



# Data analysis for neutron spectrometry with liquid scintillators: applications to fusion diagnostics

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In collaboration with  
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M. Reginatto

Data analysis for neutron spectrometry with liquid  
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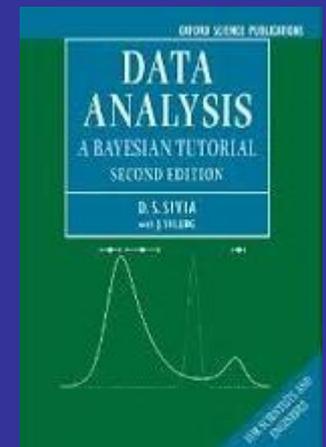
# A quote...

## Part II

### Advanced topics

*'Data analysis is simply a dialogue with the data.'*

— Stephen F. Gull, Cambridge 1994



# Contents of the talk

- Neutron spectrometry with liquid scintillation detectors
- Resolving power and superresolution of spectrometers
  - Some useful concepts from information theory
  - Backus-Gilbert representation and resolving power
  - Kozarev's approach and Shannon's superresolution limit
  - Theoretical superresolution limit vs. experimental results (PTB)
- Analysis of spectrometric measurements at JET
  - MaxEnt deconvolution
  - Bayesian parameter estimation
- Conclusions

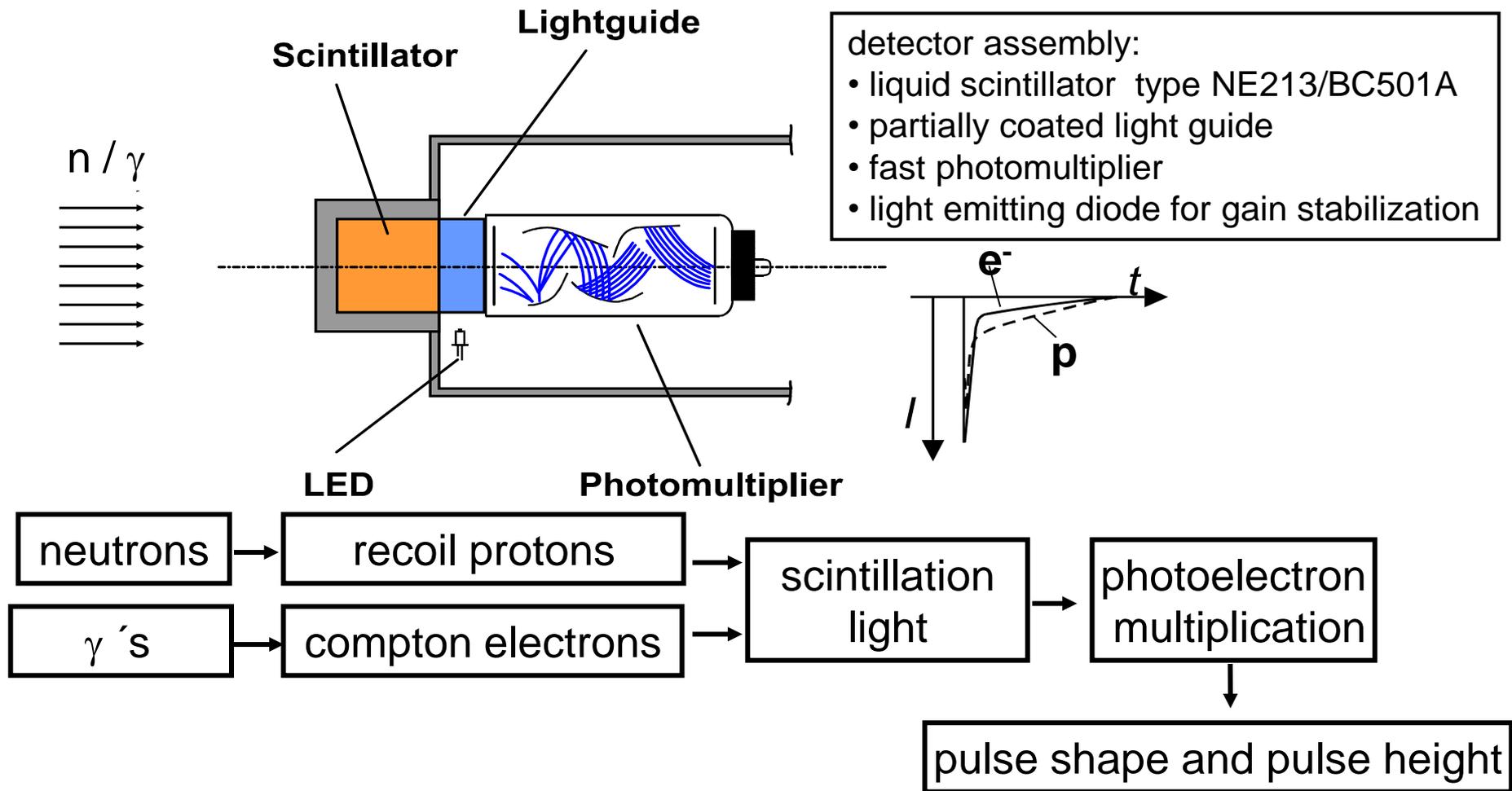
# Neutron spectrometry with liquid scintillation detectors

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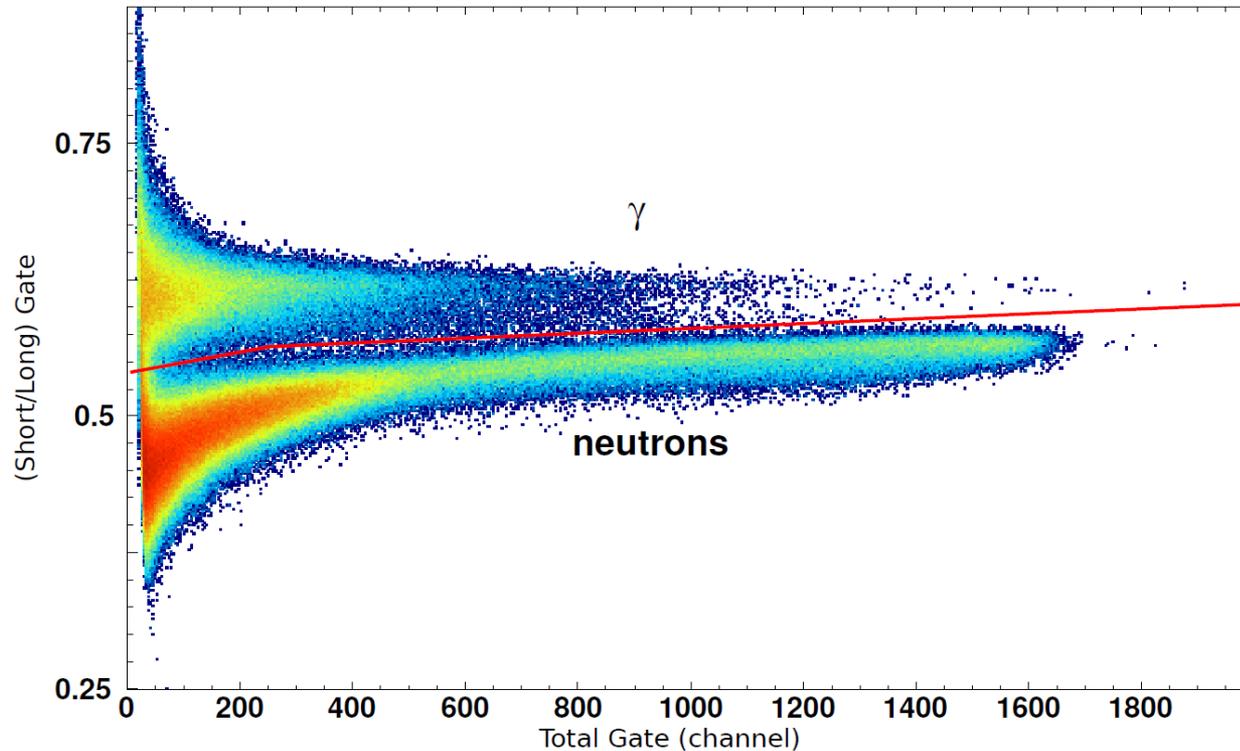
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# Organic liquid scintillator (NE-213)

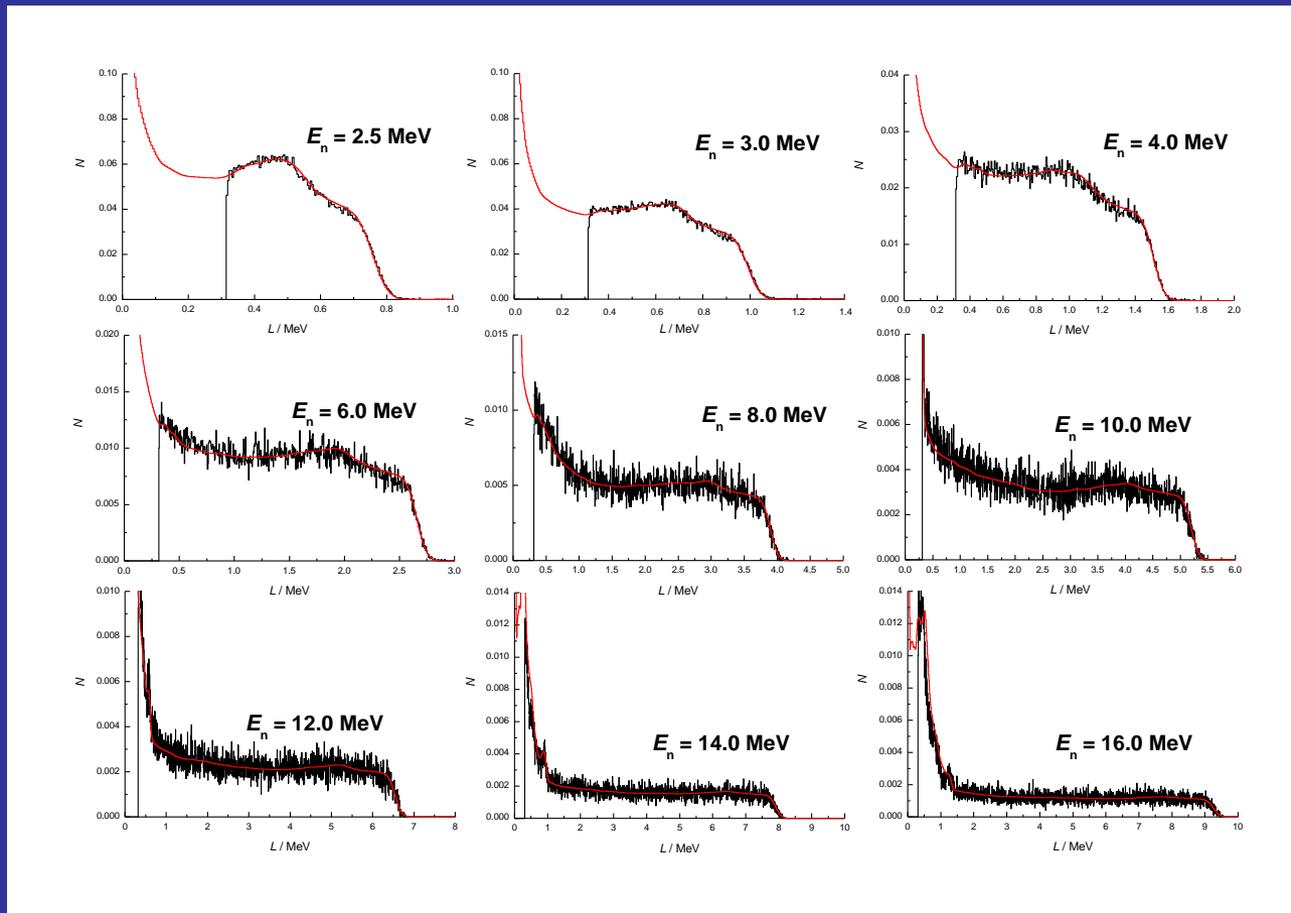


# Pulse shape (n- $\gamma$ ) discrimination



**Figure 7.** PSD identification plot. The line drawn in red separates  $\gamma$  events (top) from neutron events (bottom). For this example, data from measurements made in the 12 MeV monoenergetic neutron field were used.

