Muon relaxation functions

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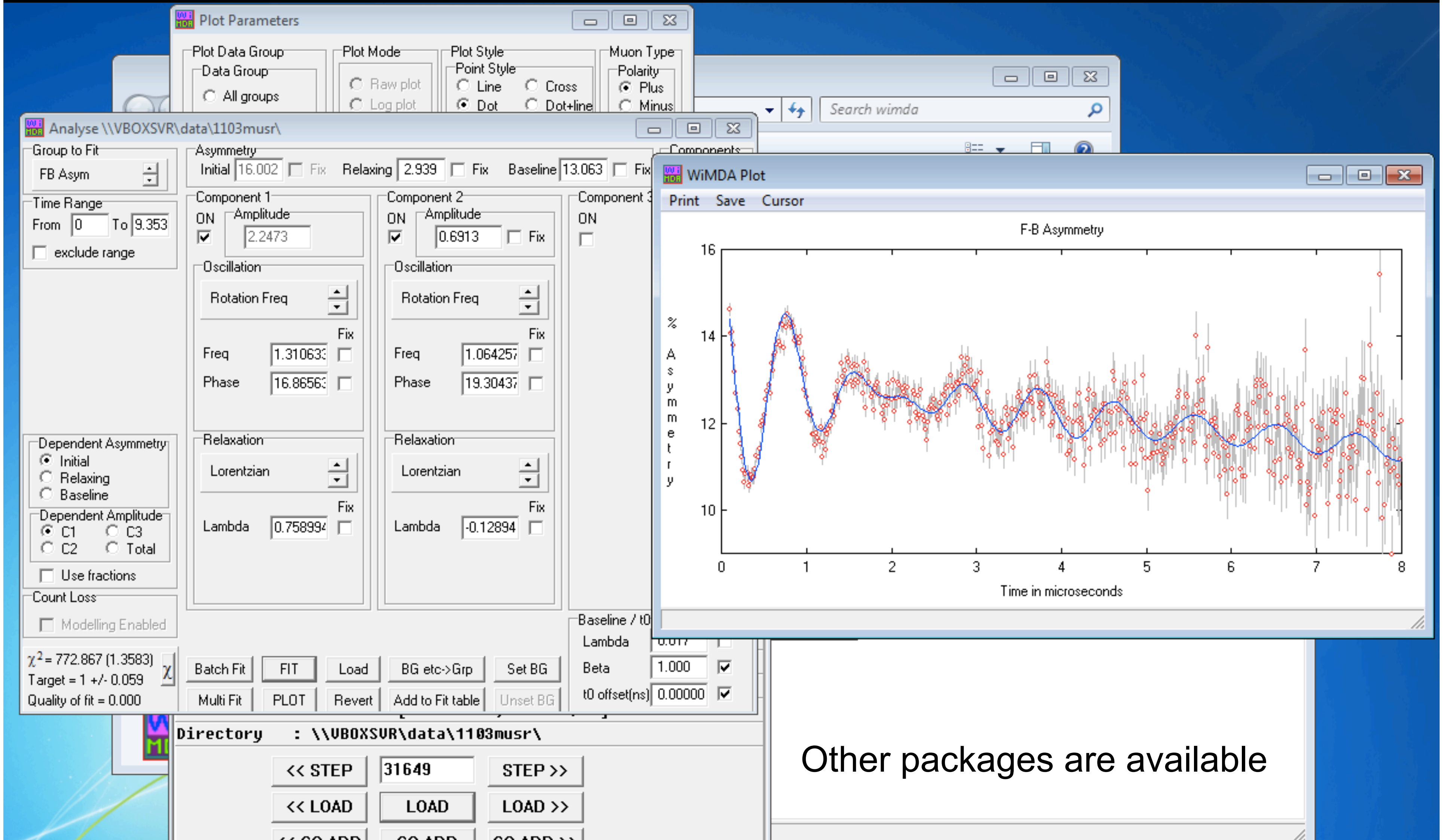
Muon training course - 2018

(Thanks to Francis Pratt for a few of the later slides on muonium-like states.)

UNIVERSITY OF OXFORD

Wimda



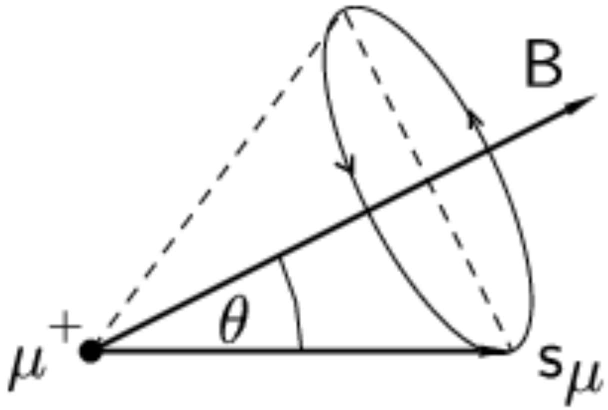
Other packages are available

see later (data analysis sessions)

Lecture plan

- Static distributions - what is a Kubo-Toyabe?
- Gaussian or Lorentzian?
- Dynamic relaxation functions - what happens when the muons get a bit jumpy?
- Stretched exponentials - dangerous evil or answer to all problems?
- When quantum mechanics shines on the experiment!
- Where is your muon?

Muon spin precession



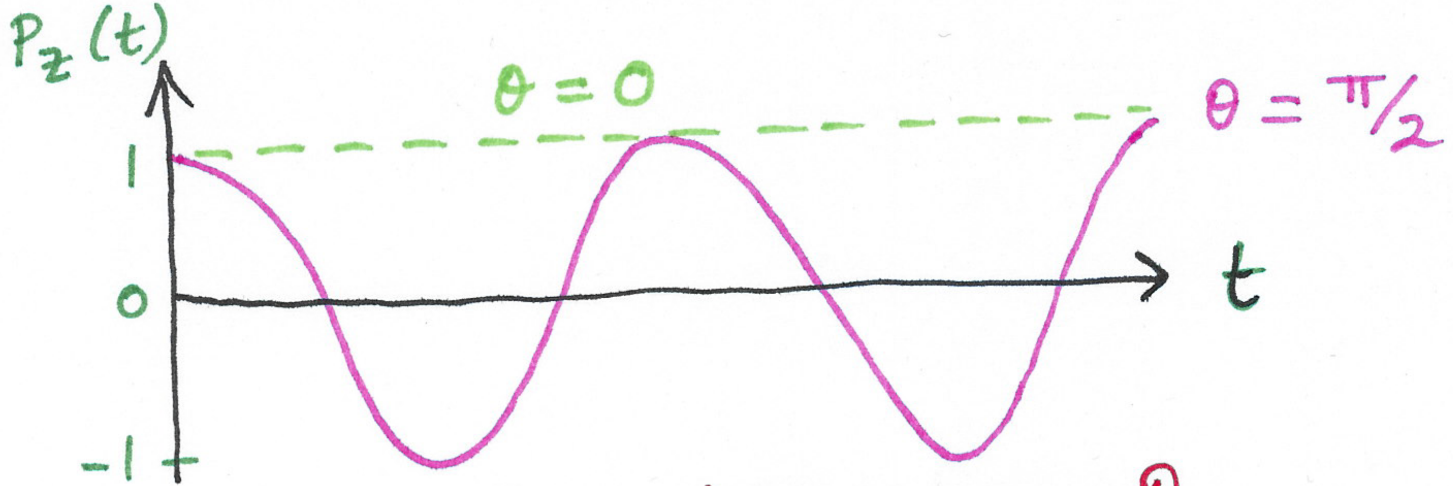
$$P_z(t) = \cos^2\theta + \sin^2\theta\cos(\gamma_\mu|B|t)$$

$|B|$ is the *modulus* of the local dipolar field

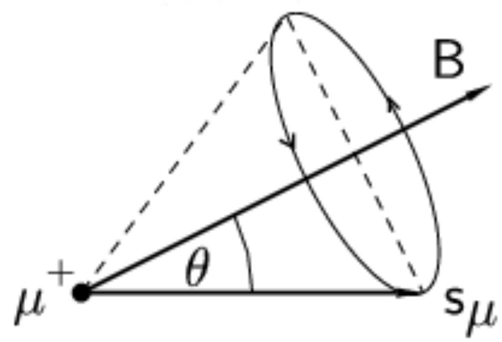
Response to a Static Field

Spin precession

$$P_z(t) = \cos^2\theta + \sin^2\theta \cos[\gamma_\mu B t]$$



depends on θ.



Response to a Static Field

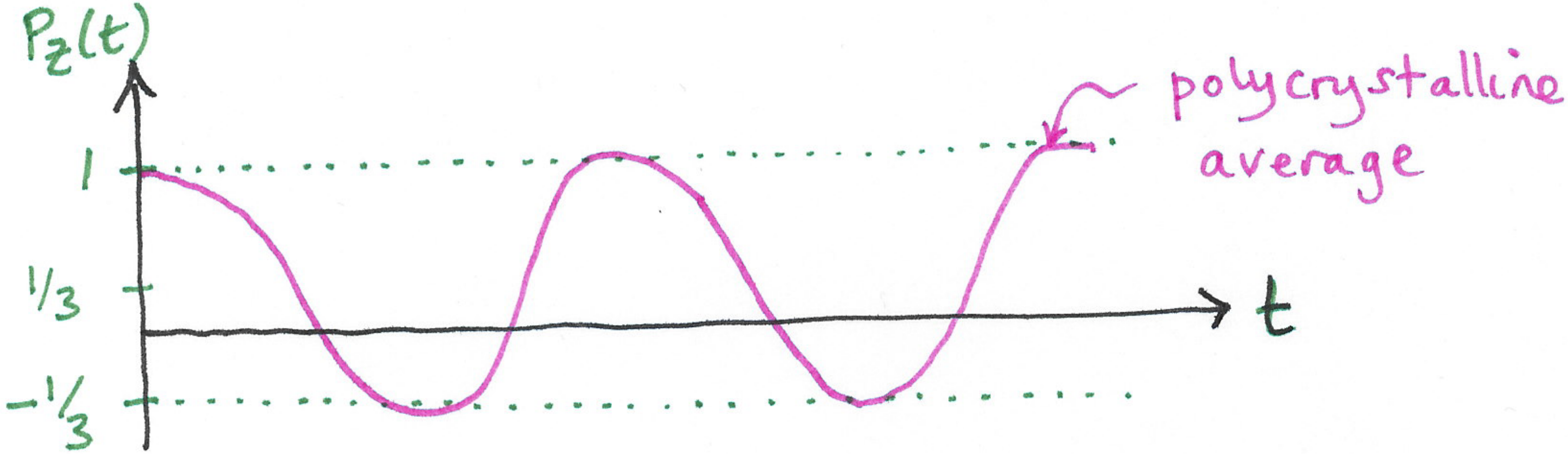
$$P_z(t) = \cos^2\theta + \sin^2\theta\cos(\gamma_\mu|B|t)$$

Angular averages: $\langle\cos^2\theta\rangle = \frac{1}{3}$

$\langle\sin^2\theta\rangle = \frac{2}{3}$

average taken over a sphere

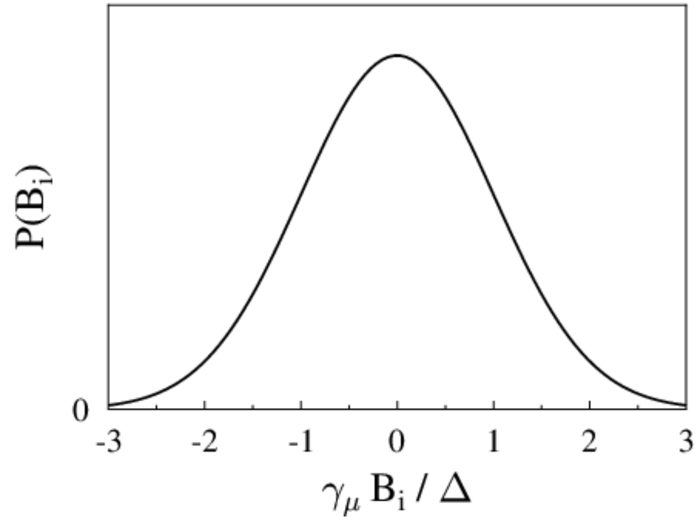
$$\therefore \quad P_z(t) = \frac{1}{3} + \frac{2}{3}\cos[\gamma_\mu B t]$$



Distribution of Static Fields

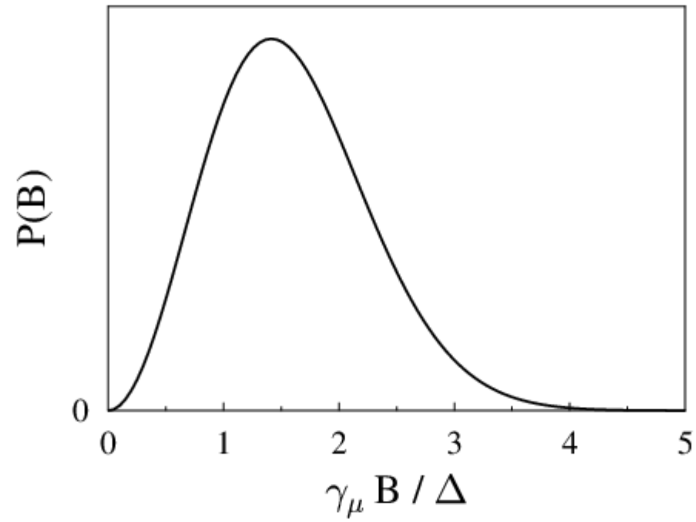
Assume that the B_x, B_y and B_z components are each distributed according to a **Gaussian** distribution, e.g.

$$P(B_x) = \frac{\gamma_\mu}{(2\pi)^{1/2}\Delta} e^{-\gamma_\mu^2 B_x^2 / 2\Delta^2}$$



The overall field distribution peaks near $2^{1/2}\Delta/\gamma_\mu$

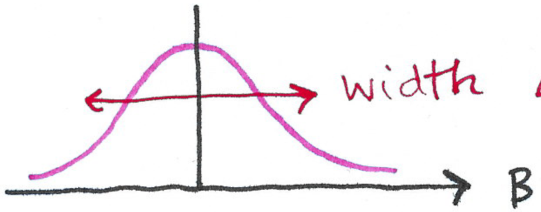
$$P(B) \propto B^2 e^{-\gamma_\mu^2 B^2 / 2\Delta^2}$$

