Practicalities of Muon Data Analysis

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ISIS Muon Training Course

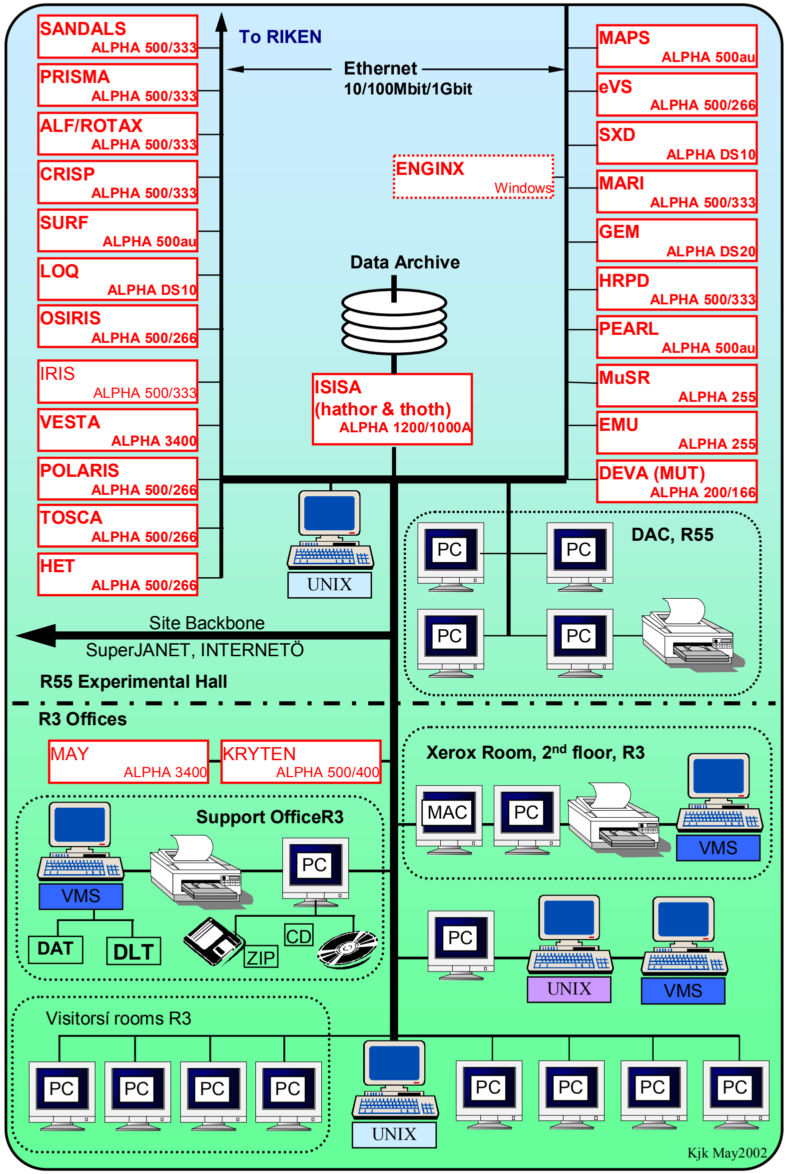
February 2005

Outline of Talk

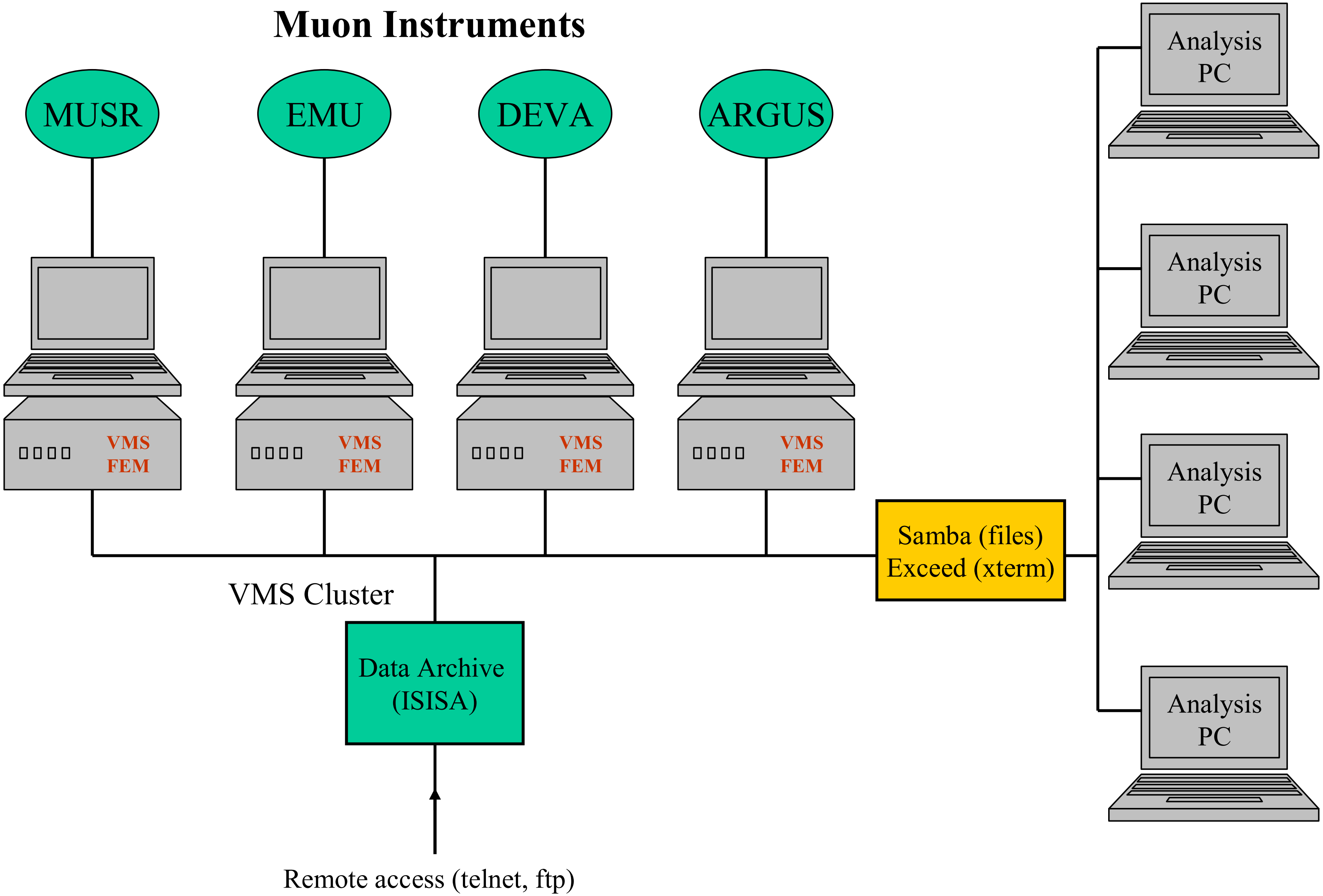
Computing infrastructure at ISIS

- Network organisation
- Front-end and data analysis machines
- Instrument control programs
- Data formats and data access

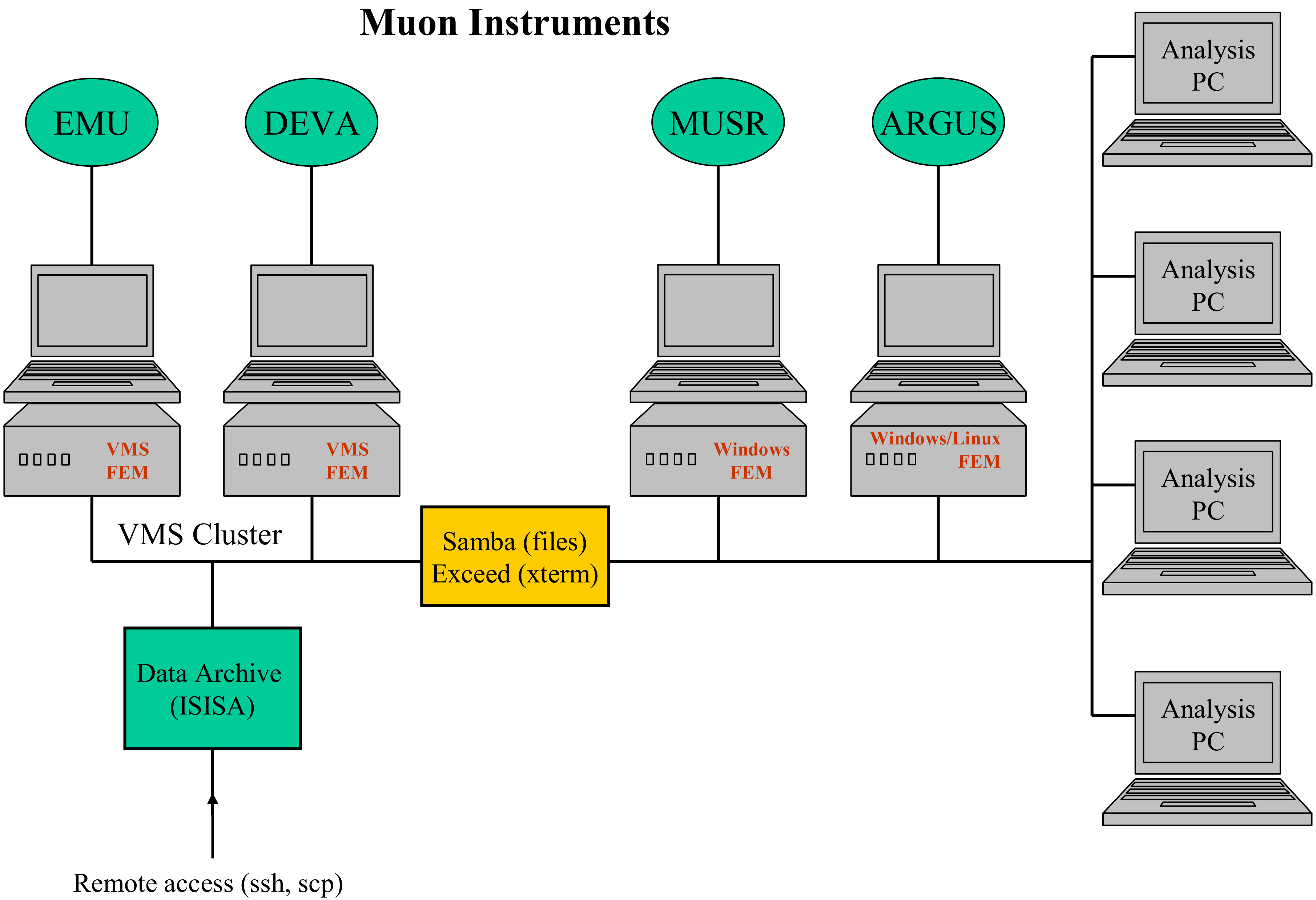
ISIS Computing (2002)



Original ISIS μSR Computing Layout



Current ISIS µSR Computing Layout



Using the ISIS Computers

- VMS alpha cluster

  Login to ISISA from an x-terminal window, use the account details available at each instrument

- Individual PCs

  Login as user: isiscnc\muontc (isismuonstc)

ISIS Computing Support can be contacted by emailing

support@isise.rl.ac.uk or ISISsupport@rl.ac.uk

or by phoning extension 1763

Using Personal Laptops at ISIS

Connecting Laptops at ISIS

Visitors to ISIS are welcome to connect their laptop to our network in the R70 hostel as well as the R55 experimental hall and R3 Offices. The ISIS internet connection is behind the CCLRC site firewall, which allows most connections going out, but connections coming in are restricted.

Physical Connections

Network sockets are available in all instrument cabins and public areas. Wireless access is also available in many parts of the R55 experimental hall (not in the MUSR or ARGUS cabins though).

IP address

IP addresses are allocated automatically using DHCP. Please set your network settings to use DHCP and reboot (if you have fixed settings for your home institution it may be worth recording their values)

Mail

Receiving mail should work immediately. Sending SMTP mail needs to go out through **outbox.rl.ac.uk**
Access to web based email will work once a proxy server has been configured.

Web

Web access off site needs to go through a proxy server. Set your browser to use the automatic configuration script **http://wwwcache.rl.ac.uk/proxy.pac**

Printers

Access to certain printers is enabled. Please ask your local contact for information on connecting to your nearest printer.

Remote Access

- All external access is via ISISA (isisa.rl.ac.uk)
  (use ssh for terminal login
  and scp for file copying)

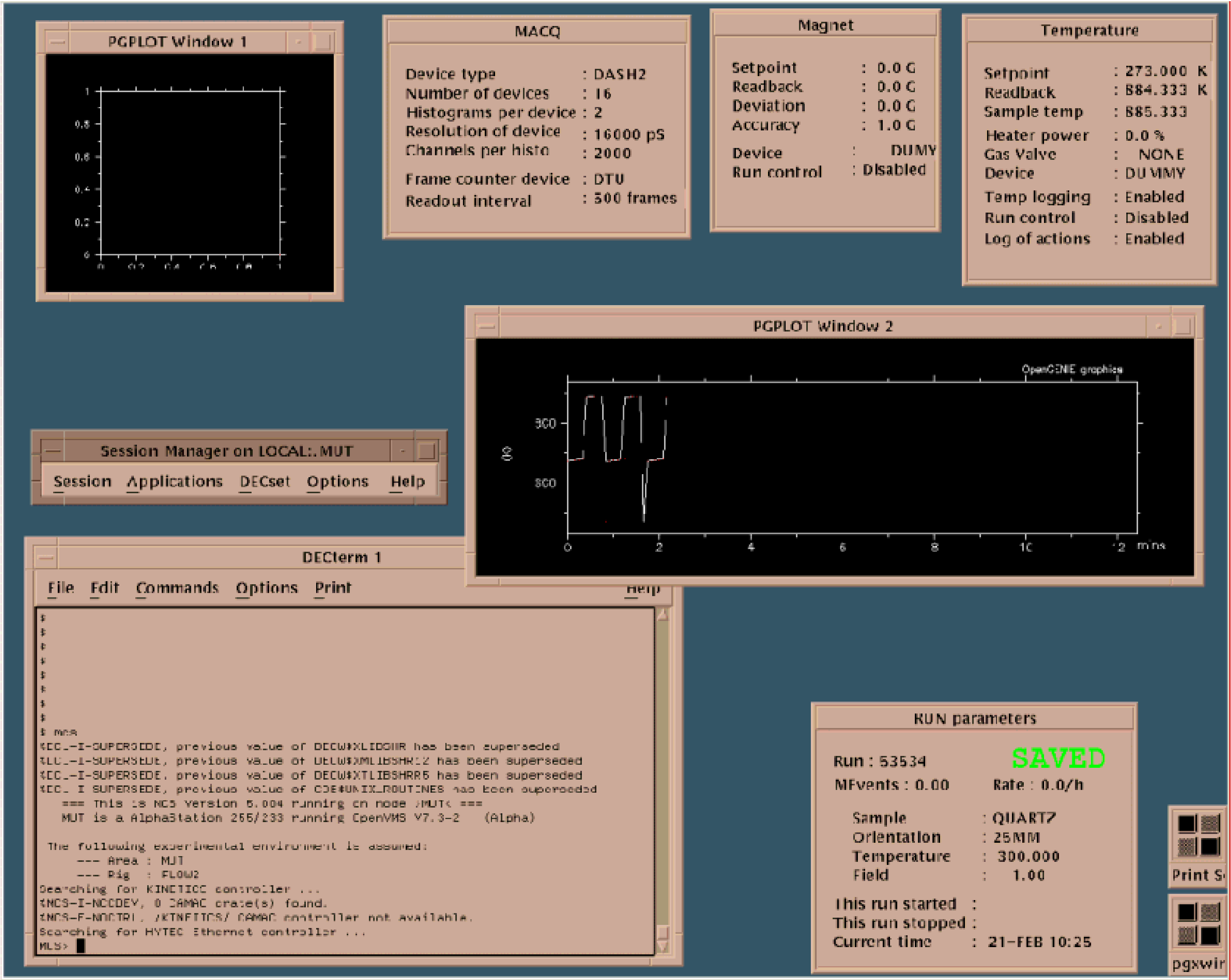
- A unified Data Portal covering all of the CLRC Facility data is under development

Data Acquisition Control Systems

Currently we have three different systems:

