Bayes Days 2000 at LANL

Three-Day Minicourse on Bayesian Analysis in Physics

Lectures presented by

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Max Planck Institute for Plasma Physics

Sponsored by
Enhanced Surveillance Program, Los Alamos National Laboratory

For more information, look on the web:
http://public.lanl.gov/kmh/course/BD2000.html

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Max-Planck-Institut für Plasmaphysik
Abteilung Oberflächenphysik

Deconvolution

V. Dose, W. von der Linden, R. Fischer
M. Donath, M. Mayer

1. Apparatus function exact

2. Apparatus function as a result of a measurement

Deconvolution

measurement

apparatus function

spectral function

$\Downarrow$ $\Downarrow$ $\Downarrow$

$$D(E) = \int_{-\infty}^{\infty} \mathrm{A}(E - E')\ f(E')\ \mathrm{d}E'$$

$\Downarrow$ $\Downarrow$ $\Downarrow$

$$\vec{D} = \mathbf{A} \cdot \vec{f}$$

$$\left.\begin{array}{l} \vec{D} = (D_1, D_2, \ldots, D_N)^T \\ \vec{f} = (f_1, f_2, \ldots, f_M)^T \end{array}\right\} \rightarrow \ \mathrm{dim}\mathbf{A} = N \times M$$

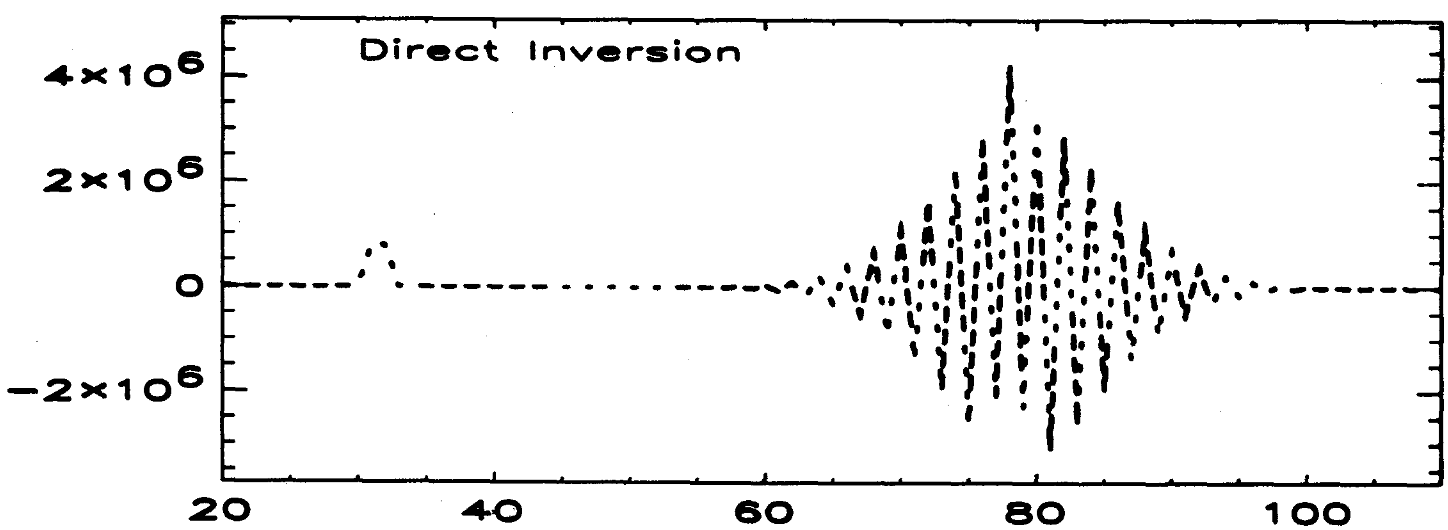
special case N=M:

$$\vec{f} = \mathbf{A}^{-1} \cdot \vec{D}$$

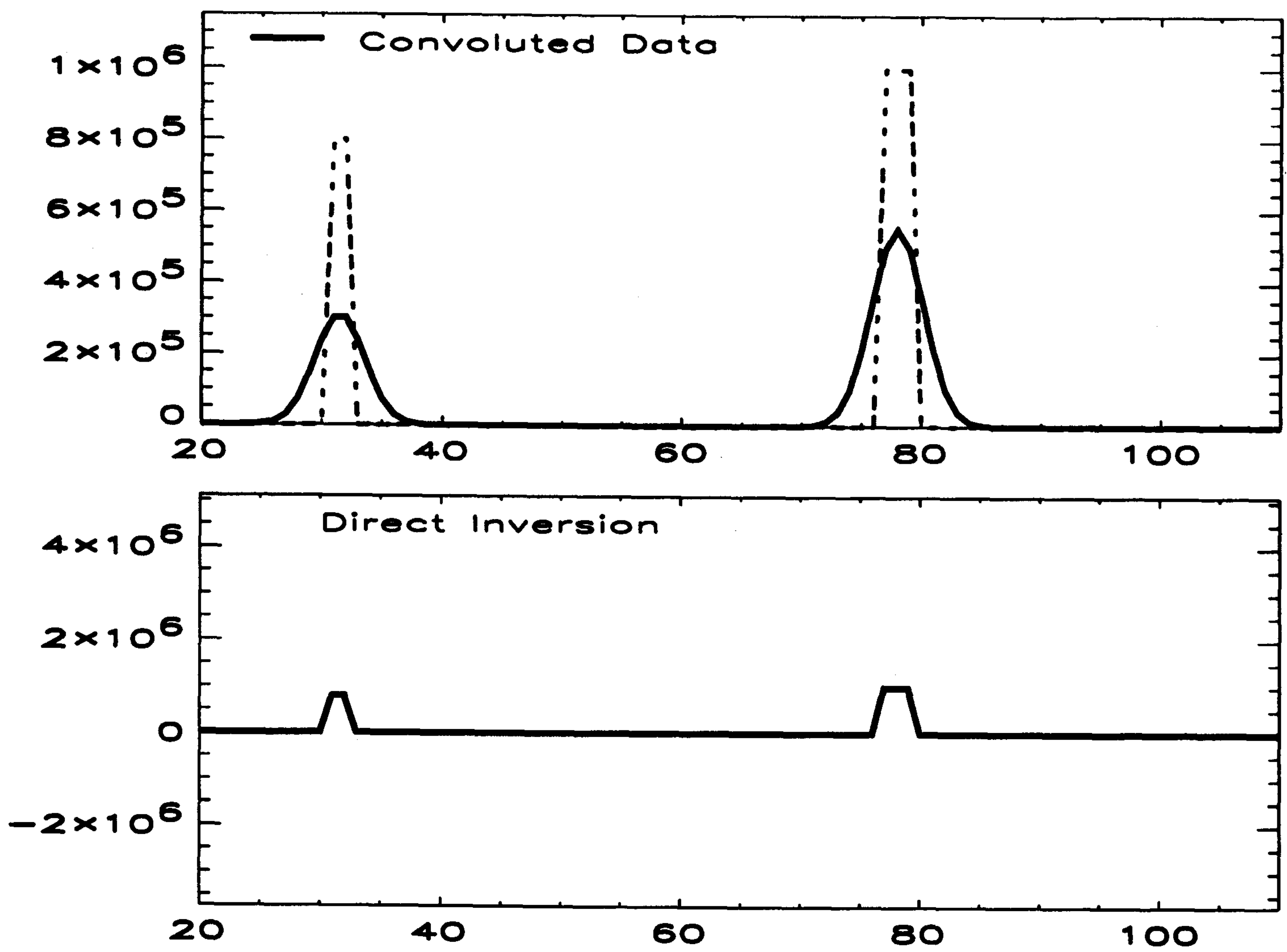
Noise,N=M:

$$\vec{D} = \mathbf{A} \cdot \vec{f} + \vec{n}_d$$

$$\vec{f} = \mathbf{A}^{-1} \cdot \vec{D}\ ?$$



Direct Inversion
4×10^6
2×10^6
0
−2×10^6
20
40
60
80
100


Convoluted Data
1×10^6
8×10^5
6×10^5
4×10^5
2×10^5
0
20
40
60
80
100
Direct Inversion
4×10^6
2×10^6
0
−2×10^6
20
40
60
80
100