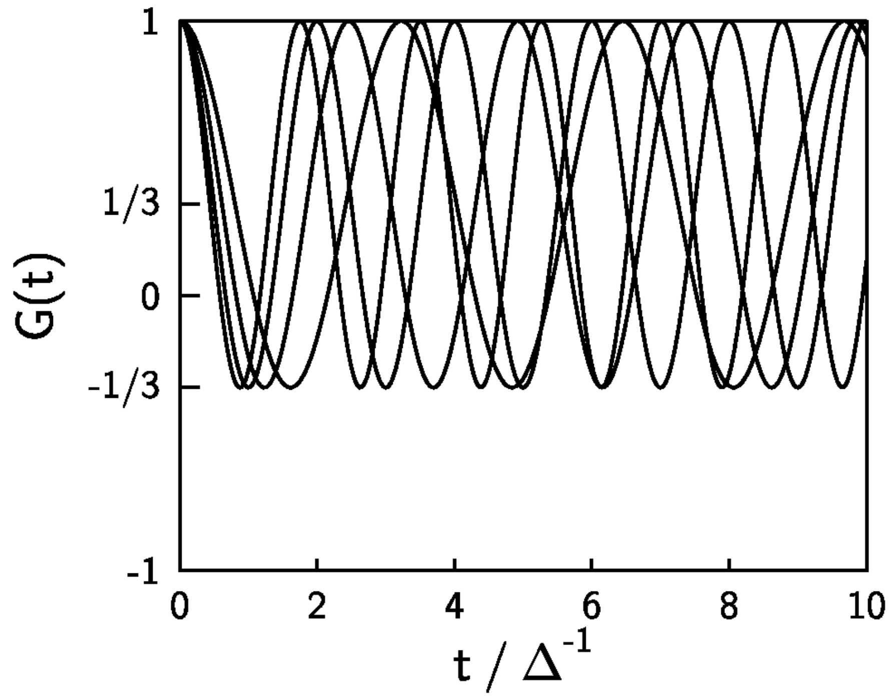


Distribution of Static Fields

Now, assume B is distributed according to a Gaussian distribution:

$$\text{prob}(B) \propto B^2 \, e^{-\gamma_\mu^2 B^2 / 2\Delta^2}$$





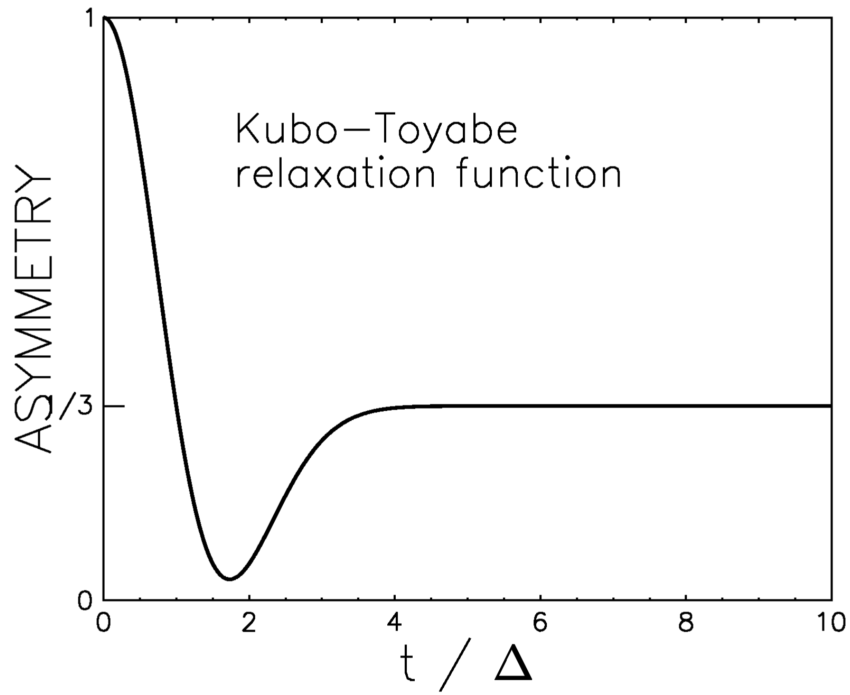
Static Kubo-Toyabe Function

Standard integrals: $\int_0^\infty x^2 e^{-a^2x^2} dx = \frac{\sqrt{\pi}}{4a^3}$ and

$$\int_0^\infty x^2 e^{-a^2x^2} \cos bx \, dx = \frac{\sqrt{\pi}}{4a^3} e^{-b^2/4a^2}\left(1-\frac{b^2}{2a^2}\right)$$

$$\Rightarrow \quad P_z(t) = \frac{1}{3} + \frac{2}{3} e^{-\frac{1}{2}\Delta^2 t^2}(1-\Delta^2 t^2)$$

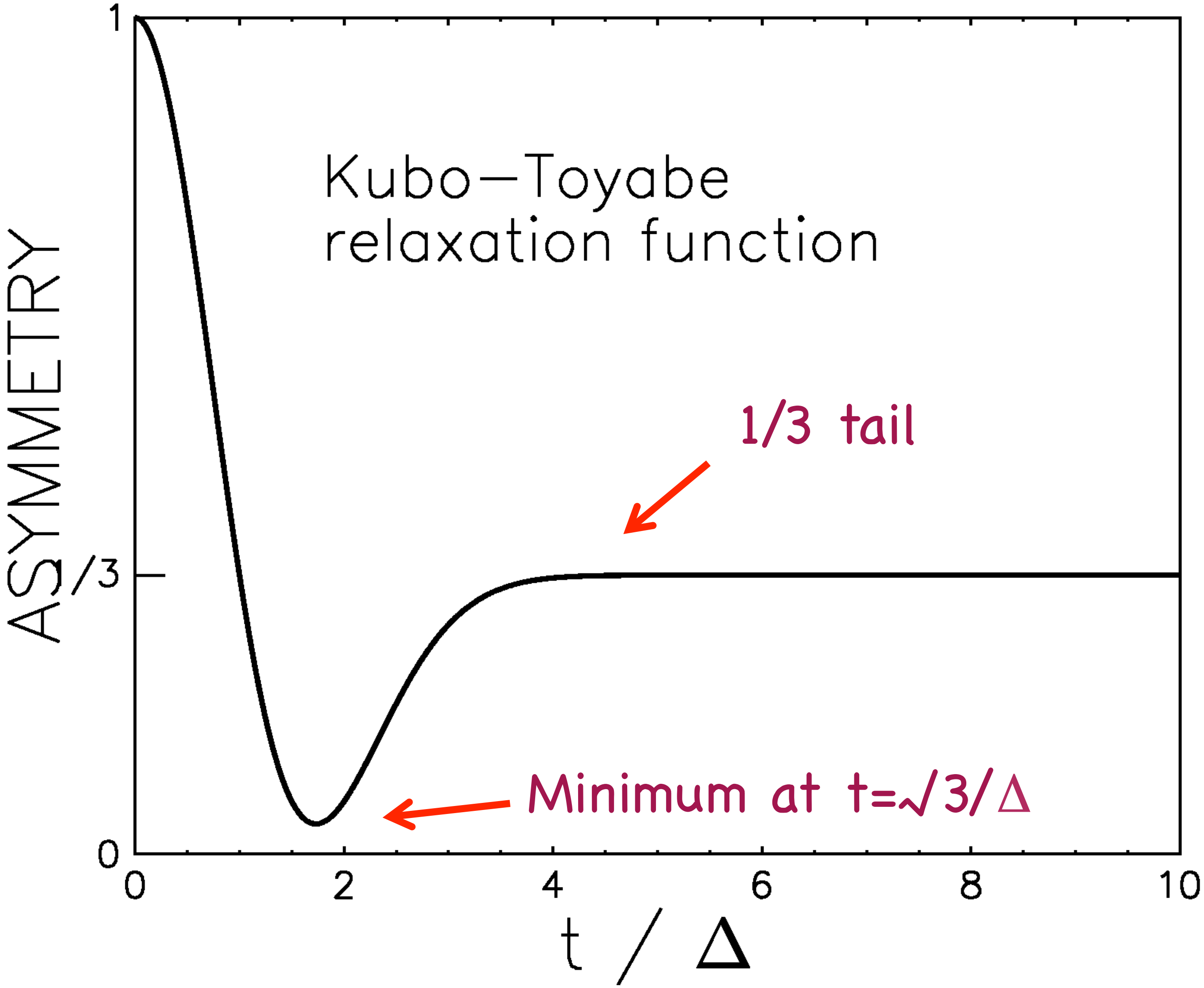
ZERO-FIELD KUBO-TOYABE FUNCTION.



Ryogo Kubo
(1920–1995)

Static Kubo-Toyabe Function

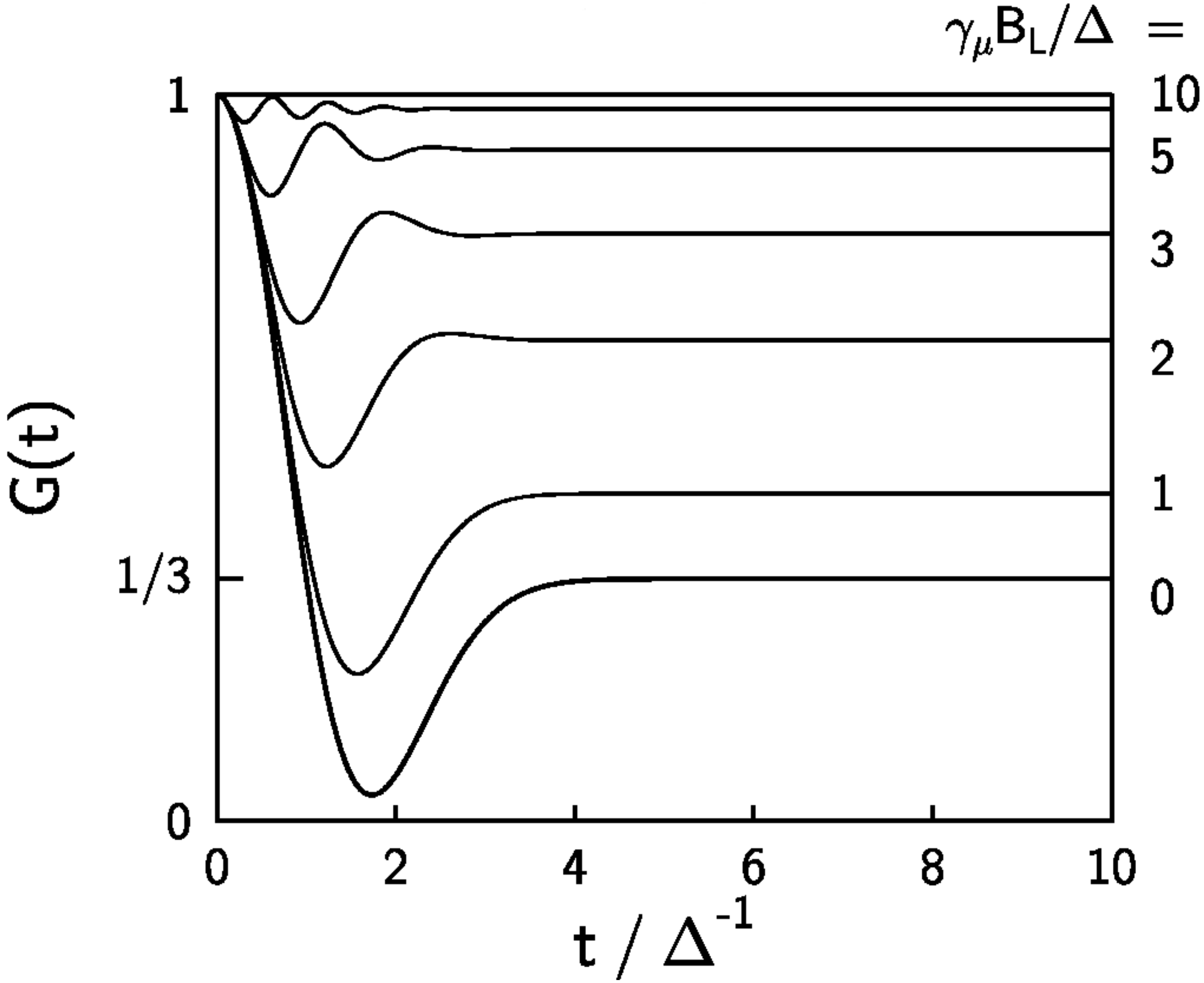
$$G(t) = 1/3 + 2/3\,(1-\Delta^2 t^2)\, e^{-\Delta^2 t^2/2}$$



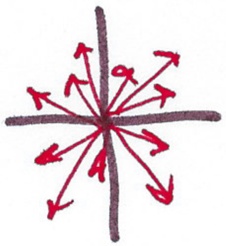
Kubo-Toyabe in Field

Apply a longitudinal field:

see a recovery of the K-T function!



Kubo-Toyabe in Longitudinal Field

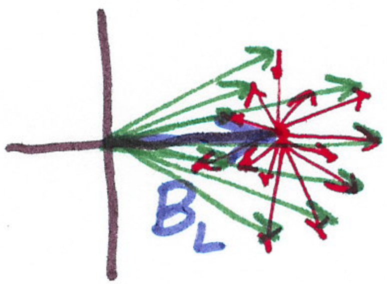


$B_L = 0$

- random fields in all directions

$\sim 1/3$ parallel or antiparallel to the muon-spin

$\sim 2/3$ perpendicular $\Rightarrow$ depolarize on a time $\sim 1/\Delta$



$B_L \neq 0$

- now add a longitudinal component

boosts the $\frac{1}{3}$ fraction along z

$$P_z(t) = \langle \cos^2\theta \rangle + \langle \sin^2\theta \cdot \cos \gamma_\mu B t \rangle$$

BOOSTED "RINGS" at $\sim \gamma_\mu B_L$.