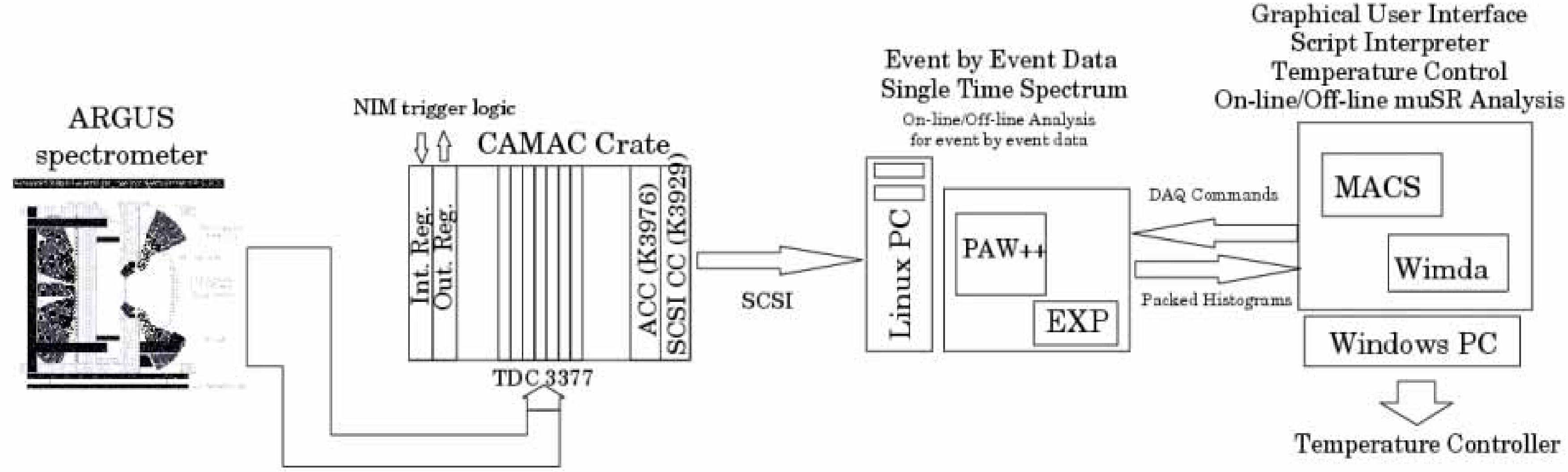
MCS	The original VMS-based system (EMU, DEVA)
MACS	PC-based system (ARGUS, 2002 on)
SECI	PC-based system (MUSR, 2004 on)

MCS



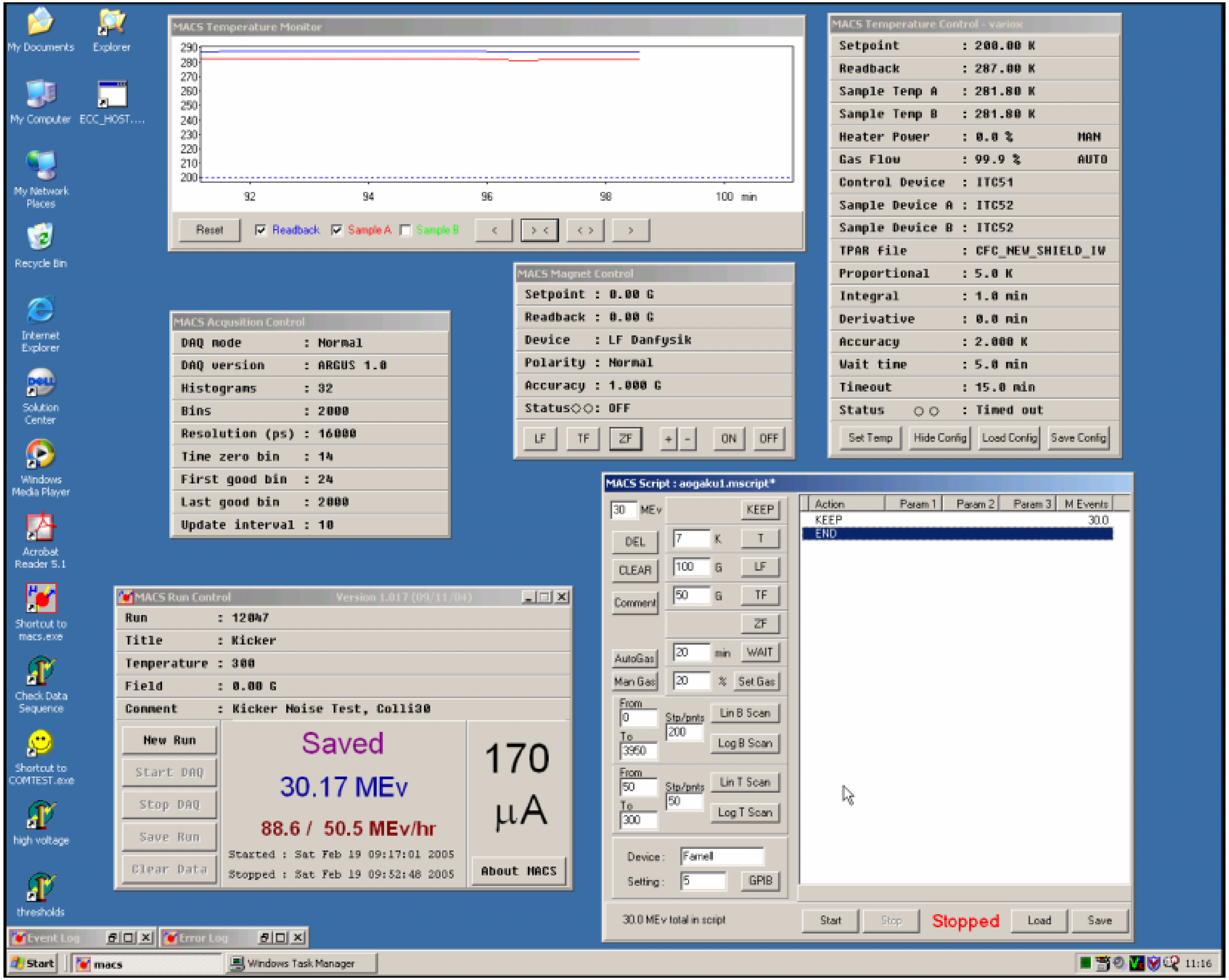
PGPLOT Window 1
MACQ
Device type : DASH2
Number of devices : 16
Histograms per device : 2
Resolution of device : 16000 pS
Channels per histo : 2000
Frame counter device : DTU
Readout interval : 500 frames
Magnet
Setpoint : 0.0 G
Readback : 0.0 G
Deviation : 0.0 G
Accuracy : 1.0 G
Device : DUMY
Run control : Disabled
Temperature
Setpoint : 273.000 K
Readback : 884.333 K
Sample temp : 885.333
Heater power : 0.0 %
Gas Valve : NONE
Device : DUMMY
Temp logging : Enabled
Run control : Disabled
Log of actions : Enabled
PGPLOT Window 2
OpenGENIE graphics
mins
Session Manager on LOCAL::MUT
Session Applications DECset Options Help
DECterm 1
File Edit Commands Options Print Help
$ mcs
MUT is a AlphaStation 255/233 running OpenVMS V7.3-2 (Alpha)
The following experimental environment is assumed:
--- Area : MUT
--- Rig : FLOW2
Searching for KINETICS controller ...
Searching for HYTEC Ethernet controller ...
MCS>
RUN parameters
Run : 53534
SAVED
MEvents : 0.00
Rate : 0.0/h
Sample : QUARTZ
Orientation : 25MM
Temperature : 300.000
Field : 1.00
This run started :
This run stopped :
Current time : 21-FEB 10:25
Print S
pgxwir

MACS



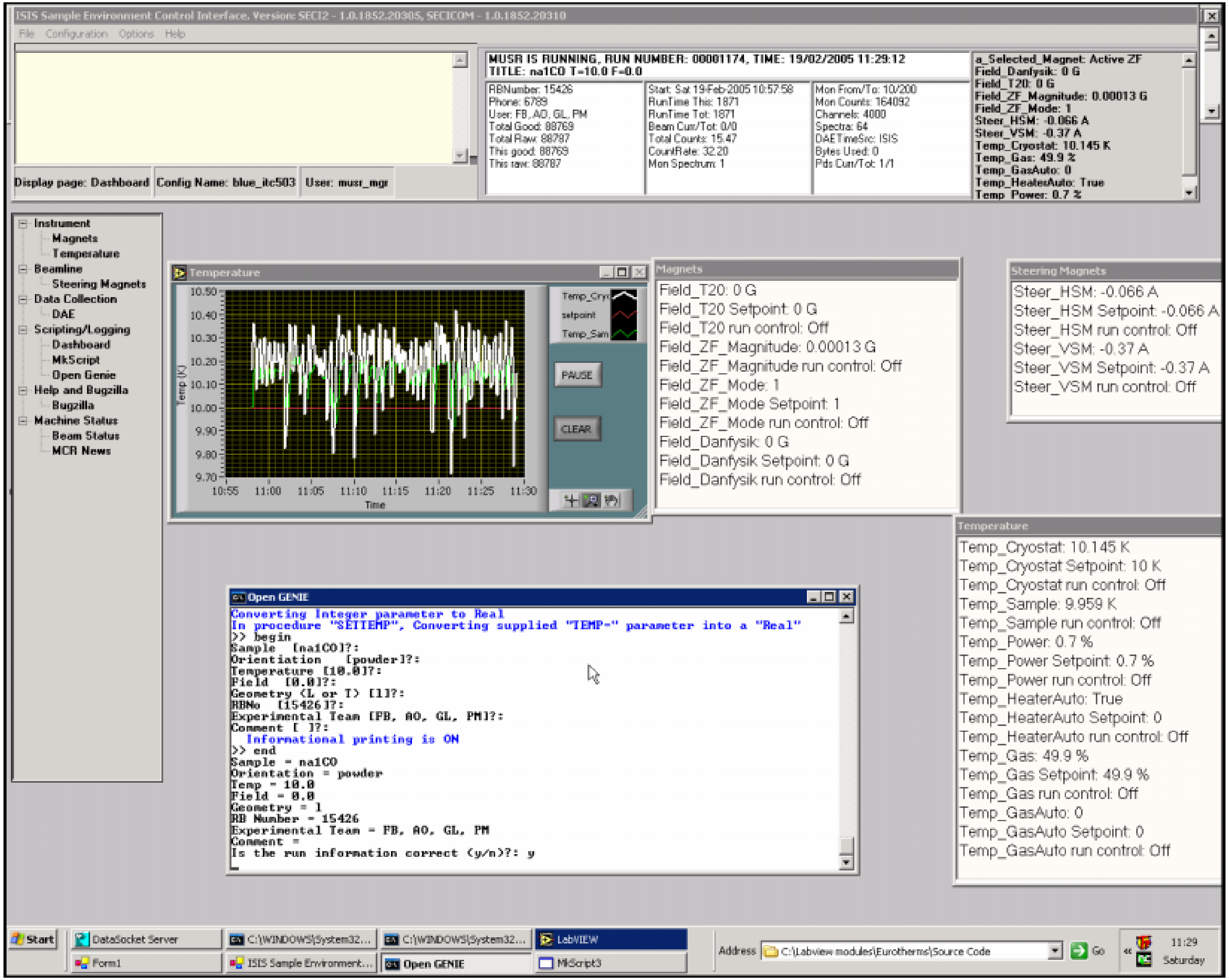
Hybrid Linux/Windows system

MACS



MACS Temperature Monitor
Reset
Readback
Sample A
Sample B
MACS Temperature Control - variox
Setpoint : 200.00 K
Readback : 287.00 K
Sample Temp A : 281.80 K
Sample Temp B : 281.80 K
Heater Power : 0.0 % MAN
Gas Flow : 99.9 % AUTO
Control Device : ITC51
Sample Device A : ITC52
Sample Device B : ITC52
TPAR file : CFC_NEW_SHIELD_IV
Proportional : 5.0 K
Integral : 1.0 min
Derivative : 0.0 min
Accuracy : 2.000 K
Wait time : 5.0 min
Timeout : 15.0 min
Status : Timed out
Set Temp
Hide Config
Load Config
Save Config
MACS Magnet Control
Setpoint : 0.00 G
Readback : 0.00 G
Device : LF Danfysik
Polarity : Normal
Accuracy : 1.000 G
Status : OFF
MACS Acquisition Control
DAQ mode : Normal
DAQ version : ARGUS 1.0
Histograms : 32
Bins : 2000
Resolution (ps) : 16000
Time zero bin : 14
First good bin : 24
Last good bin : 2000
Update interval : 10
MACS Run Control
Run : 12047
Title : Kicker
Temperature : 300
Field : 0.00 G
Comment : Kicker Noise Test, Colli30
New Run
Start DAQ
Stop DAQ
Save Run
Clear Data
Saved
30.17 MEv
88.6 / 50.5 MEv/hr
Started : Sat Feb 19 09:17:01 2005
Stopped : Sat Feb 19 09:52:48 2005
170 µA
About MACS
MACS Script : aogaku1.mscript*
Action
Param 1
Param 2
Param 3
M Events
KEEP 30.0
END
30.0 MEv total in script
Start
Stop
Stopped
Load
Save

SECI



ISIS Sample Environment Control Interface. Version: SECI2 - 1.0.1852.20305, SECICOM - 1.0.1852.20310
File Configuration Options Help
MUSR IS RUNNING, RUN NUMBER: 00001174, TIME: 19/02/2005 11:29:12
TITLE: na1CO T=10.0 F=0.0
Display page: Dashboard
Config Name: blue_itc503
User: musr_mgr
Instrument
Magnets
Temperature
Beamline
Steering Magnets
Data Collection
DAE
Scripting/Logging
Dashboard
MkScript
Open Genie
Help and Bugzilla
Bugzilla
Machine Status
Beam Status
MCR News
Temperature
Time
PAUSE
CLEAR
Magnets
Field_T20: 0 G
Field_T20 Setpoint: 0 G
Field_T20 run control: Off
Field_ZF_Magnitude: 0.00013 G
Field_ZF_Magnitude run control: Off
Field_ZF_Mode: 1
Field_ZF_Mode Setpoint: 1
Field_ZF_Mode run control: Off
Field_Danfysik: 0 G
Field_Danfysik Setpoint: 0 G
Field_Danfysik run control: Off
Steering Magnets
Steer_HSM: -0.066 A
Steer_HSM Setpoint: -0.066 A
Steer_HSM run control: Off
Steer_VSM: -0.37 A
Steer_VSM Setpoint: -0.37 A
Steer_VSM run control: Off
Temperature
Temp_Cryostat: 10.145 K
Temp_Cryostat Setpoint: 10 K
Temp_Cryostat run control: Off
Temp_Sample: 9.959 K
Temp_Sample run control: Off
Temp_Power: 0.7 %
Temp_Power Setpoint: 0.7 %
Temp_Power run control: Off
Temp_HeaterAuto: True
Temp_HeaterAuto Setpoint: 0
Temp_HeaterAuto run control: Off
Temp_Gas: 49.9 %
Temp_Gas Setpoint: 49.9 %
Temp_Gas run control: Off
Temp_GasAuto: 0
Temp_GasAuto Setpoint: 0
Temp_GasAuto run control: Off
Open GENIE
Converting Integer parameter to Real
In procedure "SETTEMP", Converting supplied "TEMP=" parameter into a "Real"
>> begin
Sample = na1CO
Orientation = powder
Temp = 10.0
Field = 0.0
Geometry = 1
RB Number = 15426
Experimental Team = FB, AO, GL, PM
Is the run information correct (y/n)?: y
Start
DataSocket Server
LabVIEW
Open GENIE
MkScript3

Data Formats for Muon Data

- MCS VMS Fortran binary (mangled by VMS ftp!)
- MACS standard binary
- SECI NeXus: hierarchical, extendable format

Typical run file is 200-600 kb in size

Data compression reduces the size by up to a factor of 7

(bzip2 is the most efficient zip algorithm for muon data)

NeXus

The NeXus hierarchical data format has three components:

A set of subroutines

to make it easy to read and write NeXus files

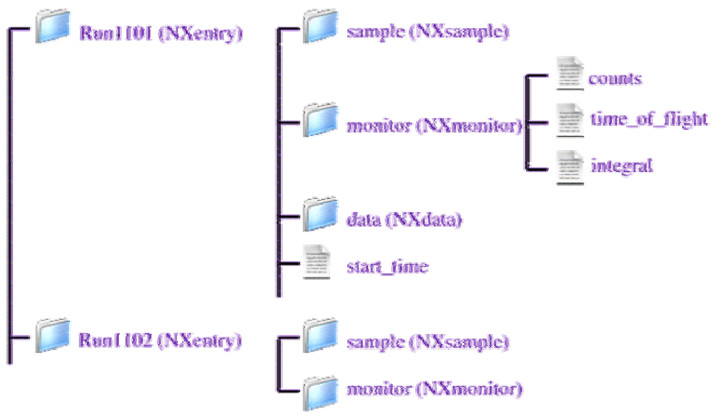
A set of design principles

to help people understand what is in them

A set of instrument definitions

to allow the development of more portable analysis software

Example part of data structure:



NeXus webpage: www.nexus.anl.gov

ISIS muons NeXus webpage: www.isis.rl.ac.uk/muons/data analysis/nexus/intro.htm

μSR Data Formats in Use Worldwide

- PSI (Switzerland)
  - .dat (VMS binary)
  - .bin (standard binary)
- TRIUMF (Canada)
  - .tri (VMS binary)
  - .mud (hierarchical)
- KEK/JPARC (Japan)
  - .kek (VMS binary)

Finding the Muon Data

ARGUS	From the ISIS network:	\\mirch\macs\argus0005634.ral
	From ISISA:	not available
DEVA	From the ISIS network:	\\ndavms\mutdata\r20000.ral
	From ISISA:	mut$disk0:[data.mut]r20000.ral
EMU	From the ISIS network:	\\ndavms\emudata\r20000.ral
	From ISISA:	emu$disk0:[data.emu]r20000.ral
MUSR	From the ISIS network:	\\ndavms\musrdata\musr00001025.nxs
	From ISISA:	musr$disk0:[data.musr]musr00001025.nxs

Special instrument (only for the muon training course practical !)