# PHS for neutrons of different energies (adjusted simulations and measurements)



# PHS and neutron spectra (JET)

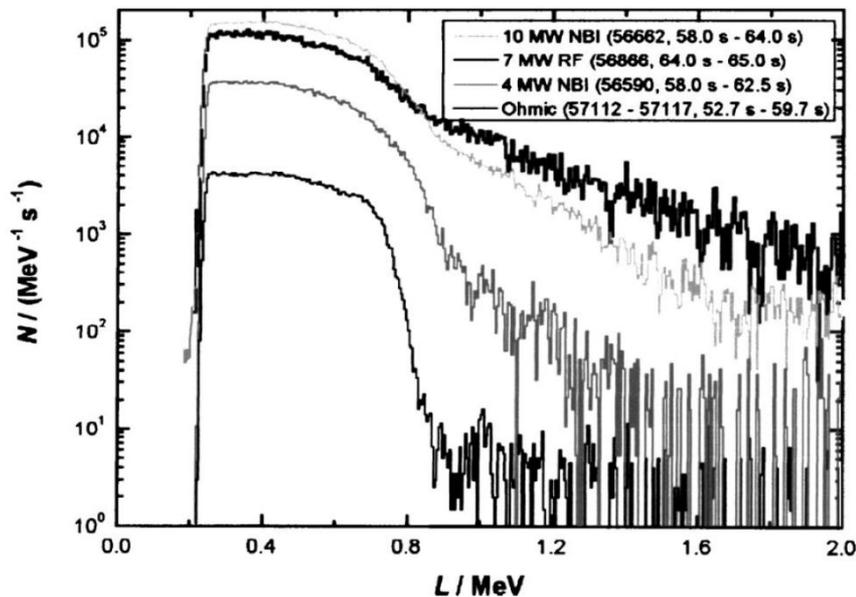


FIG. 3. PHS measured under different plasma scenarios,  $L$  = light output.

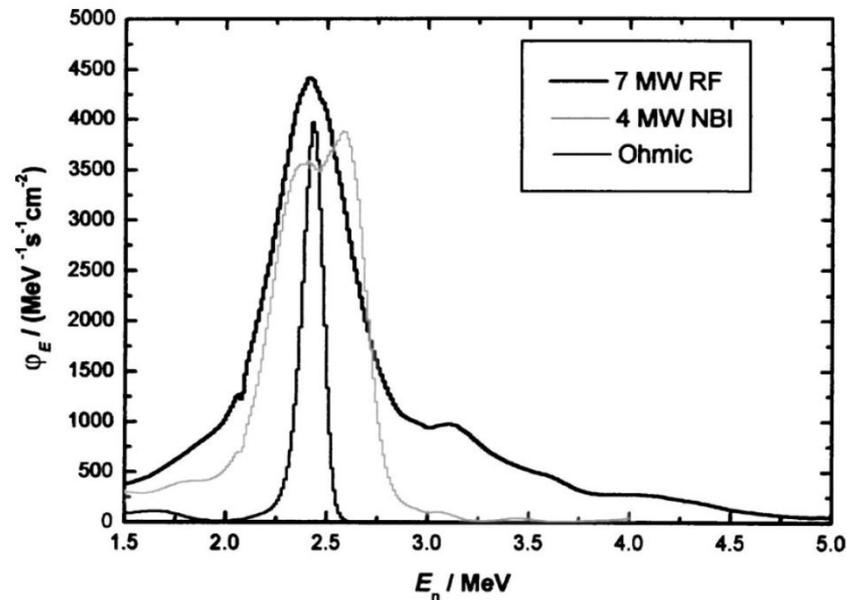


FIG. 4. Unfolded spectra for some of the PHS shown in Fig. 3.

[A. Zimbal et. al., *A compact NE213 neutron spectrometer with high energy resolution for fusion applications*, 15th Topical Conference on High-Temperature Plasma Diagnostics, San Diego, April, 2004]

# PHS and neutron spectra (JET)

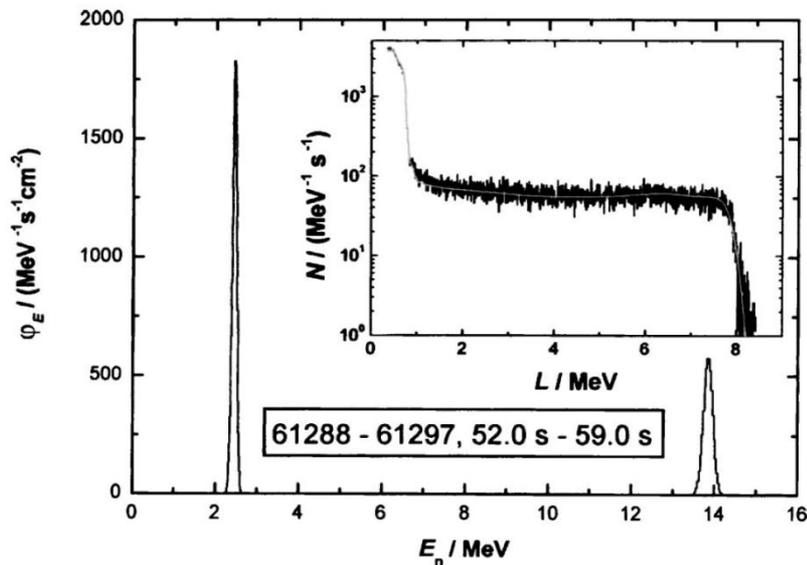


FIG. 5. Neutron spectrum produced by the reactions  $d+d \rightarrow {}^3\text{He}+n$  and  $d+t \rightarrow \alpha+n$  (TTE with pure Ohmic heating). The inset shows the measured PHS (histogram) as well as the PHS that results from folding the neutron spectrum with the response functions (line).

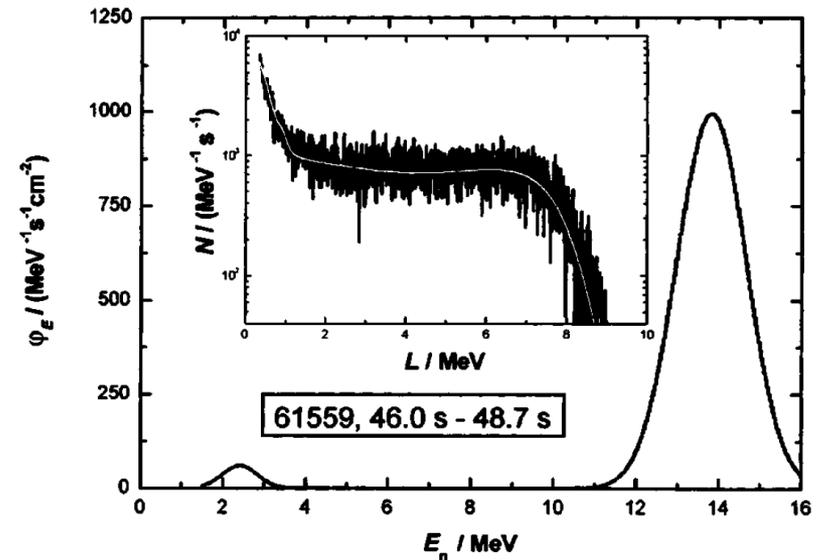


FIG. 6. Neutron spectrum produced by the reactions  $d+d \rightarrow {}^3\text{He}+n$  and  $d+t \rightarrow \alpha+n$  (ICRH fundamental T heating). The inset shows the measured PHS (histogram) as well as the PHS that results from folding the neutron spectrum with the response functions (line).

[A. Zimbal et. al., *A compact NE213 neutron spectrometer with high energy resolution for fusion applications*, 15th Topical Conference on High-Temperature Plasma Diagnostics, San Diego, April, 2004]

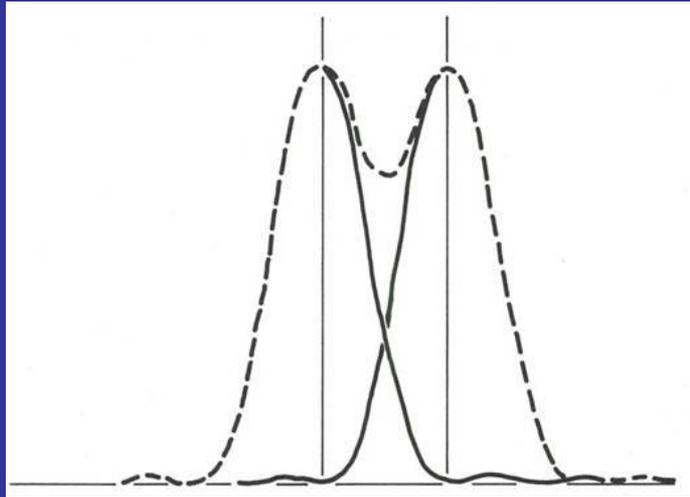
# Resolution

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# Resolution in optics: Rayleigh criterion



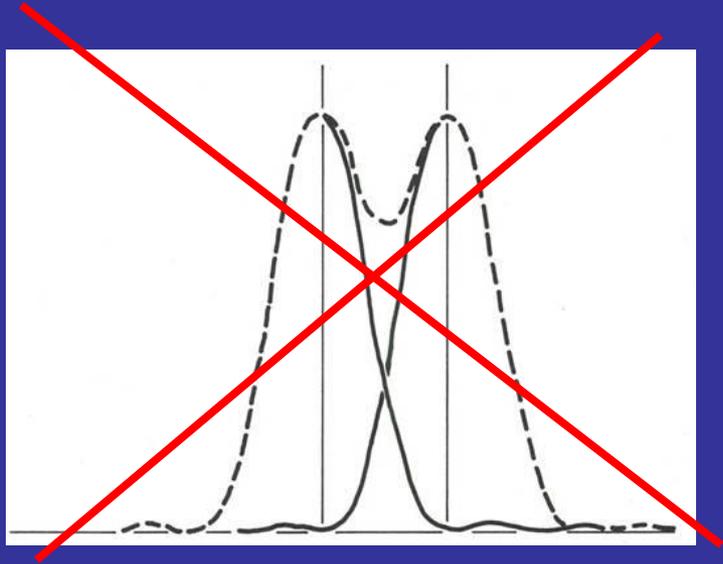
“Resolution” of an optical instrument  $\sim$  Point Spread Function (PSF).

Has been generalized and applied to other measuring devices outside of optics.

The Rayleigh criterion does not take into account the improvement achievable with algorithms for data analysis.

The ability to achieve resolution *beyond* the Rayleigh criterion is known as superresolution.