LF Kubo-Toyabe Function

Analytical calculation:

$$P(B_x) = \frac{\gamma_\mu}{(2\pi)^{1/2}\Delta} e^{-\gamma_\mu^2 B_x^2/2\Delta^2}$$

$$P(B_y) = \frac{\gamma_\mu}{(2\pi)^{1/2}\Delta} e^{-\gamma_\mu^2 B_y^2/2\Delta^2}$$

$$P(B_z) = \frac{\gamma_\mu}{(2\pi)^{1/2}\Delta} e^{-\gamma_\mu^2 (B_z^2 - B_L^2)/2\Delta^2}$$

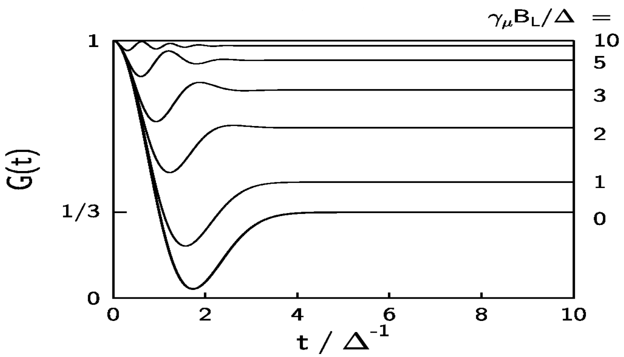
2

Gaussian distribution with offset

$$P_z(t) = \int d^3B \left[\cos^2\theta + \sin^2\theta \cos(\gamma_\mu B t)\right] P(B_x)P(B_y)P(B_z)$$

$$\Rightarrow \boxed{P_z(t) = 1 - \frac{2\Delta^2}{(\gamma_\mu B_L)^2}\left(1 - e^{-\frac{1}{2}\Delta^2 t^2}\cos\gamma_\mu B_L t\right) + \frac{2\Delta^4}{(\gamma_\mu B_L)^3}\int_0^t e^{-\frac{1}{2}\Delta^2\tau^2}\sin\gamma_\mu B_L\tau \, d\tau}$$

LONGITUDINAL-FIELD KUBO TOYABE FUNCTION



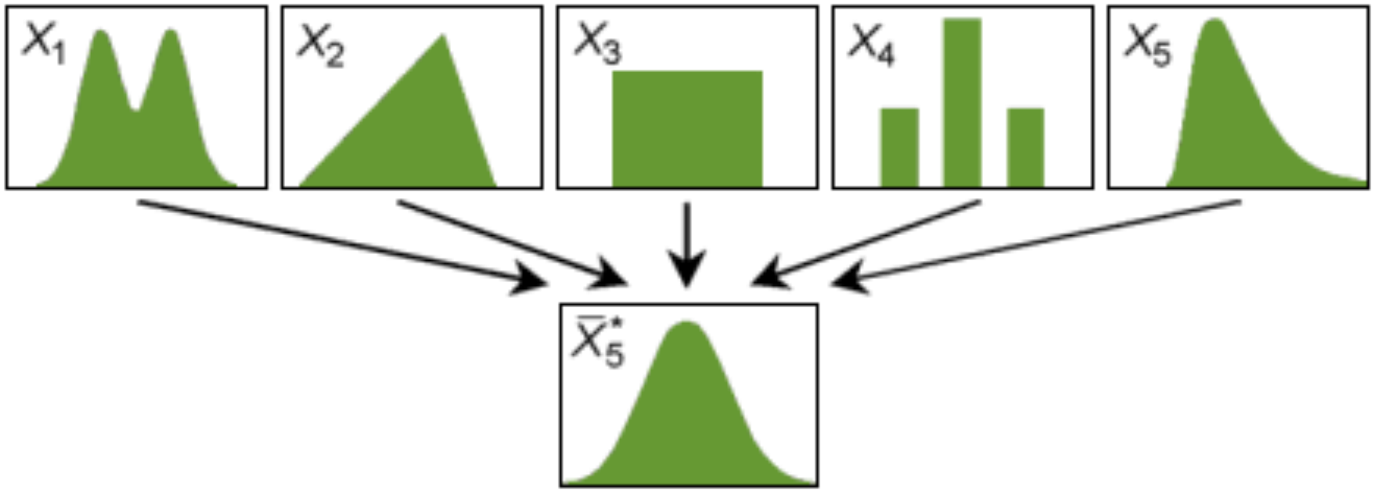
Gaussian or Lorentzian Field Distribution?

Now, assume B is distributed according to a Gaussian distribution:

$$\mathrm{prob}(B) \propto B^2 \, e^{-\gamma_\mu^2 B^2 / 2\Delta^2}$$

(Dense spins)

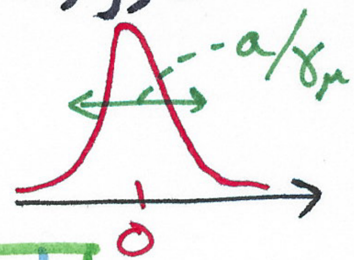
The Gaussian distribution is justified by the CENTRAL-LIMIT THEOREM; other distributions are possible.



Gaussian or Lorentzian Field Distribution?

Dilute spins: $\Rightarrow$ Lorentzian distribution

$$\mathrm{Prob}(B_i) = \frac{\gamma_\mu}{\pi} \frac{a}{a^2 + \gamma_\mu^2 B_i^2} \qquad i = x, y, z$$



and you get a similar result

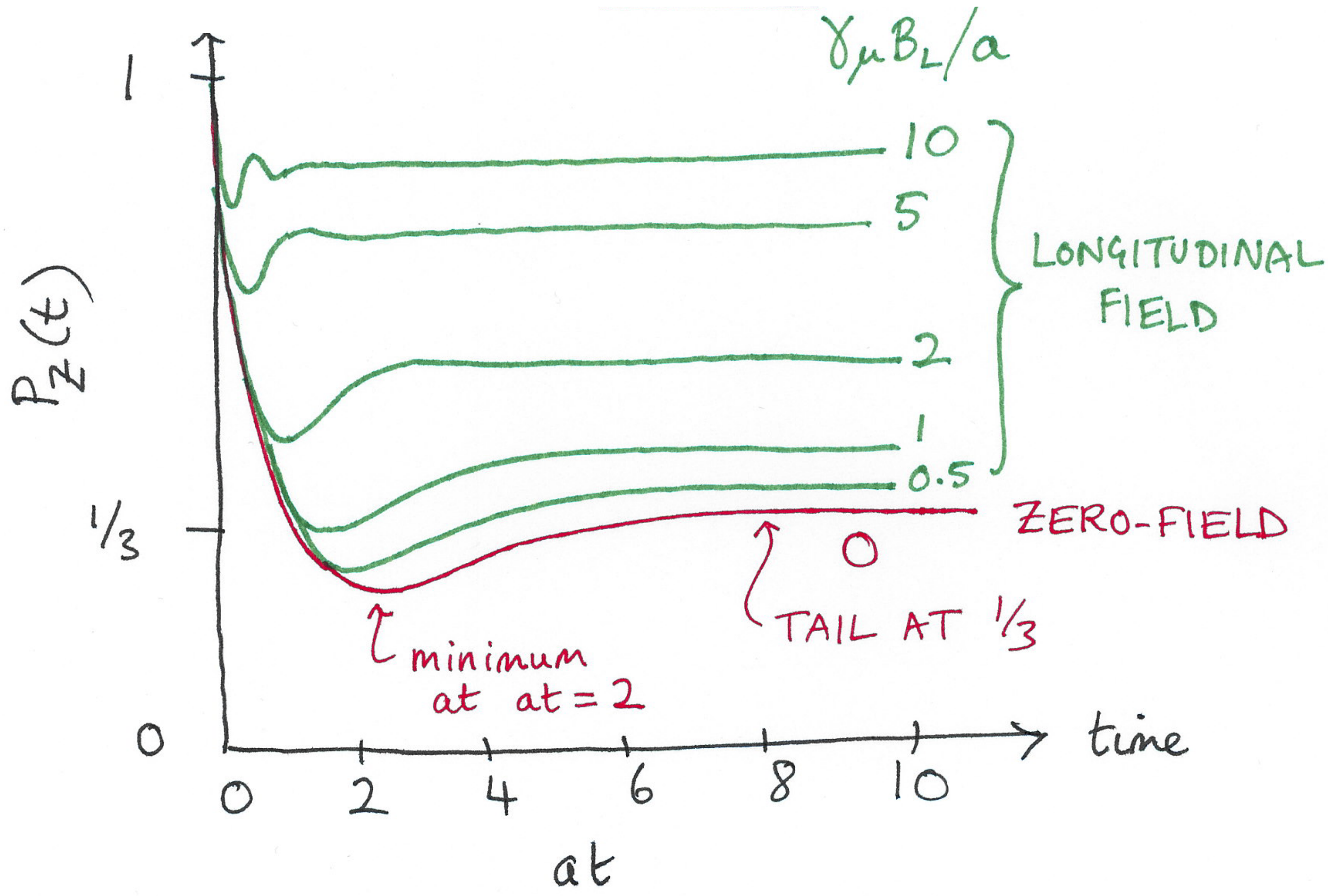
Zero field: $\boxed{P_z(t) = \frac{1}{3} + \frac{2}{3}(1 - at)e^{-at}}$

Longitudinal field:

$$\boxed{\begin{aligned} P_z(t) = {} & 1 - \frac{a}{\omega_L} j_1(\omega_L t) e^{-at} - \left(\frac{a}{\omega_L}\right)^2 \left[j_0(\omega_L t) e^{-at} - 1 \right] \\ & - \left[1 + \left(\frac{a}{\omega_L}\right)^2 \right] a \int_0^t j_0(\omega_L t) e^{-a\tau} \, d\tau \end{aligned}}$$

$\omega_L = \gamma_\mu B_L$; j_0 and j_1 are spherical Bessel functions

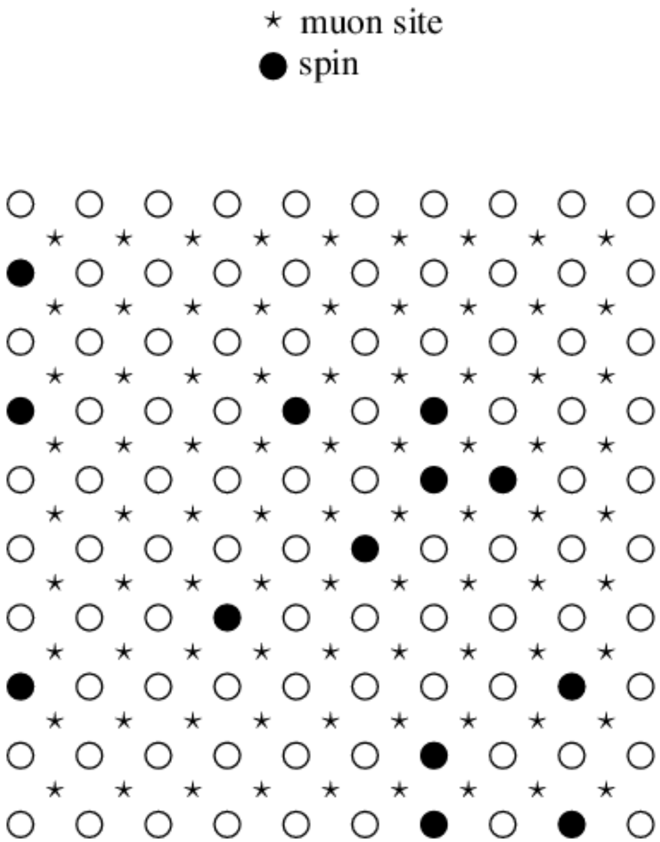
Lorentzian Kubo-Toyabe (LKT)



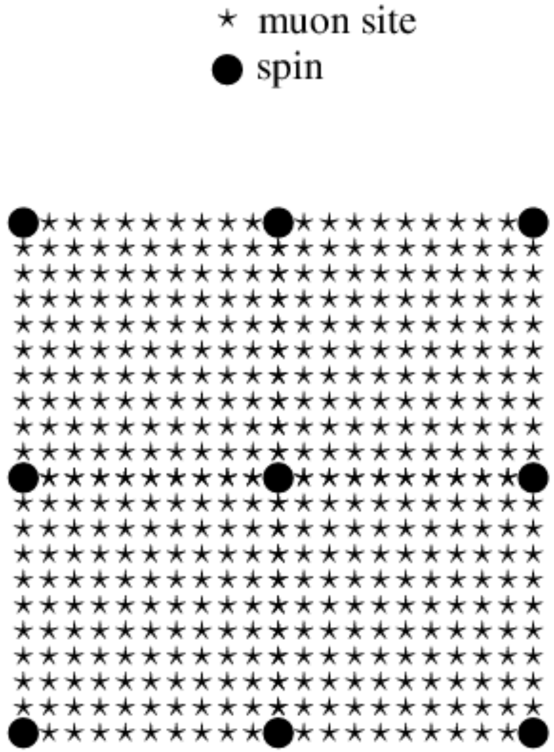
See Larkin et al. Physica B 289, 153 (2000).