Bayesian solution

$$\langle n_{d_i}^2 \rangle = \sigma_i^2, \qquad \langle n_{d_i} \rangle = 0$$

$$p\left(\vec{D}|\mathbf{A}, \vec{f}, \vec{\sigma}, I\right) = \left\{\prod_i \frac{1}{\sigma_i\sqrt{2\pi}}\right\} \exp\left\{-\frac{1}{2}\sum_i \left[\frac{D_i - \left(\mathbf{A}\vec{f}\right)_i}{\sigma_i^2}\right]^2\right\}$$

$$p\left(\vec{f}|\vec{D}, \mathbf{A}, \vec{\sigma}, I\right) = \frac{p(\vec{f}|I)}{p(\vec{D}|\mathbf{A}, \vec{\sigma}, I)} p\left(\vec{D}|\mathbf{A}, \vec{f}, \vec{\sigma}, I\right)$$

$$p\left(\vec{f}|\alpha, I\right) = \exp\left\{\alpha S(f)\right\} / Z_S$$

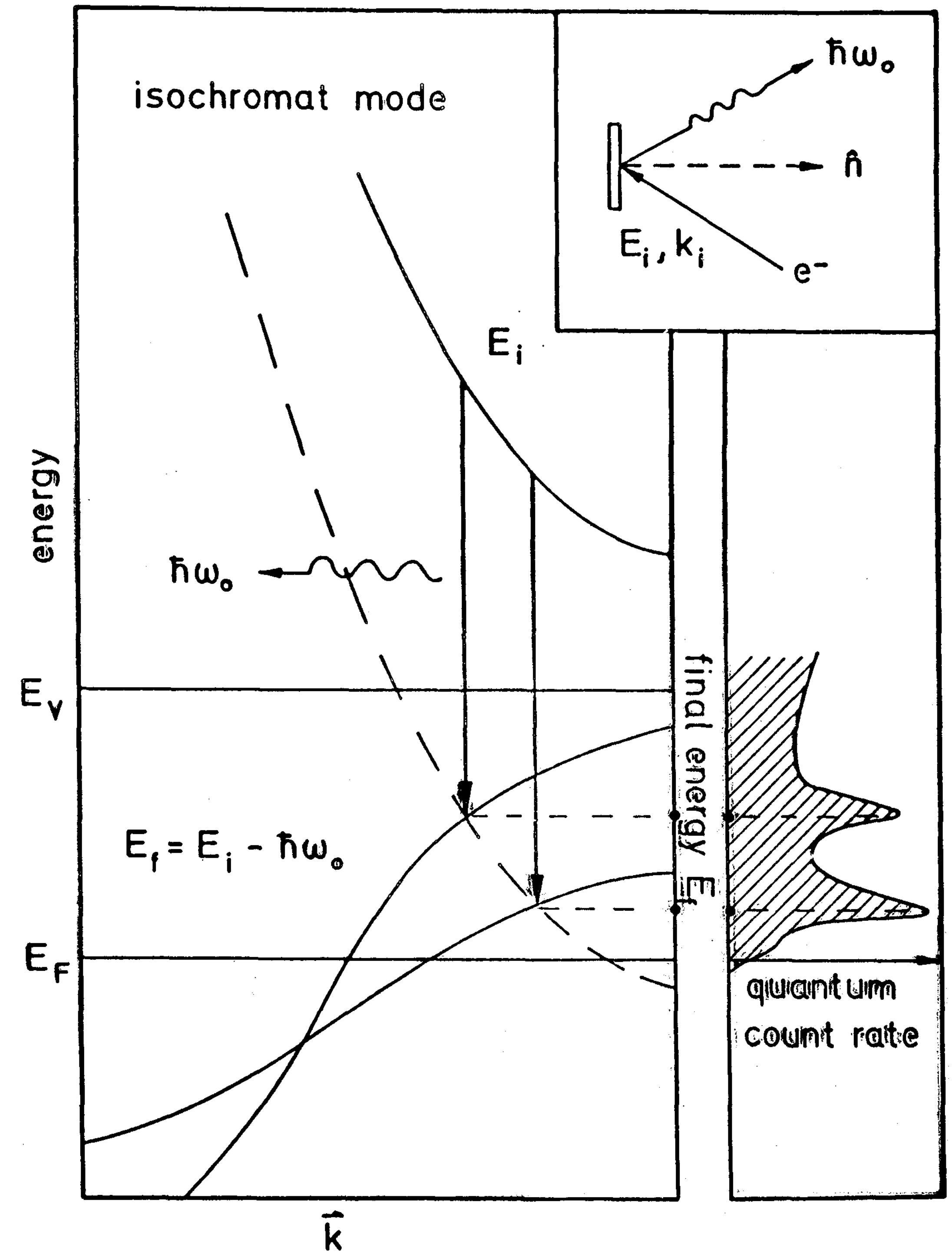
$$S(\vec{f}) = \sum_k \left[f_k - m_k - f_k \ln(\frac{f_k}{m_k})\right]$$

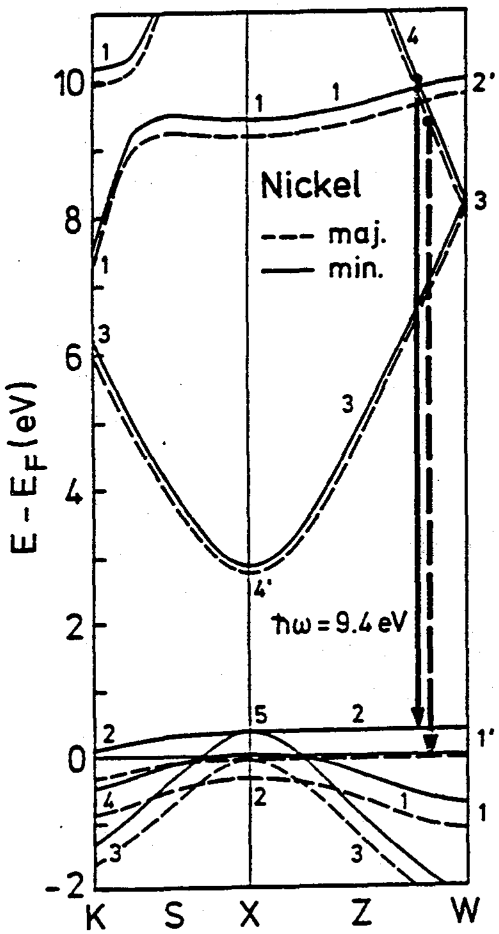
evidence approximation

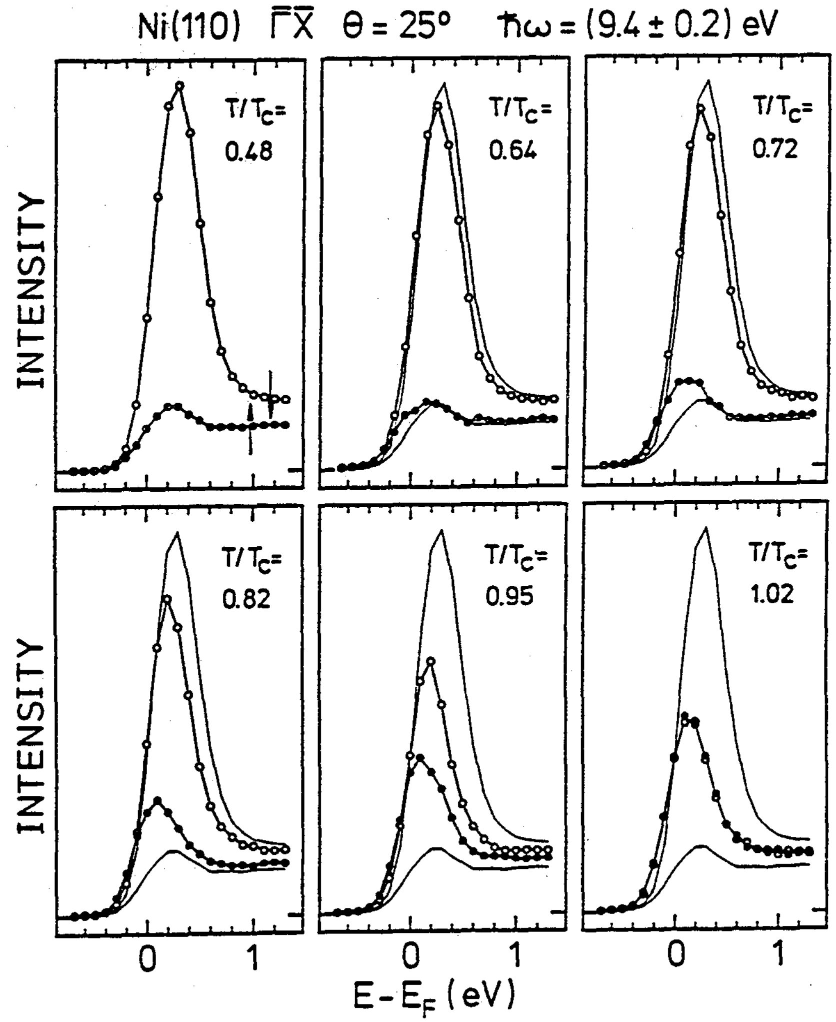
$$p\left(\alpha|\vec{D}, \mathbf{A}, \vec{\sigma}\right) = p\left(\alpha|I\right) \cdot \frac{p\left(\vec{D}|\mathbf{A}, \vec{\sigma}, \alpha, I\right)}{p\left(\vec{D}|\mathbf{A}, \sigma\right)}$$

$$\begin{aligned} p\left(\alpha|\vec{D}, \mathbf{A}, \sigma\right) &= \frac{p(\alpha|I)}{p\left(\vec{D}|\mathbf{A}, \vec{\sigma}\right)} \int p\left(\vec{D}, \vec{f}|\mathbf{A}, \vec{\sigma}, \alpha, I\right) \mathrm{d}f \\ &= \frac{p(\alpha|I)}{p\left(\vec{D}|\mathbf{A}, \vec{\sigma}\right)} \int p\left(\vec{f}|\alpha\right) \cdot p\left(\vec{D}|\mathbf{A}, \vec{f}, \vec{\sigma}, I\right) \mathrm{d}f \end{aligned}$$

inverse photoemission







M. Donath + V.D. Europhys. Lett 9 (1989) 821

$$I^{\sigma}(E,T,\mu) = j^{\sigma} \int A^{\sigma}(E')\{1 - f(E',T,\mu)\}\, g(E'-E)\, dE'$$