# Resolution for spectrometers used in radiation detection



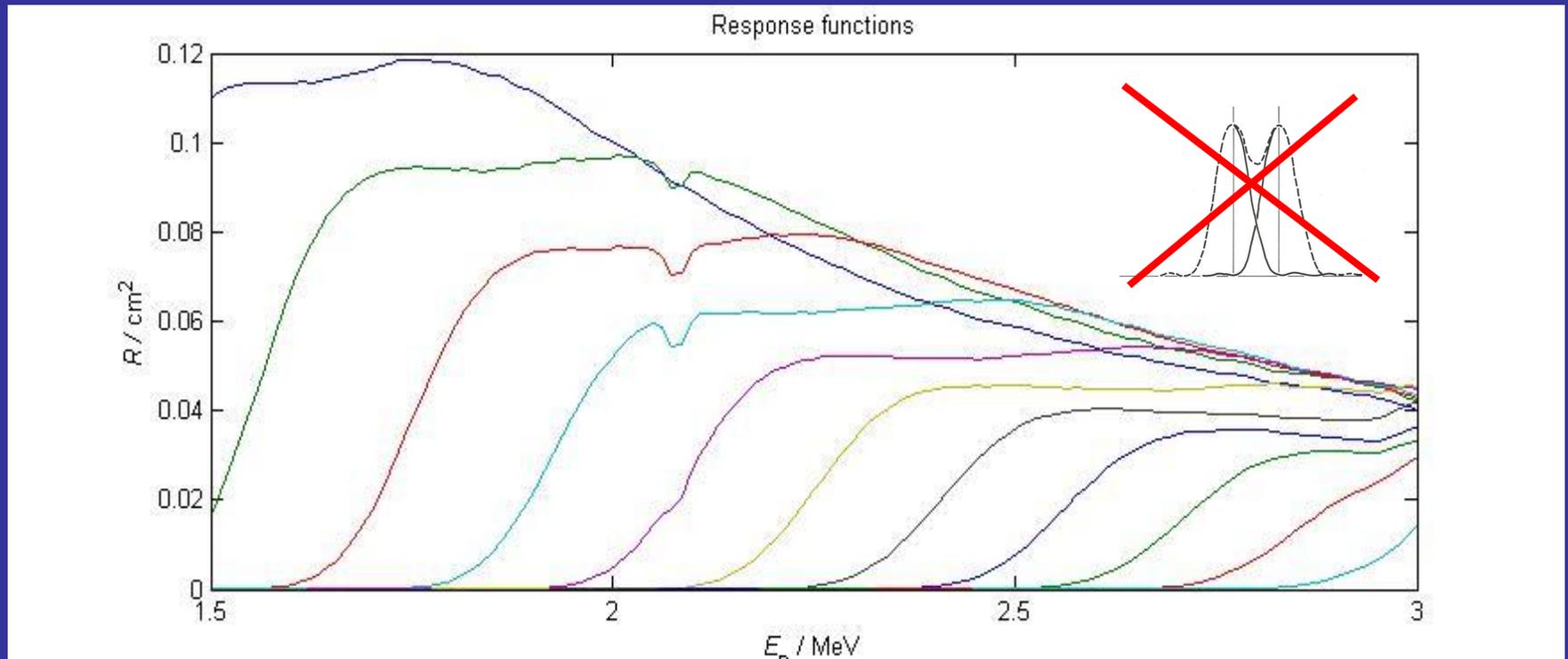
The Rayleigh criterion does *not* work for most spectrometers used in radiation detection.

A different approach is required.

The response functions (which correspond to the PSF of optics) are irregular in shape, overlap, and are not localized.

The data analysis typically requires deconvolution, and the resolution depends strongly on the data analysis.

# Spectrometer response functions for a few selected channels



The responses are irregular in shape, overlap, and they are *not* localized: ***how do you define resolution?***

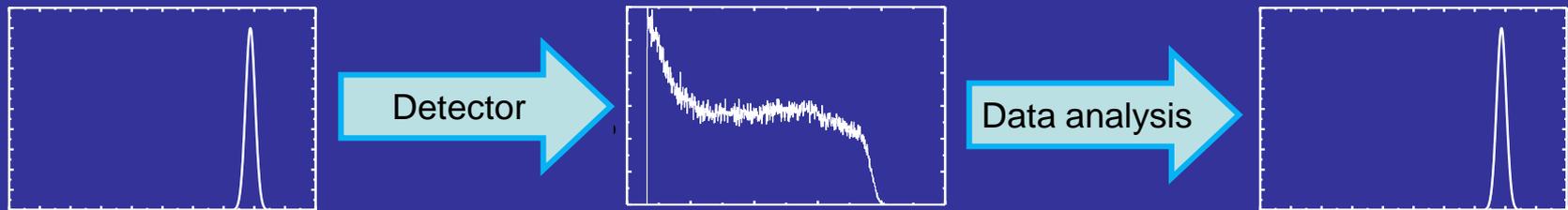
# Some useful concepts from information theory

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# Another view of a measurement



## measurement:

spectrum

*detector*

measurement

*data analysis*

spectrum

## communication system (Shannon, 1948):

message

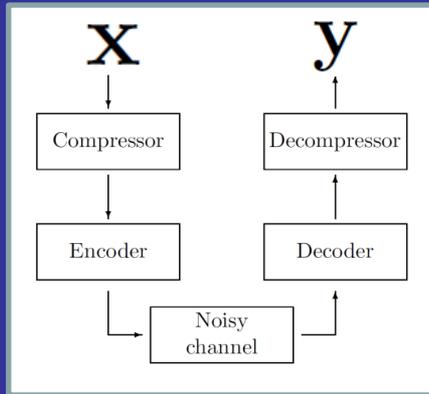
*transmitter*

(noisy) signal

*receiver*

message

# Some concepts from information theory



Joint entropy of X and Y:

Conditional entropy of X given Y:

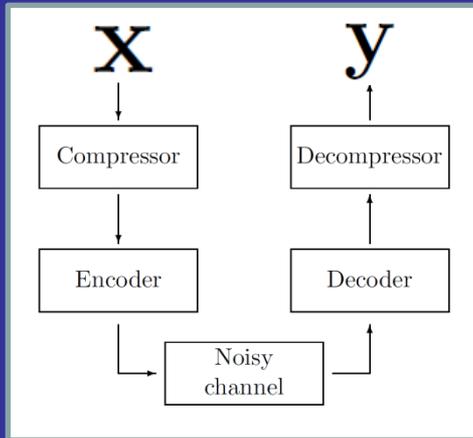
Mutual information between X and Y:

Capacity of a channel Q:

$$H(X, Y) = \sum_{x, y \in \mathcal{A}_X \mathcal{A}_Y} P(x, y) \frac{1}{\log P(x, y)}$$
$$H(X|Y) = \sum_{x, y \in \mathcal{A}_X \mathcal{A}_Y} P(x, y) \frac{1}{\log P(x|y)}$$
$$I(X; Y) = H(X) - H(X|Y)$$
$$C(Q) = \max_{\mathcal{P}_X} I(X; Y)$$

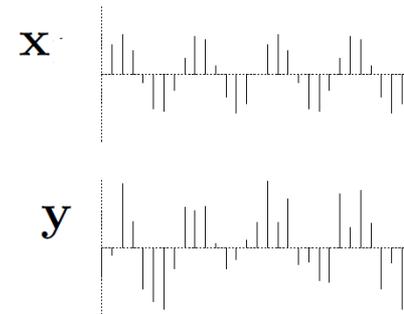
[David J. C. MacKay, *Information Theory, Inference and Learning Algorithms*, Cambridge University Press]

# Shannon's superresolution limit



Capacity of Gaussian Channel:  
(Shannon)

Shannon's superresolution limit:  
(Kozarev)



$$C = \frac{1}{2} \log \left( 1 + \frac{P_s}{P_n} \right)$$

$$SR = \frac{1}{3} \log \left( 1 + \frac{P_s}{P_n} \right)$$

$$\frac{P_s}{P_n} = \text{signal-to-noise ratio}$$

# Backus-Gilbert representation and resolving power

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# The Backus-Gilbert representation

Backus and Gilbert developed a clever way of mapping arbitrary response functions to response functions that are localized -- when that is possible!

[G. E. Backus and F. J. Gilbert, Geophys. J. R. Astron. Soc. 13, 247 (1967) and 16, 169 (1968)]

The “Backus-Gilbert” representation:

$$R_j^{BG}(E) = \sum_{k=1}^n a_{jk} R_k(E) , \quad N_j^{BG} = \sum_{k=1}^n a_{jk} N_k$$

The width of the response functions in the Backus-Gilbert representation defines the resolving power.

# The approach of Backus and Gilbert

$$A(E_i, E) = \sum_{k=1}^n a_k(E_i) R_k(E)$$

Define averaging kernels

---

$$I[A] = \int dE J(E_i, E) [A(E_i, E)]^2$$

Minimize  $I$  to find the  $a_k$

$$J(E_i, E) \sim (E - E_i)^2$$

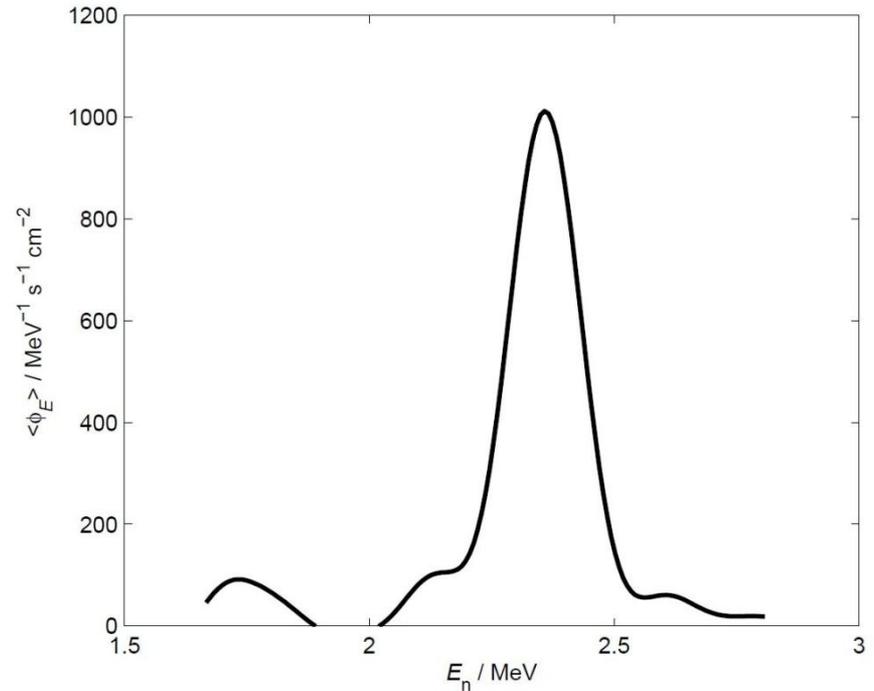
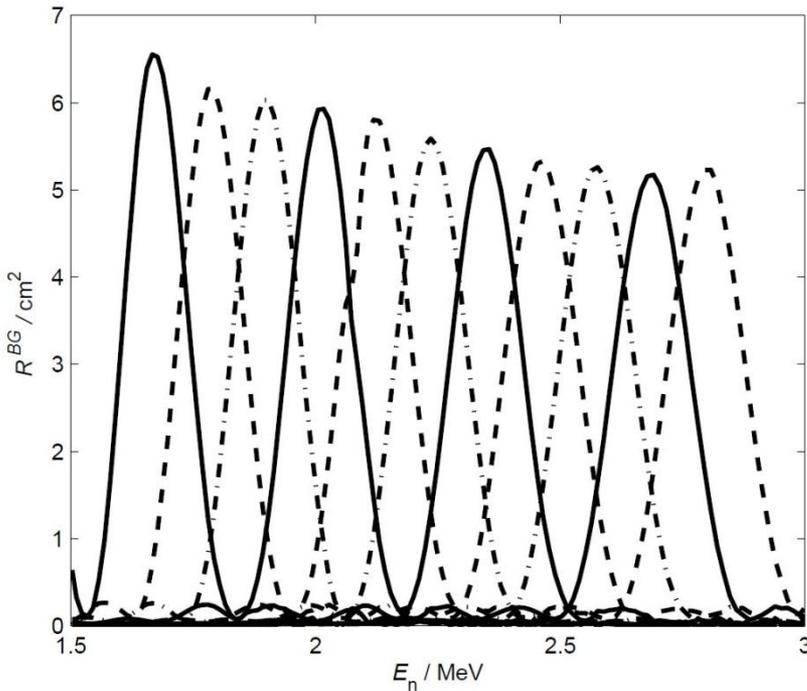
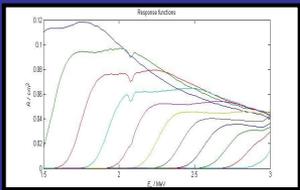
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$$\sum_{j=1}^n \int dE [J(E_i, E) R_k(E) R_j(E)] a_j(E_i) + \lambda \int dE R_k(E) = 0$$