The ‘Dilute’ Spin Condition

A broad range of couplings from the muon to the nearest spin is the key here

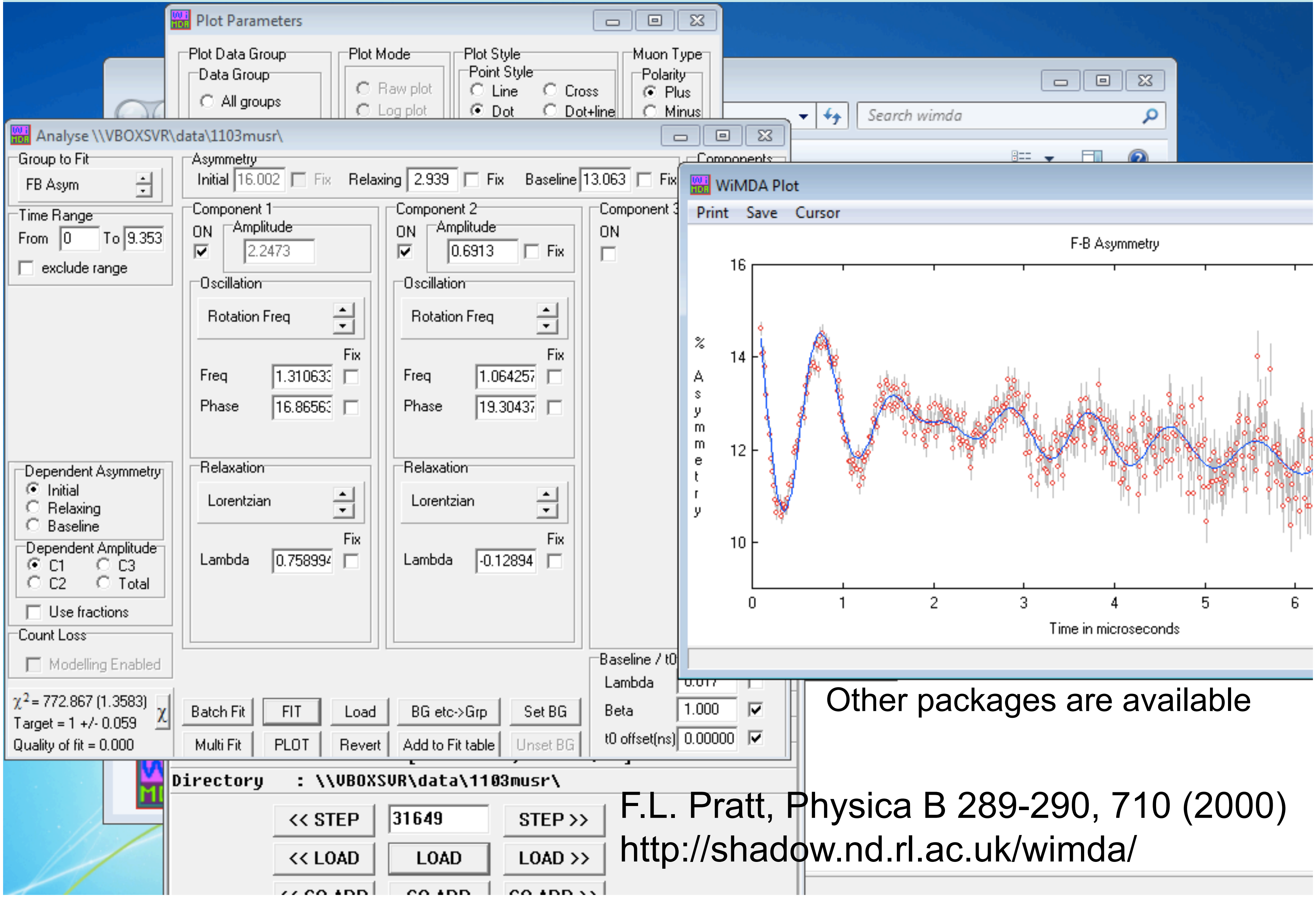


e.g. metallic random alloy spin glasses



e.g. complex molecular magnets

All these functions available in Wimda

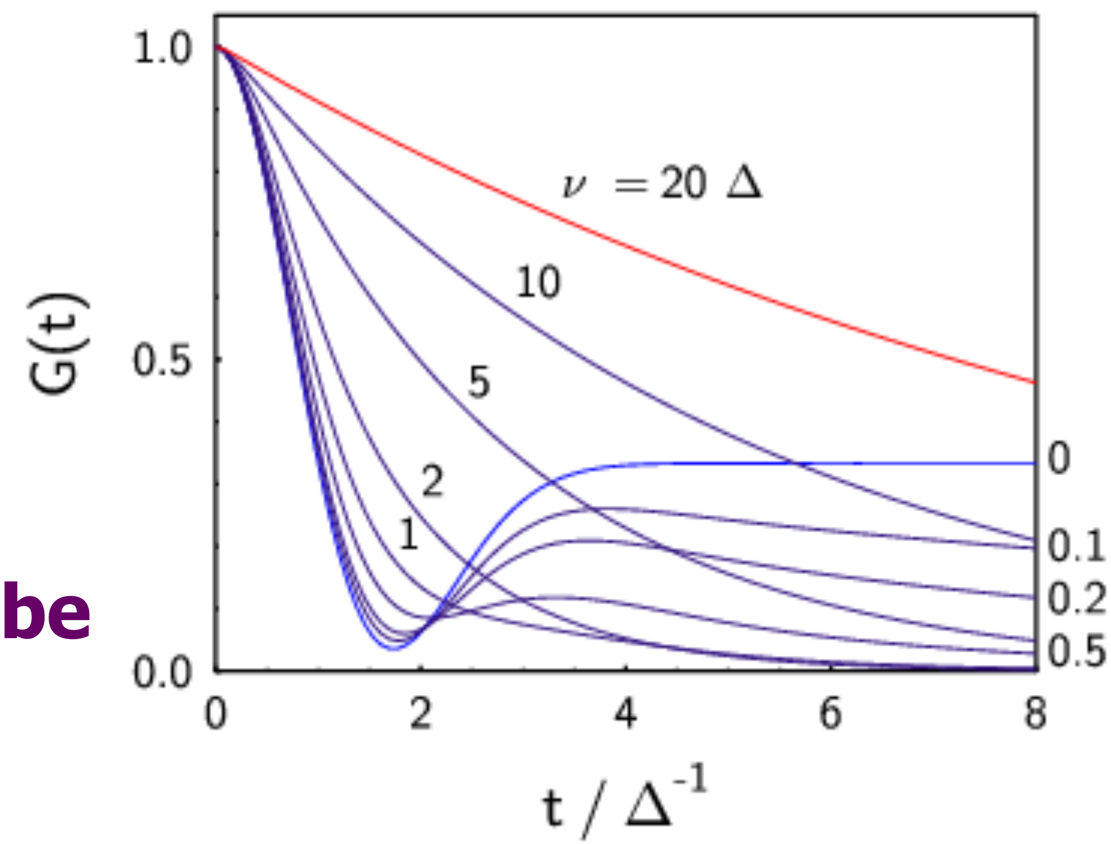


Other packages are available

F.L. Pratt, Physica B 289-290, 710 (2000)
http://shadow.nd.rl.ac.uk/wimda/

Introduce Dynamics

One can interpolate between statics and dynamics using a **dynamical Kubo-Toyabe function**



Introduce Dynamics

"Strong collision" approximation

(How to get a dynamic relaxation function from a static one)

Assume

1. local field on μ^+ is suddenly changed by a "collision", after which it is randomly distributed with no correlation with field before collision.
2. Collision takes place at rate ν

A Markov process:

$$\frac{\langle B(t)B(0)\rangle}{\langle [B(0)]^2\rangle} = e^{-\nu t}$$

Introduce Dynamics

Dynamic relaxation function

$$G_z(t,\nu) = \text{muons that don't collide up to time } t$$
$$+$$
$$\text{muons that do one collision}$$
$$+$$
$$\text{muons that do two collisions}$$
$$+ \ldots$$

$$= \sum_{n=0}^{\infty} g_z^{(n)}(t)$$

no jumps

$$g_z^{(0)}(t) = e^{-\nu t} \quad g_z(t)$$

the static relaxation function

fraction of muons not hopped up to time t

Introduce Dynamics

one jump at t_1

$$g_z^{(1)}(t) = \int_0^t \underbrace{(\nu\, dt_1)}_{\text{jumping probability}} \underbrace{e^{-\nu(t-t_1)} g_z(t-t_1)}_{\text{after jump}} \underbrace{e^{-\nu t_1} g_z(t_1)}_{\text{before jump}}$$

jumping probability between t_1 and $t_1 + dt_1$

Sum up all single jumps between 0 and t

two jumps

$$g_z^{(2)}(t) = \int_{t_2}^{t} \int_0^{t_2} \nu^2\, dt_2\, dt_1\, e^{-\nu(t-t_2)} g_z(t-t_2)\, e^{-\nu(t_2-t_1)} \cdot$$

$$\times\ g_z(t_2-t_1)\, e^{-\nu t_1} g_z(t_1)$$

Introduce Dynamics

SUMMING UP

$$G_Z(t,\nu) = e^{-\nu t}\Big[g_Z(t) + \nu \int_0^t g_Z(t_1)\, g_Z(t-t_1)\, dt_1 + \nu^2 \int_0^t \int_0^{t_2} g_Z(t_1)\, g_Z(t_2-t_1)\, g_Z(t-t_2)\, dt_1 dt_2 + \dots \Big]$$

Analytic solutions can be found by Laplace transforms.

BASIC IDEA: $G_Z(t) = \sum_{n=0}^{\infty} g_Z^{(n)}(t)$ with

$$g_Z^{(n)}(t) = \nu^n \int_{t_n}^{t} \dots \int_0^{t_2} dt_n \dots dt_1 \, e^{-\nu t} g_Z(t-t_n) \dots g_Z(t_1)$$

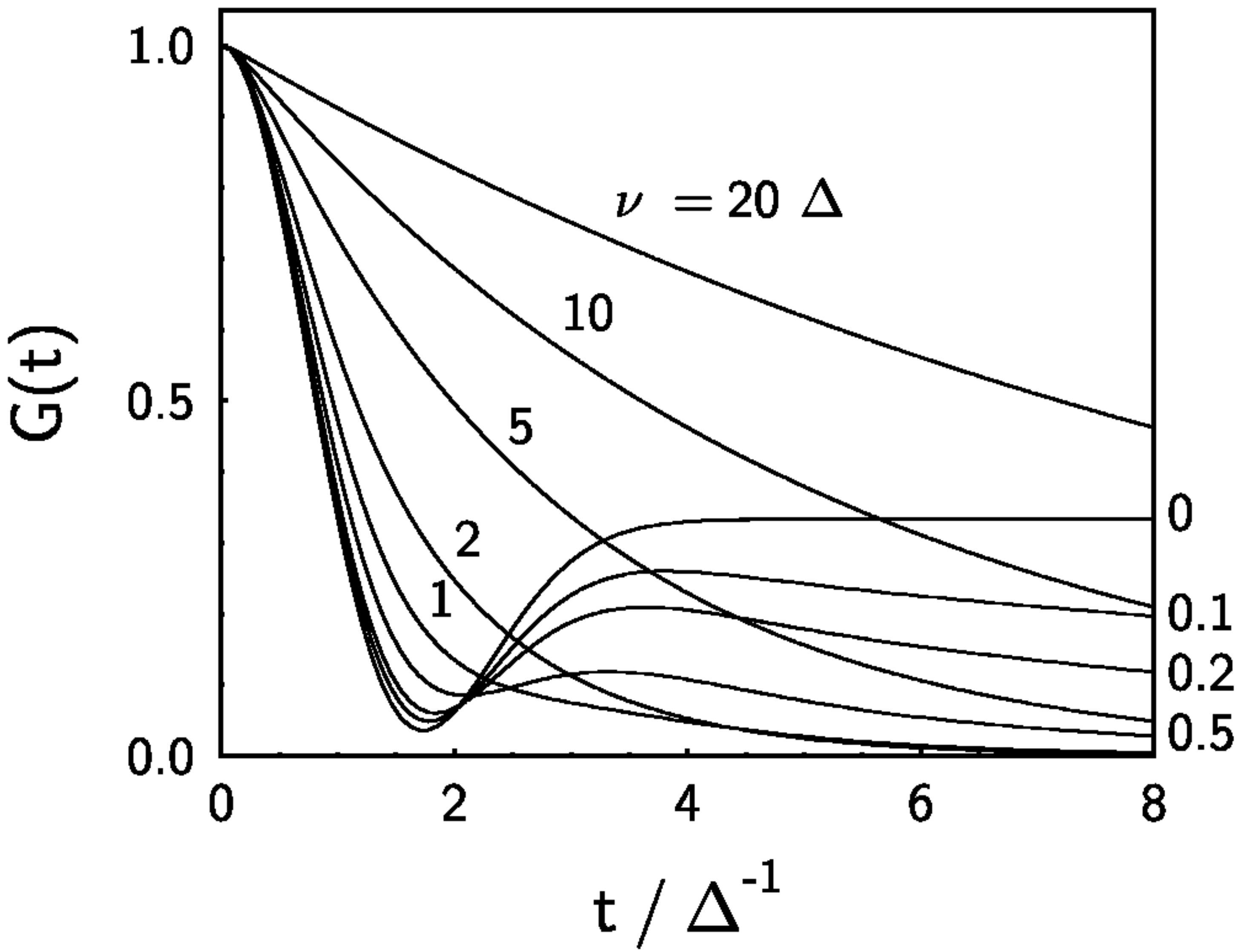
(a convolution!)

Write $f_Z^{(n)}(s) = \int_0^\infty g_Z^{(n)}(t)\, e^{-st}\, dt = \nu^n \left[f_Z(s) \right]^{n+1}$

$$\Rightarrow \quad F_Z(s) = \int_0^\infty G_Z(t)\, e^{-st}\, dt = \sum_{n=0}^{\infty} \nu^n \left[f_Z(s) \right]^{n+1} = \frac{f_Z(s)}{1 - \nu f_Z(s)}$$

Sum of an infinite geometric progression

Dynamical Kubo-Toyabe (DKT)



Dynamical Kubo-Toyabe (DKT)

A route to the dynamic Kubo-Toyabe function

$$g_z(t) = \frac{1}{3} + \frac{2}{3}\left(1 + \Delta^2 t^2\right) \exp\left(-\frac{1}{2}\Delta^2 t^2\right)$$

$$\Rightarrow f_z(s) = \frac{1}{3s} + \frac{2s}{3\Delta^2}\left[1 - s\int_0^\infty \exp\left[-\frac{1}{2}\Delta^2 t^2 - st\right] dt\right]$$

$$\Rightarrow F_z(s) = \frac{f_z(s)}{1 - \nu f_z(s)} \xrightarrow[\text{inverse Laplace transform}]{\text{numerically}} G_z(t)$$

In fact, numerically it's easier to work with

$$G_z(t,\nu) = g_z^{(0)}(t) + \nu \int_0^t dt_1\, g_z^{(0)}(t - t_1)\, G_z(t_1, \nu)$$

[though note that what you want is on the LHS and RHS!]

Since the G_z integral depends only on G_z at earlier times and the known static function g_z , it can be built up sequentially in time

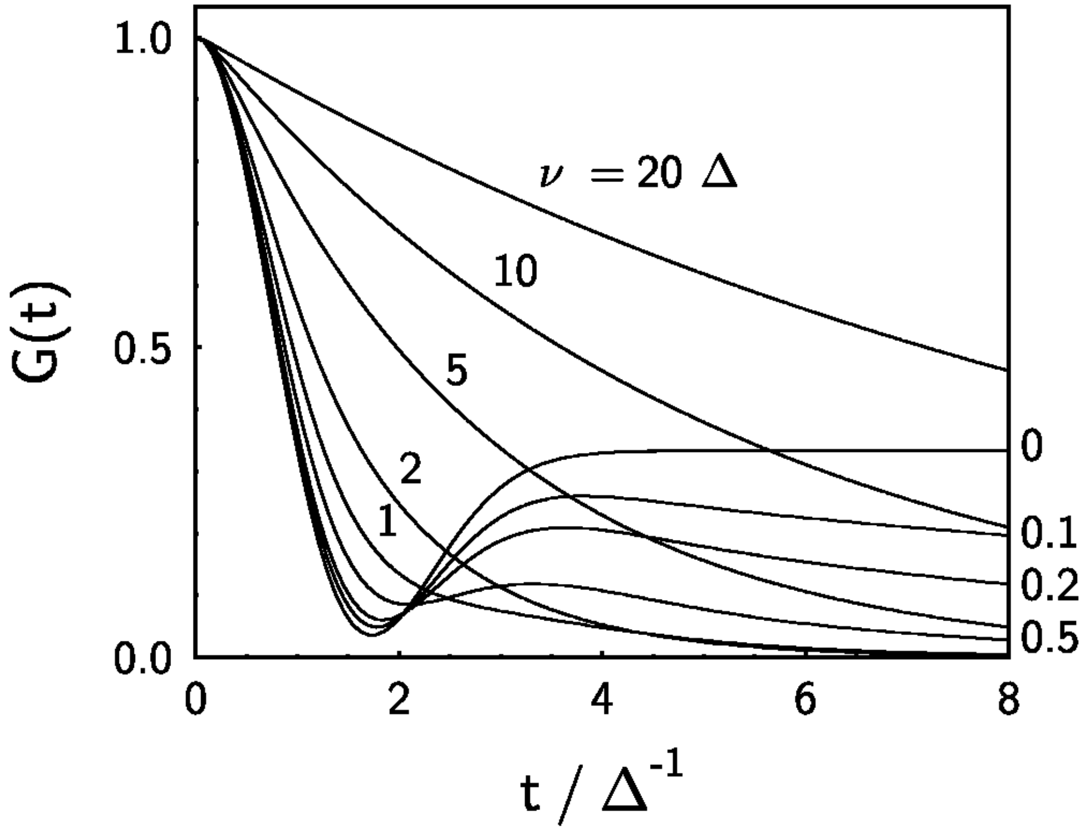
Slow Hopping

Main effect is in the tails !