MUONTC	From the ISIS network:	\\ndavms\muontc_data\r20000.ral
	From ISISA:	muontc$disk0:[data.muontc]r20000.ral

Temperature Logs

- Usually stored in a tlog subdirectory within the data directory.

  Same name as the data file but with extension .tlog

- NeXus files store the tlog data internally

Taking Data Away

- Copy to own laptop
- Burn CD using PC in instrument cabin
- Send to remote system back home – pushing is easier than pulling!
- Fetch using remote login from home

Retrieving Older Data

Restoring files from the ISIS Data Archive

Archiver Restore Times

Restores for last cycle within 10 minutes. Restores for relatively recent data within 1 hour.

Older runs are restored from tape starting at 10:00 am for requests placed during the previous 24hrs (excluding weekends).

Restoring RAW Files

In order to restore ISIS RAW files, simply type **RESTISIS** from the DCL command prompt.

usage:

```
RESTISIS [options] inst_name low_run high_run
```

options:

- -l is used to retrieve (T)LOG files
- -s is used to retrieve SAV files.
- -v will produce a verbose (diagnostic) output.
- -d can be used to specify a restore directory.

e.g.:

```
RESTISIS -l -d SYS$SCRATCH MUSR 12345 12350
```

Muon Data Analysis Software Used at ISIS

UDA (VMS, General Purpose)

RUMDA (VMS, General Purpose)

MESA (VMS, Maximum Entropy for TF Studies)

WiMDA (Windows, General Purpose)

many user groups have also developed their own programs

Muon Data Analysis Software Used at ISIS

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MESA (VMS, Maximum Entropy for TF Studies)

WiMDA (Windows, General Purpose) - practical session

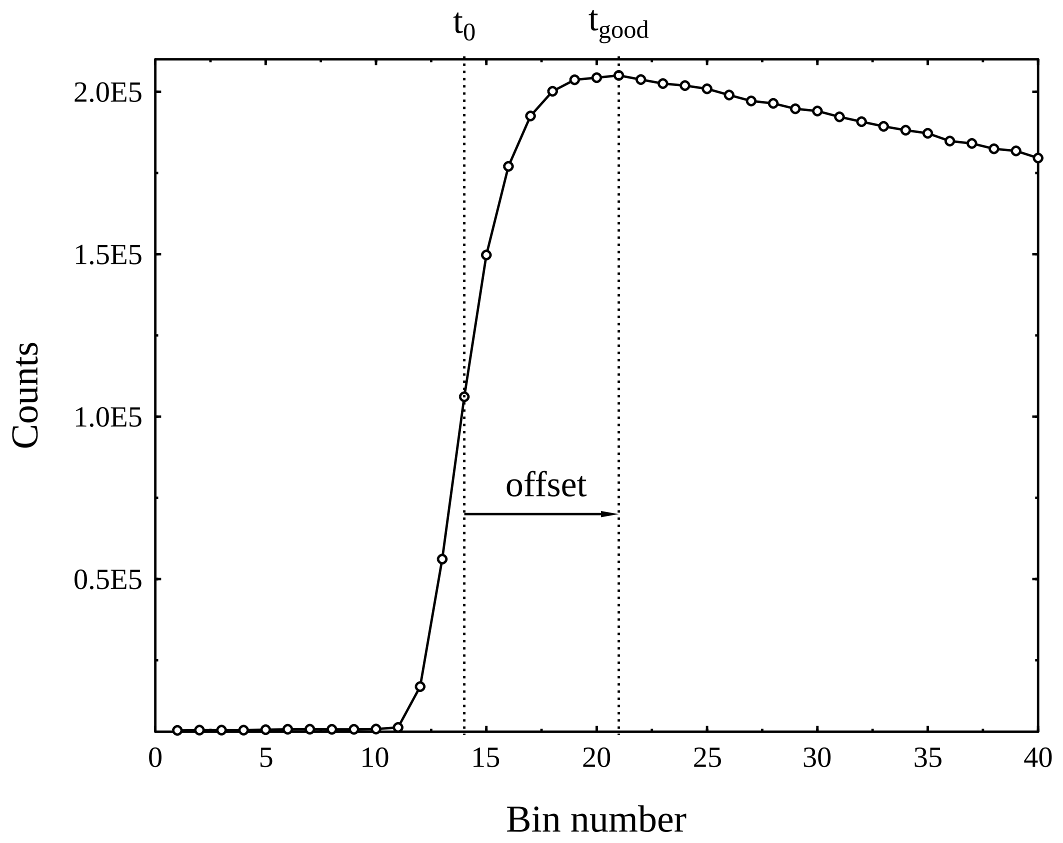
many user groups have also developed their own programs

Main Stages in Muon Data Analysis

1. Preparing the data to be analysed, 'setting up'
2. Fitting the measured asymmetry to a chosen relaxation function; 'analysing'
3. Assessing the fitted relaxation parameters, which may involve a further stage of fitting these parameters to an appropriate model; 'modeling'
4. Preparing plots of the results of analysing and modelling the data, 'plotting'

1. Setting Up the Data

a) Checking the time origin t_0 and the time of the first and last good data points



1. Setting Up the Data

b) Defining the detector grouping

e.g.

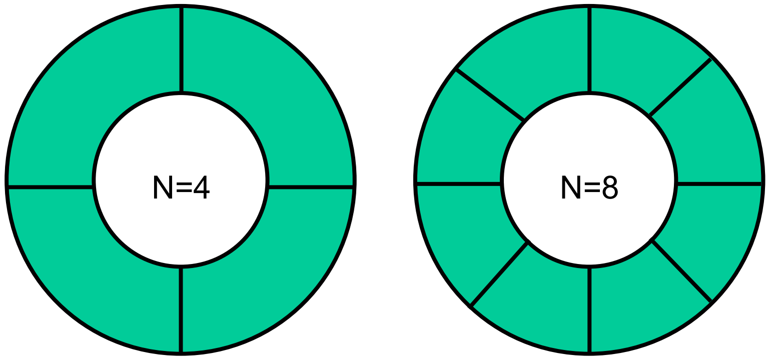
for LF/ZF :	Forward group	1-16	
	Backward group	17-32	
for TF :	Group1	1-4,	17-20
	Group2	5-8,	21-24
	Group3	9-12,	25-28
	Group4	13-16,	29-32

Notes:

ARGUS has 192 detectors (usually pregrouped to 32 histograms in the data file)

MUSR has 64 detectors (conveniently pregrouped to 32 histograms in the data analysis software)

Note that a dephasing effect will reduce the asymmetry of TF data if not enough groups are used:



Dephasing factor = $\sin(\pi/N) / (\pi/N)$

TF Groups	Dephasing Factor
16	99 %
8	98 %
4	90 %
2	64 %

i.e. 8 TF groups are sufficient for most purposes

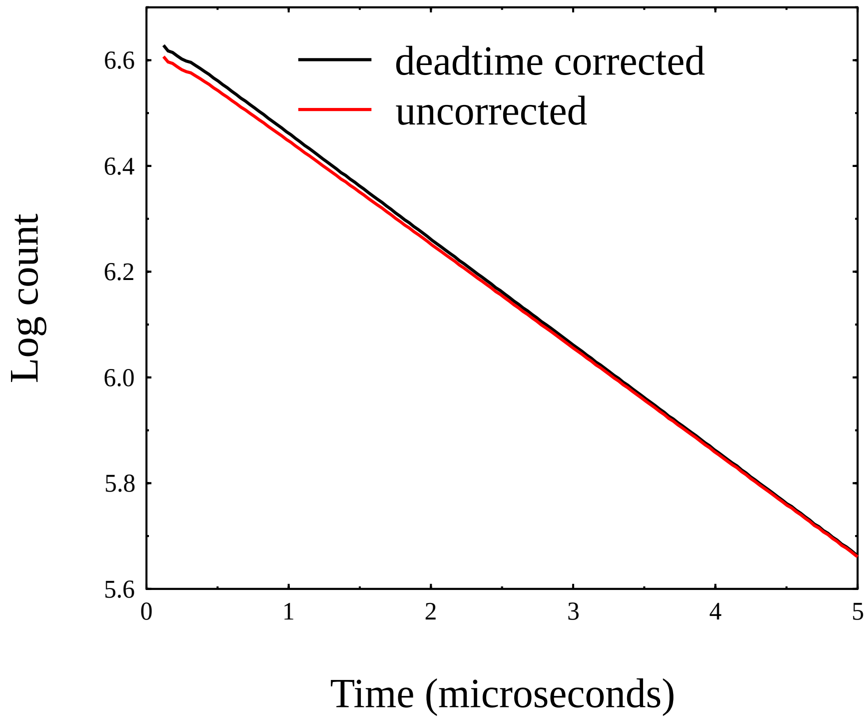
c) Corrrection for counting loss due to counter deadtime

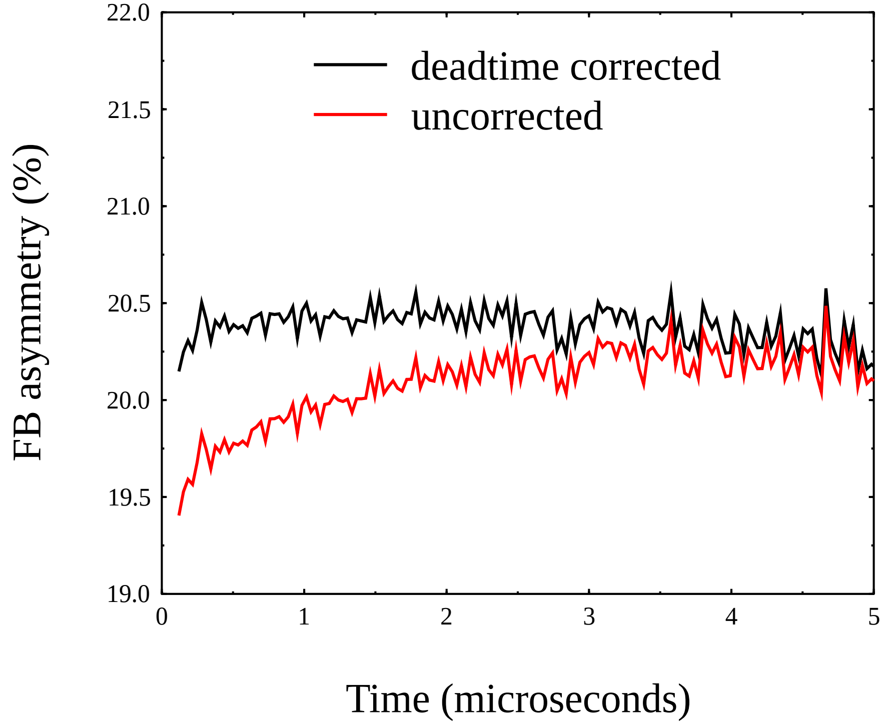
characterised by a deadtime τ for each detector channel, typically $\tau \sim 10$ ns

deadtimes for particular instruments are obtained from high statistics calibration runs using Ag

data rate correction to the observed rate r_{ob} is applied to give the true rate r

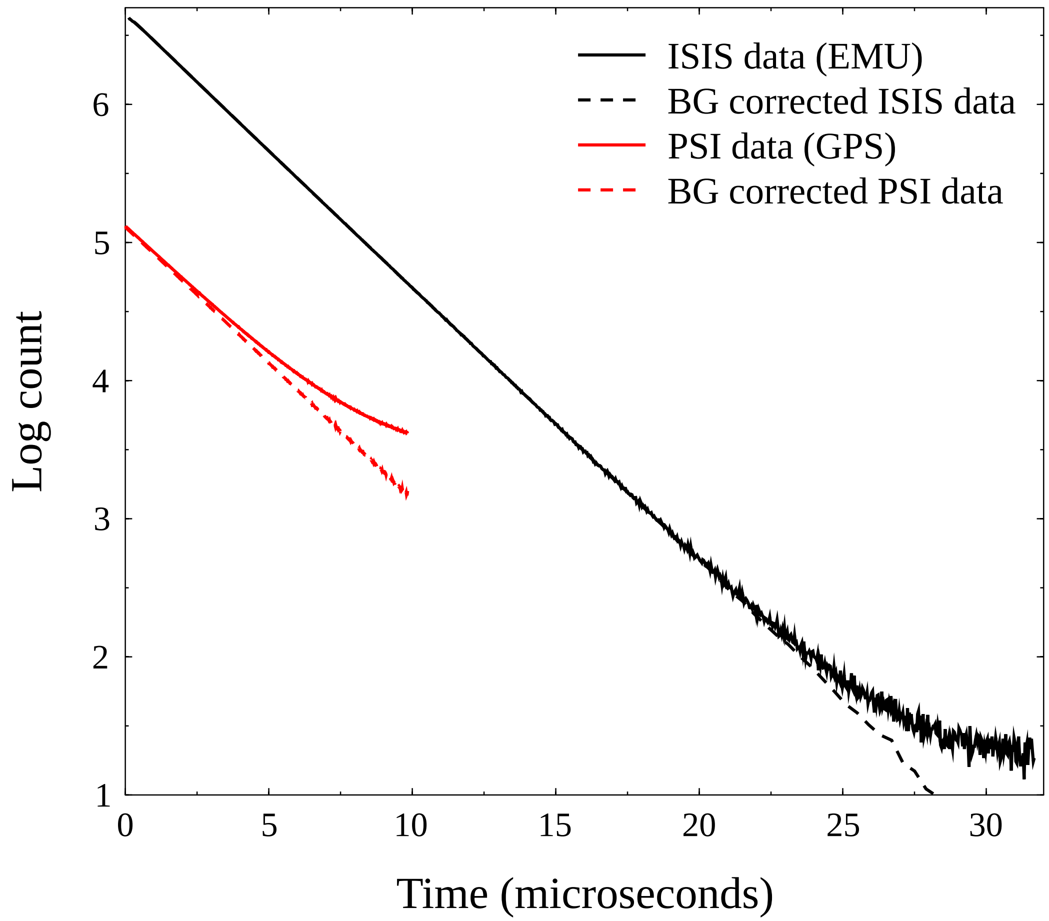
the simplest form of correction is $r = r_{ob} / (1 - r_{ob}\tau)$





d) Correction for steady background count rate

can be included as part of the fitting procedure



e) Choice of binning:

The standard raw time bin for ISIS data is 16 ns. It is often useful to choose to increase the bin size for data analysis

bin width :	tradeoff between number of points and fitting speed
	allows separate focus on fast and slow parts of the relaxation
fixed/variable:	variable binning compensates for the deteriorating signal-to-noise at longer times
	best to keep to fixed binning for weakly damped oscillations, e.g. TF studies