$$\sum_{j=1}^n \int dE R_j(E) a_j(E_i) = 1$$

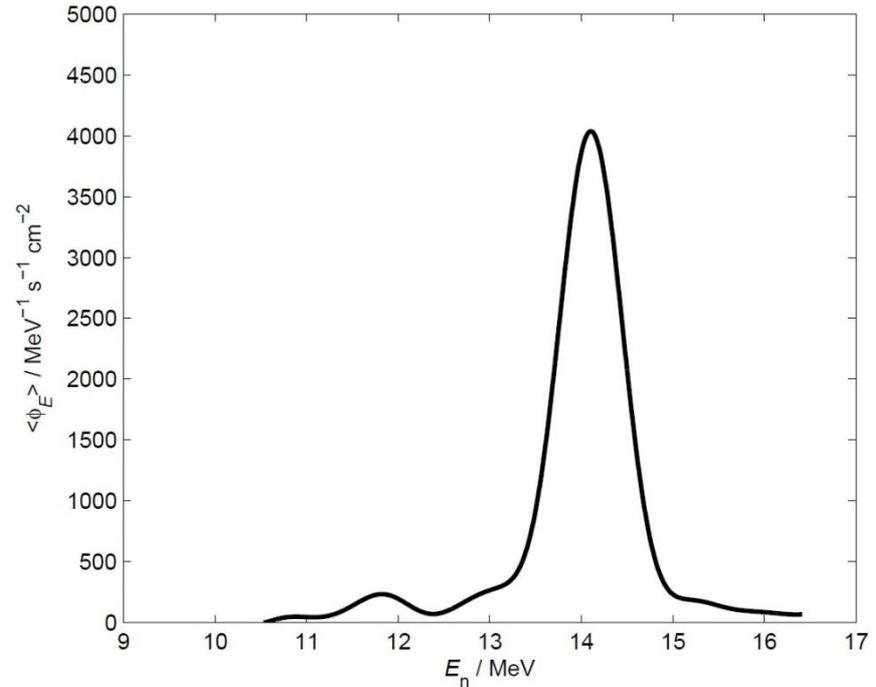
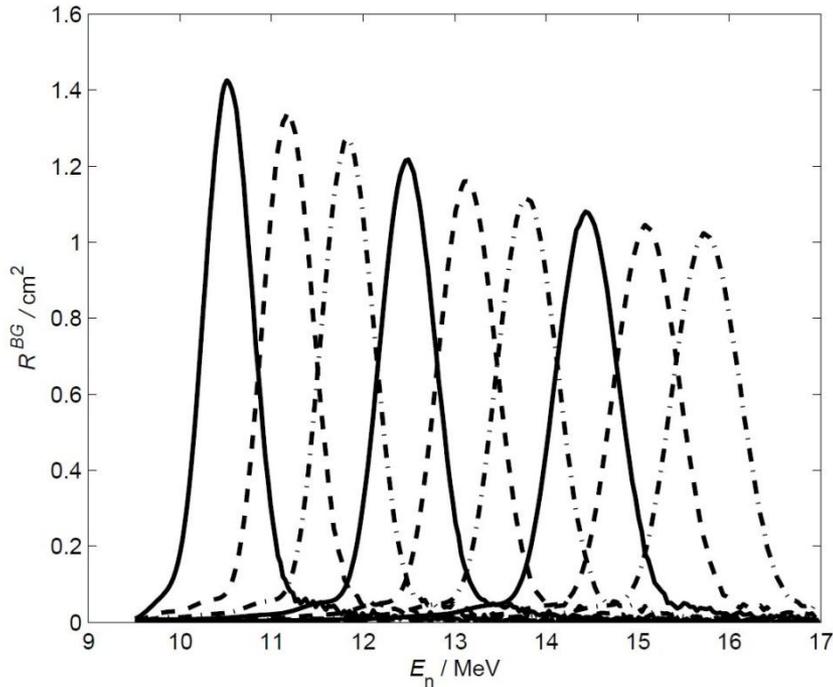
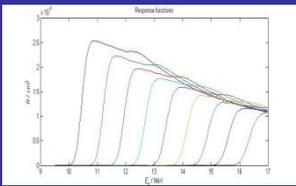
Linear equations for the  $a_k$ !

# Backus-Gilbert representation



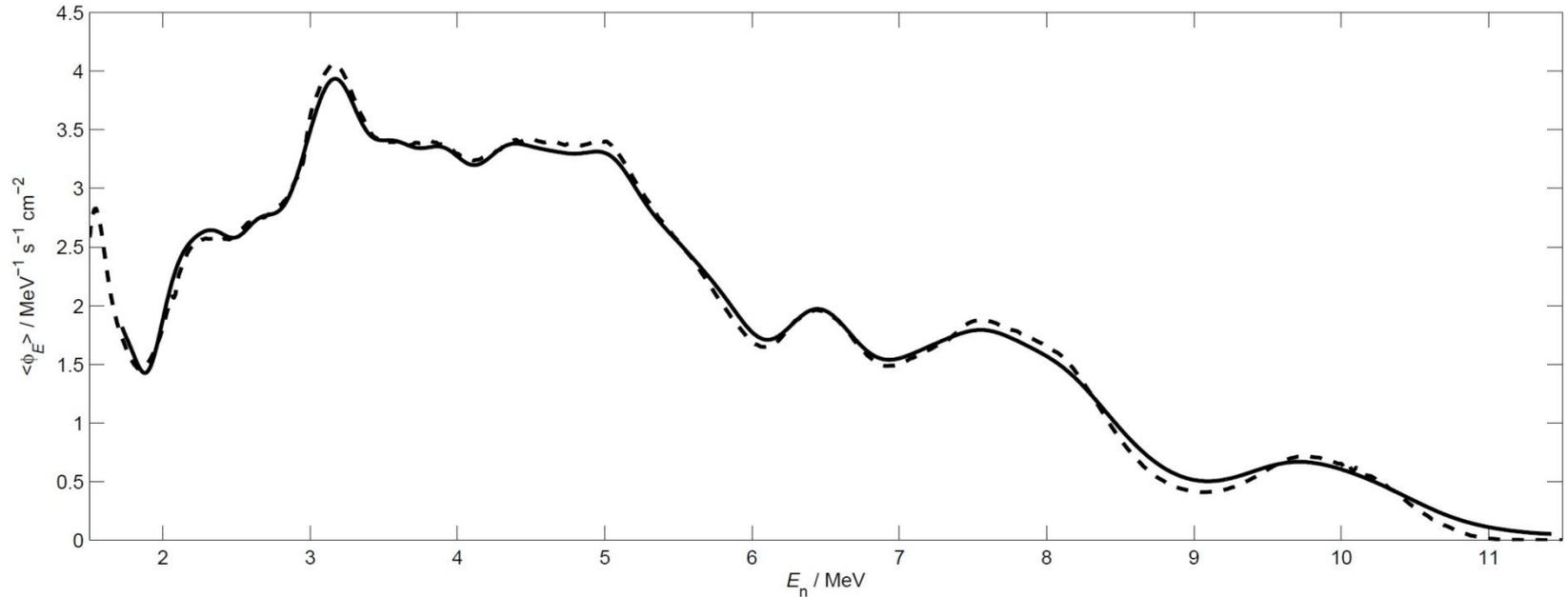
**FIGURE 2.** Response functions  $R_j^{BG}(E)$  for energies  $E_n \sim 2.5$  MeV (left) and PHS (right), both in the Backus-Gilbert representation. For clarity, only a few of the 143  $R_j^{BG}(E)$  that were calculated are shown.

# Backus-Gilbert representation



**FIGURE 3.** Response functions  $R_j^{BG}(E)$  for energies  $E_n \sim 14$  MeV (left) and PHS (right), both in the Backus-Gilbert representation. For clarity, only a few of the 1022  $R_j^{BG}(E)$  that were calculated are shown.

# Backus-Gilbert representation: more results



**FIGURE 4.** PHS in the Backus-Gilbert representation (solid line) compared to the neutron spectrum derived using maximum entropy deconvolution [10] (dashed line) for an  $^{241}\text{AmBe}(\alpha,n)$  source.

[M. Reginatto and A. Zimbal, *Superresolution of a compact neutron spectrometer*, in *Bayesian Inference and Maximum Entropy Methods in Science and Engineering*, eds. A. Mohammad-Djafari, J.-F. Bercher, and P. Bessiere, American Institute of Physics (2010)]

# What did we learn?

- The “Backus-Gilbert” representation is very useful!
- The resolving power of the NE213 spectrometer is about 0.18 MeV (or better) at  $\sim 2.5$  MeV, and about 0.93 MeV (or better) at  $\sim 14$  MeV.
- The response functions in the Backus-Gilbert representation are localized; therefore, the PHS in the Backus-Gilbert representation looks like the neutron spectrum.
- The response functions in the Backus-Gilbert are approximately Gaussian in shape.

# Kozarev's approach and Shannon's superresolution limit

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# Proof of superresolution

Maximum entropy unfolding, compared to calculation.

Resolving power  $\sim 0.18$  MeV

FWHM of peak  $\sim 0.08$  MeV

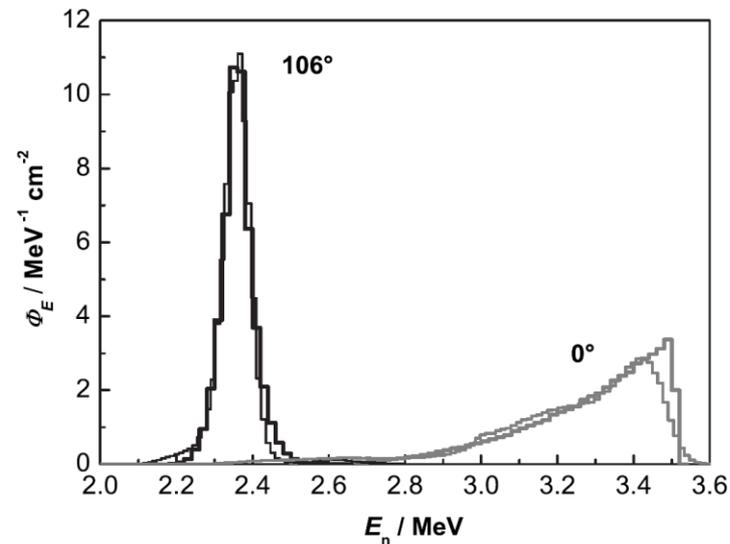


FIG. 4. Calculated (thick line) and measured (thin line) energy distribution for neutrons using the  $d+d \rightarrow {}^3\text{He}+n$  reaction at different positions of the detector (neutron emission angles of  $106^\circ$  and  $0^\circ$  relative to the incoming deuteron beam). The calculations have been normalized to match the total fluence of the measurements.

Inverse Problems **6** (1990) 55–76. Printed in the UK

## Shannon's superresolution limit for signal recovery†

E L Kosarev

Institute for Physical Problems, USSR Academy of Sciences, 117334 Moscow, USSR

Received 3 May 1989, in final form 30 October 1989

Dedicated to Professor C E Shannon on the occasion of the 40th anniversary of his theorem

**Abstract.** It is shown there is an absolute limit for resolution enhancement in comparison with the Rayleigh classic diffraction limit. The maximum value of superresolution which can be obtained in principle is determined by noise and may be computed via the Shannon theorem concerning the maximum information transmission speed through the connecting channel having noise. A restoration algorithm based on the maximum likelihood method which has Shannon's supremum superresolution is described. Numerical tests of this algorithm are presented and results of its application to a nuclear magnetic resonance experiment are shown. The close connection of superresolution power and the uncertainty principle is discussed. Superresolution depends logarithmically on the signal-to-noise ratio.