The Kubo-Toyabe "$\frac{1}{3}$" becomes (at long times)

$$G_z(t) \longrightarrow \frac{1}{3}\, e^{-\frac{2}{3}\nu t}$$

LOOKS THE RIGHT WAY ROUND



Fast Hopping

Fast fluctuation limit

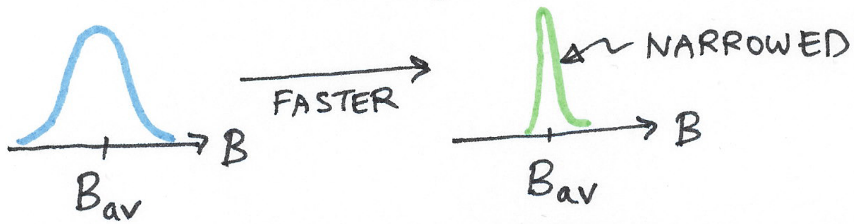
$$G_z(t) \to e^{-\lambda t}$$

EXPONENTIAL

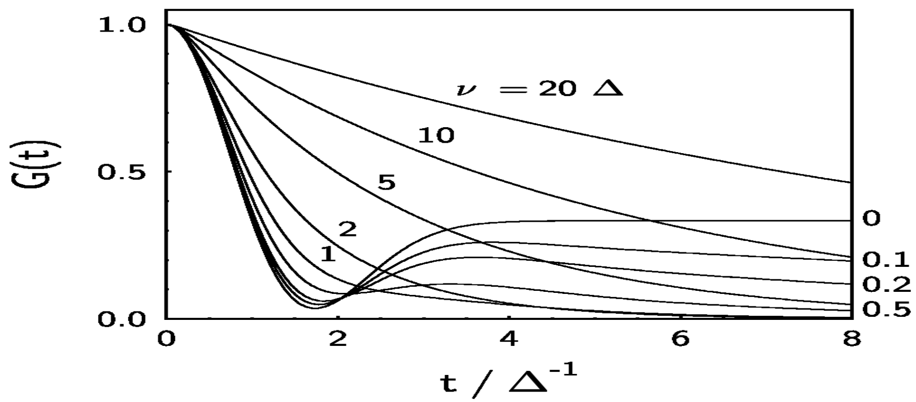
RELAXATION RATE $\lambda = \dfrac{2\Delta^2}{\nu}$ FLUCTUATION RATE

LOOKS THE WRONG WAY ROUND

(TRICKY JARGON: MOTIONAL NARROWING



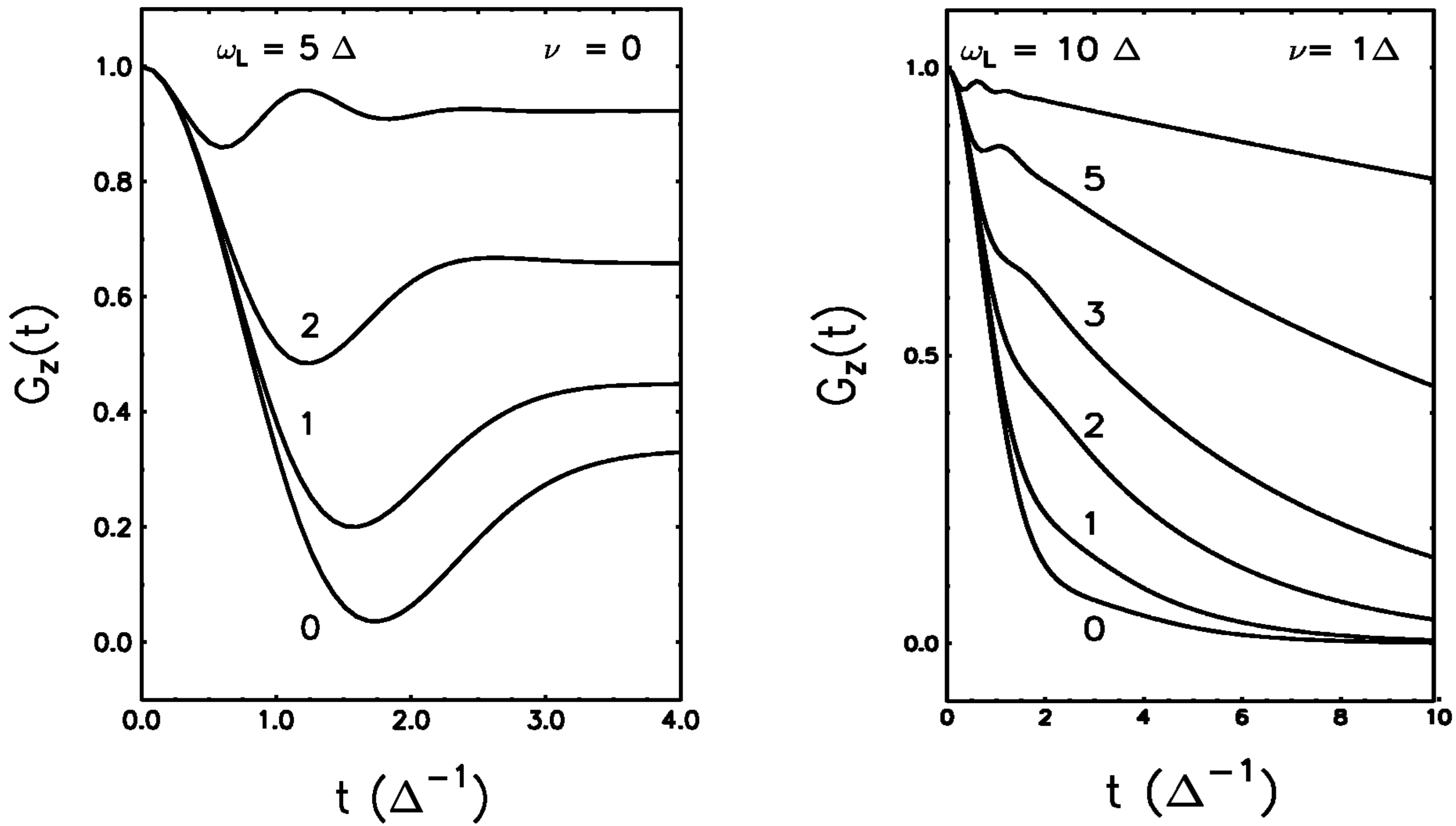
Muon "sees" more of an average field when moving fast – its effective field distribution narrows)



Effect of Longitudinal Field

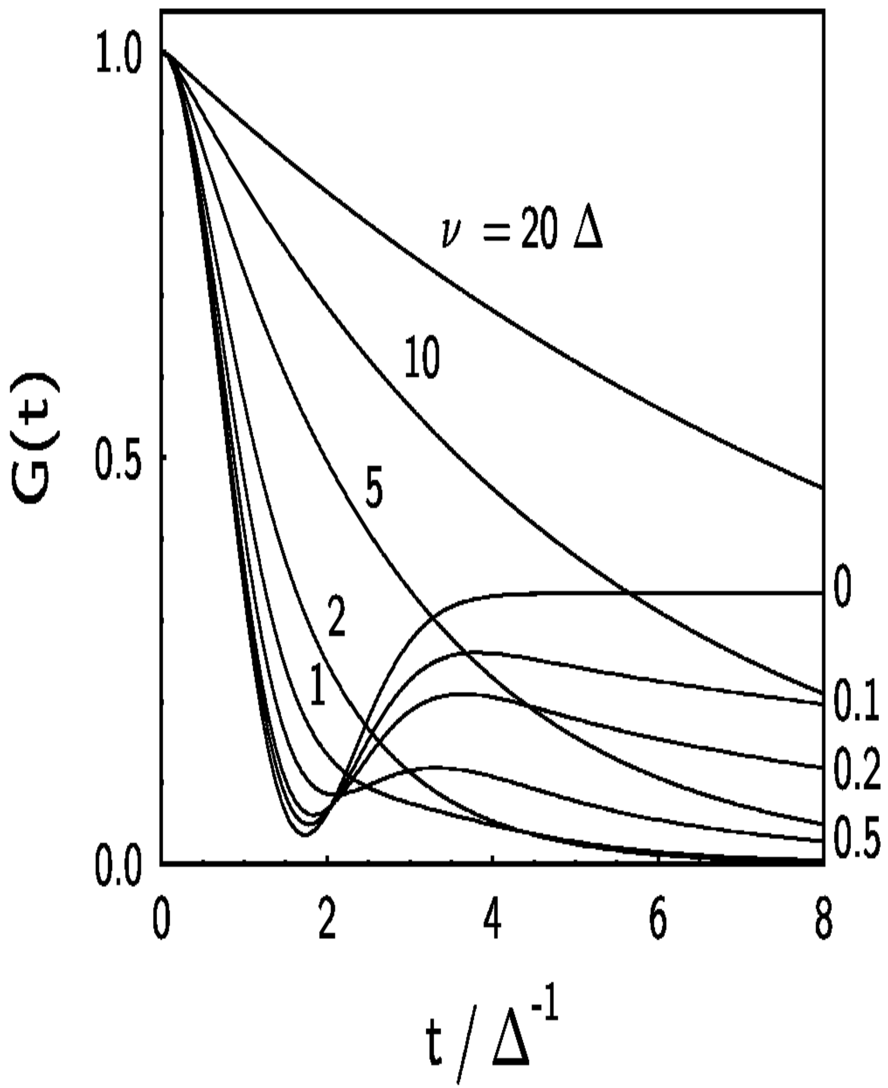
Static

Dynamic

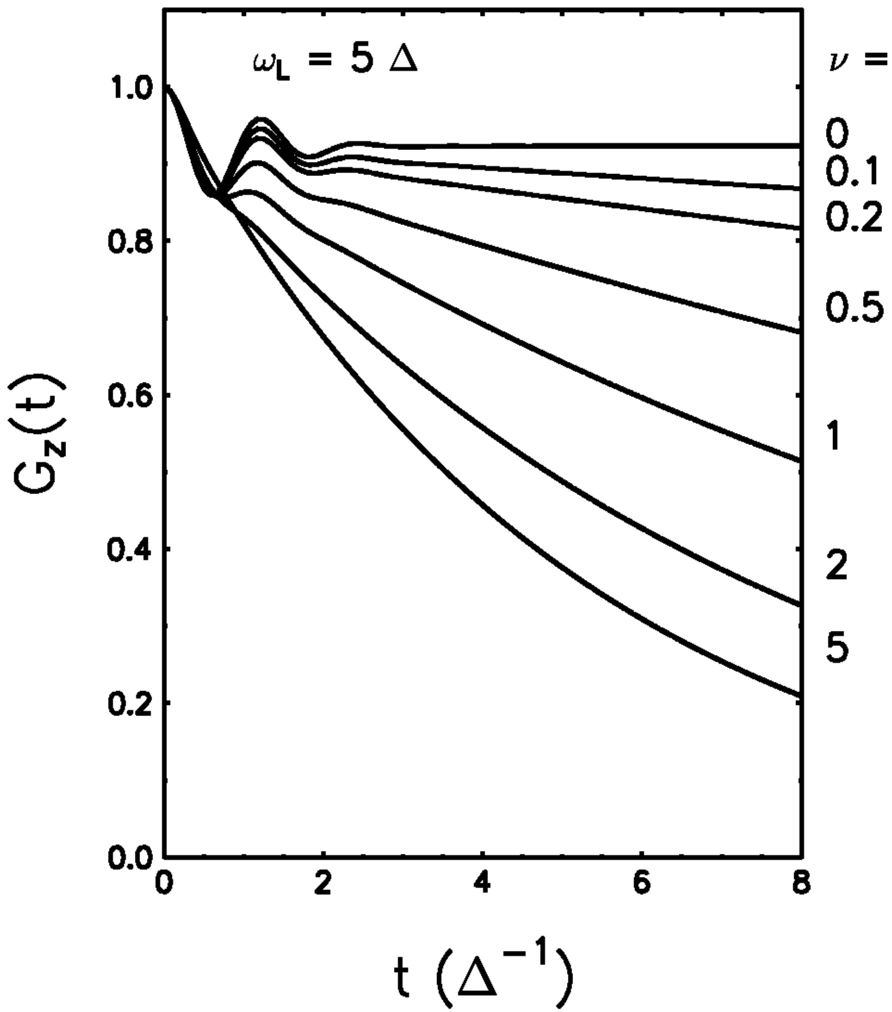


Effect of Dynamics

Zero-field



Longitudinal-field



The Keren Function

Perturbation expansion for $P_z(t)$ gives an **analytical** result valid for $\nu > \Delta$

$$P_z(t) = P_z(0)\exp\left[-\Gamma(t)t\right]$$

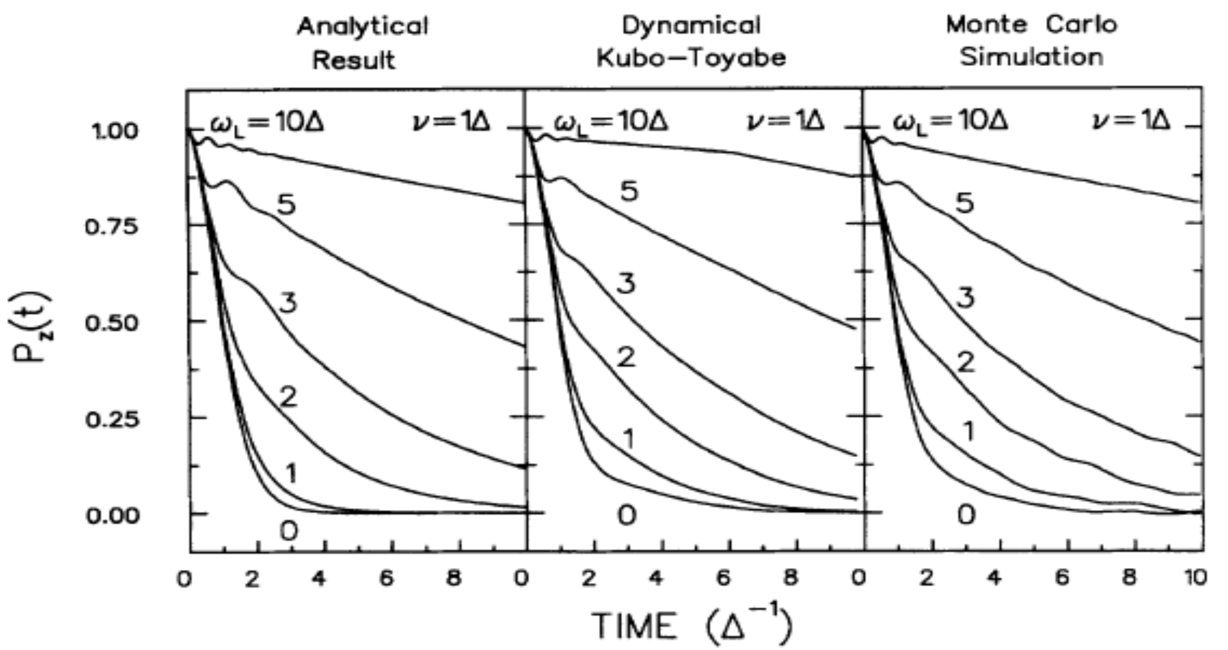
$$\Gamma(t)t = 2\Delta^2 \frac{\{[\omega_L^2+\nu^2]\nu t + [\omega_L^2-\nu^2][1-e^{-\nu t}\cos(\omega_L t)] - 2\nu\omega_L e^{-\nu t}\sin(\omega_L t)\}}{(\omega_L^2+\nu^2)^2}$$

PRB 50,10039 (94)

ZF limit: (LF Abragam) $\Gamma(t)t = \frac{2\Delta^2}{\nu^2}(e^{-\nu t} - 1 + \nu t)$

Fast ν limit: ($\nu > \omega_L$) $\Gamma(t)t = \frac{2\Delta^2 \nu}{\omega_L^2+\nu^2} t$