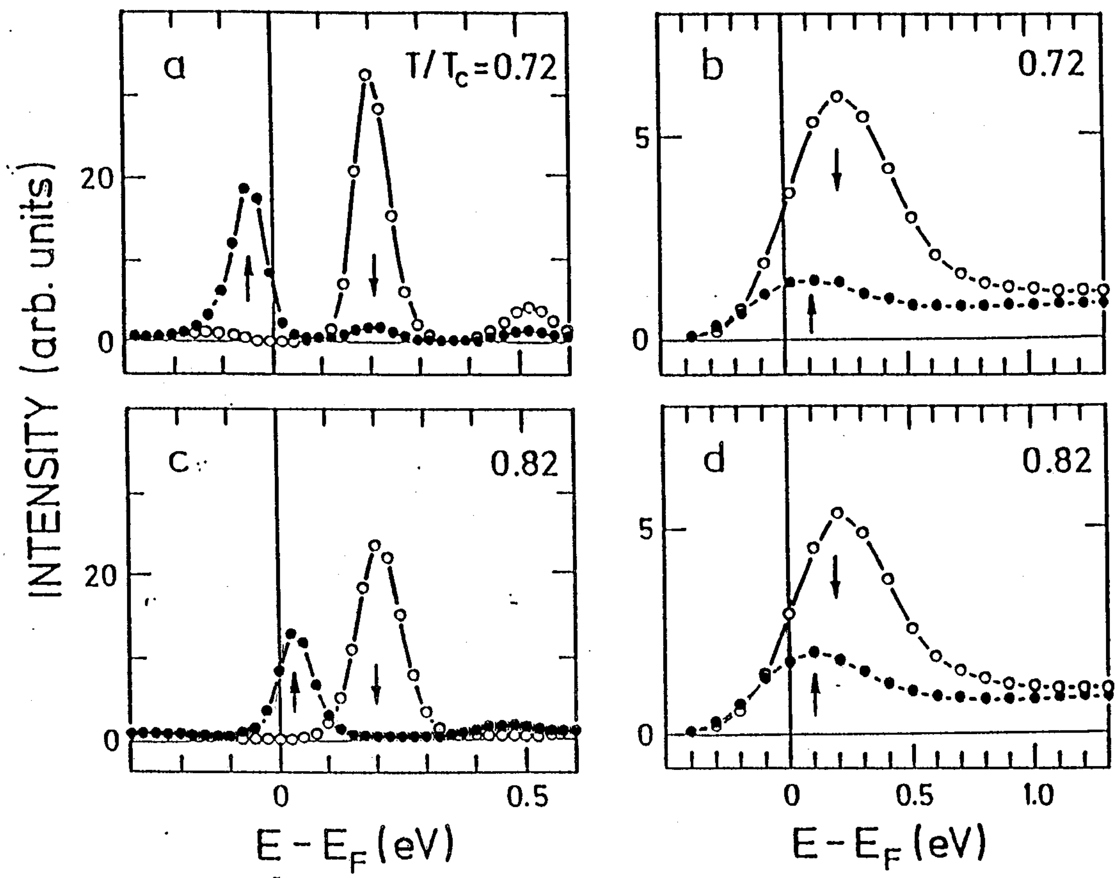
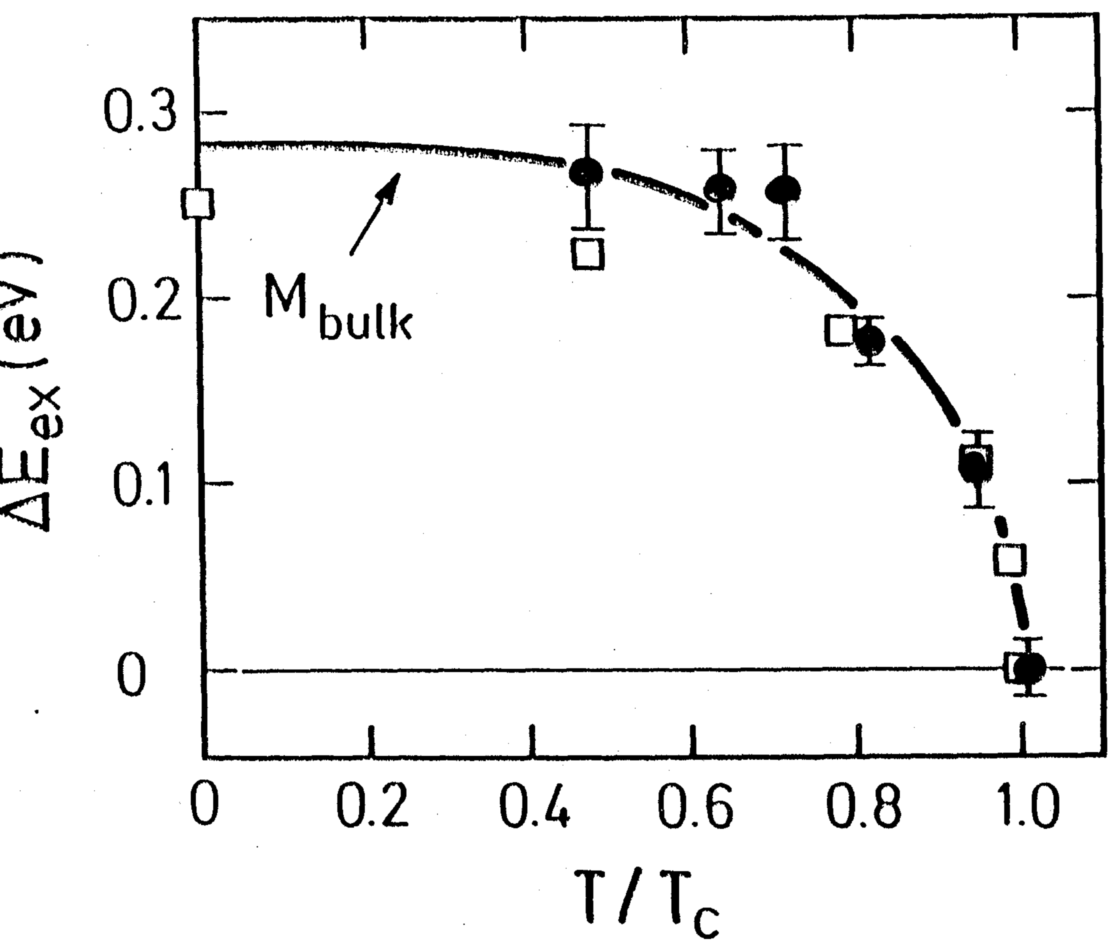