# Kozarev's paper on superresolution

PROBLEM: To apply Kozarev's result, you need response functions that are translationally invariant.

SOLUTION: Introduce a new representation, the "Gaussian representation" where

$$R_j^G(E) = G(E_j - E) = \sum_{k=1}^n g_{jk} R_k(E)$$

and the width of the Gaussians  $\sim$  resolving power.

# Calculation of the superresolution

Transform the response functions, the signal (data), and the noise (statistics of the data) to the Gaussian representation.

Estimate the power of the signal and the power of the noise.

Calculate the superresolution using

$$SR = \frac{1}{3} \log \left( 1 + \frac{P_s}{P_n} \right)$$

$P_n$  and  $P_s$  are the power of the signal and of the noise

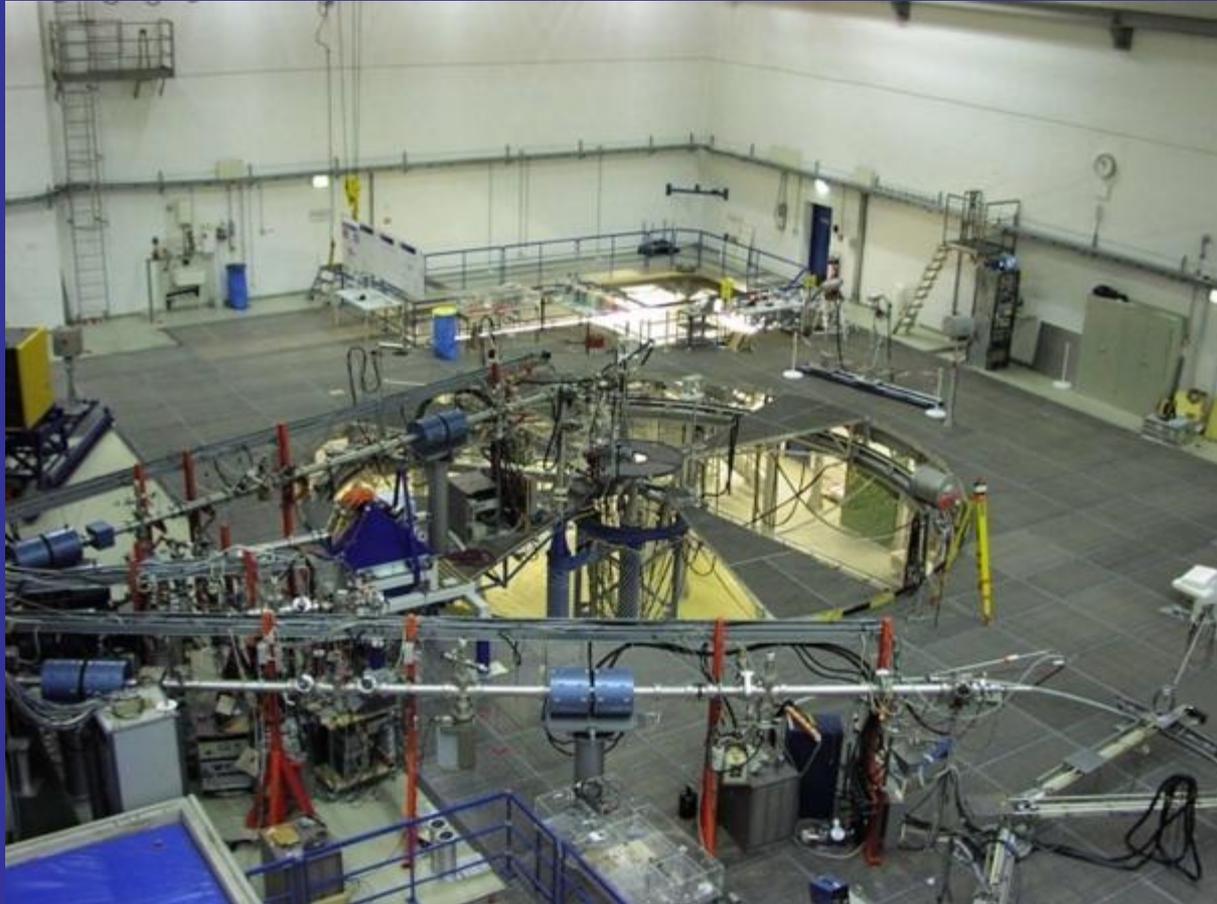
# Theoretical superresolution limit vs. experimental results

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# PTB accelerator facility: low scatter hall

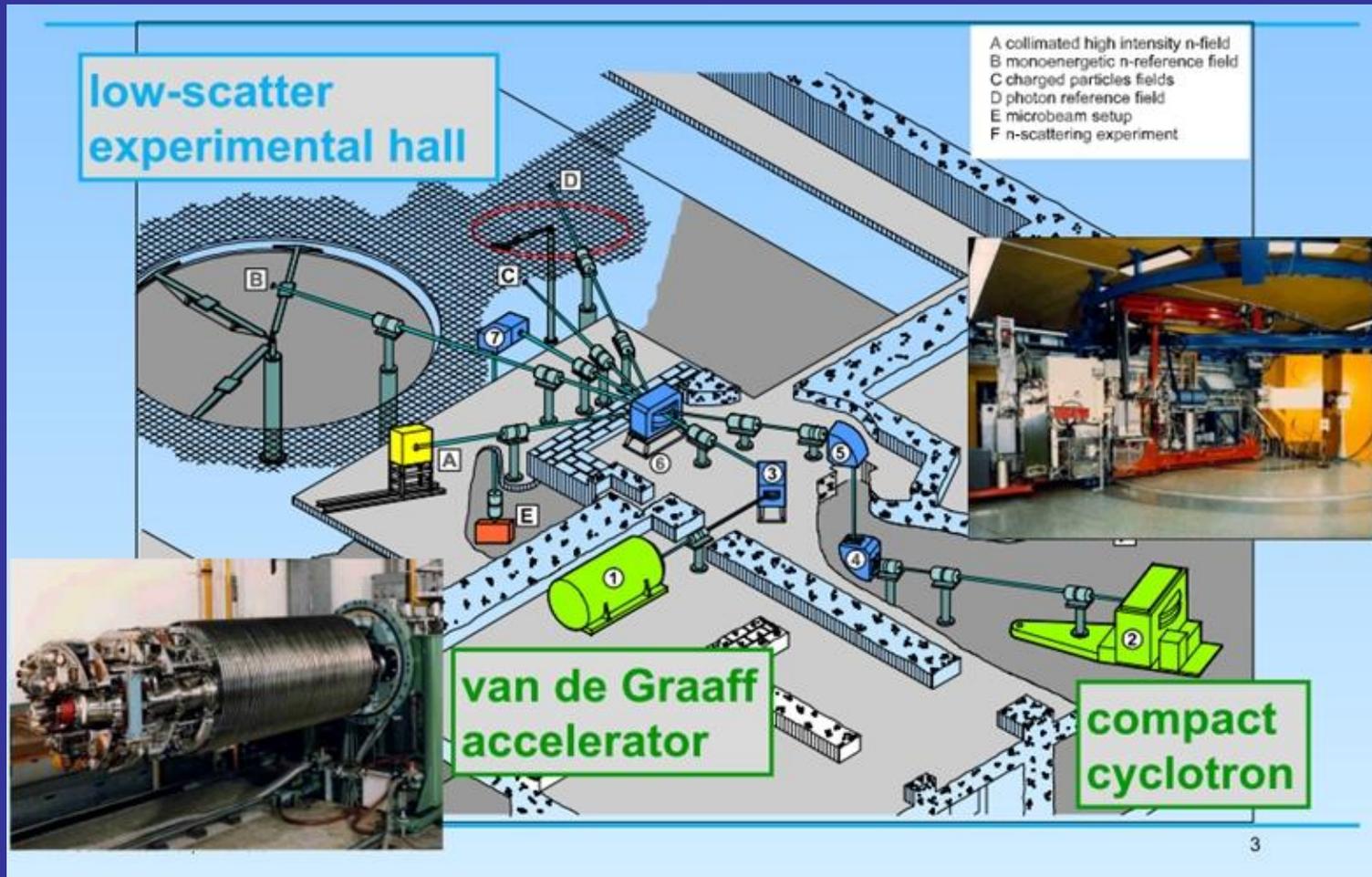


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# PTB accelerator facility: overview