Amit Keren



Stretched Exponential Functions

$$e^{-(\lambda t)^{\beta}}$$

stretch parameter

STRETCHED EXPONENTIALS FIT EVERYTHING

Stretched Exponential Functions

$$e^{-(\lambda t)^{\beta}}$$

lineshape parameter

Gaussian	$\beta=2$
Lorentzian	$\beta=1$
Stretched	$\beta<1$

Stretched exponentials generally arise from:

1) *Distribution of relaxation times*

2) *Distribution of couplings*

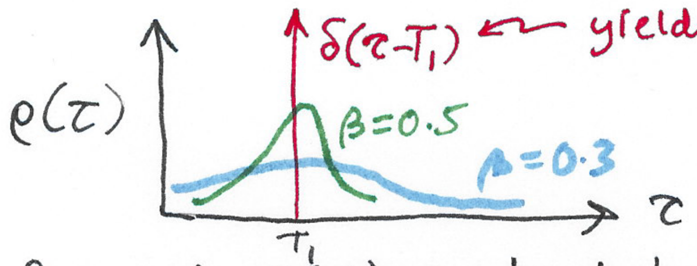
Distribution of Relaxation Time

$$e^{-t/\tau} \longrightarrow \int_0^\infty \rho(\tau)\, e^{-t/\tau}$$

This yields a STRETCHED EXPONENTIAL $\quad e^{-(t/T_1)^\beta}$

if $$\rho(\tau) = -\frac{1}{\pi\tau}\sum_{l=1}^{\infty} \frac{(-1)^l\,\Gamma(1+l\beta)}{l!}\left(\frac{\tau}{T_1}\right)^{\beta l}\sin(\pi\beta l)$$

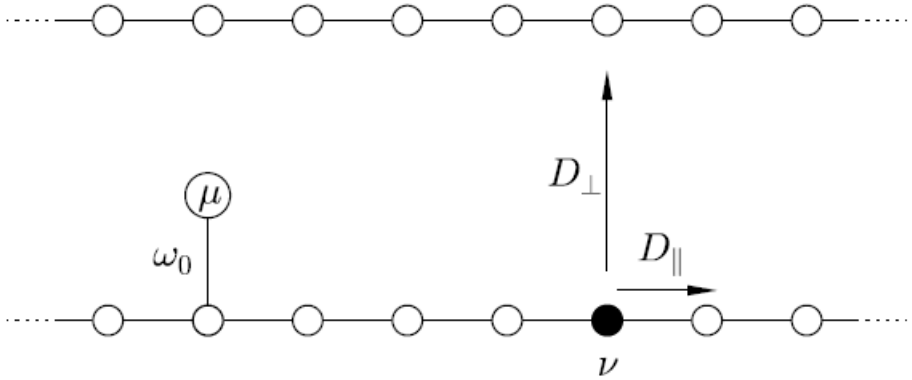
[see Steer, Blundell et al, Physica B 326, 513 '03]



The form of $\rho(\tau)$ is hard to justify physically in most cases, but broad distributions of τ lead to smaller β.

Distribution of Relaxation Times: Diffusion

1D:

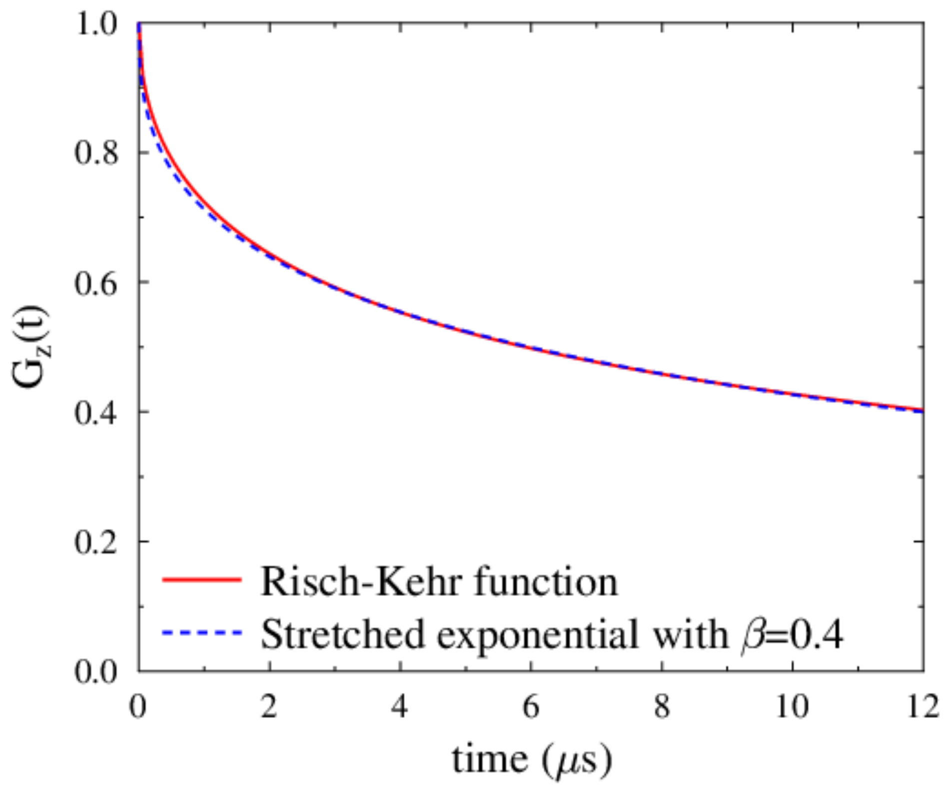


Risch-Kehr function

$$G_z(t) = \mathrm{e}^{\Gamma t}\,\mathrm{erfc}\,\sqrt{\Gamma t}$$

PRB 46, 5246 (1992)

Klaus Kehr
(1934-2000)



B-dependent Relaxation and Spectral Density

Correlation function for field fluctuations:

$$\Phi(t) = \frac{\langle B(t)B(0)\rangle}{\langle [B(0)]^2\rangle} = e^{-\nu t}$$

Fourier transform of $\Phi(t)$ gives the spectral density $S(\omega)$

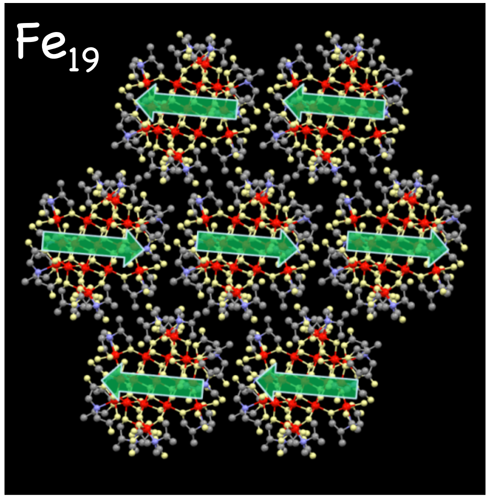
$$S(\omega) = \nu \;/\; (\nu^2 + \omega^2)$$

λ is proportional to $S(\omega_L)$

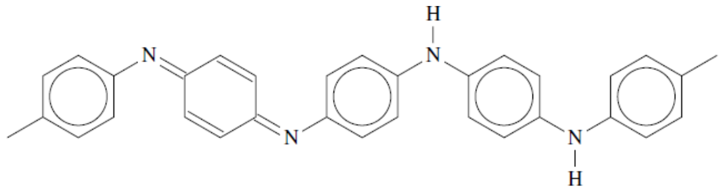
Complex relaxation processes such as those based on diffusion typically give power laws for $\Phi(t)$ and $S(\omega)$

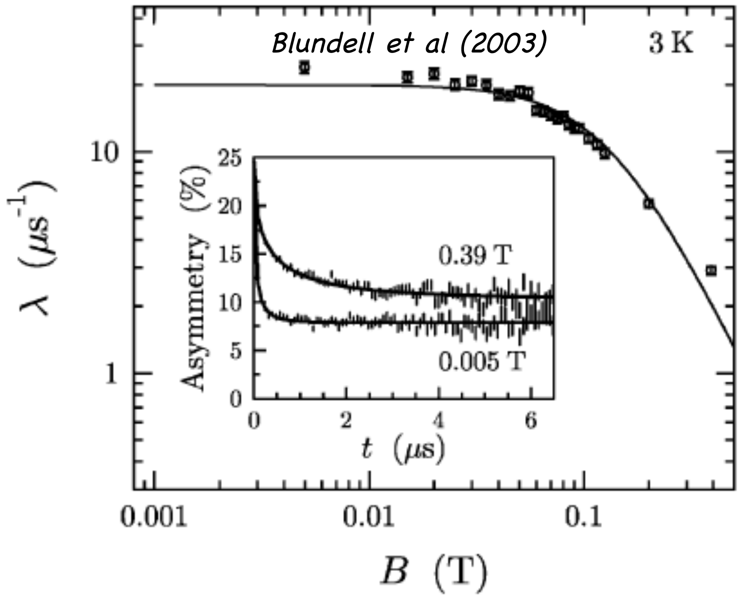
B-dependent Relaxation and Spectral Density

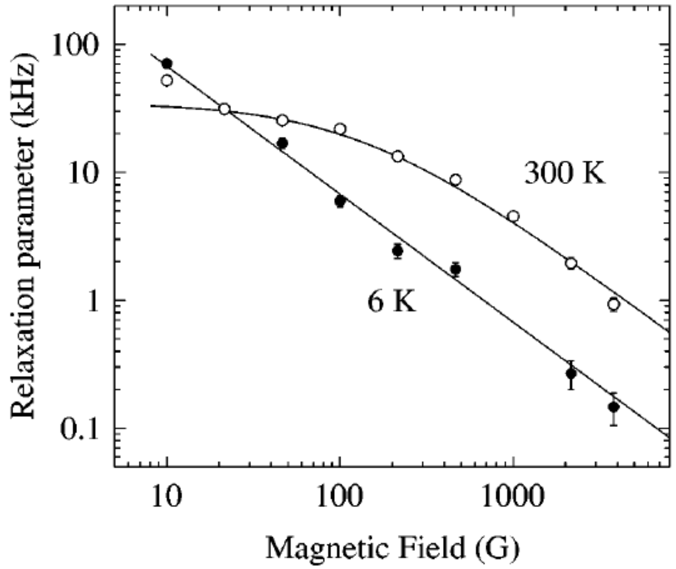
Single molecule magnet



Polyaniline







Stretched relaxation is due to the coupling distribution

Stretched relaxation is due to the 1D diffusion process

Distribution of Couplings

Spin Glasses

Muons that stop closer to magnetic ions "see" a wider local field distribution (which extends to higher fields) than muons which stop at a greater distance

Y.J. Uemura et al, PRB **31**, 546 (1985)

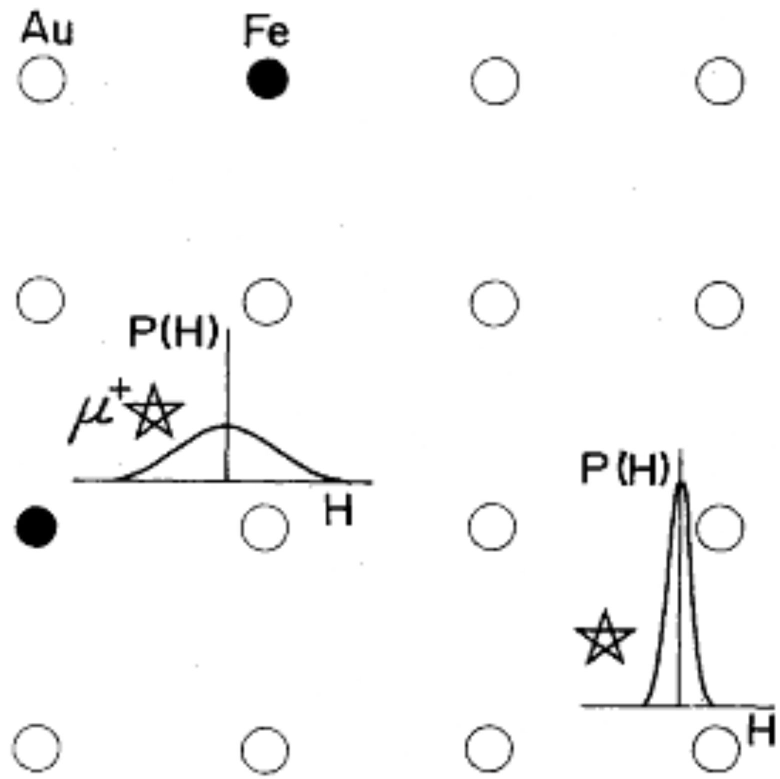


FIG. 3. Schematic view of different variable ranges of random local fields at different muon sites in dilute-alloy spin glasses. When Fe (or Mn) moments fluctuate, the local field at muon sites closer to the magnetic ions will be modulated in a wider range.

Distribution of Couplings

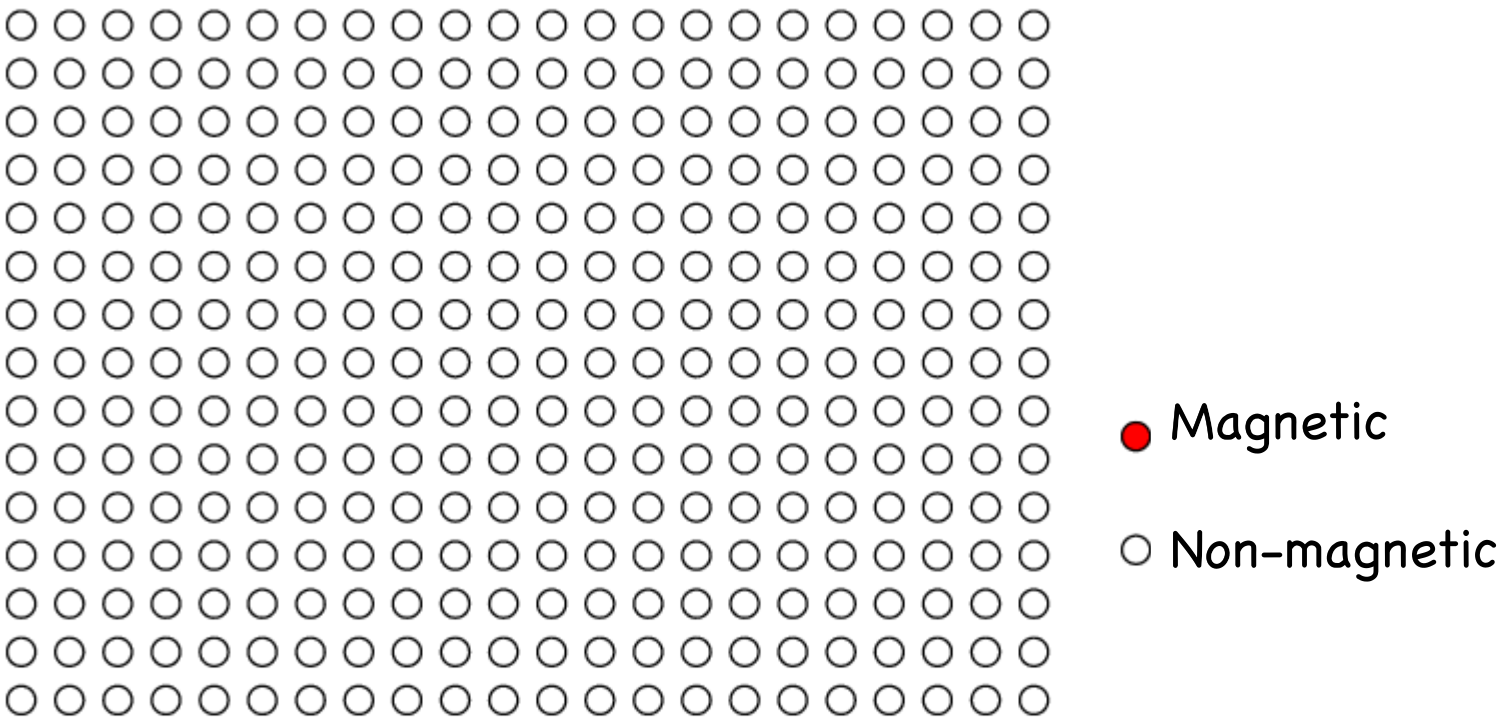
The correct relaxation function must therefore be an average over distribution widths Δ.