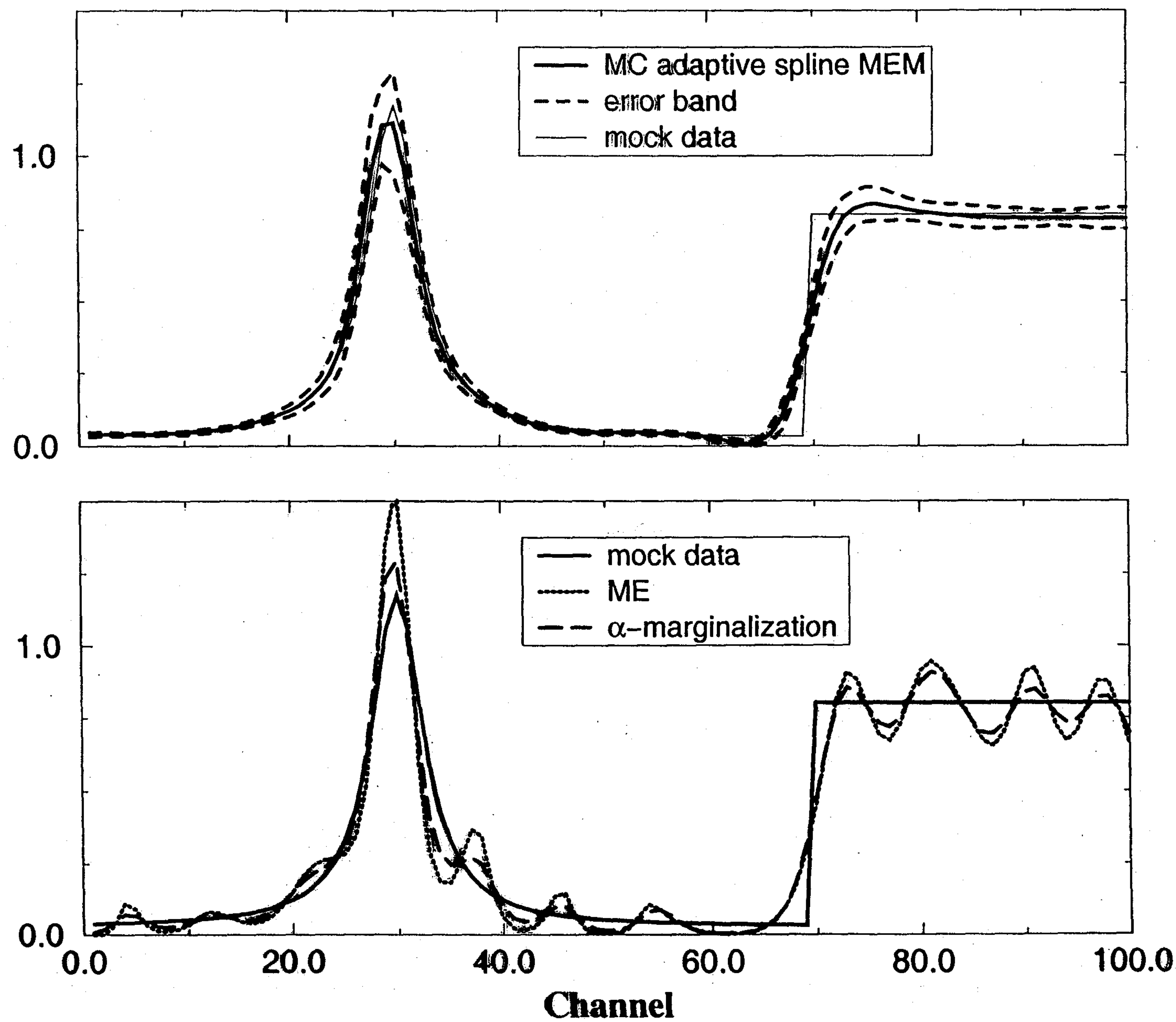
Fig. 2: Spin-dependent quasiparticle spectral density (a,c) and experimental IPE data (b,d) of the $Z_4 \rightarrow Z_2$-transition in Ni for two temperatures $T/T_C = 0.72$ (a,b) and 0.82 (c,d).

v. d. Linden et al. PRL 71 (1993) 899



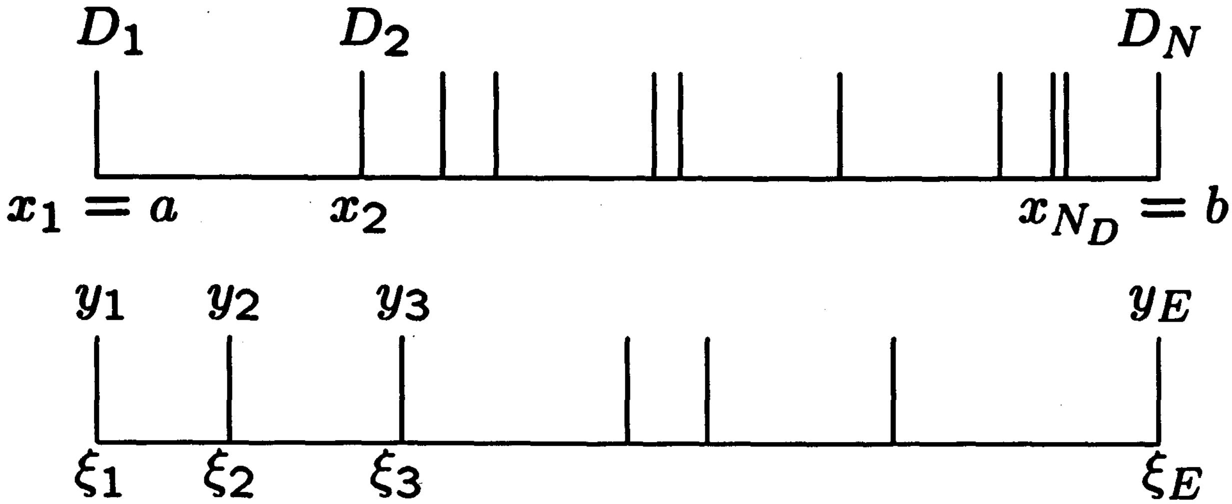
v. d. Linden et al PRL 71 (1993) 899

Borgiel, Nolting, Donath SSC 72 (1989) 825



MC adaptive spline MEM
error band
mock data
1.0
0.0
mock data
ME
α–marginalization
1.0
0.0
0.0
20.0
40.0
60.0
80.0
100.0
Channel

Adaptive interpolation model



$$f(x) = f^S\left(x|E, \vec{\xi}, \vec{y}\right)$$

Model : $$M = M\left(E, \vec{\xi}\right)$$

$$p\left(M|\vec{D}, I\right) = \frac{p(M|I)}{p\left(\vec{D}|I\right)} p\left(\vec{D}|M, I\right)$$

$$\begin{aligned} p\left(\vec{D}|M, I\right) &= \int p\left(\vec{D}, \vec{y}|M, I\right) \mathrm{d}\vec{y} \\ &= \int p\left(\vec{y}|M, I\right) p\left(\vec{D}|\vec{y}, M, I\right) \mathrm{d}\vec{y} \end{aligned}$$

$$p\left(\vec{D}|\vec{y}, M, I\right) = \left(\prod_i \frac{1}{\sigma_i\sqrt{2\pi}}\right) \exp\left\{-\frac{1}{2}\sum_i^N \left(\frac{D_i - f(x_i)}{\sigma_i}\right)^2\right\}$$

Priors I

$$p(M|I) = p\left(\vec{\xi}|E,I\right) p(E|I)$$

$$p(E|I) = \frac{1}{N}$$

choose $p\left(\vec{\xi}|E,I\right)$ =flat

$$Z = \int_a^b \mathrm{d}\xi_2 \int_{\xi_2}^b \mathrm{d}\xi_3 \ldots \int_{\xi_{E-2}}^b \mathrm{d}\xi_{E-1} = \frac{(b-a)^{E-2}}{(E-2)!}$$

$$p\left(\vec{\xi}|E,I\right) (\Delta\xi)^{E-2} = \frac{(E-2)!}{(b-a)^{E-2}} (\Delta\xi)^{E-2}$$

$$\frac{p\left(\vec{\xi}|E+1,I\right)}{p\left(\vec{\xi}|E,I\right)} = \frac{(E-1)\,\Delta\xi}{b-a}$$

alternatively:

$$p\left(\vec{\xi}|E,I\right) = \frac{(E-2)!\prod_{i=2}^{E} \Theta\left[\xi_{i-1} + \Delta\xi \leq \xi_{i-1}\right]}{(b-a-(E-1)\Delta\xi)^{E-2}}$$

Posterior estimates

$$p\left(\vec{f}|\vec{D}, E_0, x, \vec{\xi}, I\right) = \int p\left(\vec{f}, \vec{y}|\vec{D}, E_0, \vec{x}, \vec{\xi}, I\right) \mathrm{d}^E y$$

$$= \int p\left(\vec{f}|\vec{D}, E_0, \vec{y}, \vec{x}, \vec{\xi}, I\right) p\left(\vec{y}|\vec{D}, E_0, \vec{\xi}, I\right) \mathrm{d}^E y$$

$$p\left(\vec{f}|\vec{D}, E_0, \vec{y}, \vec{x}, \vec{\xi}, I\right) = \delta\left(\vec{f} - \mathrm{S}(x, \vec{\xi})\vec{y}\right)$$

Bayes theorem:

$$p\left(\vec{y}|\vec{D}, E_0, \vec{x}, \vec{\xi}, I\right) = \frac{p\left(\vec{y}|E_0, \vec{\xi}, I\right)}{p\left(\vec{D}|I\right)} p\left(\vec{D}|\vec{y}, E_0, \vec{x}, \vec{\xi}, I\right)$$

$$\langle g\left(\vec{f}\right)\rangle = \int g\left(\vec{f}\right) p\left(\vec{f}|\vec{D}, E_0, \vec{x}, \vec{\xi}, I\right) \mathrm{d}^{E_0} f$$

in particular

$$g(f) = f \qquad g(f) = f^2$$

Priors II

$$p\left(\vec{y}|M,I\right) = \exp\left\{-\Phi\left(f\left(\vec{y}\right)\right)\right\}/Z(M)$$

for a general quadratic log prior

$$p(f) = \exp\left\{-\frac{\lambda}{2}\vec{f}^T \mathrm{A}\vec{f}\right\}/Z\left(\lambda, f\right)$$

consistent with spline

$$\Phi = \int_a^b |f''|^2 \mathrm{d}x$$

$$f^S = \mathrm{S}\vec{y}$$

$$p\left(\vec{y}|M,\lambda,I\right) = \left(\frac{\lambda}{2\pi}\right)^{E/2}\sqrt{\det \mathrm{S}^T \mathrm{AS}}\exp\left\{-\frac{\lambda}{2}\vec{y}^T \mathrm{S}^T \mathrm{AS}\vec{y}\right\}$$