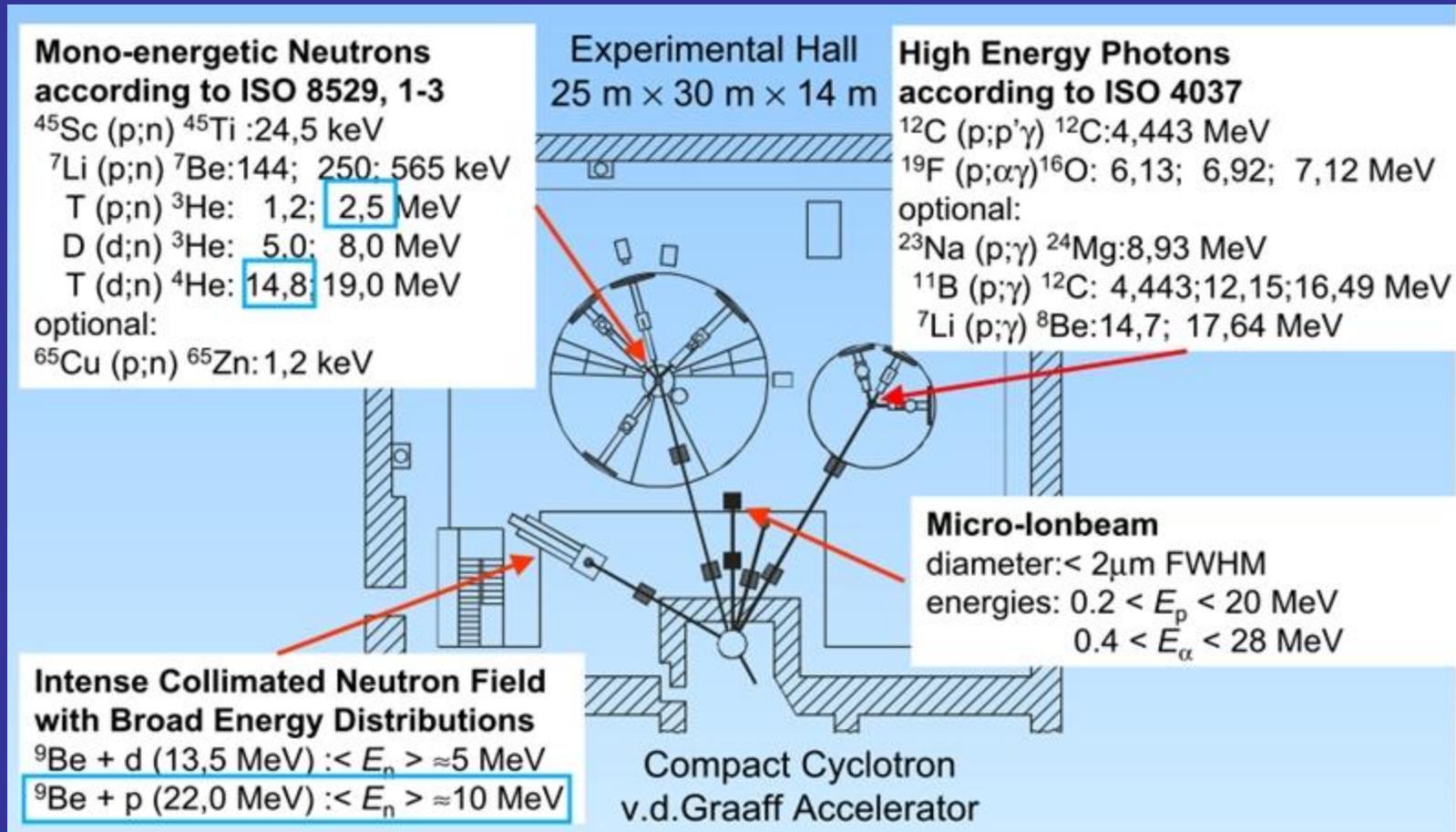


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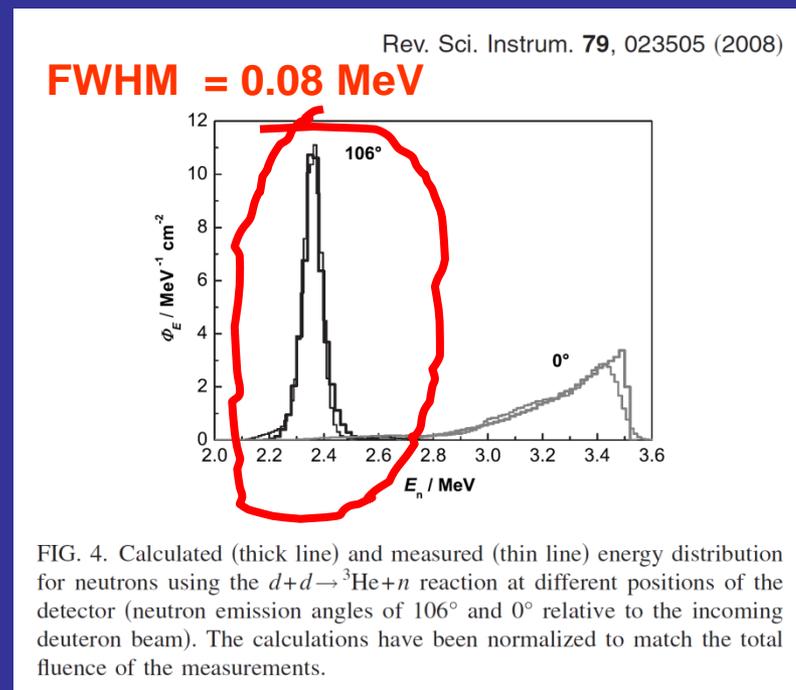


# PTB accelerator facility: radiation fields



# Superresolution for NE213

FWHM (MeV) EXPERIMENT  (PHS + MaxEnt deconvolution)	FWHM (MeV) THEORY  (superresolution factor )
0.08	0.04
0.111	0.067
0.127	0.080
0.133	0.083



FWHM (experiment) / FWHM (theoretical limit)  $\sim 1.6$ .

# Remarks

The Rayleigh criterion is *not* well suited to describe the resolution of spectrometers used in radiation detection.

The procedure presented here *is* generally applicable:

- (1) Backus-Gilbert representation and resolving power,
- (2) Superresolution limit based on Kozarev's approach.

The superresolution achieved for NE-213 measurements with different signal-to-noise ratios was close to the theoretical limit.

Within 60 % of the theoretical value for the data sets considered in this work.

The method presented here provides a useful estimate of the superresolution that is achievable in practice.

# Analysis of measurements at JET: MaxEnt deconvolution and Bayesian parameter estimation

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# Measurement conditions

- Two shots: 82723 (NBI 21.0 MW) and 82724 (NBI 17.5 MW)

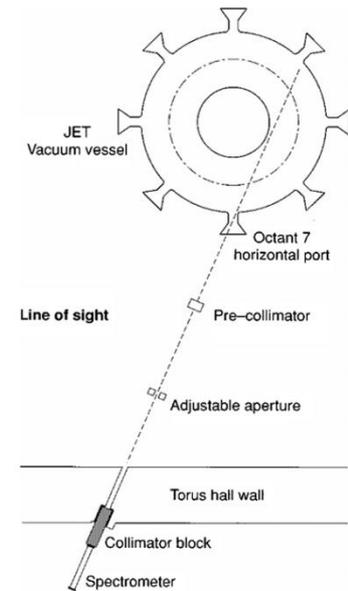
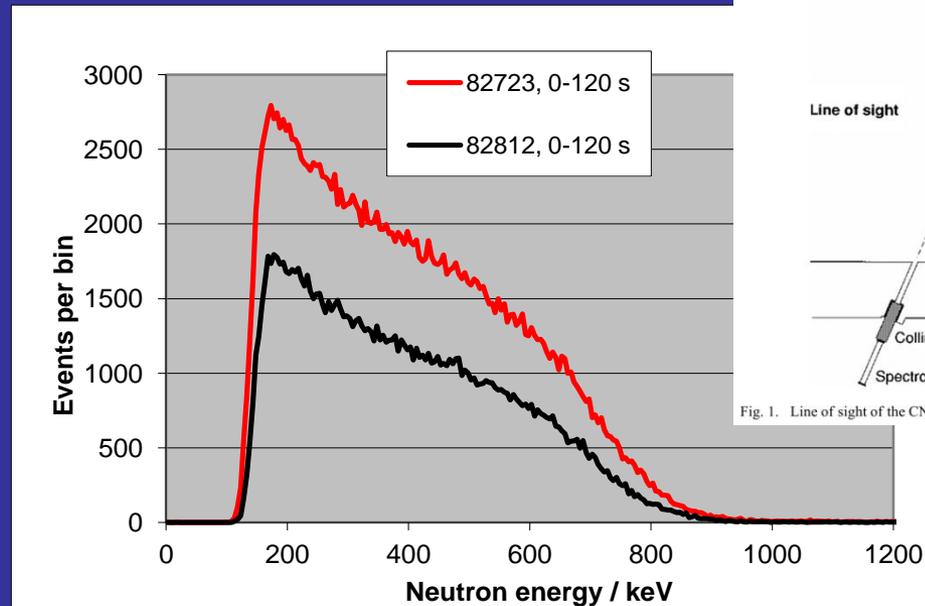
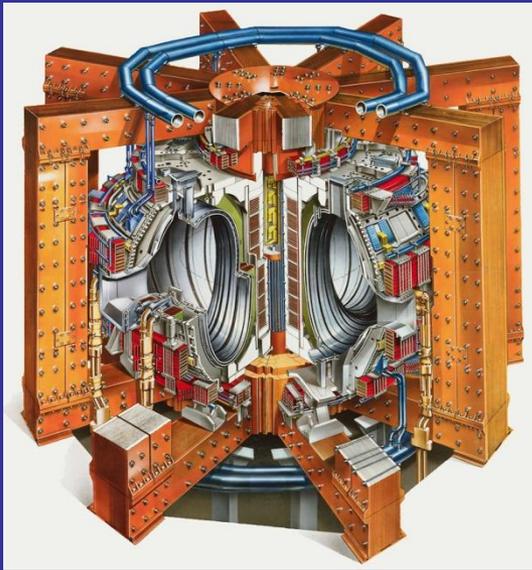


Fig. 1. Line of sight of the CNS as installed at JET (from [1]).

# MaxEnt

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# Why do we apply different methods?

The choice of method depends on the information that is available and the question that is being asked

MaxEnt deconvolution is a non-parametric estimation method – e.g., best estimate of the neutron spectrum with few assumptions?

Bayesian parameter estimation makes use of a parameterized neutron spectrum – e.g., what is the ion temperature?

# Maximum entropy principle (MaxEnt)

1. Start with your best estimate of the spectrum,  $\Phi^{DEF}(E)$
2. From all the spectra that fit the data, choose as solution spectrum  $\Phi(E)$  the one that is “closest” to  $\Phi^{DEF}(E)$
3. “Closest” means: the spectrum  $\Phi(E)$  that maximizes the relative entropy,

$$S = -\int \left\{ \Phi(E) \ln \left( \frac{\Phi(E)}{\Phi^{DEF}(E)} \right) + \Phi^{DEF}(E) - \Phi(E) \right\} dE$$

# MaxEnt solutions

The solution spectrum can be written in closed form:

$$\Phi_i = \Phi_i^{DEF} e^{-\sum_k \lambda_k R_{ki}}$$

It is possible to give a Bayesian justification of the solution

The analysis was carried out with MAXED, a code originally developed for neutron spectrometry, part of the UMG 3.3 package available from RSICC and the NEA data bank

# MAXED: Software for MaxEnt

UMG package: available from RSICC and NEA data bank



The screenshot shows the NEA website interface. At the top left is the AEN/NEA logo and the text 'Agence pour l'énergie nucléaire / Nuclear Energy Agency'. At the top right is the OECD/OCDE logo. A navigation bar contains links for Home, About, Themes, Data Bank, Publications, Press Room, and Search. The main content area features a title 'NEA-1665 UMG 3.3 (Abstract last modified 22-SEP-2004)' and a description: 'UMG 3.3, Analysis of data measured with spectrometers using unfolding techniques'. Below this is an 'Abstract Table of Contents' with links for NAME, COMPUTER, PROBLEM, SOLUTION, RESTRICTIONS, CPU, FEATURES, AUXILIARIES, STATUS, REFERENCES, REQUIREMENTS, LANGUAGE, OPERATING SYSTEM, OTHER RESTRICTIONS, AUTHOR, MATERIAL, and CATEGORIES. A list of program versions follows, with a note that a password and special authorization are required to request or retrieve programs. A table lists the program names, package IDs, and their status (Obsolete or Tested). At the bottom, a section titled 'Machines used:' provides details on the original computer (IBM PC, PC Windows) and the test computer (HP 9000, Linux-based PC, PC Windows, DEC ALPHA W.S.).

[[Program Service](#) | [Recent programs](#)]

**NEA-1665 UMG 3.3 (Abstract last modified 22-SEP-2004)**

UMG 3.3, Analysis of data measured with spectrometers using unfolding techniques

**Abstract Table of Contents:**  
[NAME](#) | [COMPUTER](#) | [PROBLEM](#) | [SOLUTION](#) | [RESTRICTIONS](#) | [CPU](#) | [FEATURES](#) | [AUXILIARIES](#) | [STATUS](#) | [REFERENCES](#) | [REQUIREMENTS](#) | [LANGUAGE](#) | [OPERATING SYSTEM](#) | [OTHER RESTRICTIONS](#) | [AUTHOR](#) | [MATERIAL](#) | [CATEGORIES](#) |

1. NAME OR DESIGNATION OF PROGRAM - UMG 3.3.  
2. COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHER MACHINE VERSION PACKAGES AVAILABLE -

To request or retrieve programs click on the one of the active versions below. A password and [special authorization](#) is required.

Explanation of the [status codes](#).

Program-name	Package-ID	Status
UMG 3.3	NEA-1665/01	Obsolete
UMG 3.3	NEA-1665/02	Obsolete
<a href="#">UMG 3.3</a>	<a href="#">NEA-1665/03</a>	<a href="#">Tested</a>

Machines used:

Package-ID	Orig.Computer	Test Computer
NEA-1665/03	IBM PC,PC Windows	HP 9000, Linux-based PC, PC Windows, DEC ALPHA W.S.