This leads to a root-exponential relaxation function: $G(t) = G(0)\exp(-(\lambda t)^{1/2})$

where the relaxation rate λ is inversely proportional to the fluctuation rate ν.

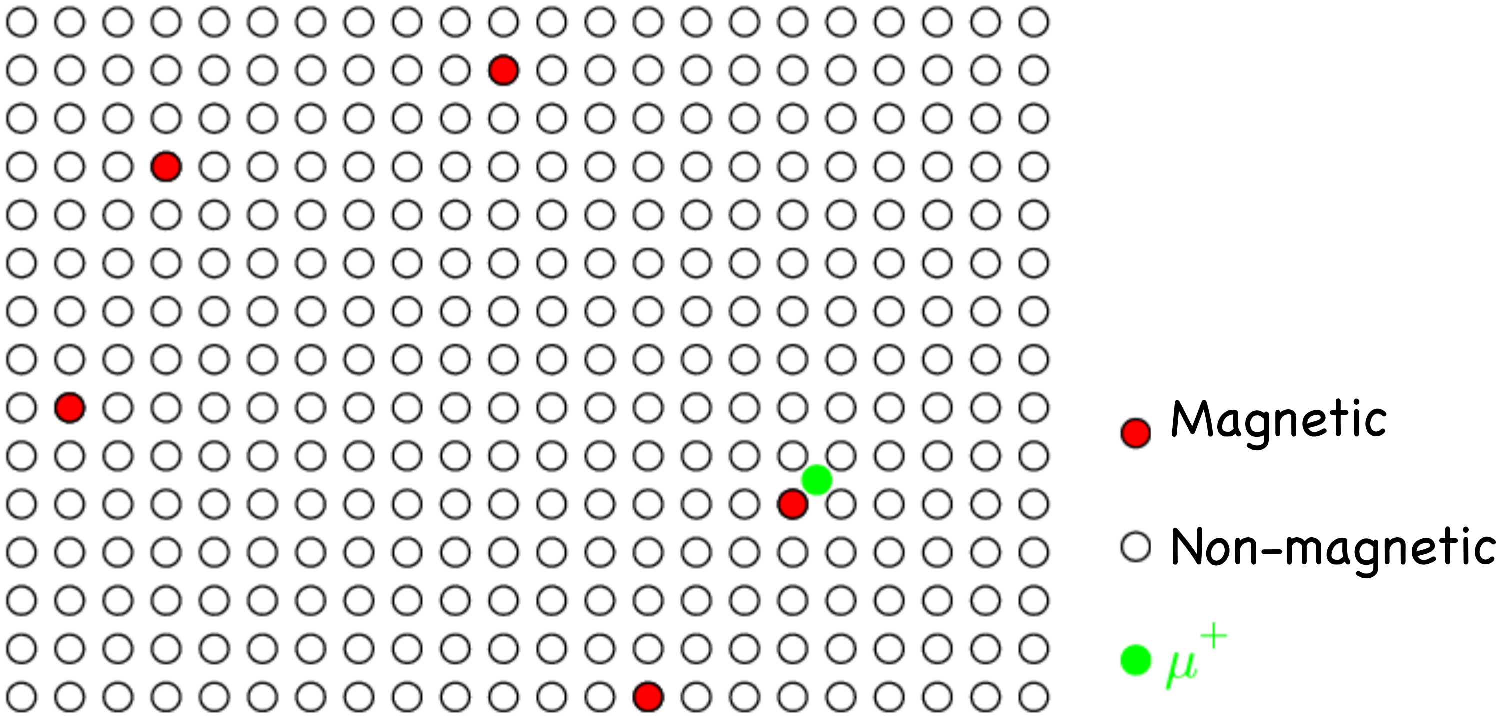
Distribution of Couplings

Non-magnetic host



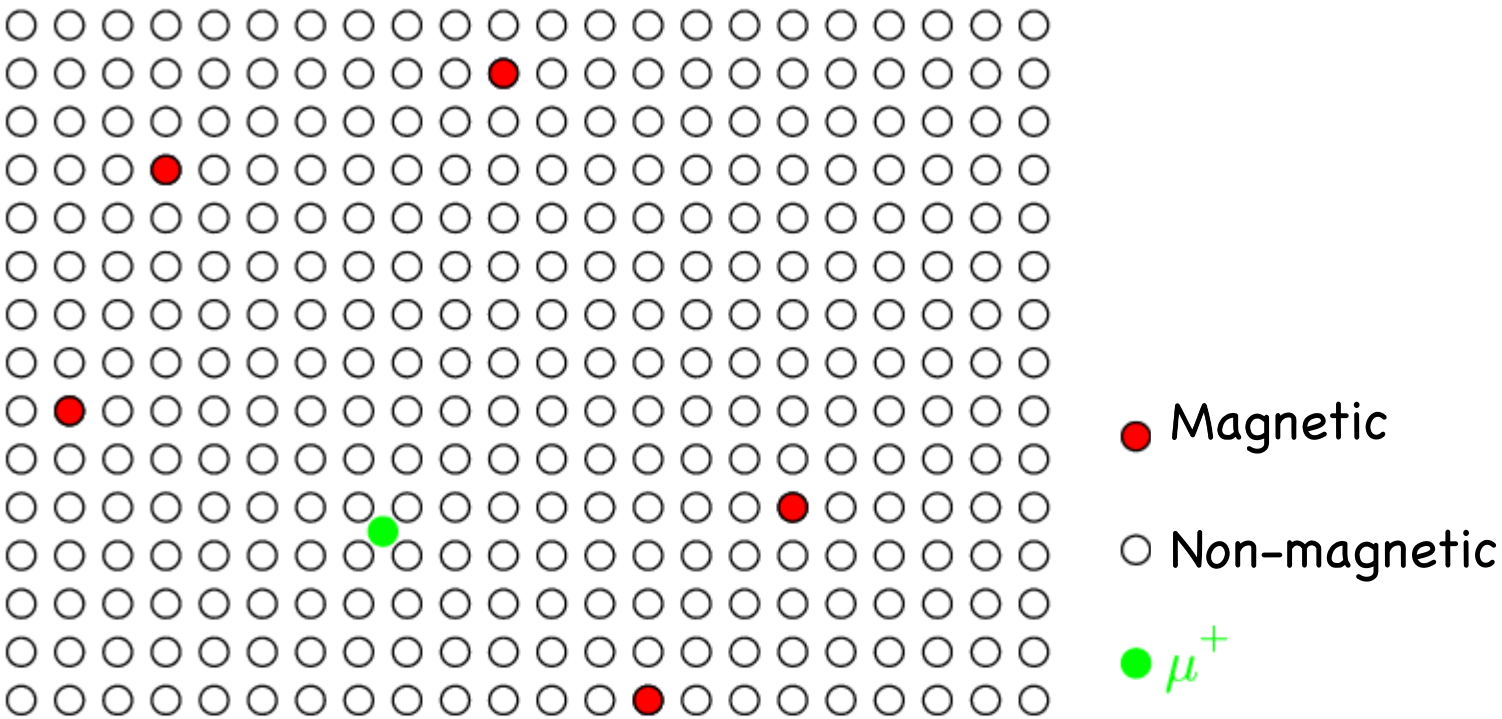
Spin glass

Muon stops close to magnetic ion



Spin glass

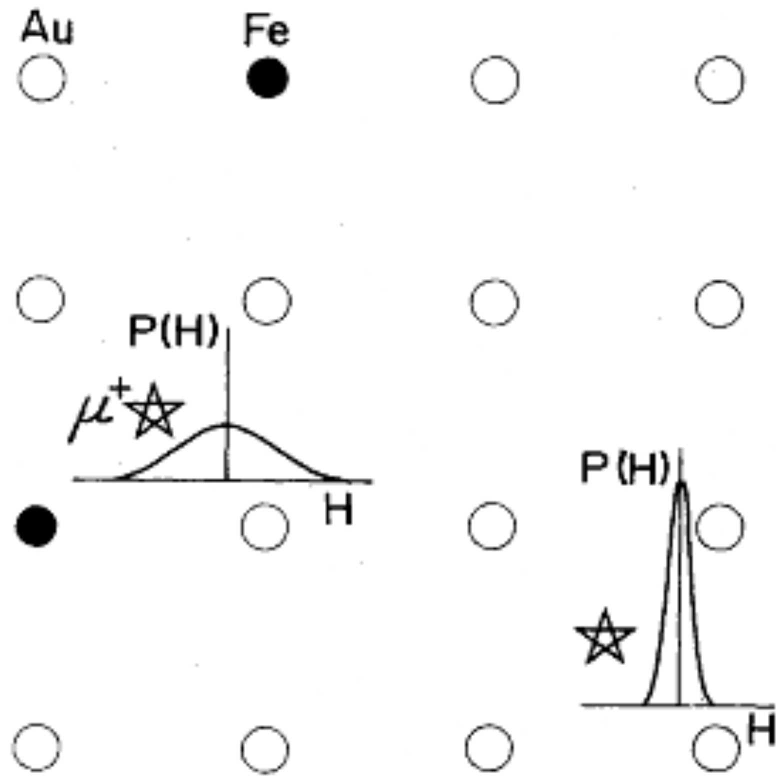
Muon stops well away from magnetic ion



Distribution of Couplings

Spin Glasses

Muons that stop closer to magnetic ions "see" a wider local field distribution (which extends to higher fields) than muons which stop at a greater distance



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Y.J. Uemura et al, PRB **31**, 546 (1985)

Distribution of Couplings

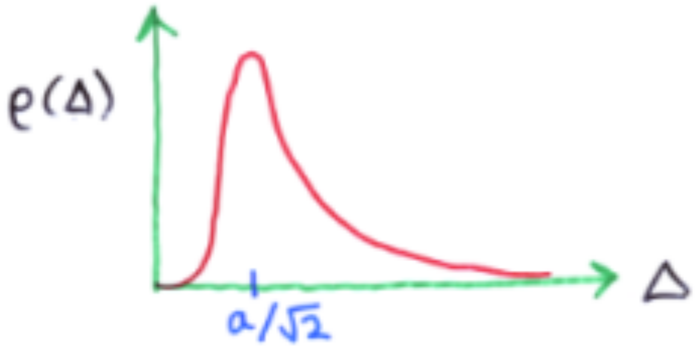
Range of coupling strengths

i.e. distribution of Δ

PRB 31 546 '85
PRB 50 10039 '94

$$\rho(\Delta) = \sqrt{\frac{2}{\pi}}\,\frac{a}{\Delta^2}\,e^{-a^2/2\Delta^2}$$

$\langle\Delta\rangle \sim a$



so that

$$P(t) = \int_0^\infty e^{-\Gamma t}\,\rho(\Delta)\,d\Delta$$

$$= \exp\left[-(\lambda t)^{1/2}\right] \quad \text{where } \lambda = \frac{2a^2\Gamma}{\Delta^2}$$

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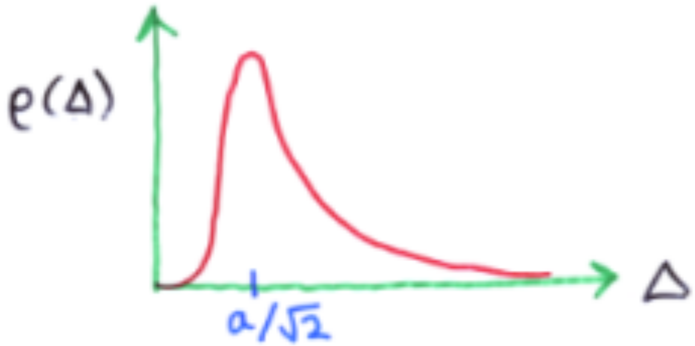

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……**but is the dogma correct?**

Distribution of Couplings

Monte-Carlo calculation of distribution of Δ

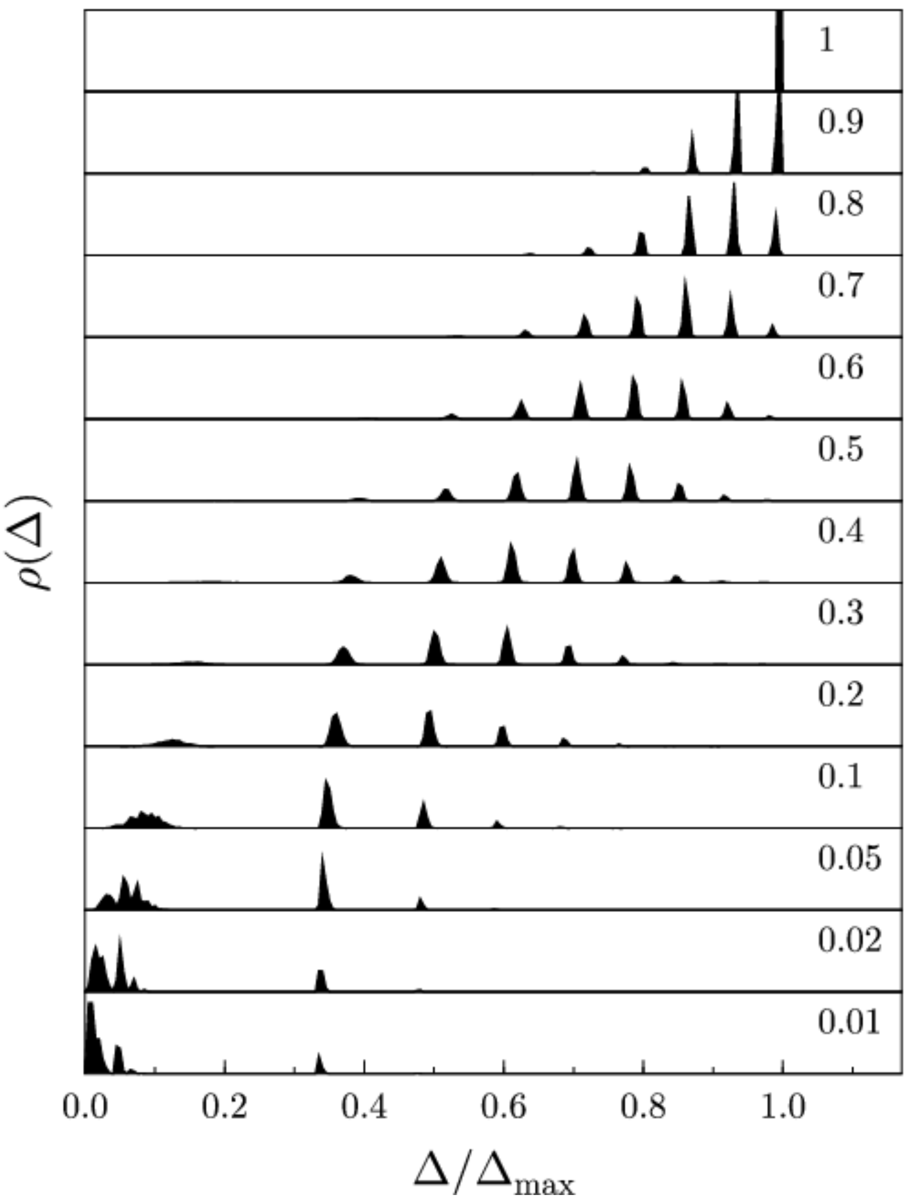
$$\boxed{\Delta^2 = \frac{2}{3}S^2\hbar^2\gamma_\mu^2\gamma_e^2\sum_k \frac{1}{r_k^6}}$$

r_k is the distance from the muon to the $k^{\rm th}$ spin

the sum is taken over sites occupied with probability c

- If $c = 1$, $\rho(\Delta) = \delta(\Delta - \Delta_{\rm max})$.
- For $c = 0.01$, substantial departures from

$$\rho(\Delta) = \sqrt{\frac{2}{\pi}}\left(\frac{a}{\Delta^2}\right) e^{-a^2/2\Delta^2}.$$