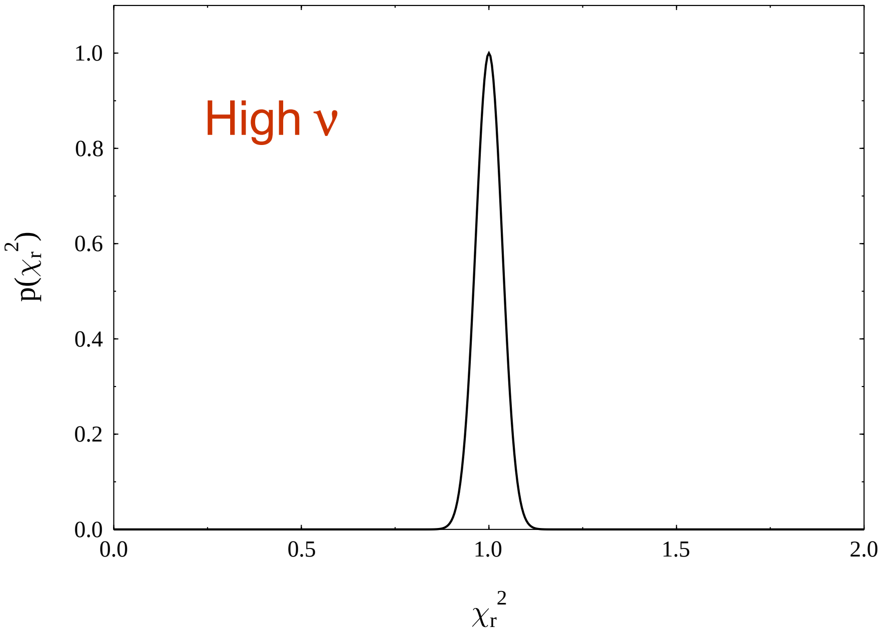
2. Analysing the Relaxation

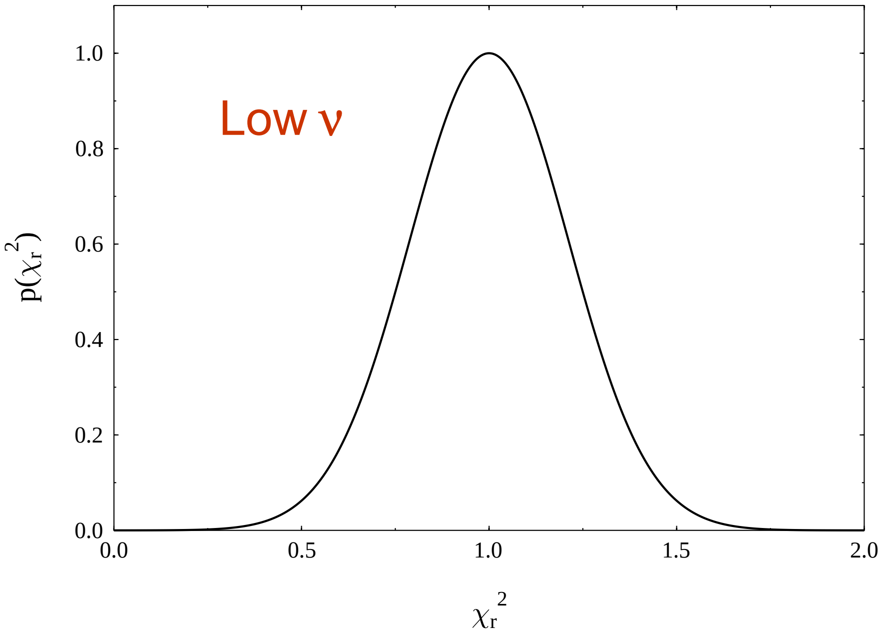
- Try fitting to possible alternative relaxation functions
- Look for systematic deviations of the fit from the data ñ are additional relaxation components needed?
- Use the reduced chi-squared χ_r^2 to judge the quality of the fit and appropriateness of the model

$$\chi_r^2 = \sum_{i=1}^{N} \left(\frac{y_i - y(x_i; p_1, p_2 .. p_m)}{\sigma_i} \right)^2 \Big/ (N - m)$$

N-m = ν is the number of degrees of freedom

Expected standard error of χ_r^2 is $(2/\nu)^{1/2}$





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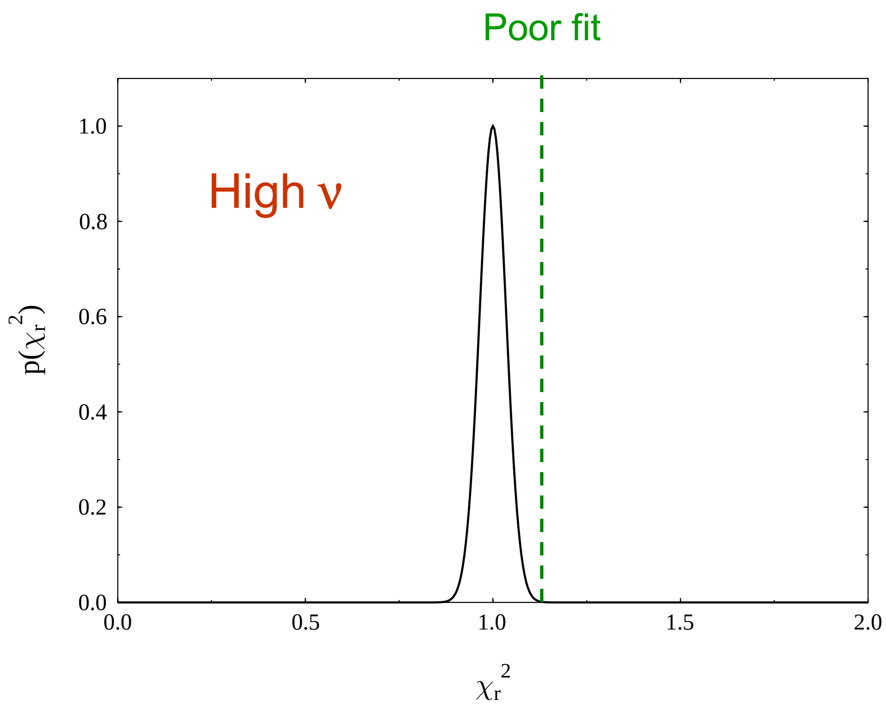

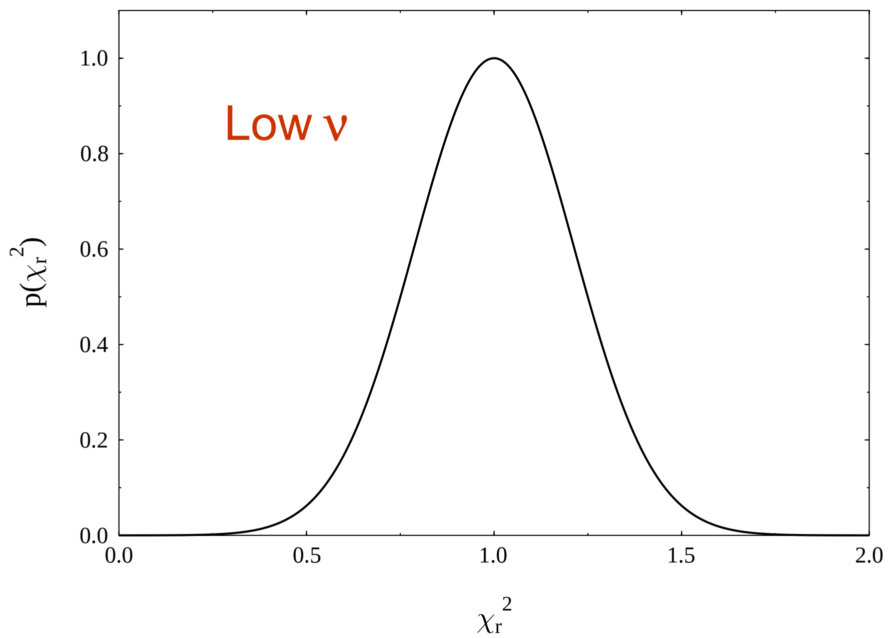

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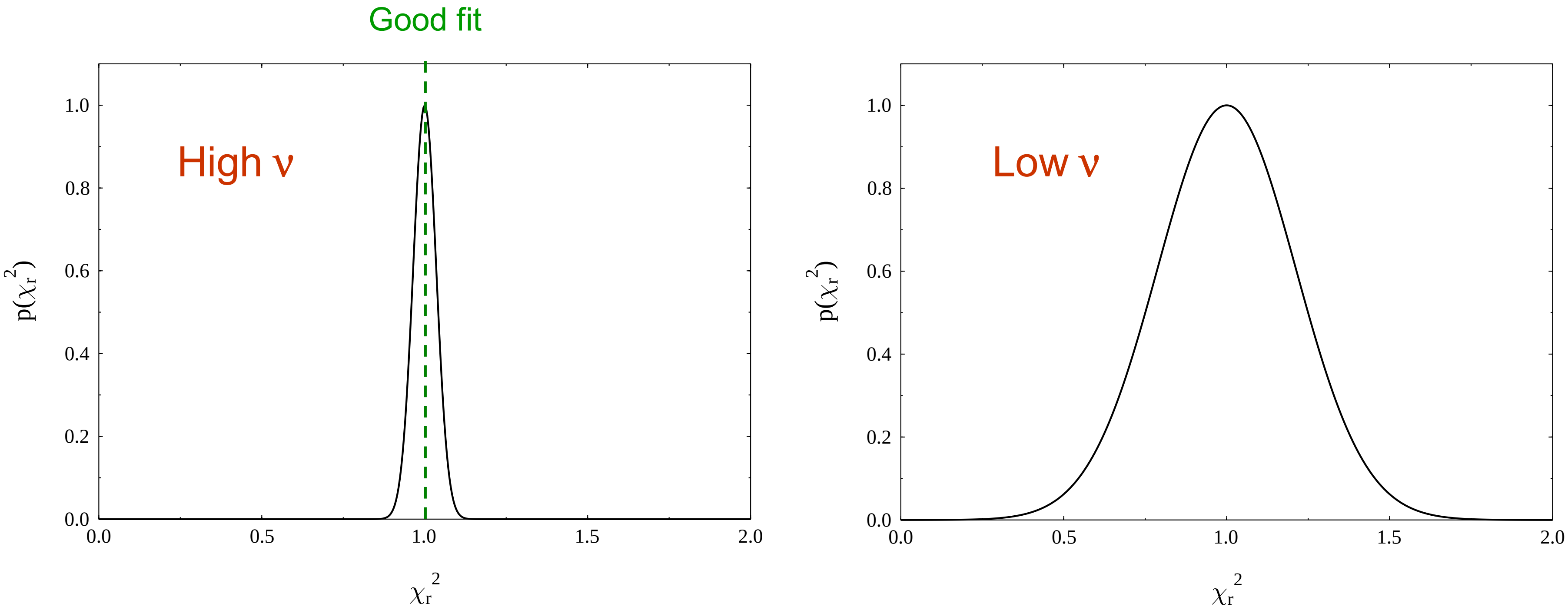

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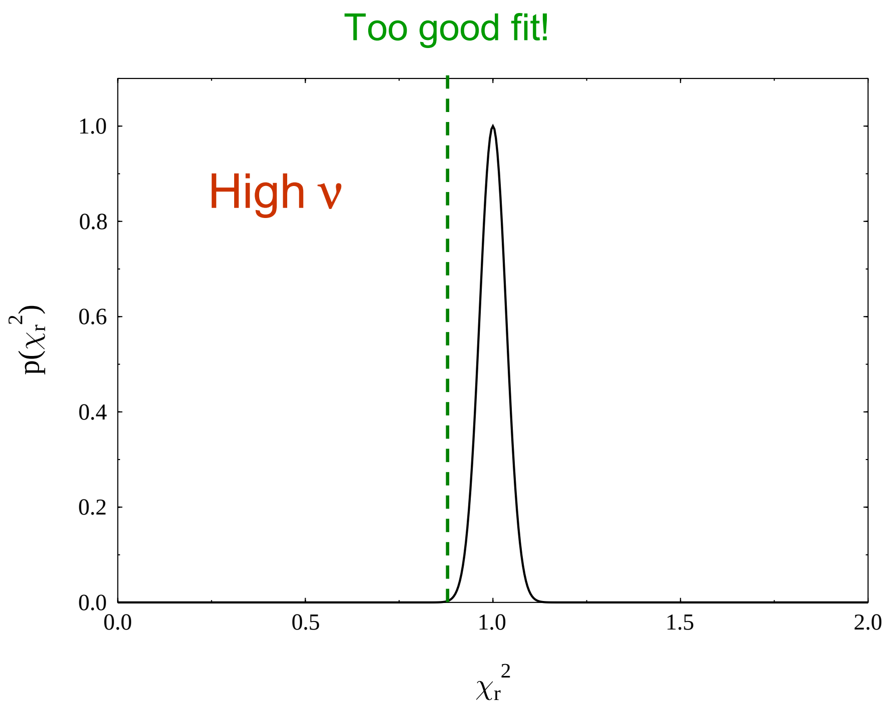

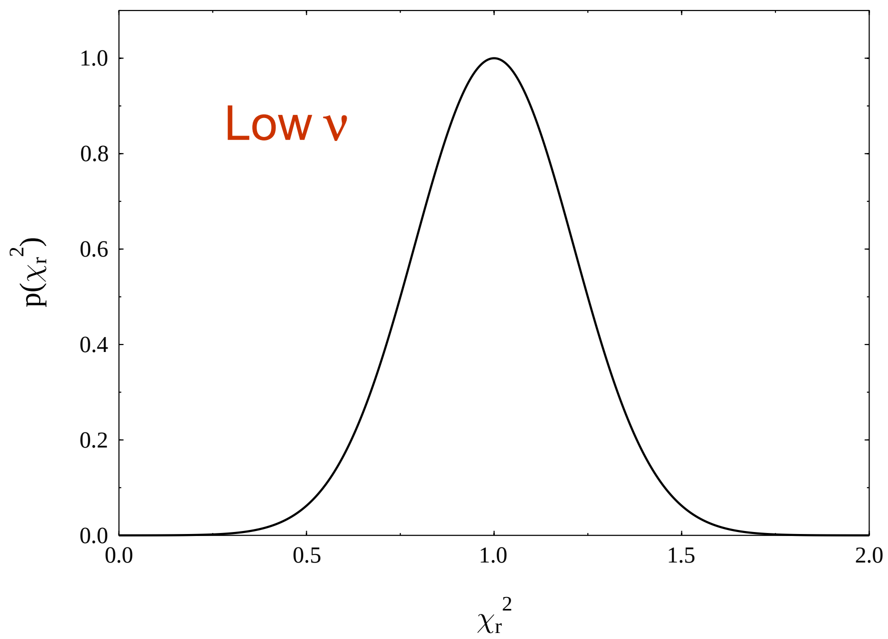

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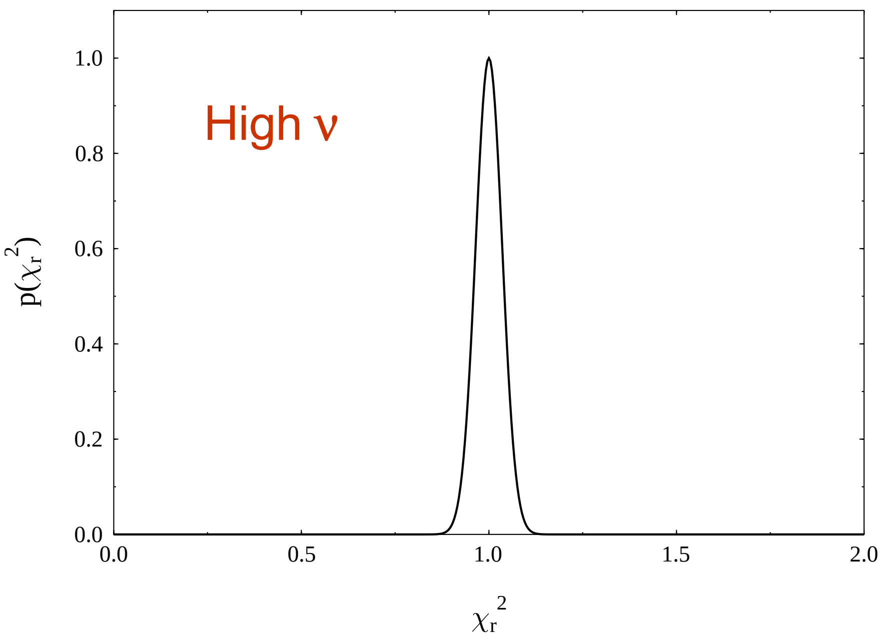
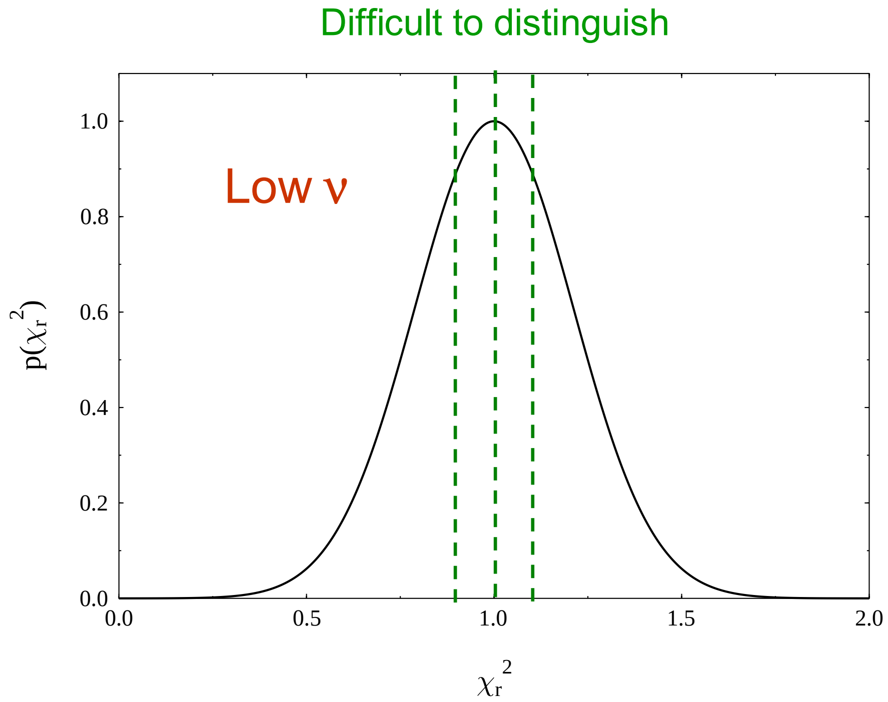




3. Modelling Fitted Parameter Sets

- A further stage of fitting involves modelling the fitted parameters for a related set of runs:

  e.g. following the temperature dependence of a
  precession frequency within a magnetic phase

  or fitting the field dependence of a relaxation rate to
  an appropriate model

4. Plotting the Results

Close integration with the fitting process is desirable for rapid feedback on:

the data quality

the state of the analysis

the progress of the experiment

WiMDA/GLE	used in the data analysis workshop
Origin	popular general-purpose Windows plotting package

Analysis of Complex Rotation Spectra

1. Fourier and All Poles transforms
2. Maximum Entropy spectral analysis
3. Time domain analysis versus frequency domain analysis

Fourier and All-Poles Transforms

FFT (Fast Fourier Transform) is the standard way to convert from time domain to frequency domain.