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# Algorithm of MAXED

1. Define the set of admissible solutions using two conditions:

$$N_k + \varepsilon_k = \sum_i R_{ki} \Phi_i \qquad \sum_k \frac{\varepsilon_k^2}{\sigma_k^2} = \chi^2$$

2. To get the MaxEnt solution, optimize the Lagrangian

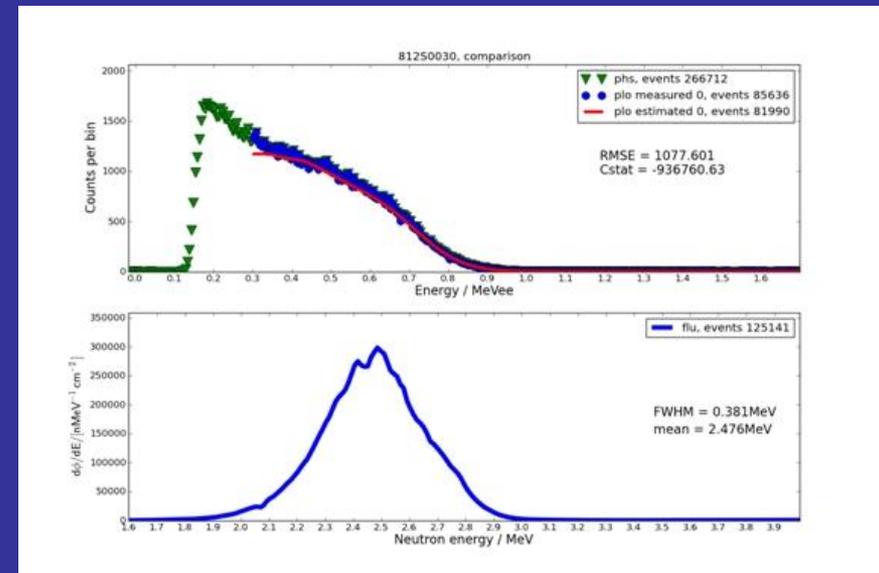
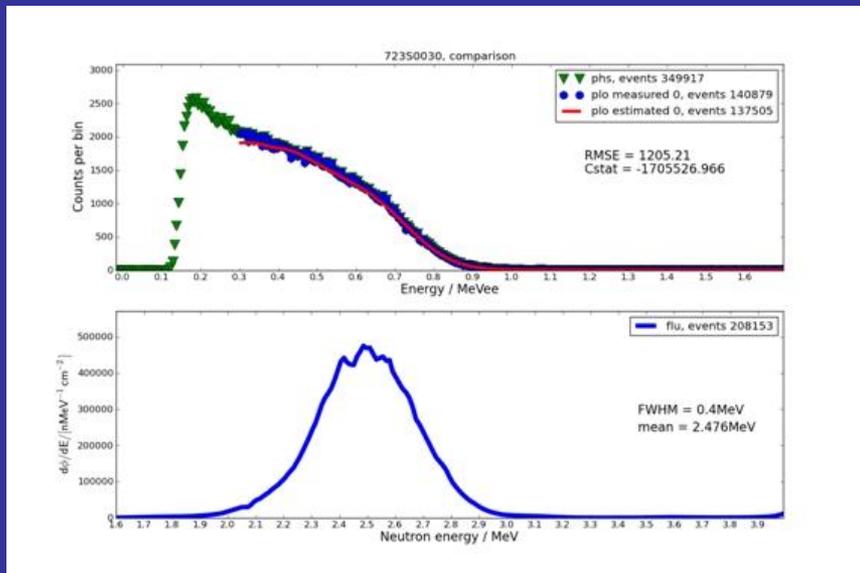
$$L(\Phi_i, \varepsilon_k, \lambda_k, \mu) = S - \sum_k \lambda_k \left[ \sum_i \{R_{ki} \Phi_i\} - N_k - \varepsilon_k \right] - \mu \left[ \sum_k \left\{ \frac{\varepsilon_k^2}{\sigma_k^2} \right\} - \chi^2 \right]$$

or, equivalently, the potential function

$$Z(\lambda_k) = - \sum_i \left\{ \Phi_i^{DEF} \exp \left( - \sum_k \lambda_k R_{ki} \right) \right\} - \left[ (\chi^2) \sum_k (\lambda_k \sigma_k)^2 \right]^{1/2} - \sum_k N_k \lambda_k$$

# MaxEnt deconvolution: PRELIMINARY results

MaxEnt deconvolution of shots 82723 and 82812



# Bayesian parameter estimation

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# Bayesian parameter estimation

1. Introduce a model of the PHS

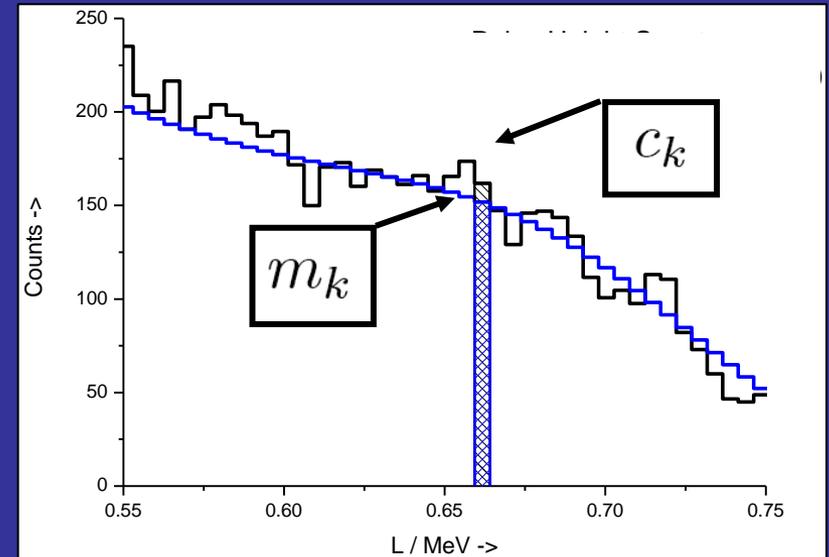
2. Calculate the likelihood

$$\begin{aligned} \rightarrow P(m_1, m_2, \dots | FWHM, I) \\ = \prod_k \frac{e^{-c_k} c_k^{m_k}}{m_k!} \approx e^{-(\chi^2/2)} \end{aligned}$$

3. Introduce priors

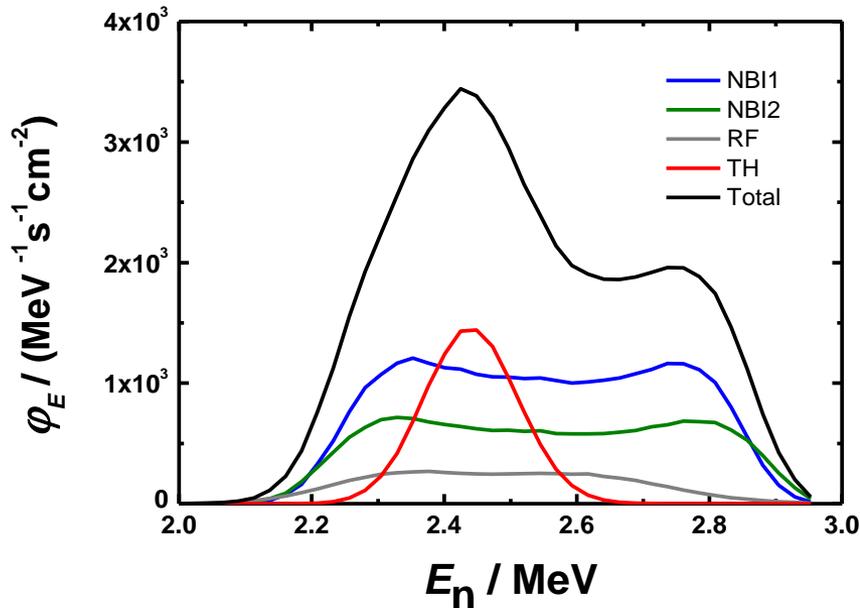
4. Use Bayes' theorem to estimate the probability given the data,

$$\rightarrow P(FWHM | m_1, m_2, \dots, I) \sim P(m_1, m_2, \dots | FWHM, I) P(FWHM | I)$$

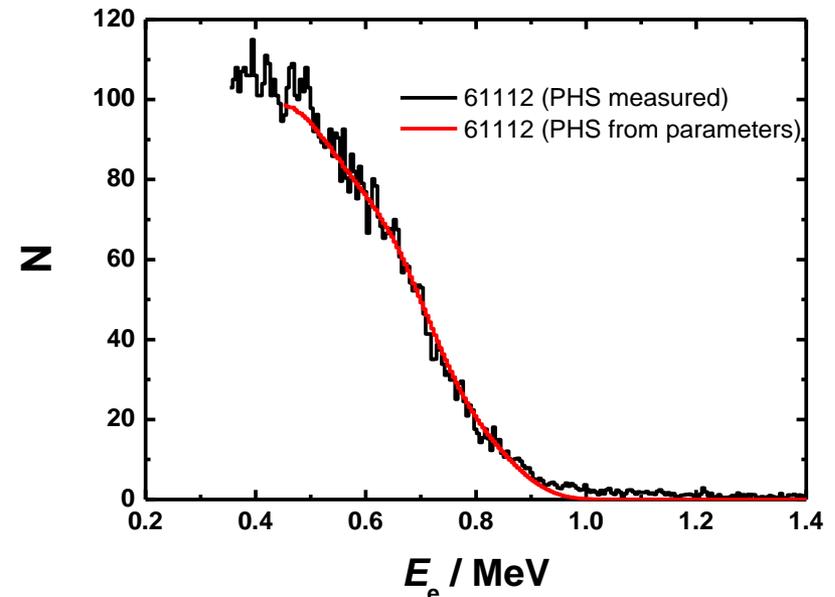


# Simple example: sum of 4 components

Most probable spectrum

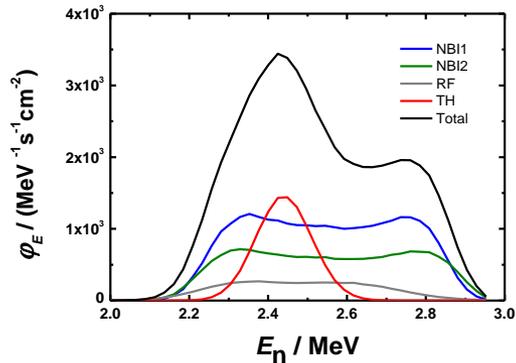


Check!: folding of spectrum

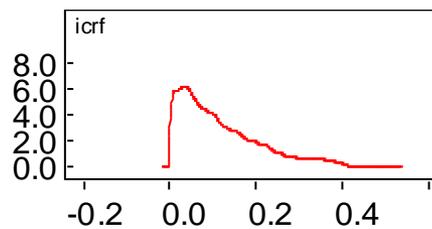
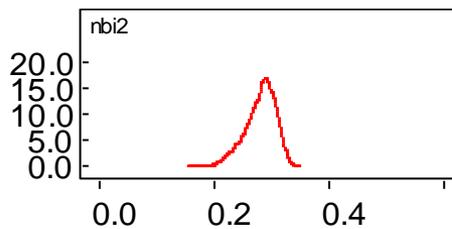
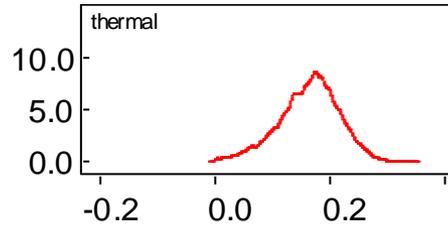
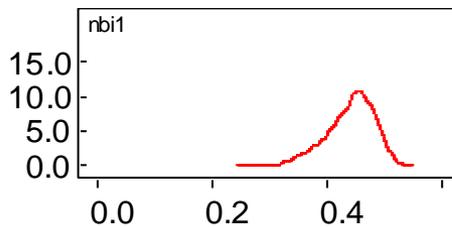


[L. Bertalot et. al., *Neutron Energy Measurements of Trace Tritium Plasmas with NE213 Compact Spectrometer at JET*, EFDA-JET-CP(05)02-17]