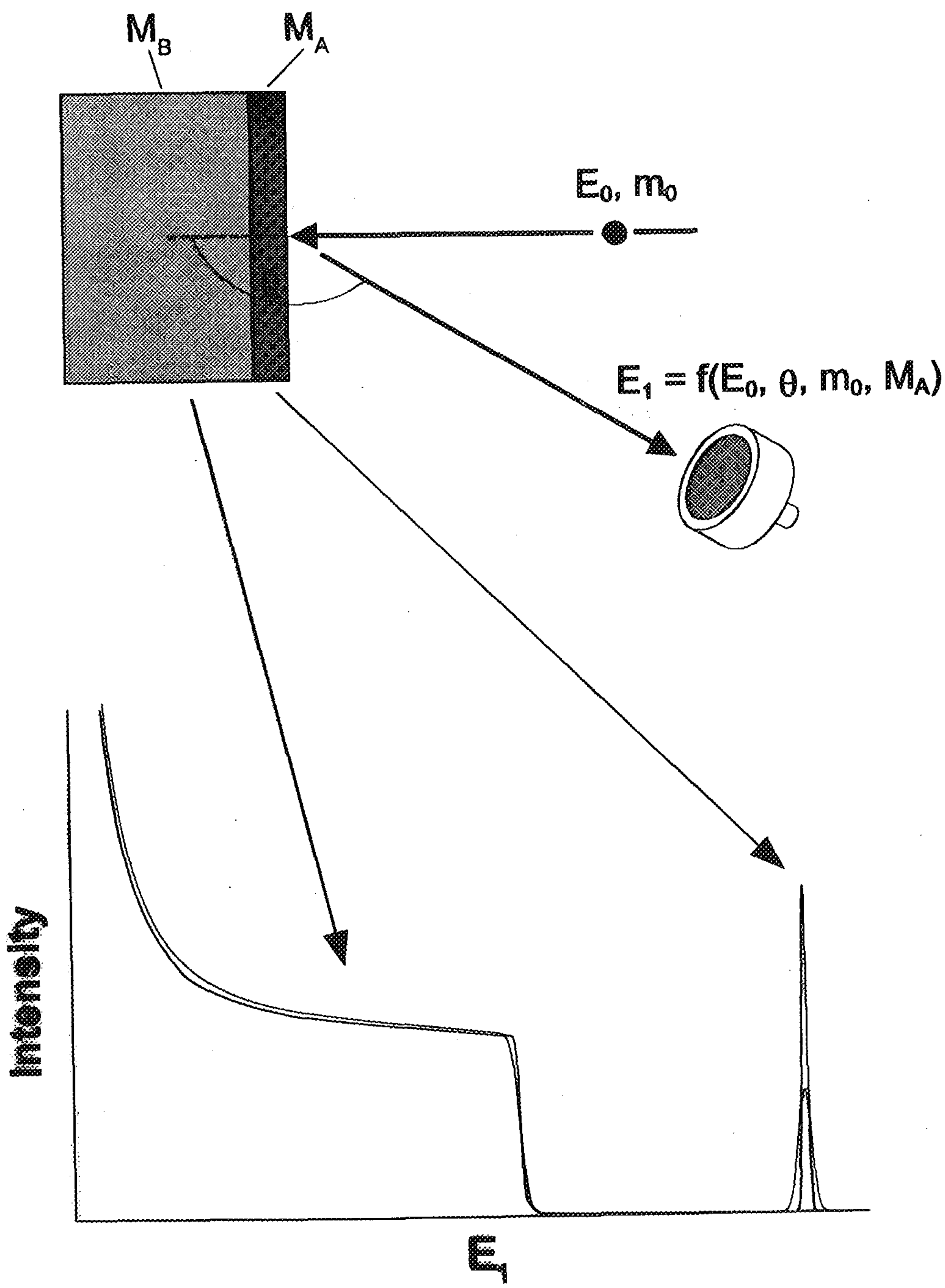
$$p\left(\vec{y}|M,I\right) = \int p\left(\vec{y}|M,\lambda,I\right)p\left(\lambda|I\right)\mathrm{d}\lambda$$

Jeffrey's prior

$$p(\lambda|I) = \frac{\mathrm{d}\lambda}{\lambda} \;\rightarrow\; p(\lambda|I) = \frac{a^\gamma}{\Gamma(\gamma)}\lambda^{\gamma-1}\mathrm{e}^{-a\lambda}$$

