, dm, cm values adopted in the symmetric fit. The fitting function is :

- for $\left\{ \text{or} \begin{array}{l} X_i \leq cm - dmleft \\ X_i \geq cm + dmright \end{array} \right.$ $\qquad Y_i \pm \sigma Y_i = 0 \qquad (11)$
- for $cm - dmleft \leq X_i \leq cm$ $\qquad Y_i \pm \sigma Y_i = ym \left(1 - \dfrac{cm - X_i \pm \sigma X_i}{dmleft} \right) \qquad (12)$
- for $cm \leq X_i \leq cm + dmright$ $\qquad Y_i \pm \sigma Y_i = ym \left(1 - \dfrac{X_i \pm \sigma X_i - cm}{dmright} \right) \qquad (13)$

The fitting procedure and iterative phase are quite similar to those described in § 5.3 and 5.4, but there are 4 parameters $P(1, 2, 3, 4)$ instead of 3 to be fitted. An evaluator of this dissymmetry(Fig. 1, 5) is then calculated which is the difference between right and left slopes divided by the uncertainty on this difference. This evaluator is one of the criteria which allow to appreciate the quality of the settings. It must be lower than 2.

6 Harmonic Ratio Determination

In order to determine $\mathcal{H}$ (which is a half-integer) without any ambiguity, it is necessary to get an uncertainty $\sigma\mathcal{H} \leq .2$.

6.1 Direct measurement

During MISTRAL first measurements, many harmonic ratios $\mathcal{H}$ were carefully determined by recording mass peaks for the same ions at 2 different frequencies corresponding to the harmonics $\mathcal{H}$ and $(\mathcal{H} + i)$:

$$\mathcal{H} = \frac{i \times f_{\mathcal{H}}}{f_{\mathcal{H}+i} - f_{\mathcal{H}}} \tag{14}$$

$$\sigma\mathcal{H} = \sqrt{2}\frac{\mathcal{H}^2}{i}\frac{\sigma f}{f} \tag{15}$$

It is worth noting that these measurements require a very high accuracy : *e.g.*, for $\mathcal{H}\simeq 2000$ and $i = 1$, $\sigma\mathcal{H} \leq .2$ requires $\sigma f/f \leq 4.10^{-8}$. However the possibility to use $i\simeq 6$–8 instead of 1 was very helpful.

6.2 Field Calibration

Later on, these $\mathcal{H}$ determinations allowed to calibrate the magnetic field mesurement which is performed by Nuclear Magnetic Resonance, so that $\mathcal{H}$ is now obtained through a very simple procedure :

$$\mathcal{H} = \frac{f}{f_c} = f \times \frac{2\pi(m - m_e + V)}{X_{cal}Bc^2} \tag{16}$$

$$\sigma\mathcal{H} = \mathcal{H}\sqrt{\left(\frac{\sigma f}{f}\right)^2 + \left(\frac{\sigma B}{B}\right)^2} \tag{17}$$

$m - m_e + V$ is the mass of the ion with kinetic energy V.
B is the value measured by RMN.
X_{cal} is the calibration parameter which introduces a correction of the order of 10^{-4} due to the fact that the RMN gauge may only be positioned on the external side of the magnetic field.
The same typical value $\mathcal{H}\sim 2000$ requires now a $\sim 10^{-4}$ accuracy for f and B. For f, such an accuracy is trivial, and for B, it is easily achieved by the RMN measurement. $\mathcal{H}$ is then rounded to the nearest half-integer.

7 Some other tools

Some other tools have been developed to help to prepare and to drive the experiment during data taking periods.

7.1 Mass Table comparisons : *DRAW_MASS, CALC_MASS*

Since the analysis is linked with the Atomic Mass Evaluation —AME— [3], the measured values are compared to the adjusted data from AME, and the subsequent calibration factors are calculated by the code.

7.2 B Resonance frequency prediction : *CALC_FREQB*

Using the measured resonance frequency of A and the AME estimation of B mass, it is possible to calculate the resonance frequencies of B which are the nearest from those of A.

7.3 Montecarlo Simulations : *SIMU*

The MISTRAL code provides montecarlo simulations of triangular peaks.
ym, dm, cm, $SIGY$, $SIGB$, ... are chosen by the user. The simulation uses Poisson distributions in order to be able to test what occurs for low counting rates. Such simulations were first performed to test the validity of the fitting procedure. They also allowed to study the final accuracy according to the different parameters. In particular, the possibility to group together a large number of measures with counting rates as low as 0.1 count/cycle at top of the peak, was first tested in the simulation. This possibility has been very useful later on (Fig. 3). They also allow many other studies such as the influence of drifts.

References

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[2] A. Coc, R. Le Gac, M. de Saint Simon, C.Thibault and F. Touchard, Nucl. Instr. Meth. **A271** (1988) 512

[3] ftp://csnftp.in2p3.fr/pub/AMDC/masstables/mass_rmd.mas95