FFT assumes frequency spectrum is well represented by array of evenly spaced points, which works well for spectra containing broad spectral features.

However, if the spectrum contains very narrow features, other types of frequency transform can work better.

The All-Poles (maxent) method is one such method, which makes an expansion of the data in terms of a series of sharp frequencies

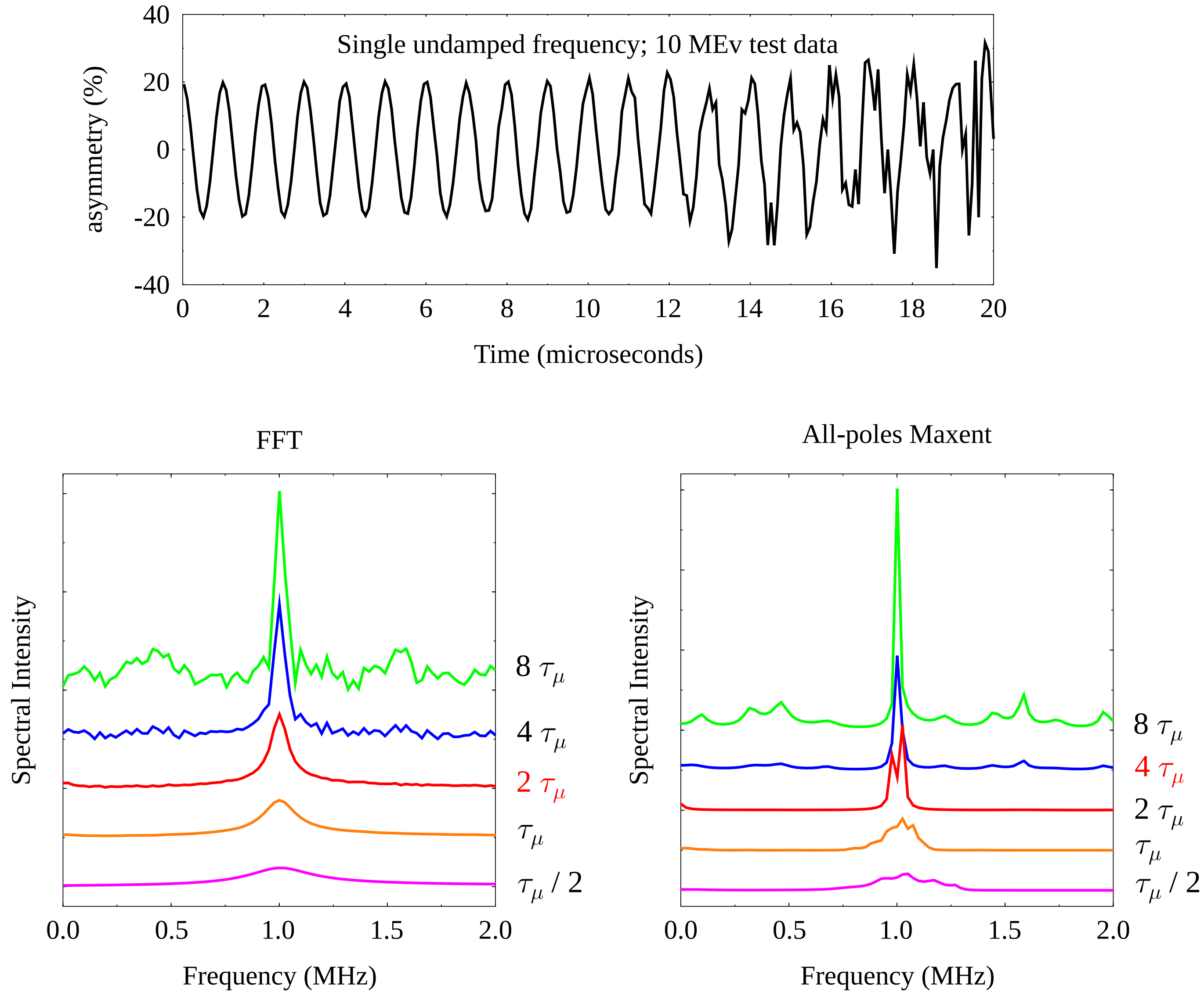
See Press et al, Numerical Recipes, CUP for further details of the All-Poles transform

All transform methods assume that the data error is independent of time, which is clearly not the case for μSR data.

Data filtering (apodization) is essential before transforming.

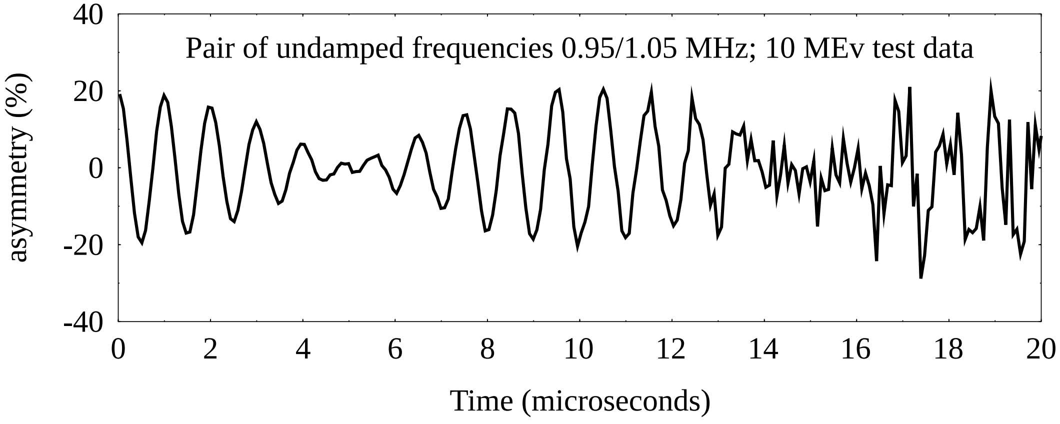
Fourier and All-Poles Transforms

Optimal filtering time constant for a single undamped test frequency

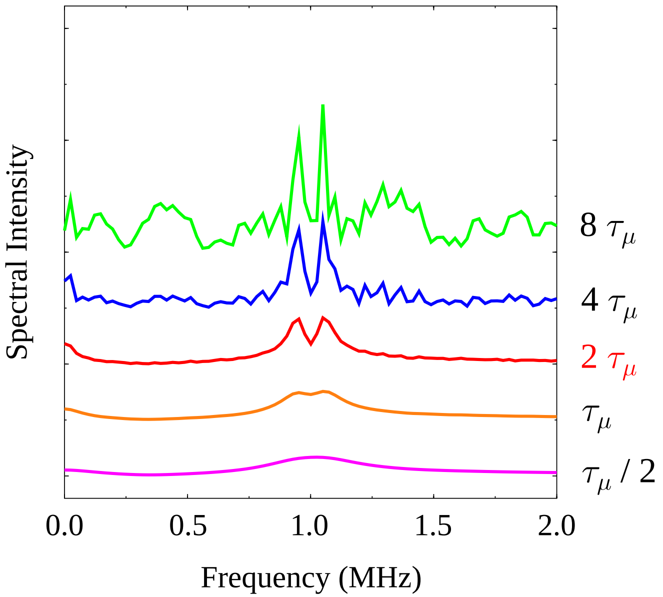


Fourier and All-Poles Transforms

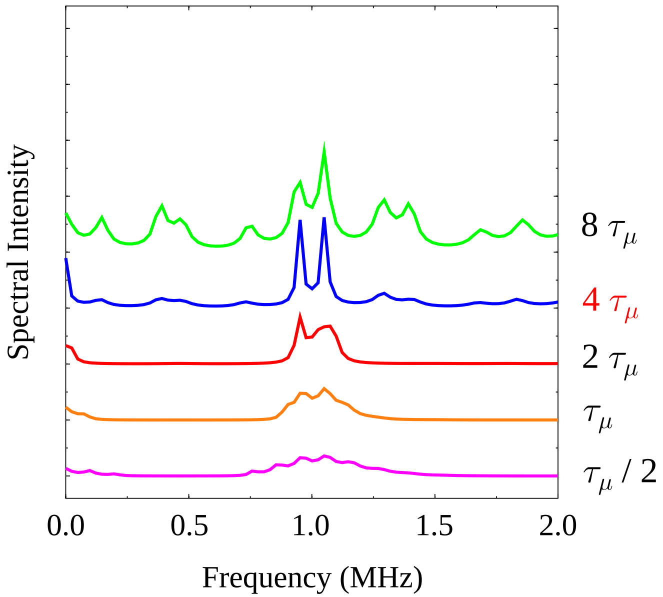
A close pair of undamped test frequencies



FFT



All-poles Maxent



The Maximum Entropy Method

Avoids the noise problem and need for filtering; takes data errors fully into account

Iterative procedure for constructing the frequency spectrum with the minimum structure (i.e. maximum entropy) that is consistent with the measured data

Entropy here is determined from the frequency spectrum p_k

$$S = -\sum_k \frac{p_k}{b} \log \frac{p_k}{b}$$

The procedure involves maximising S ñ $\lambda \chi^2$, where λ is a Lagrange multiplier

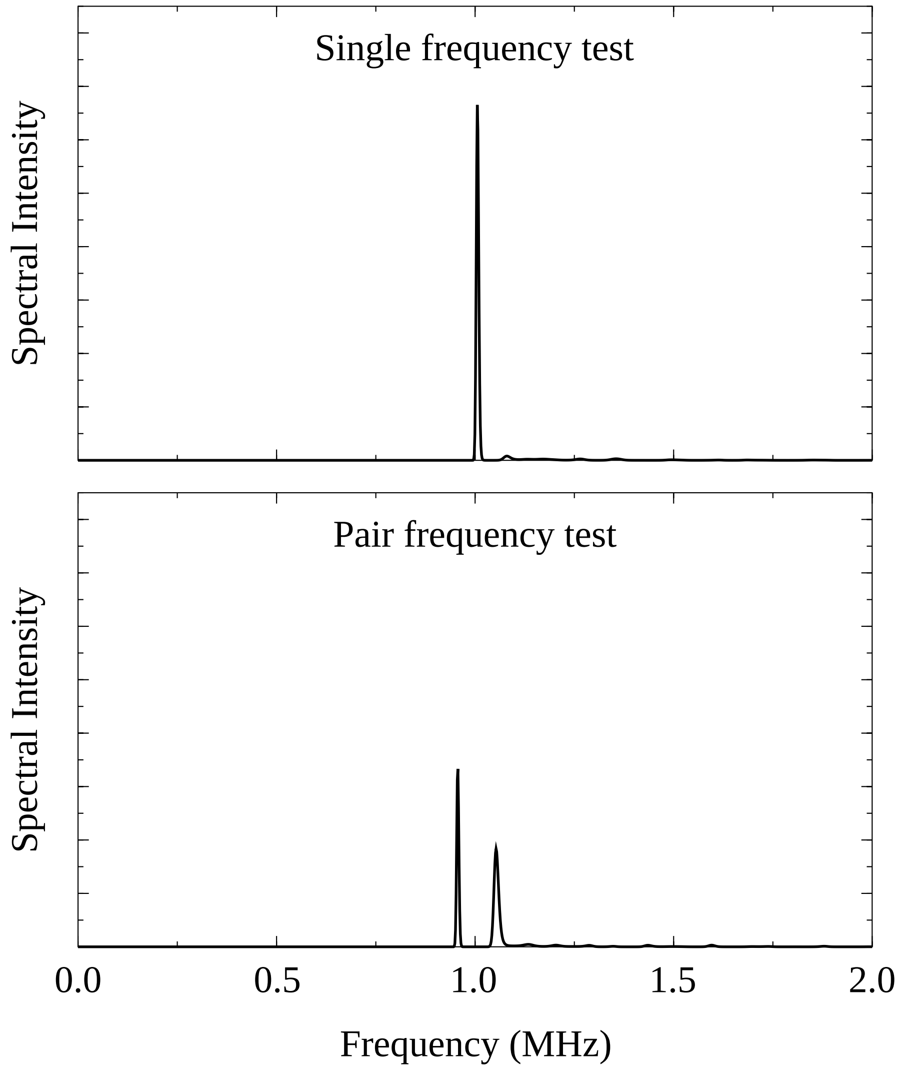
See Rainford and Daniell, Hyperfine Interactions 87, 1129 (1994)
for a detailed discussion of using Maximum Entropy in μSR

for a general reference see:

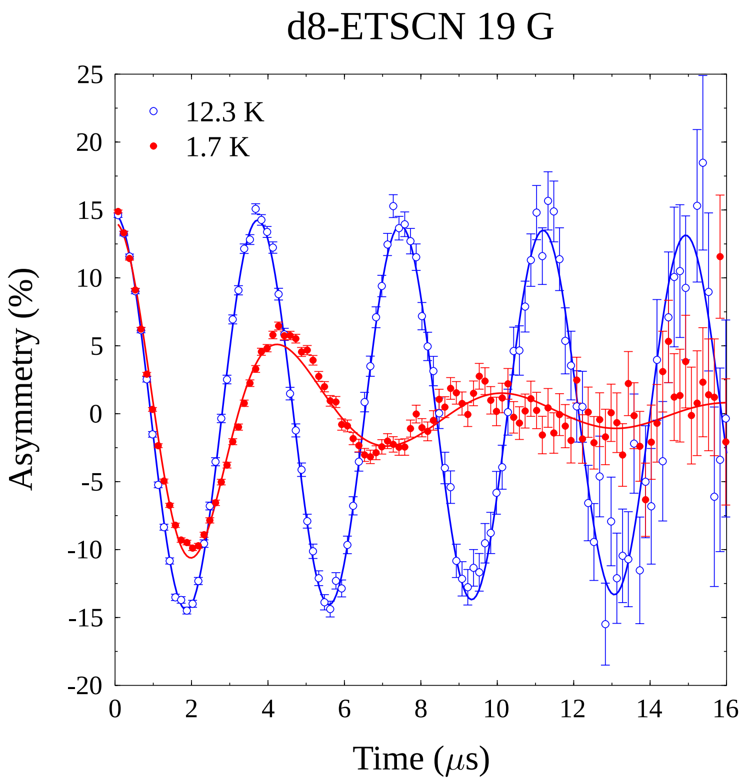
ìMaximum Entropy in Actioní, Buck and Macaulay, OUP (1991)