$$(a \rightarrow 0, \gamma \rightarrow 1)$$

1a



Broadening mechanismus

1. incident beam energy
   at E_0=2.6 MeV $\approx$ 13 keV

2. detector resolution at
   $E_1 \approx$2 MeV $\approx$ 15 keV

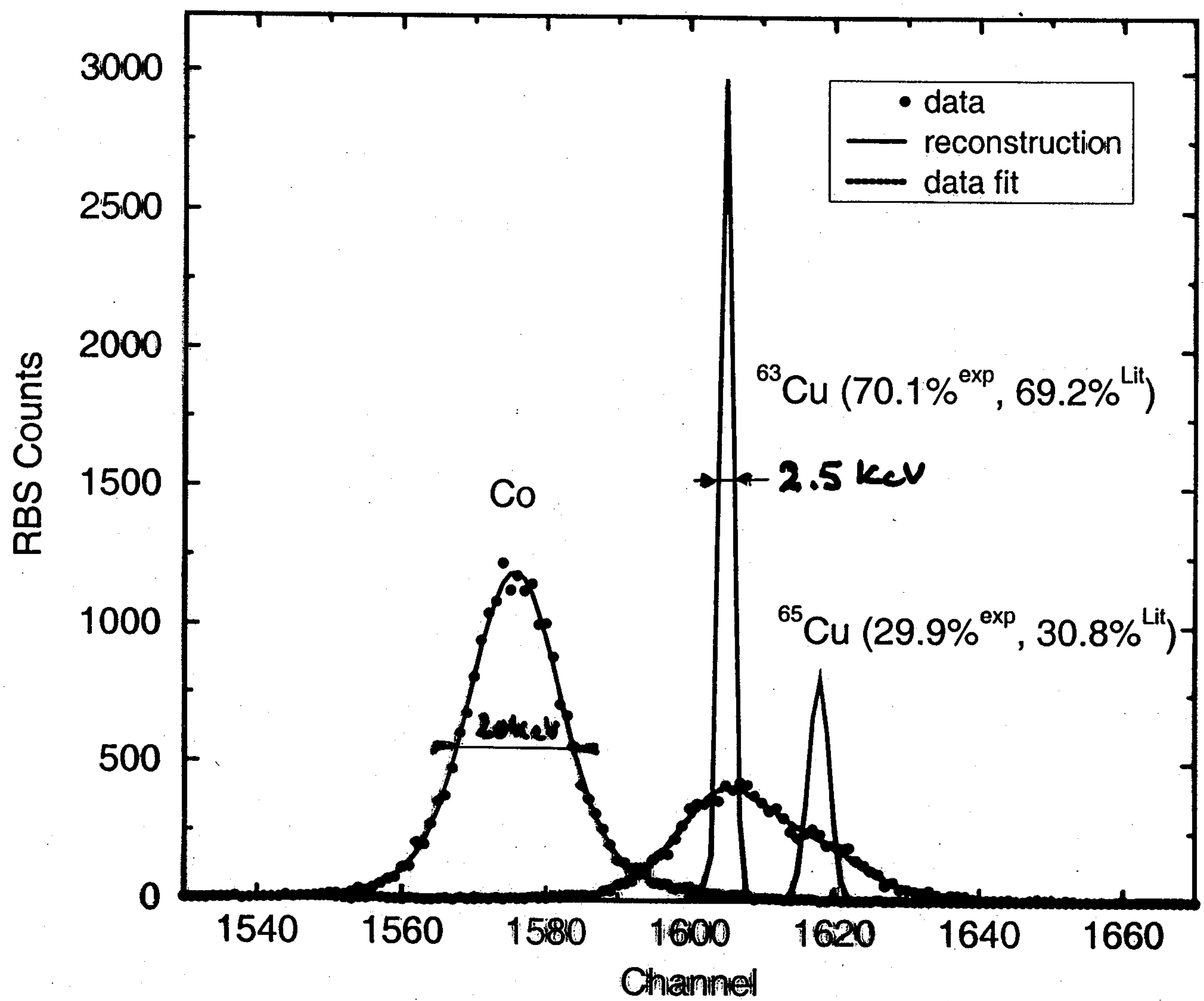
3. electronic noise $\approx$ 5 keV

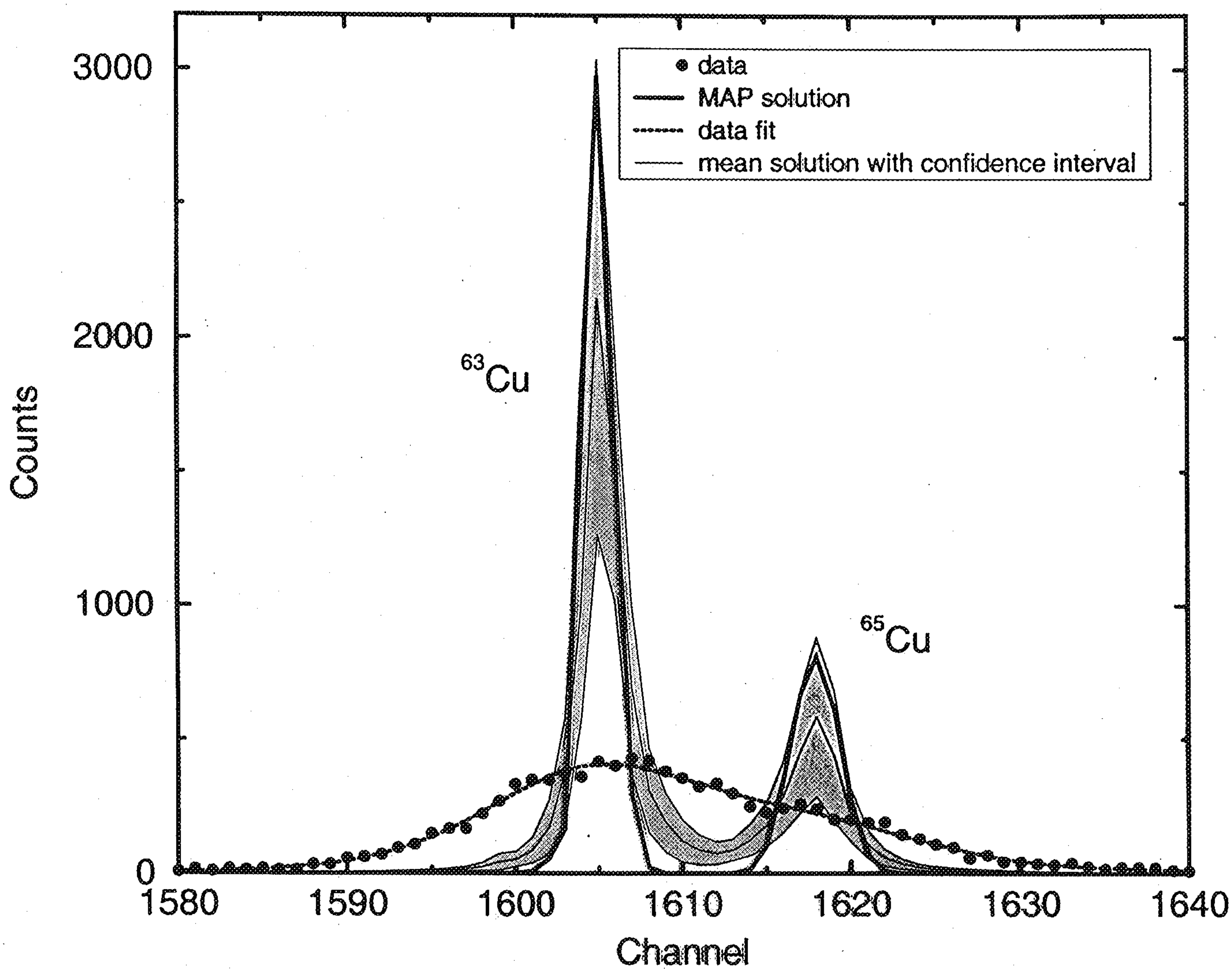
4. detector solid angle, beam spot size,
   finite film thickness $\approx$ 3 keV

overall resolution 20.6 keV

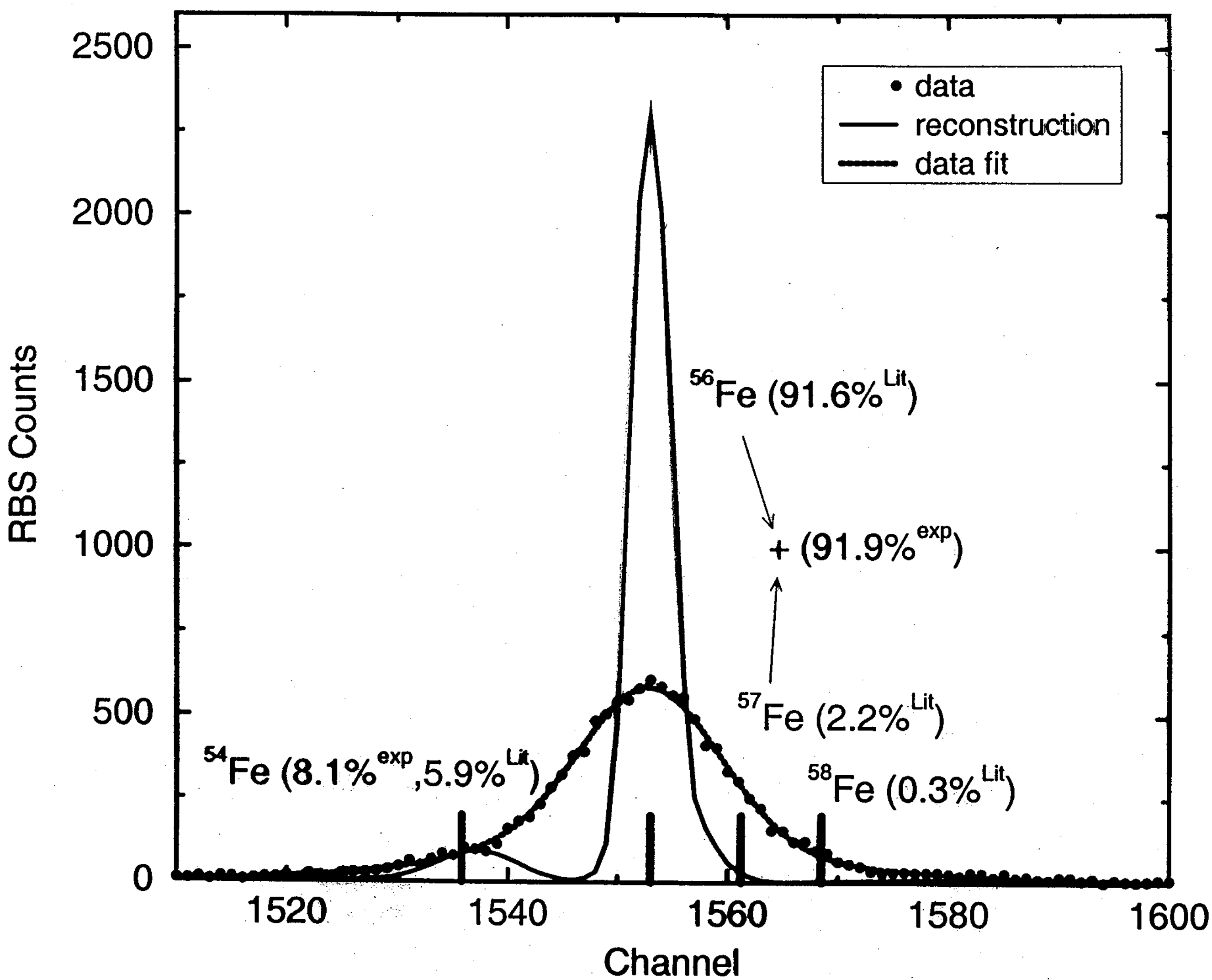
$$D(E) = \int f\left(E'\right) \mathrm{A}\left(E - E'\right) \mathrm{d}E'$$