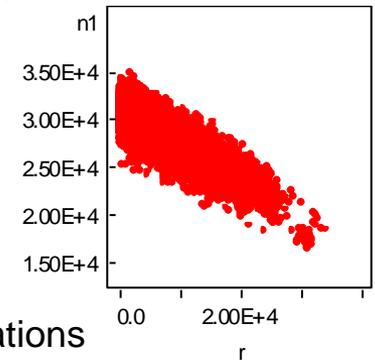
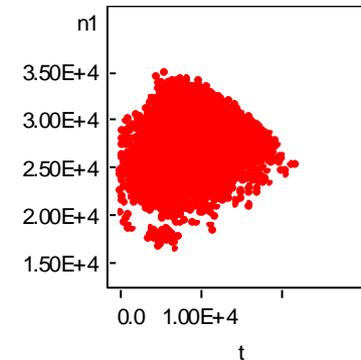
# Simple example: results



nbi 1	45 %
icrf	9 %
thermal	17 %
nbi 2	29 %



Posterior probabilities



Correlations

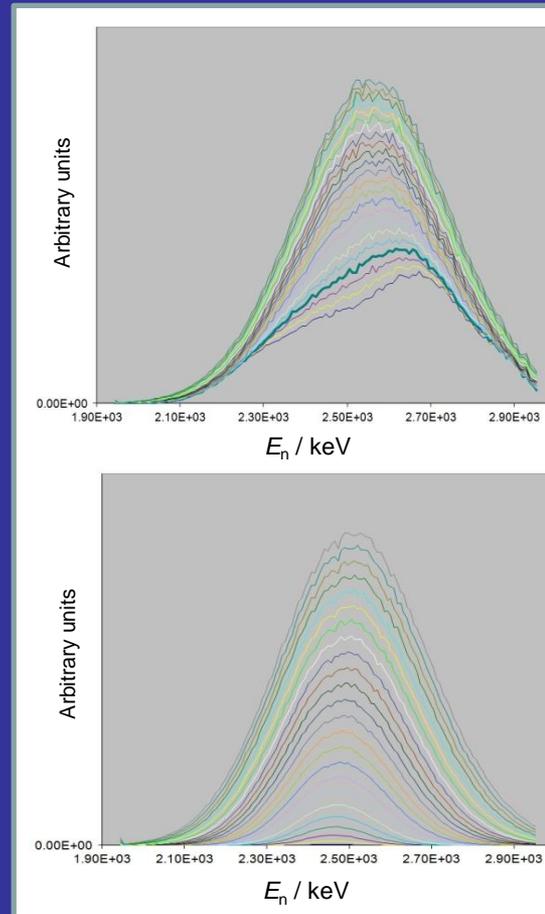
# Simulations for shots 82723 and 82724: PRELIMINARY results

“NBI-Bulk”:  
Simulations of reactions involving NBI 130 kV injected deuterons into thermal plasmas with  $T_i \sim 3\text{-}25$  keV.

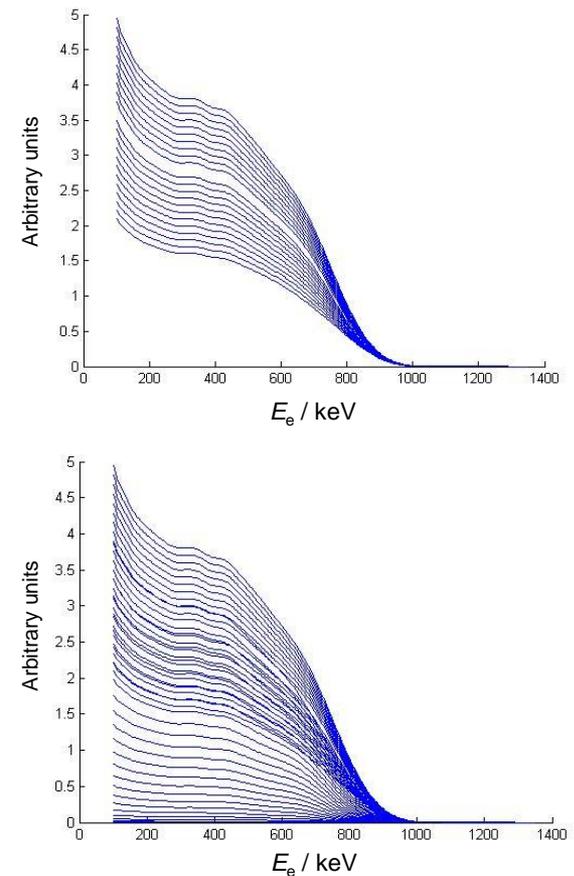
“Bulk-Bulk”:  
Simulations of reactions involving thermal deuterons with  $T_i \sim 2\text{-}25$  keV.

Assume that the spectrum is a sum of components, one for each  $T_i$

Neutron spectra

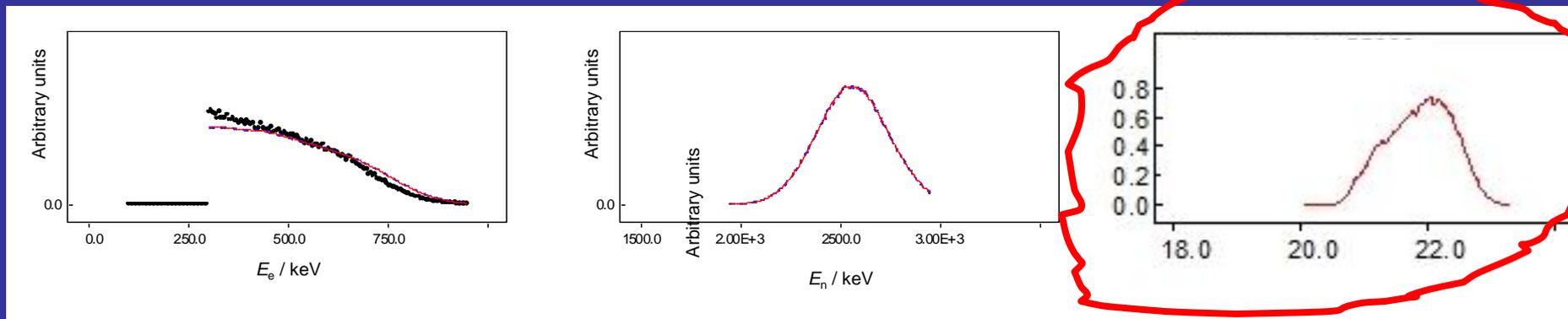


PHS

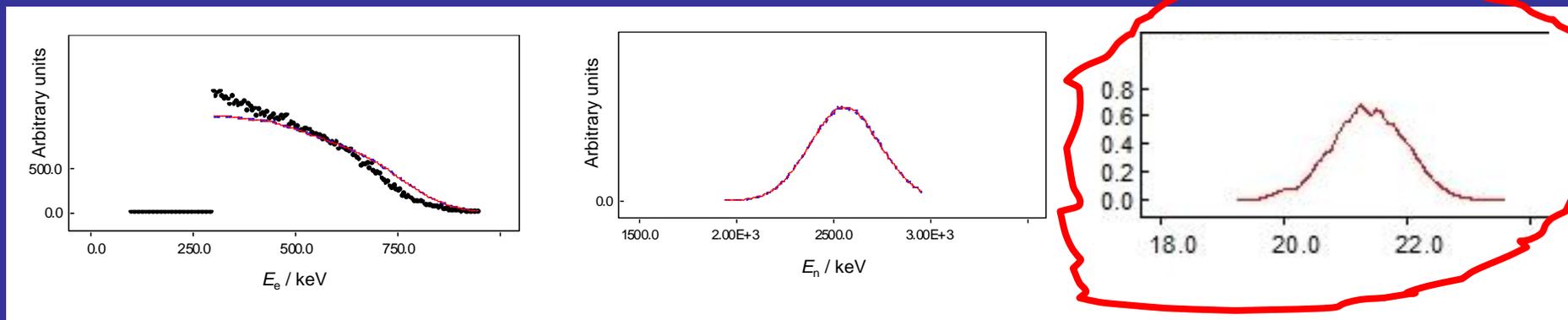


# Bayesian analysis: PRELIMINARY results (I)

82723: PHS, neutron spectrum and probability of  $T_i$

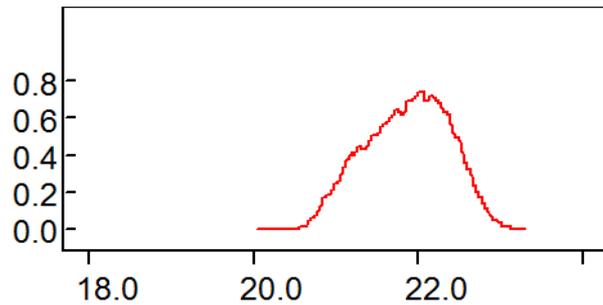


82812: PHS, neutron spectrum and probability of  $T_i$

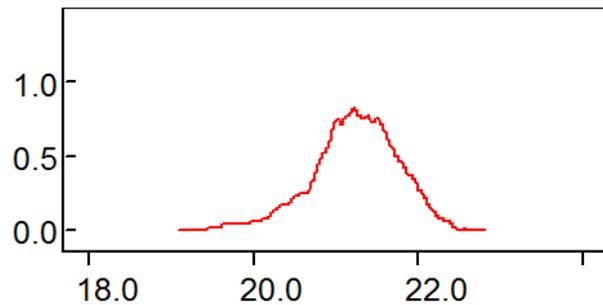


# Bayesian analysis: PRELIMINARY results (II)

Probability of  $T_i$  - shot 82723

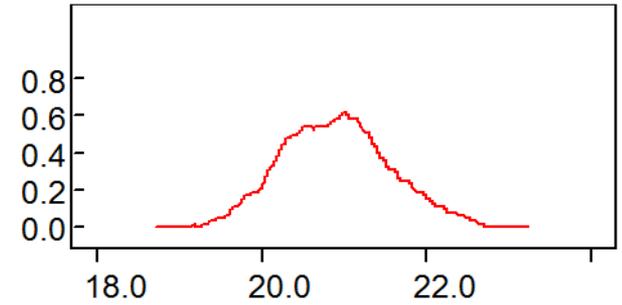
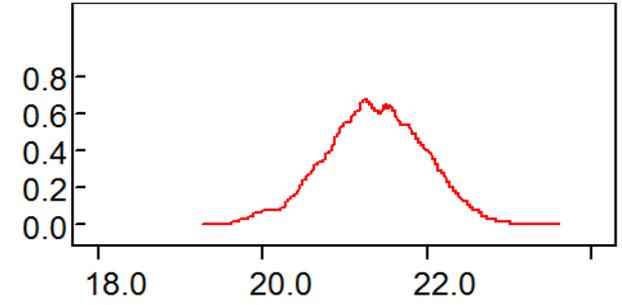


Ratio 1:9



Ratio 2:8

Probability of  $T_i$  - shot 82812



# Conclusions

M. Reginatto

Data analysis for neutron spectrometry with liquid scintillators: applications to fusion diagnostics



# Conclusions

- Neutron spectrometry with liquid scintillation detectors can provide information that may be difficult to obtain with other diagnostic tools. But appropriate methods of data analysis should be used!
- The classical concept of resolution is not always applicable (or useful) for many of the detectors that are used for spectrometry. But information theory can provide the tools that are necessary to develop better ways of describing the capabilities of spectrometers.
- The Backus-Gilbert representation can be used to define the detector's resolving power, while Kozarev's approach can be used to calculate the superresolution that is theoretically achievable (i.e., the Shannon limit).
- Superresolution values that are close to the Shannon limit have been achieved for liquid scintillation detectors using maximum entropy deconvolution
- Preliminary results of the analysis of recent measurements carried out at JET show that the spectrometer and the methods of data analysis give good results, providing reliable estimates of the neutron spectrum and of the ion temperature.

Thank you for your attention!

M. Reginatto

Data analysis for neutron spectrometry with liquid  
scintillators: applications to fusion diagnostics