The Maximum Entropy Method

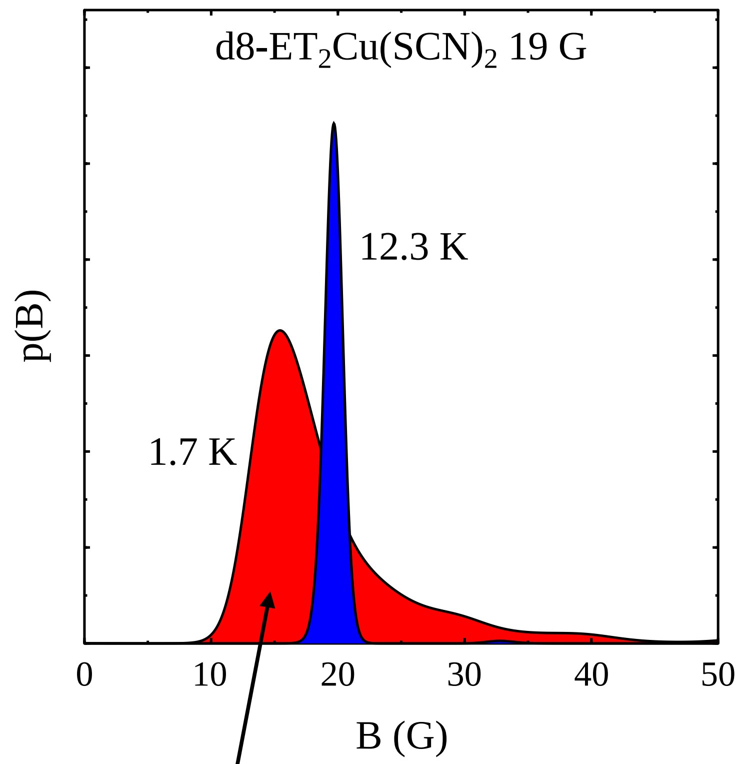
Demonstration using the test data for the transforms



Organic Superconductor Example

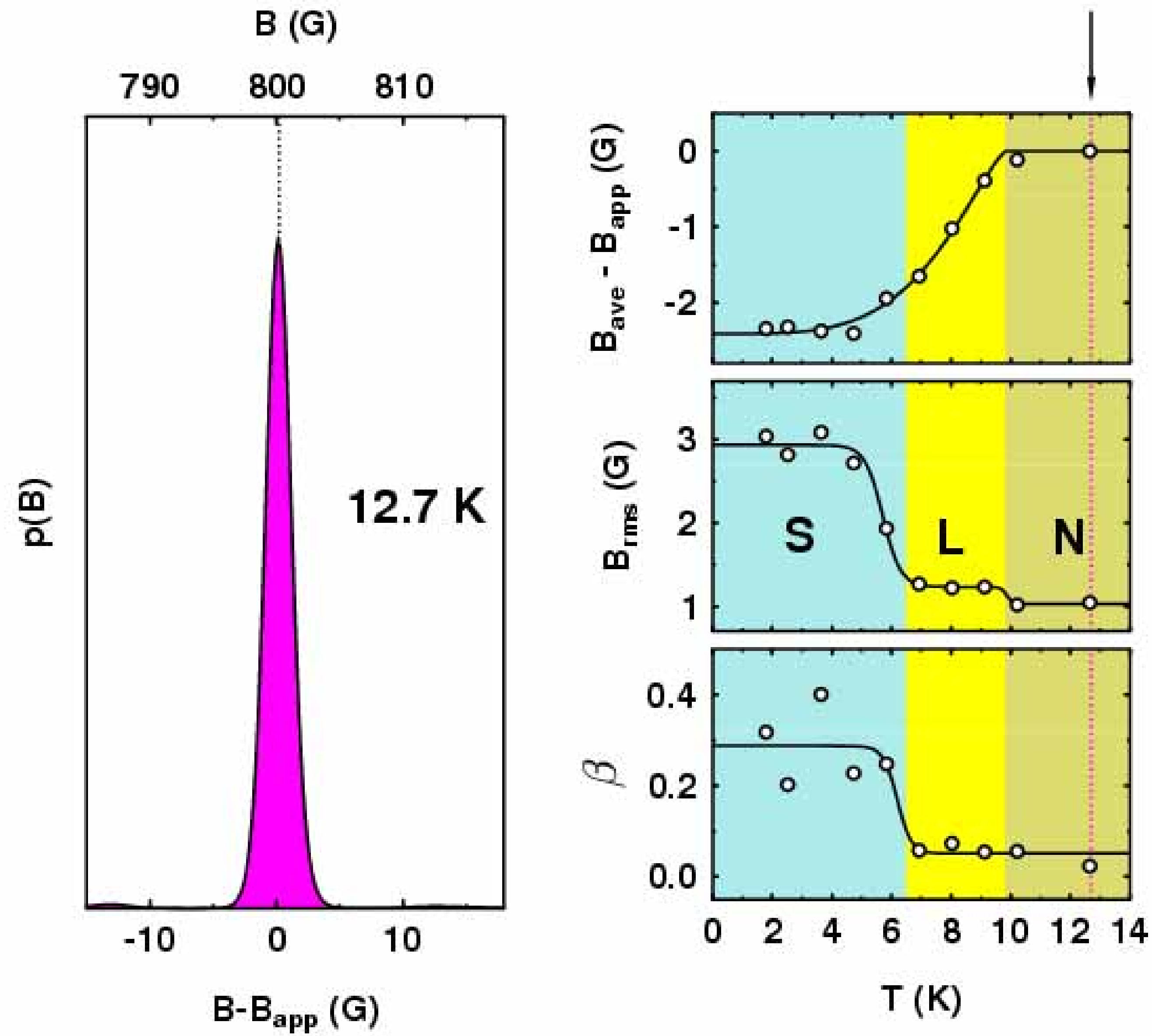


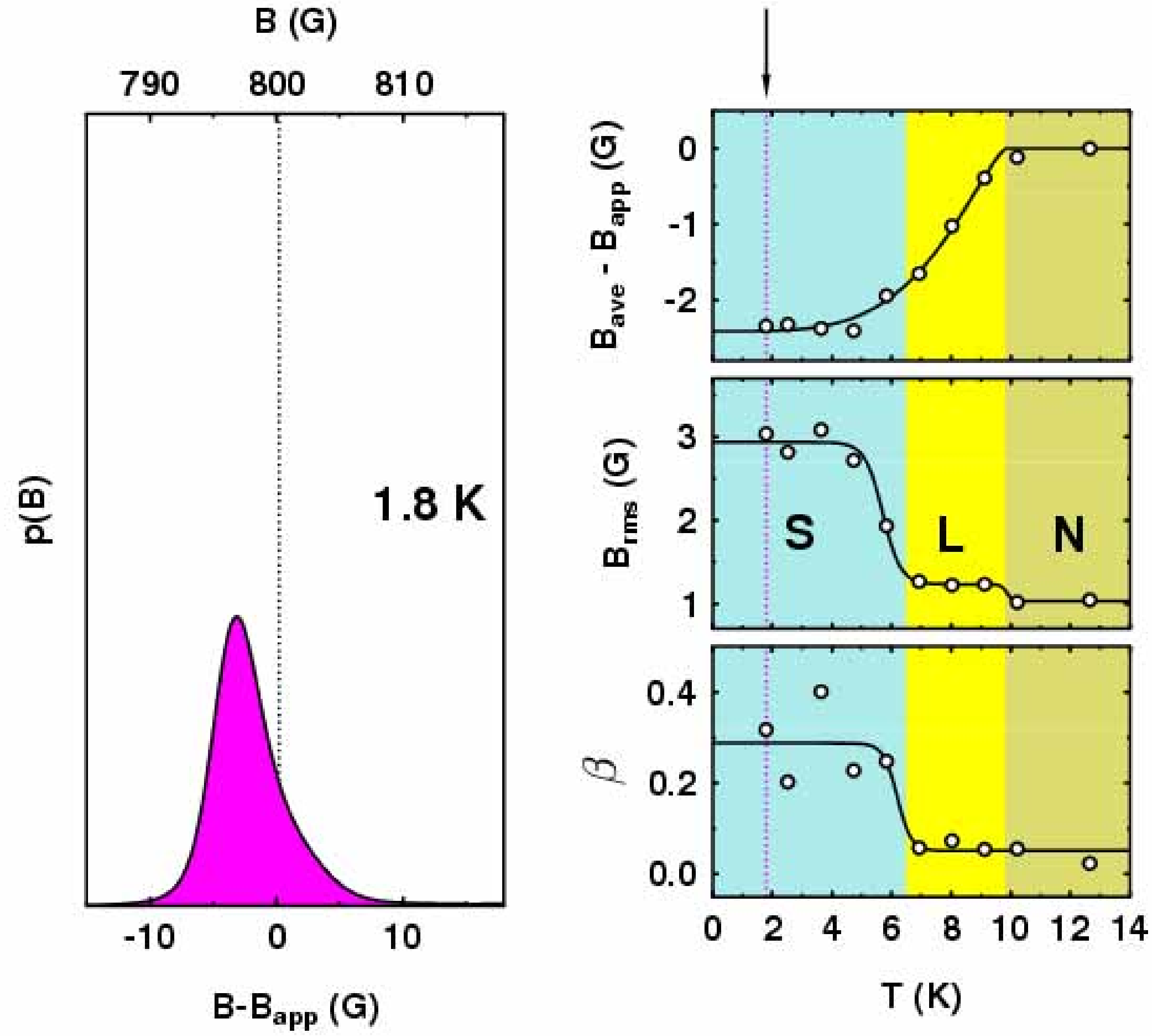
Maximum Entropy Spectra



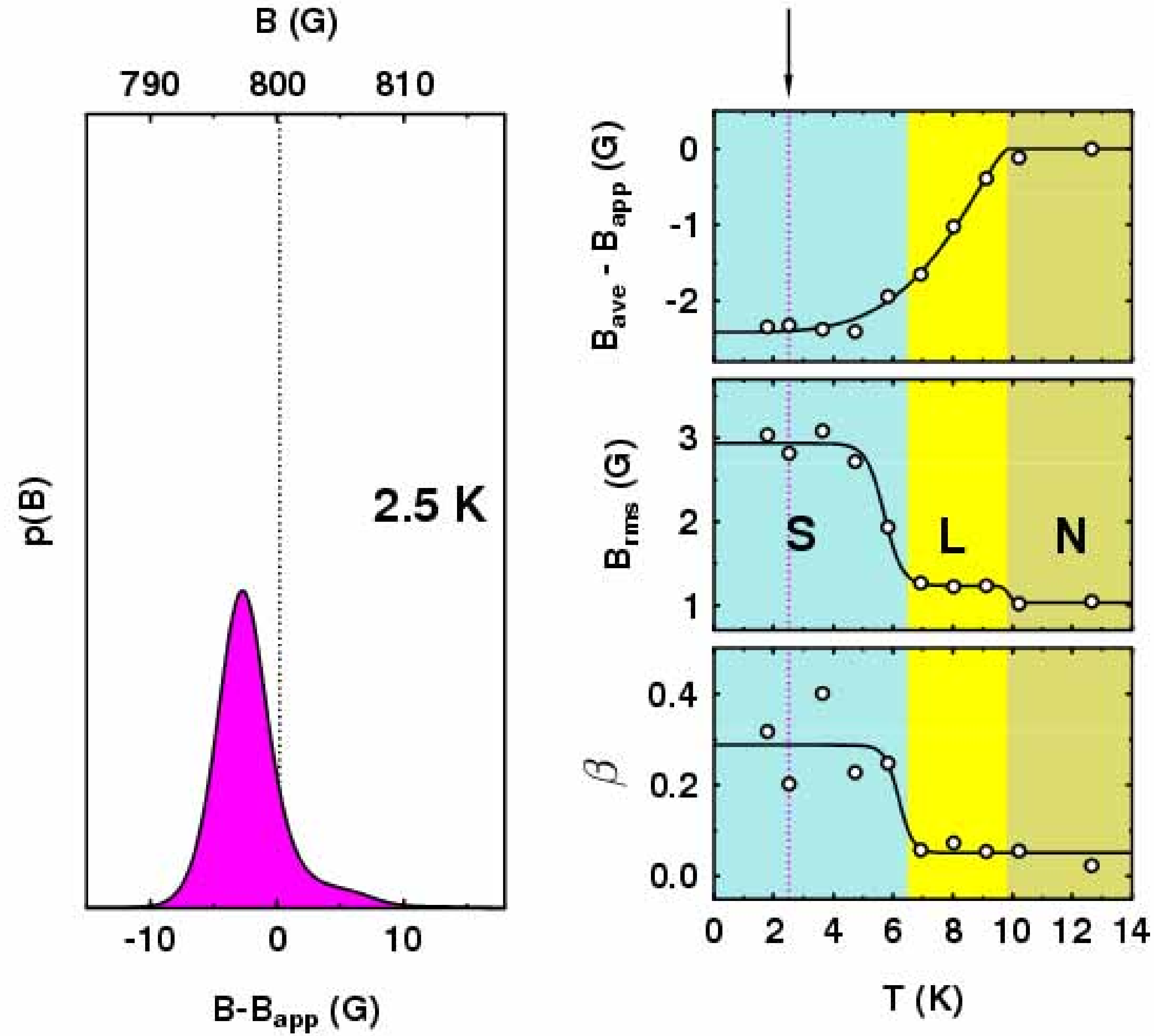
Characteristic field distribution
due to vortex lattice

Melting of the Vortex Lattice

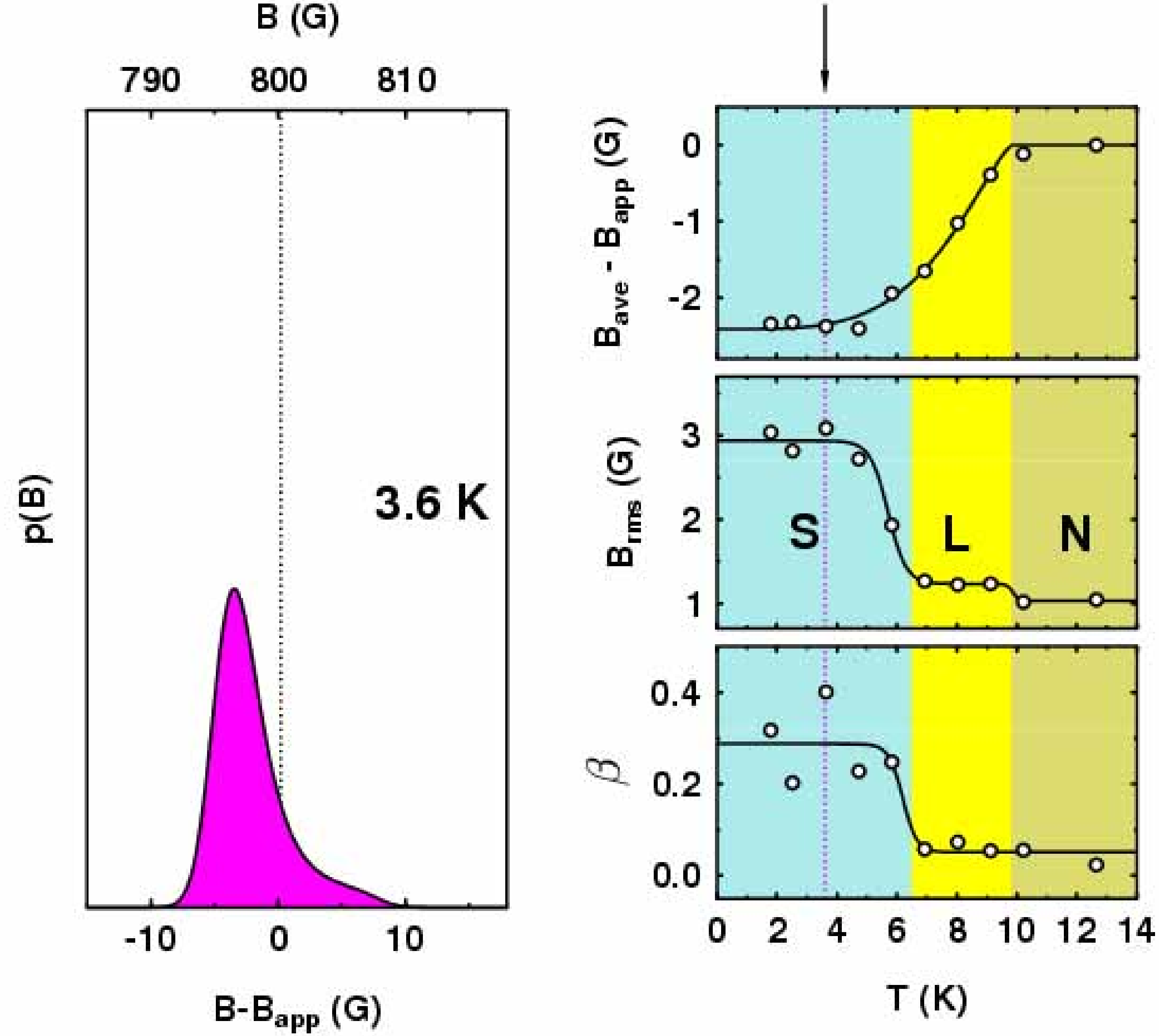

B (G)
790
800
810
p(B)
12.7 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
B$_{rms}$ (G)
β
S
L
N
T (K)
0 2 4 6 8 10 12 14