MAP - Solution

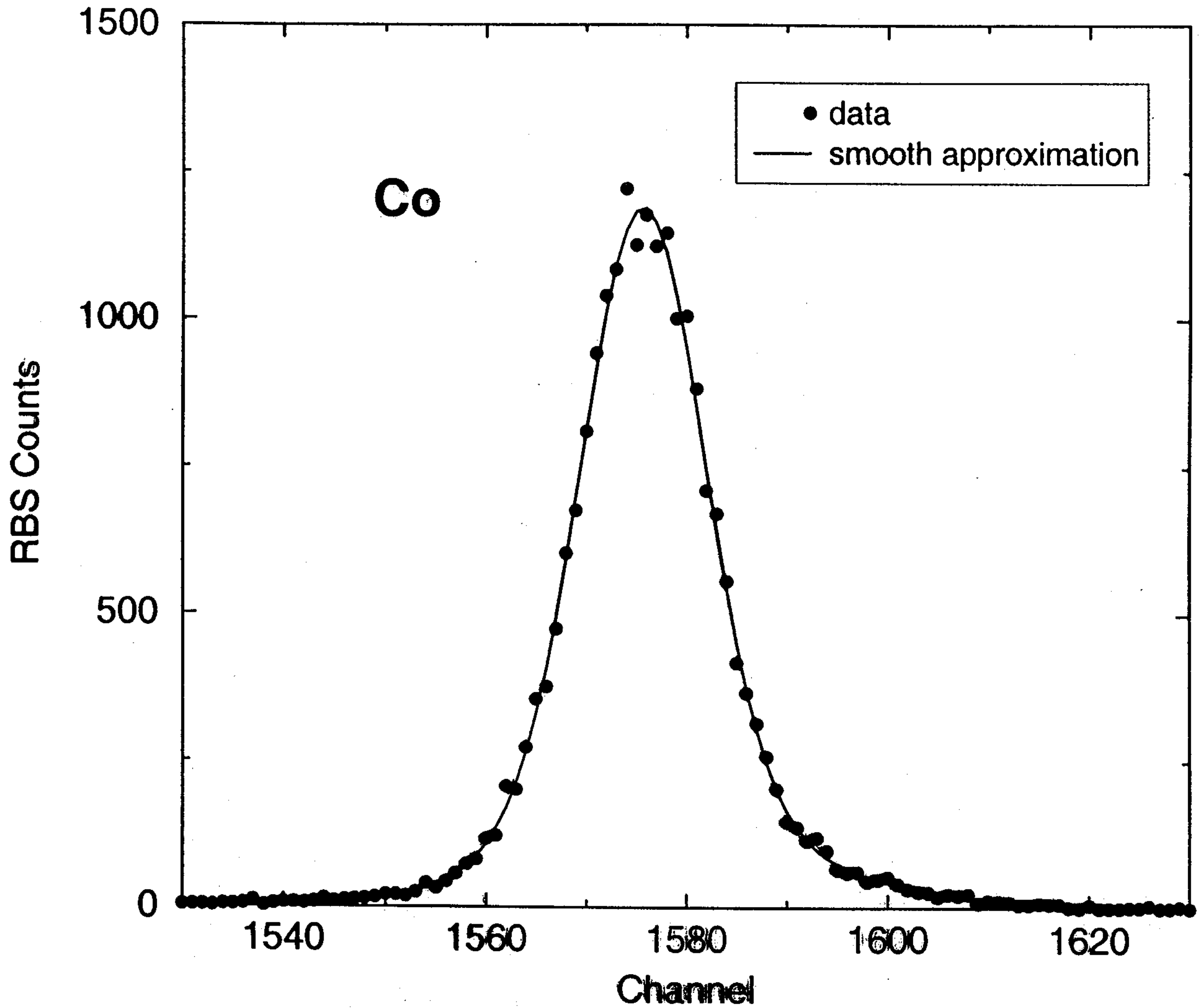




data
MAP solution
data fit
mean solution with confidence interval
^{63}Cu
^{65}Cu
Counts
Channel
3000
2000
1000
0
1580
1590
1600
1610
1620
1630
1640



2500
2000
1500
1000
500
0
RBS Counts
1520
1540
1560
1580
1600
Channel
data
reconstruction
data fit
56Fe (91.6%Lit)
+ (91.9%exp)
57Fe (2.2%Lit)
54Fe (8.1%exp,5.9%Lit)
58Fe (0.3%Lit)



1500
1000
500
0
RBS Counts
data
smooth approximation
Co
1540
1560
1580
1600
1620
Channel

$$\vec{D} = \mathbf{A}\vec{f} + \vec{n}_d$$

now: apparatus function $\mathbf{A}$ also noise corrupted: $\tilde{\mathbf{A}}$

$$p\left(\vec{D}|\vec{f},\mathbf{A},\vec{\sigma},I\right) = \exp\left\{-\frac{1}{2}\sum_i \left(\frac{D_i - \sum_k a_{ik}f_k}{\sigma_i}\right)^2\right\} / Z_L$$

$$p\left(\vec{D}|\vec{f},\tilde{\mathbf{A}},\vec{\sigma},\delta,I\right) = \int \mathrm{d}a_{ik}\, p\left(\mathbf{A}|\tilde{\mathbf{A}},\delta,I\right) p\left(\vec{D}|\mathbf{A},\vec{f},\vec{\sigma},I\right)$$

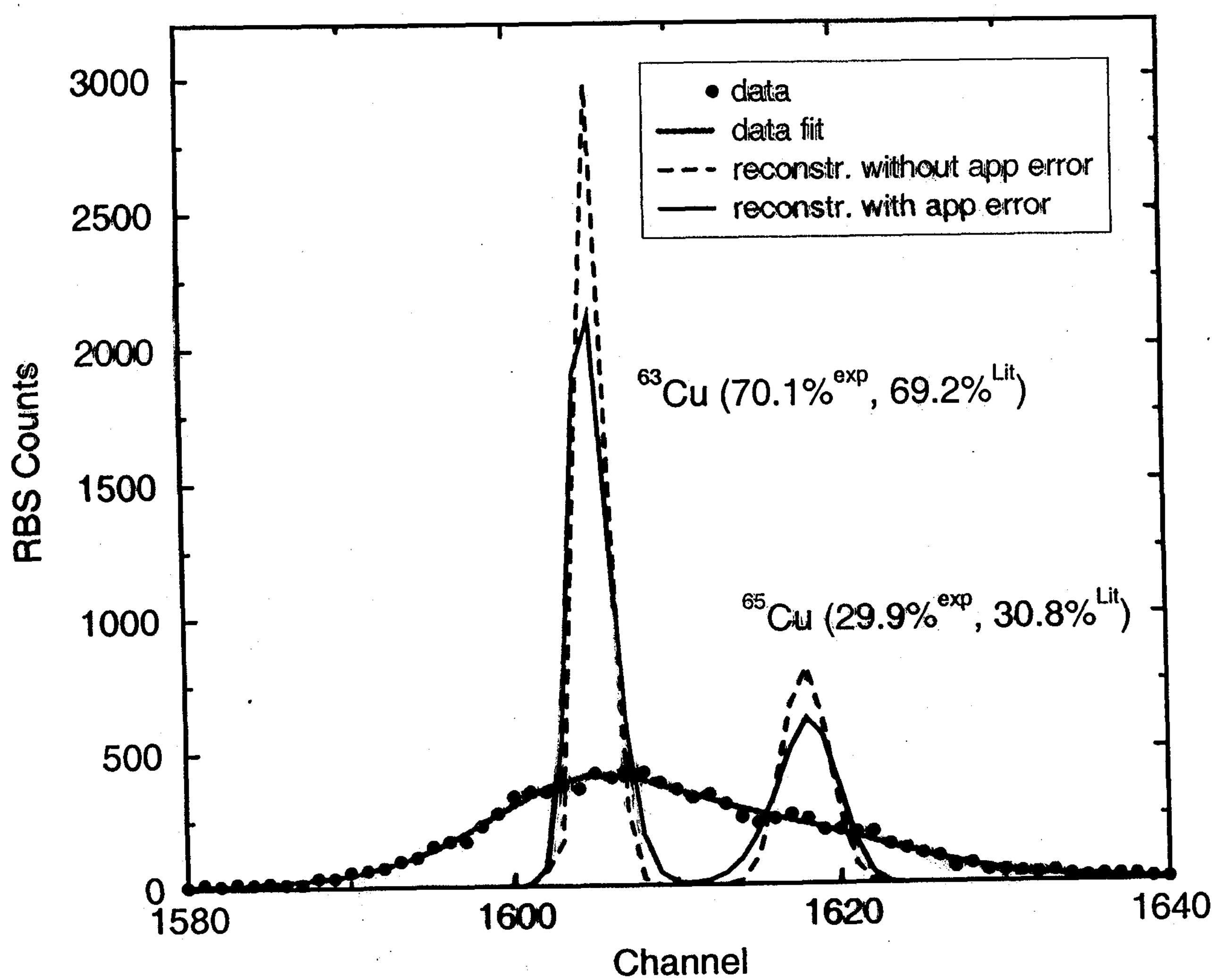
$$p\left(\mathbf{A}|\tilde{\mathbf{A}},\delta,I\right) = \exp\left\{-\frac{1}{2}\sum_{i,k}\left(\frac{a_{ik}-\tilde{a}_{ik}}{\delta_{ik}}\right)^2\right\} / Z_P$$

$$p\left(\vec{D}|\vec{f},\tilde{\mathbf{A}},\delta,\vec{\sigma},I\right) = \exp\left\{-\frac{1}{2}\sum_i \frac{\left[D_i - \left(\tilde{\mathbf{A}}\vec{f}\right)_i\right]^2}{\sigma_i^2 + \sum_k f_k^2\delta_{ik}^2}\right\} / Z$$

$$\Sigma_i^2 = \underbrace{\sigma_i^2}_{\text{measurement of data D}} + \underbrace{\sum_k f_k^2\delta_{ik}^2}_{\text{measurement of apparatus function }\tilde{\mathbf{A}}}$$

measurement of data D

measurement of apparatus function $\tilde{\mathbf{A}}$



data
data fit
reconstr. without app error
reconstr. with app error
63Cu (70.1%exp, 69.2%Lit)
65Cu (29.9%exp, 30.8%Lit)
RBS Counts
0
500
1000
1500
2000
2500
3000
1580
1600
1620
1640
Channel