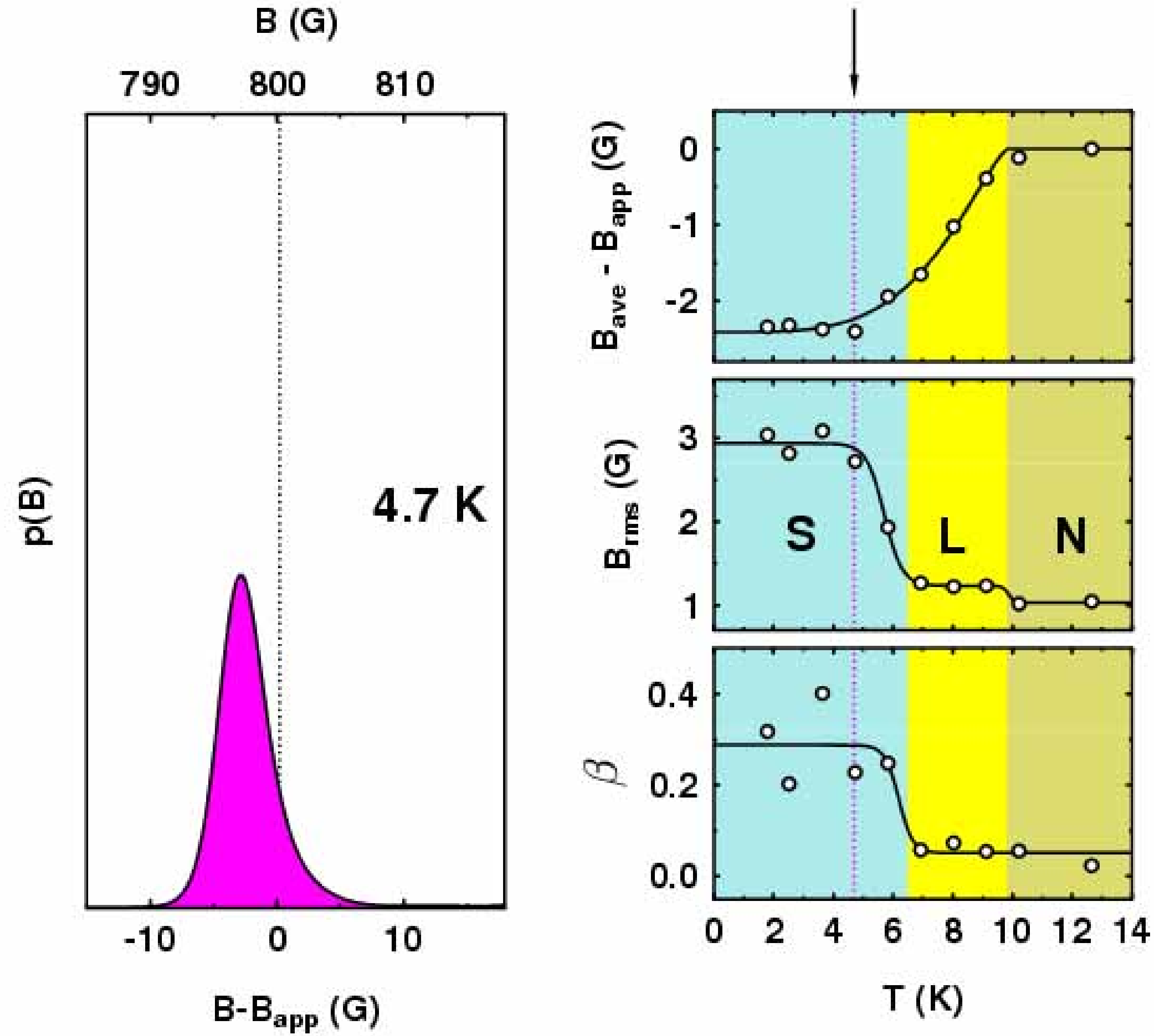
B (G)
790
800
810
p(B)
1.8 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



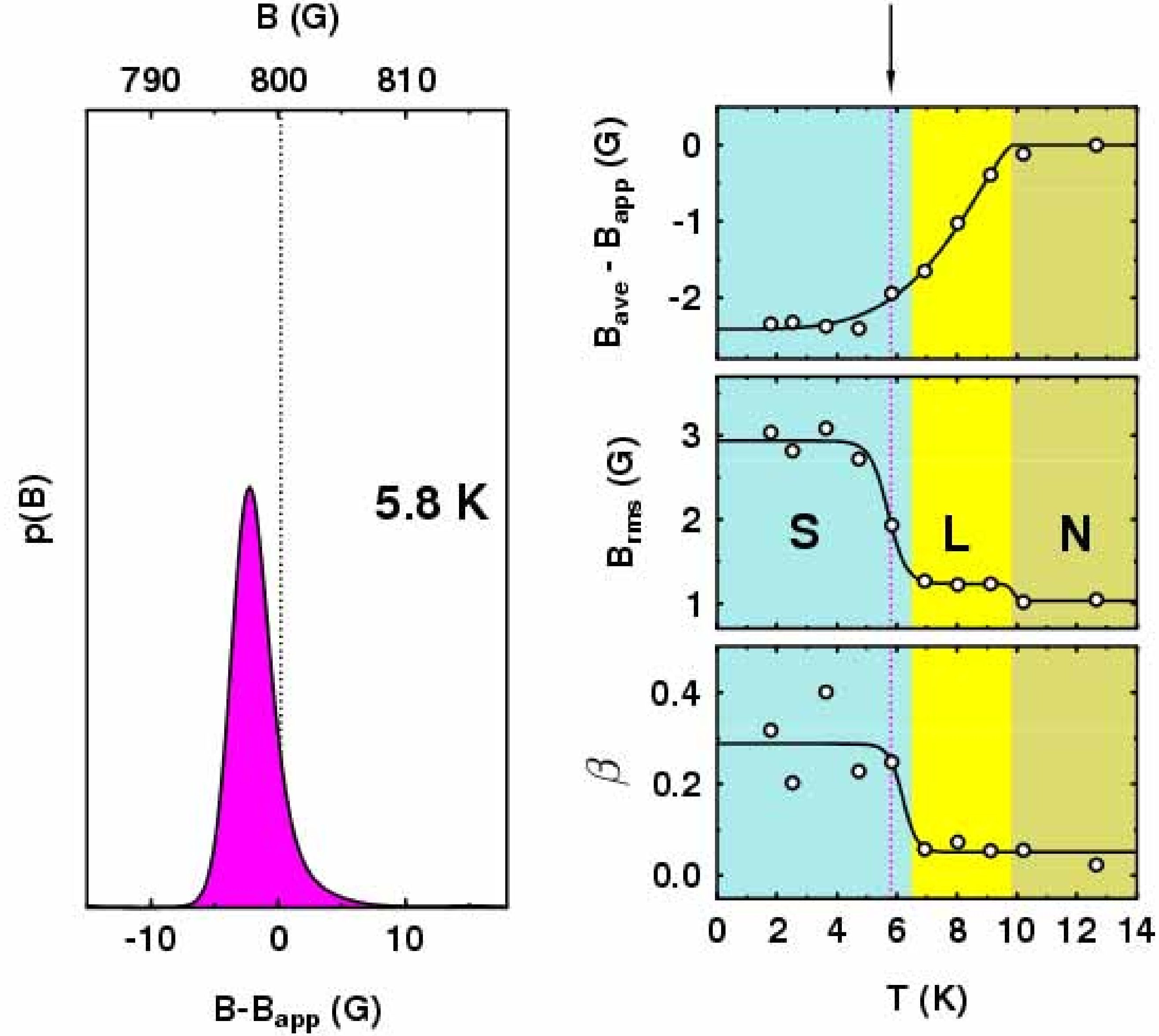
B (G)
790
800
810
p(B)
2.5 K
-10
0
10
B-B_{app} (G)
B_{ave} - B_{app} (G)
0
-1
-2
B_{rms} (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



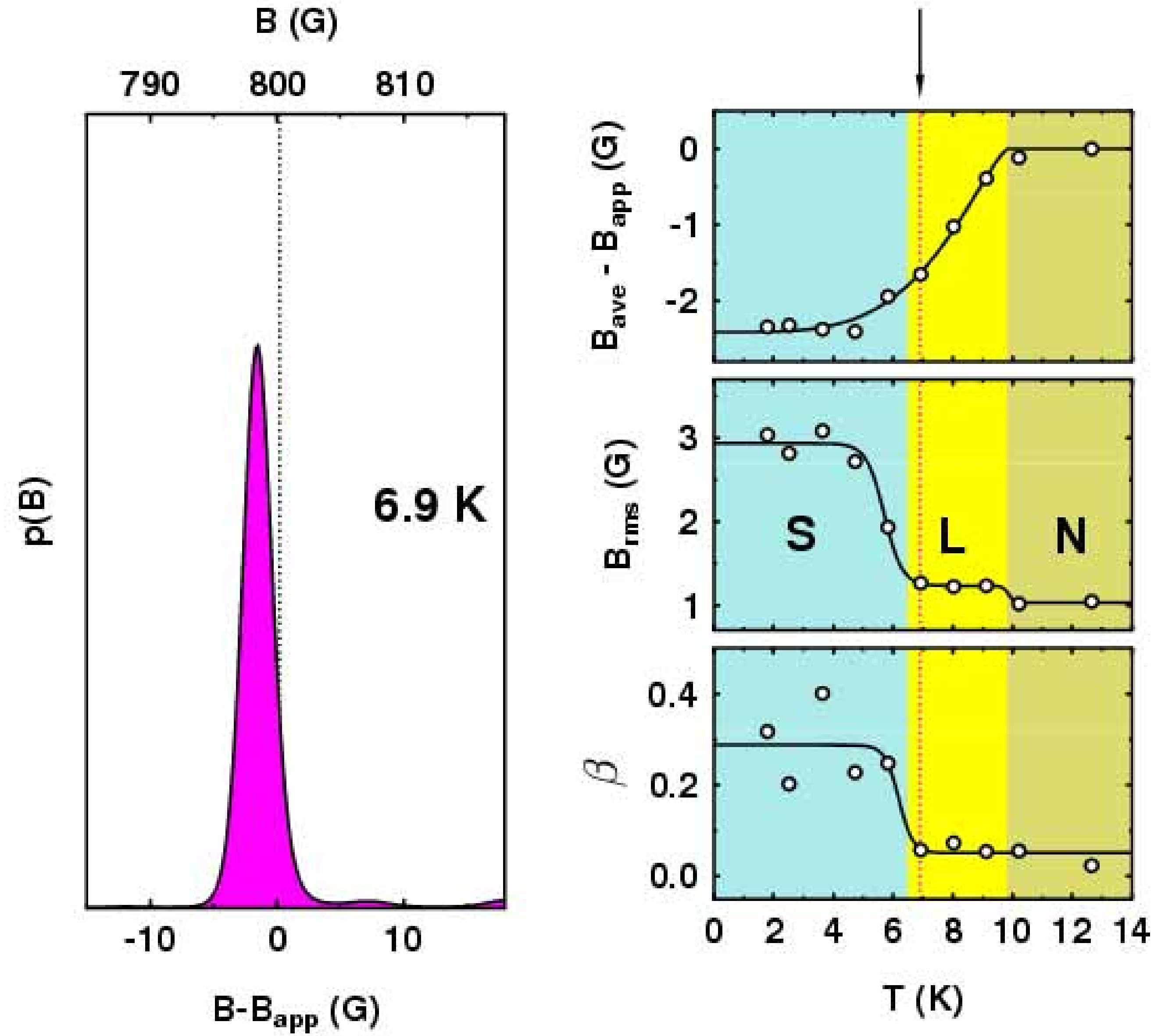
B (G)
790
800
810
p(B)
3.6 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)

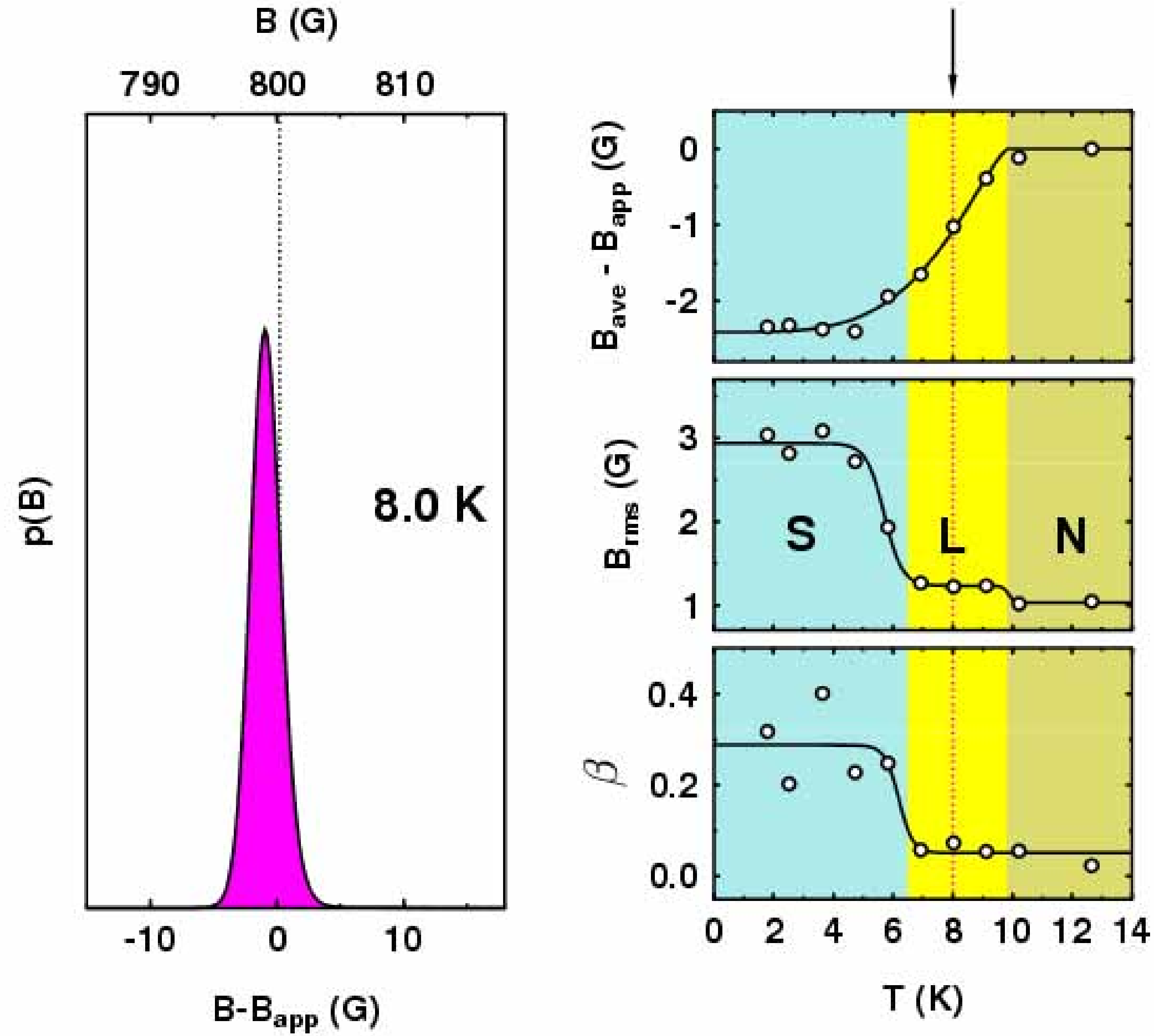


B (G)
790
800
810
p(B)
4.7 K
-10
0
10
B-B_app (G)
B_ave - B_app (G)
0
-1
-2
B_rms (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)

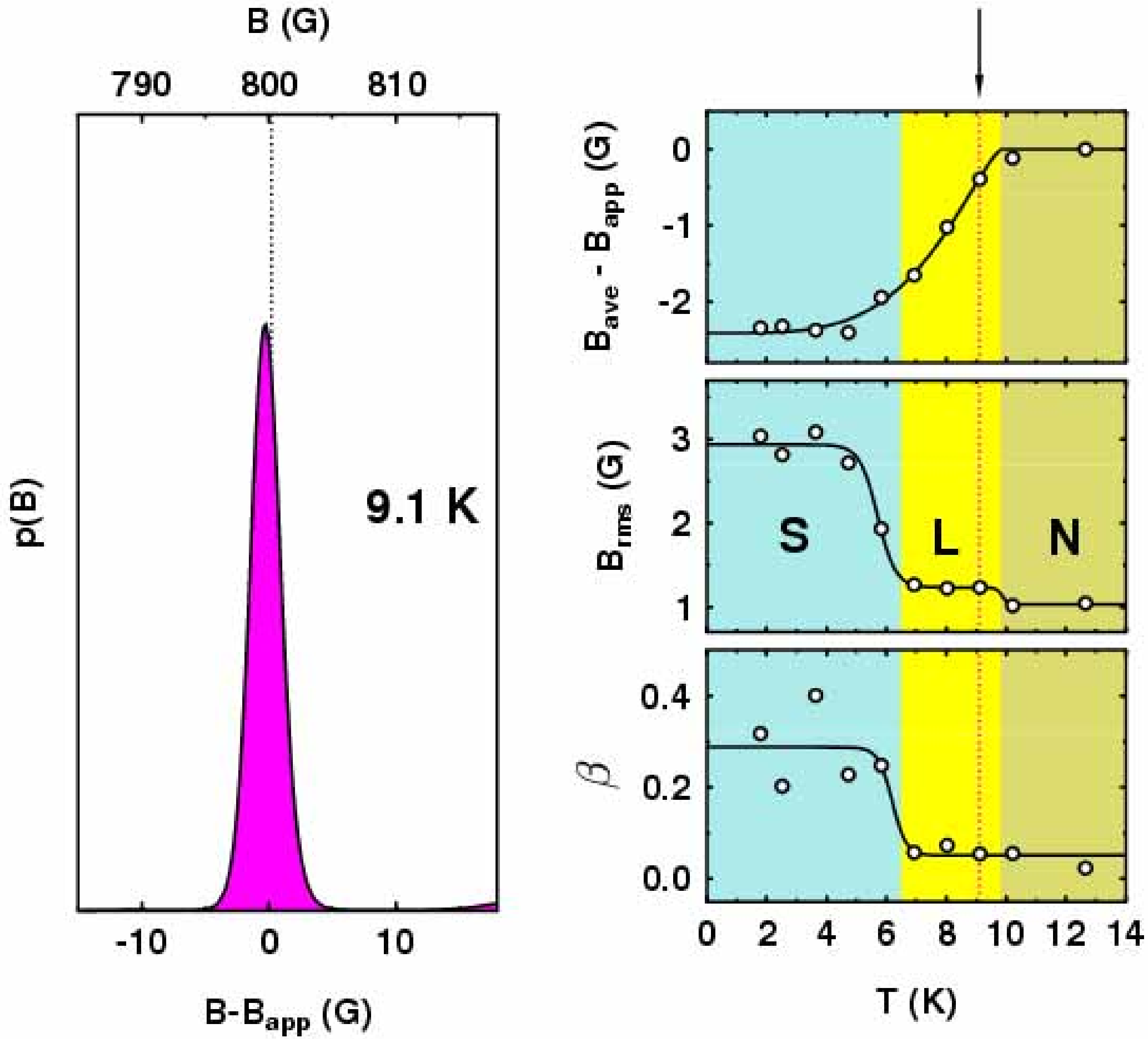


B (G)
790
800
810
p(B)
5.8 K
-10
0
10
B-B_app (G)
B_ave - B_app (G)
0
-1
-2
B_rms (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)

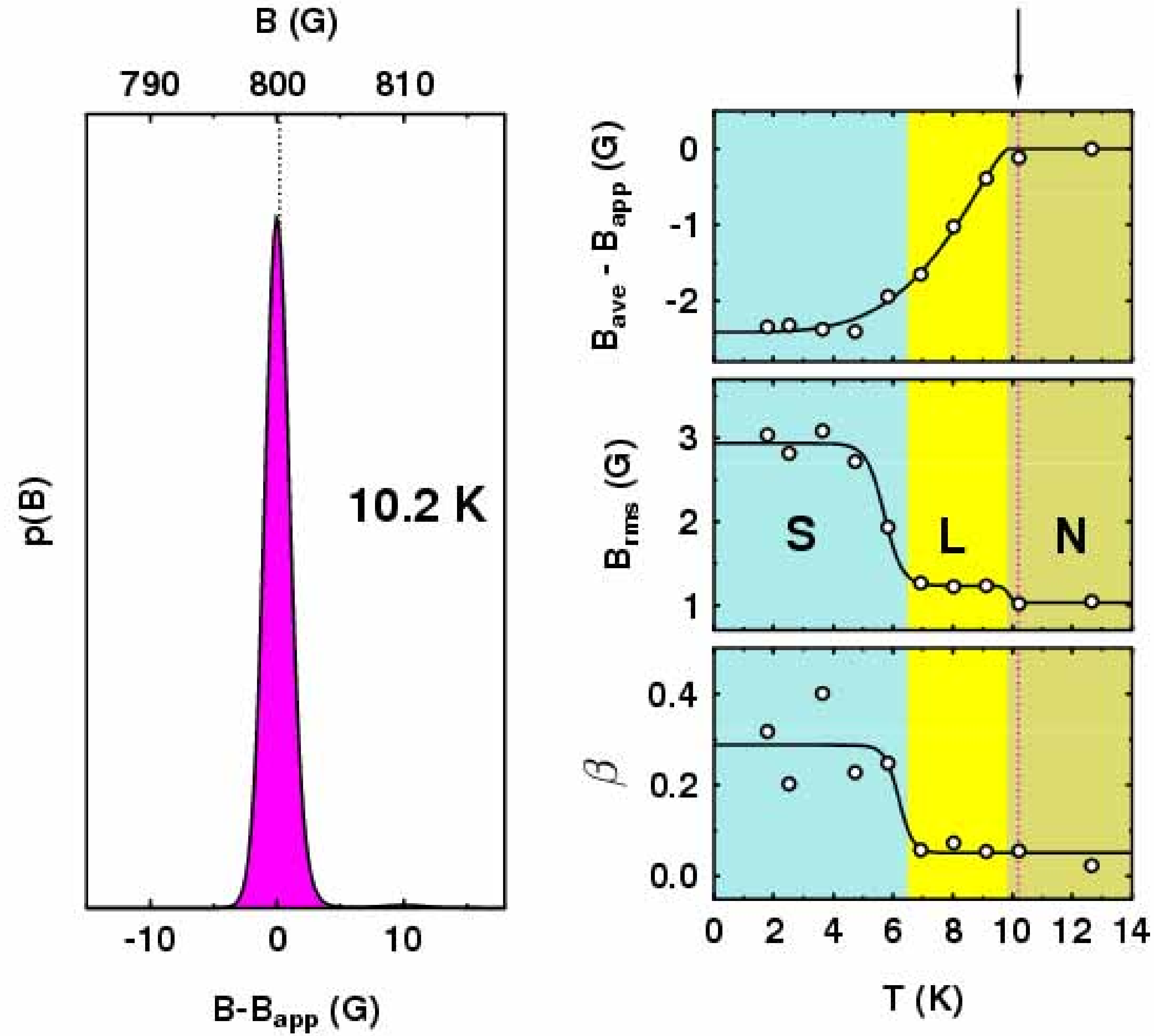

B (G)
790
800
810
p(B)
6.9 K
-10
0
10
B-B_app (G)
B_ave - B_app (G)
0
-1
-2
B_rms (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



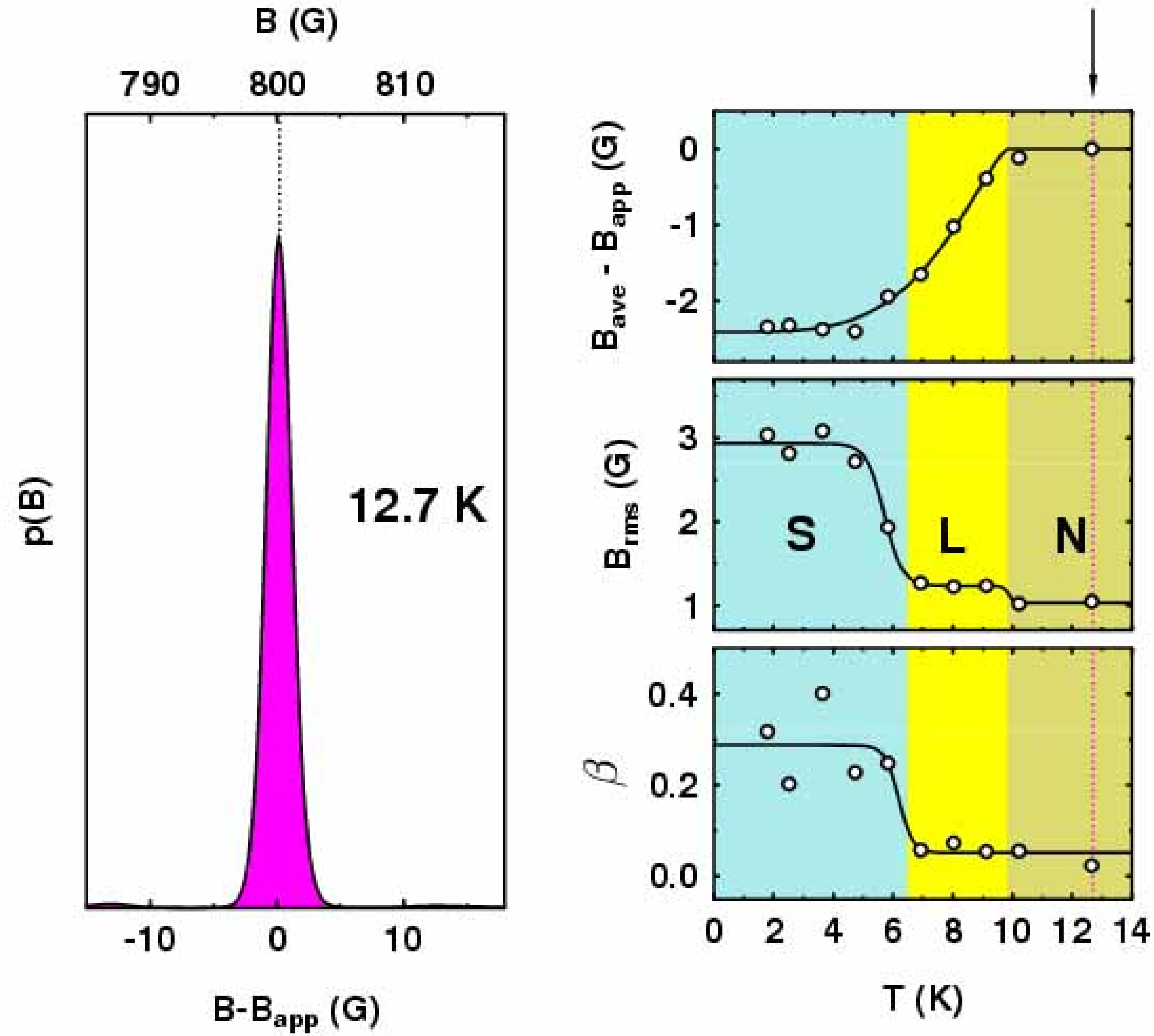
B (G)
790
800
810
p(B)
8.0 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



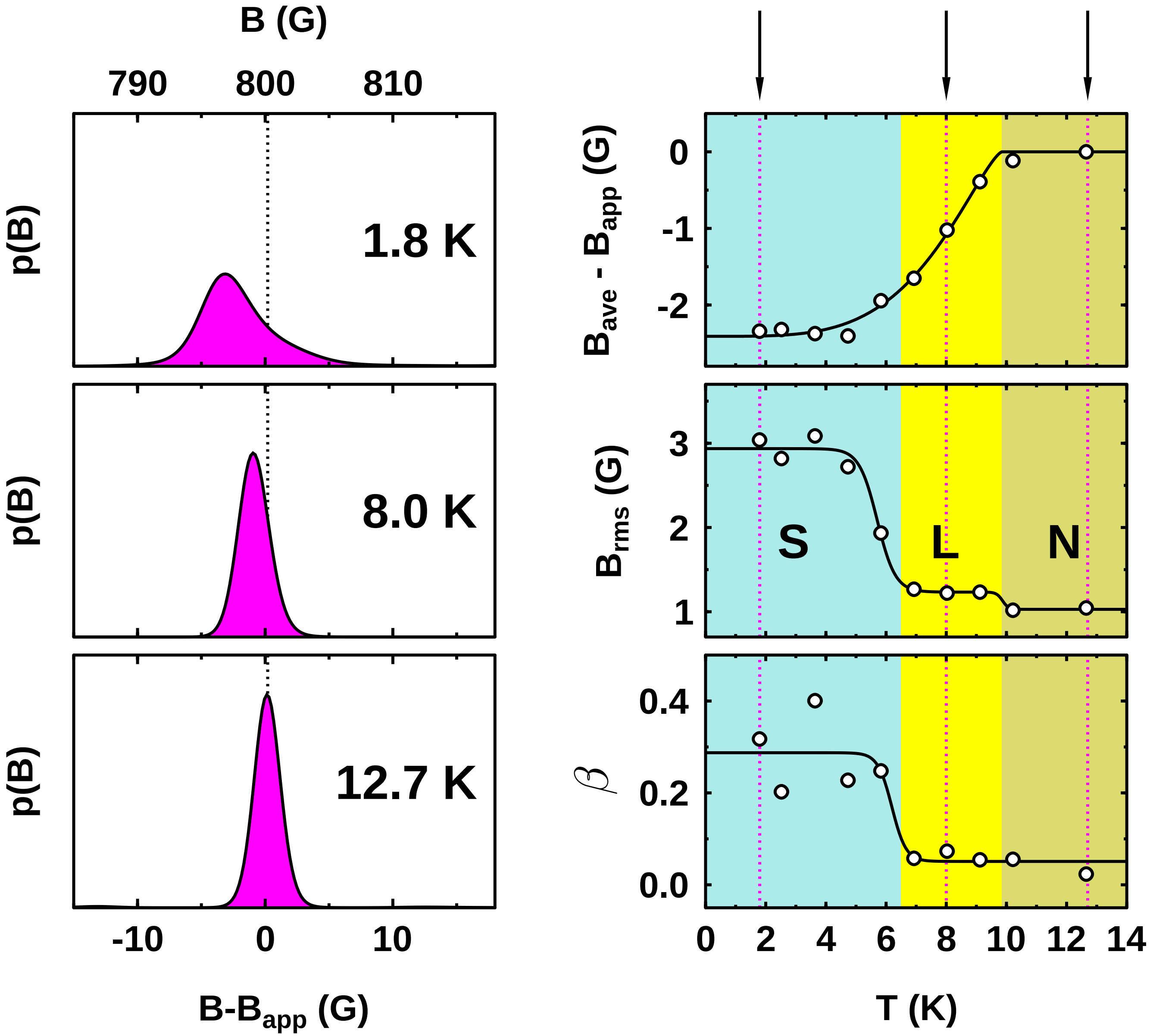
B (G)
790
800
810
p(B)
9.1 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



B (G)
790
800
810
p(B)
10.2 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



B (G)
790
800
810
p(B)
12.7 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)



B (G)
790
800
810
p(B)
1.8 K
8.0 K
12.7 K
-10
0
10
B-B$_{app}$ (G)
B$_{ave}$ - B$_{app}$ (G)
0
-1
-2
B$_{rms}$ (G)
3
2
1
S
L
N
β
0.4
0.2
0.0
0
2
4
6
8
10
12
14
T (K)

Time Domain Analysis versus Frequency Domain Analysis

Single Frequency

	Freq (MHz)	Width (MHz)
Test Data	1.0000	0.000
Time domain fit	0.9998(1)	0.001(1)
Maximum Entropy	1.006	0.003

Pair of Frequencies

	Freq (MHz)		Width (MHz)	
Test Data	0.9500,	1.0500	0.000,	0.000
Time domain fit	0.9493(1)	1.0499(3)	0.003(3)	0.004(3)
Maximum Entropy	0.956	1.054	0.002	0.005

Time Domain Analysis versus Frequency Domain Analysis

Summary

Transforms are good for determining a qualitative picture of data:

FFT best for spectra containing relatively broad features

All-poles transform best for spectra composed of sharp features

Maximum Entropy gives an ëunbiasedí view of the data but Time Domain Fitting gives best ultimate accuracy, provided the correct model is being used.

Combination of Frequency Domain and Time Domain analysis works best

Next:

Practical Data Analysis Workshop

back in R78