Convolution theorem

$$h(E) = \int f\left(E'\right) A\left(E - E'\right) \mathrm{d}E'$$

$$M^n(h) = \int E^n h(E) \mathrm{d}E = \int E^n \mathrm{d}E \int f\left(E'\right) A\left(E - E'\right) \mathrm{d}E'$$

$$\text{Let } E = E' + y \rightarrow E^n = \sum_{i=0}^{n} \binom{n}{i} y^i (E')^{n-i}$$

$$M^n(h) = \sum_{i=0}^{n} \binom{n}{i} M^i(A) M^{n-i}(f)$$

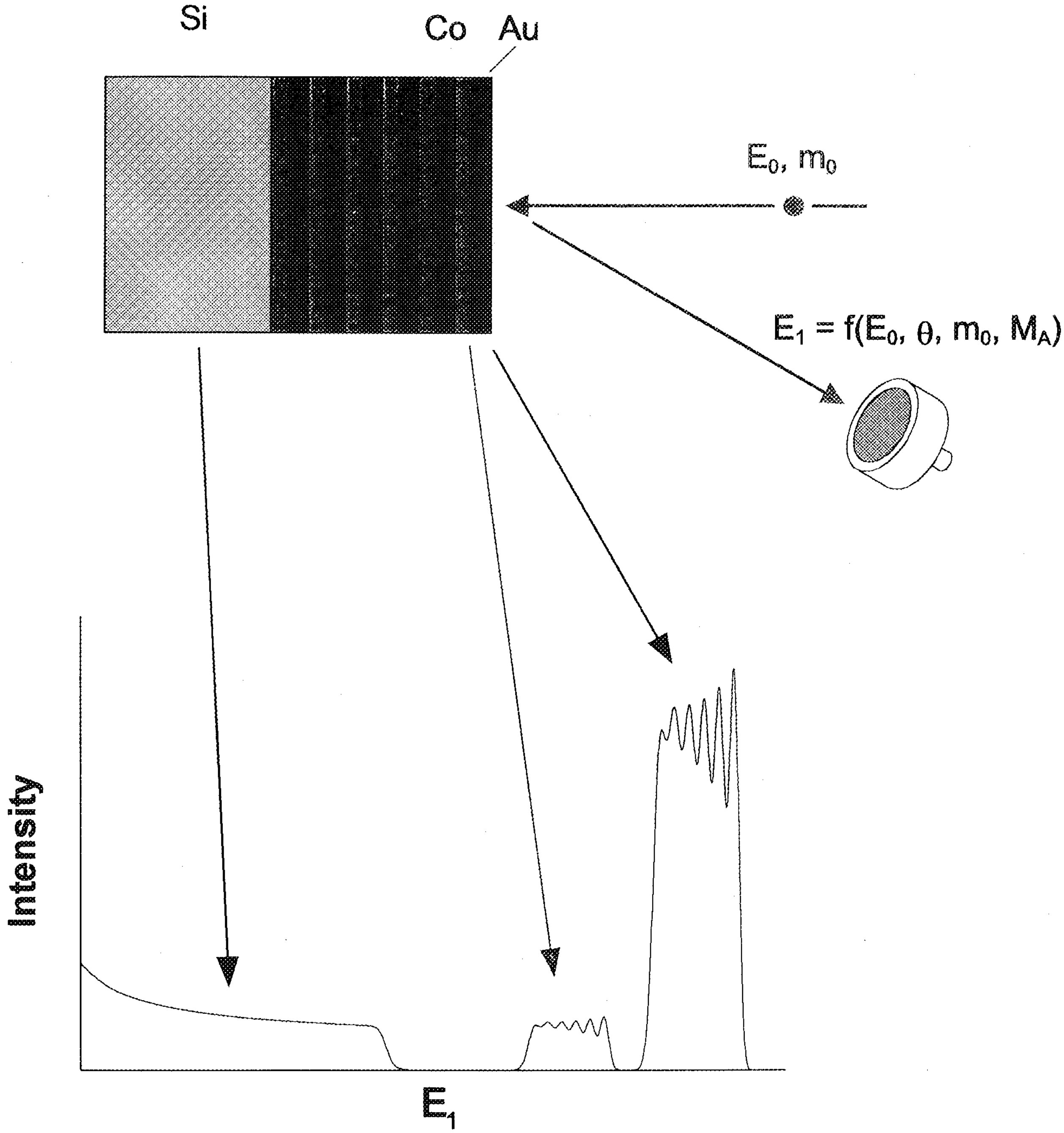
normalized functions, centred moments:

$$\mathrm{var}(h) = \mathrm{var}(A) + \mathrm{var}(f)$$

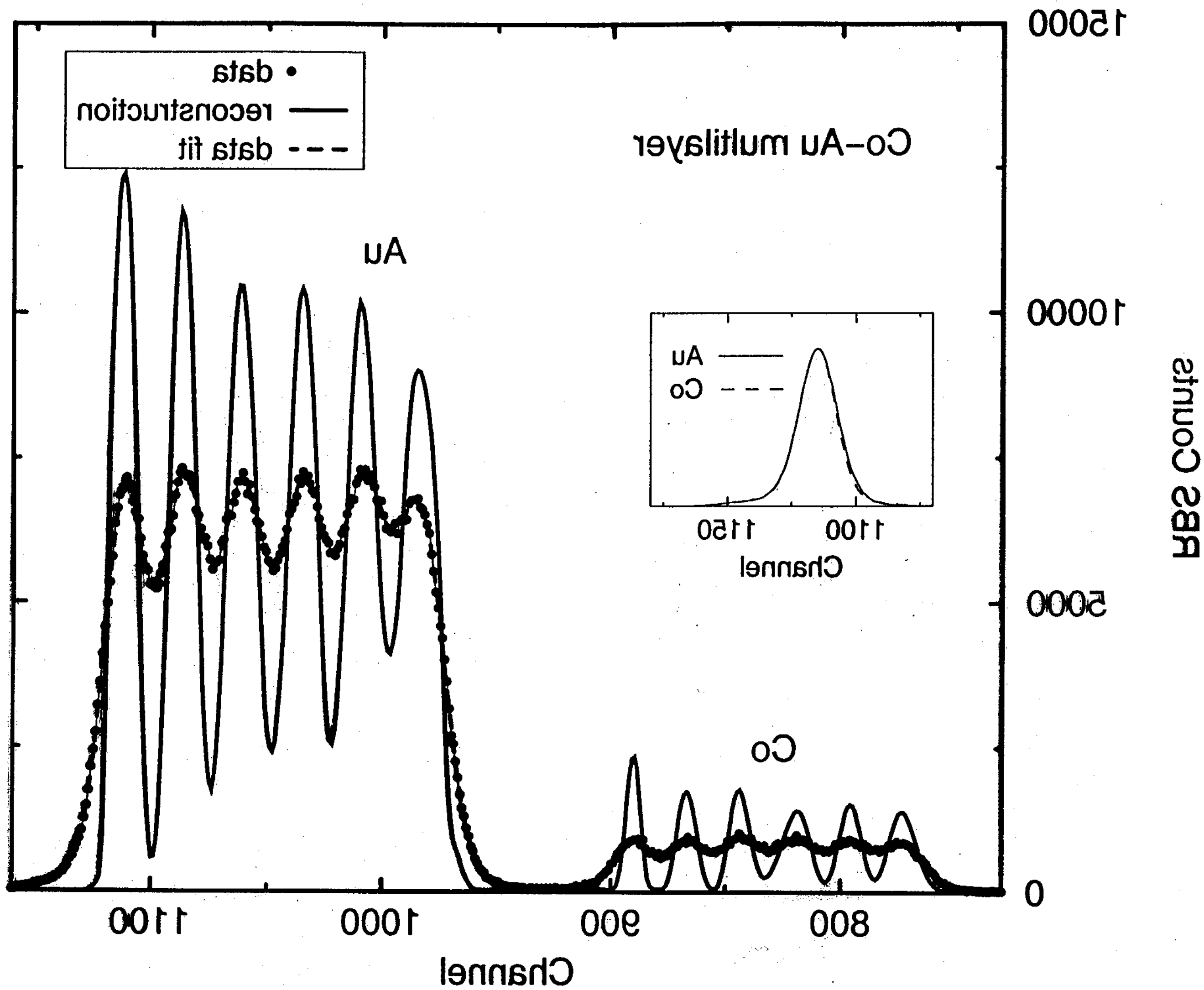
let width of image $f \approx \alpha \cdot$ (width of measurement h), $\alpha < 1$:

$$\mathrm{var}(h) = \mathrm{var}(A) + \alpha^2 \mathrm{var}(h)$$

$$\frac{\mathrm{width}(A)}{\mathrm{width}(h)} = \sqrt{1 - \alpha^2} = \begin{cases} 0.986, \alpha = \frac{1}{6} \\ 0.992, \alpha = \frac{1}{8} \end{cases}$$



Si
Co
Au
E_0, m_0
$E_1 = f(E_0, \theta, m_0, M_A)$
Intensity
E_1



Co–Au multilayer
data
reconstruction
data fit
Au
Co
RBS Counts
Channel
0
5000
10000
15000
1100
1000
900
800
Au
Co
1150
1100
Channel