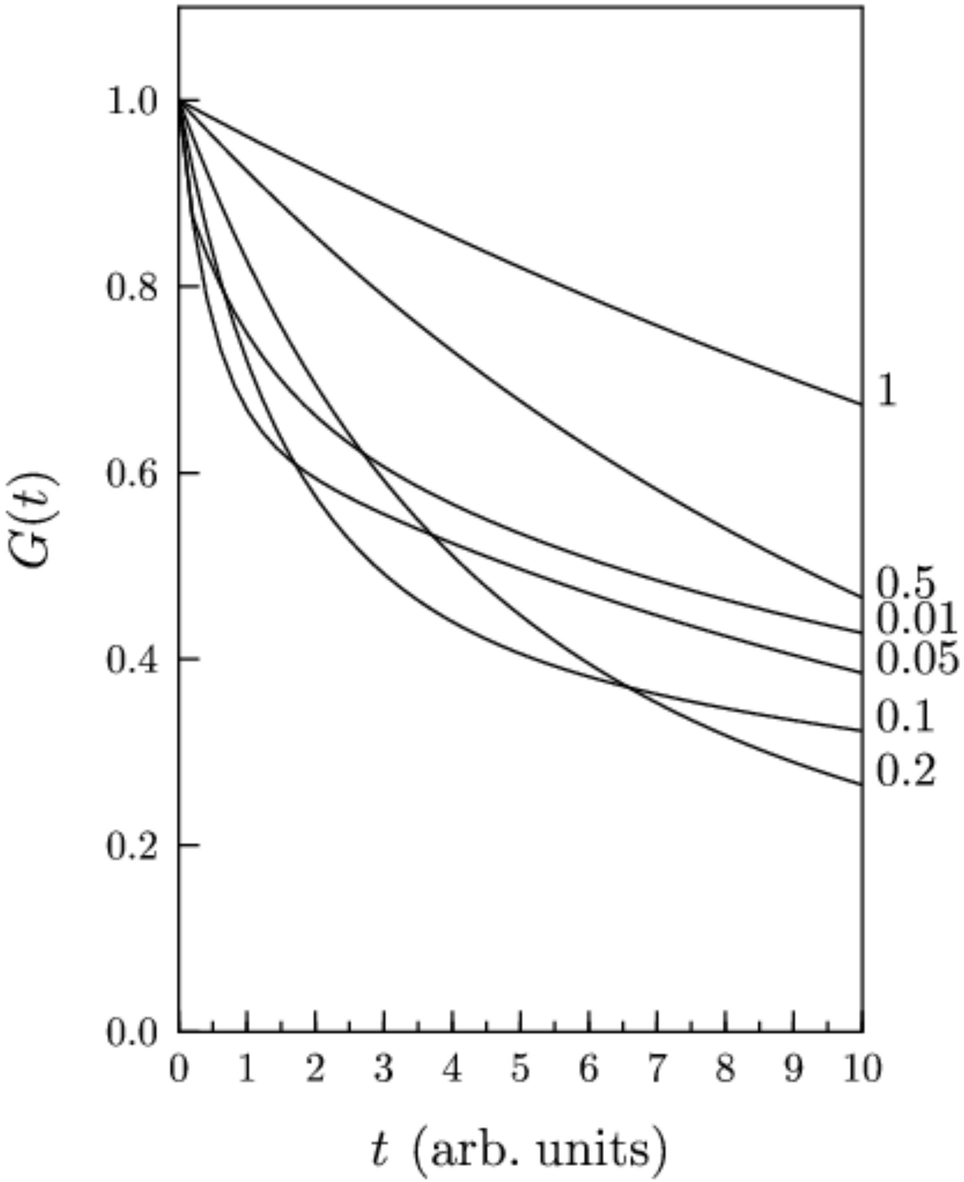
S. J. Blundell, T. Lancaster, F. L. Pratt, C. A. Steer, M. L. Brooks and J. F. Letard, J. Phys. IV France **114**, 601 (2004)

Distribution of Couplings

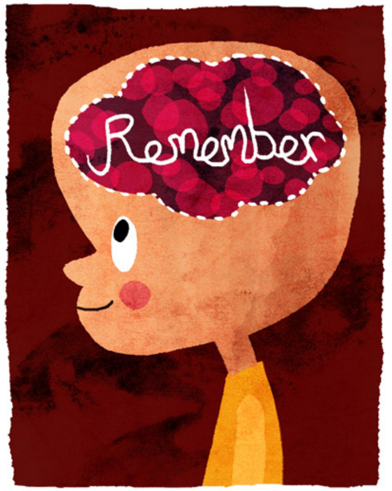
The μSR function can be obtained from $\rho(\Delta)$ using

$$G(t) = \int_0^\infty \exp(-2\Delta^2 t/\nu)\rho(\Delta)\,\mathrm{d}\Delta.$$

- Adjust the fluctuation frequency as $\nu \propto c^2$ to crudely simulate the effect of the slowing down of the remaining spins as c decreases.
- If $c = 1$, simple exponential relaxation results.
- If $c \ll 1$, the relaxation is similar to the observed root exponential behaviour.



S. J. Blundell, T. Lancaster, F. L. Pratt, C. A. Steer, M. L. Brooks and J. F. Letard, J. Phys. IV France **114**, 601 (2004)



Some things to REMEMBER.

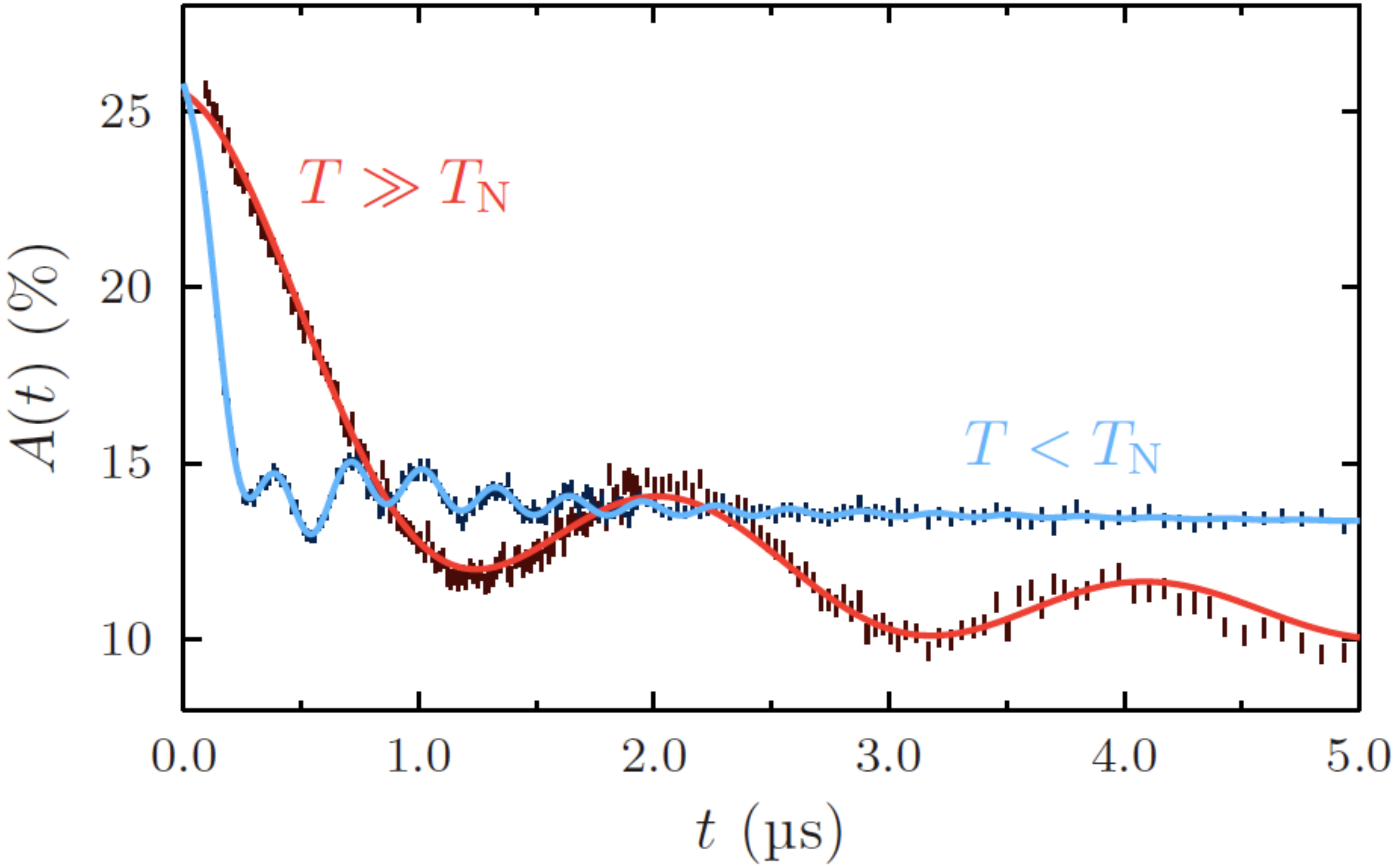
1. The standard fit functions (particularly $e^{-(\lambda t)^\beta}$) may "work" – but what does it mean?

2. Fluctuations in magnets are often CORRELATED
i.e. not Markov!

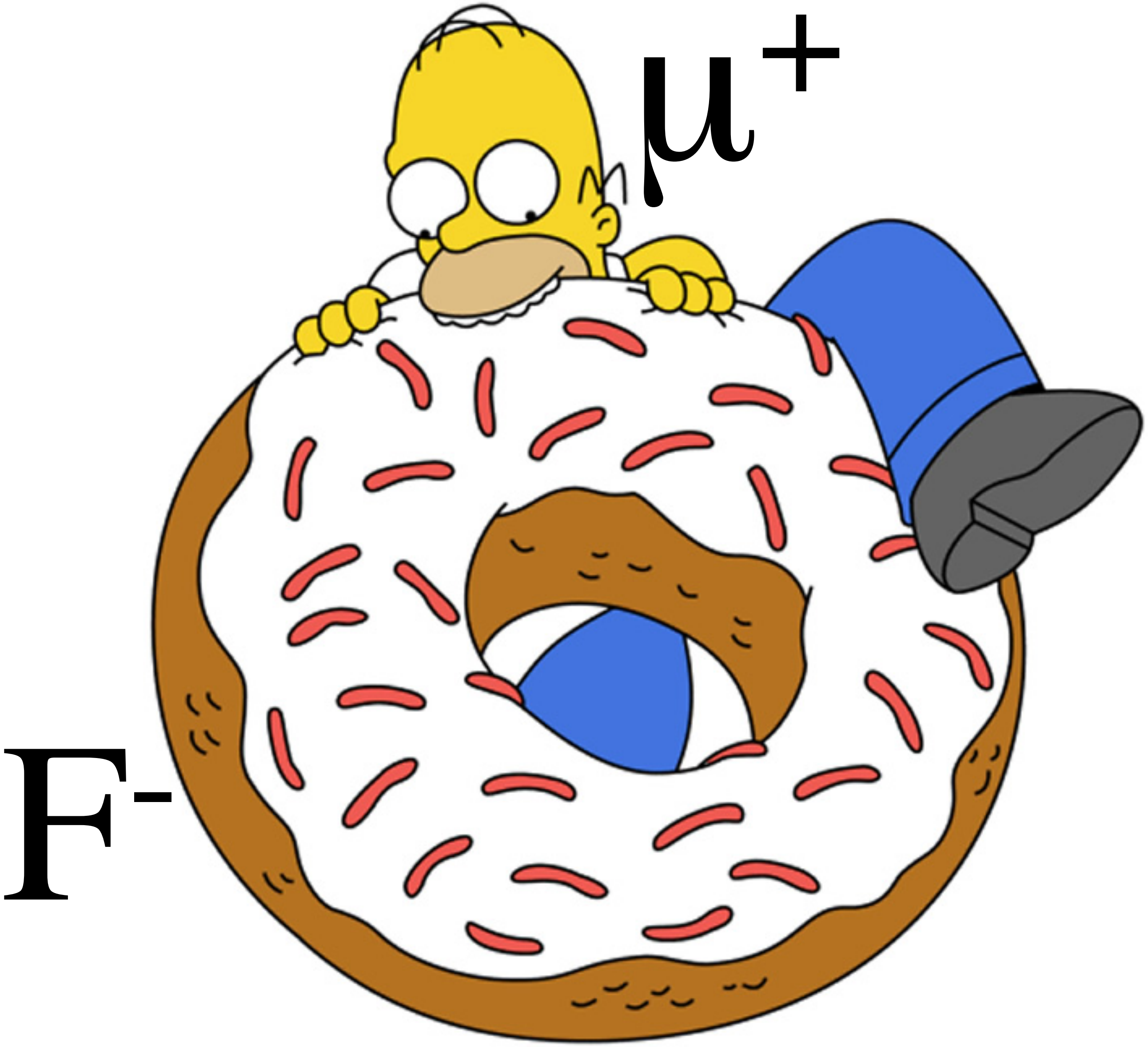
see Keren et al. PRB 64 054403 '01 (beautiful paper)

3. Beware the hints of quantum coherence!
(see work of Celio & Meier.)

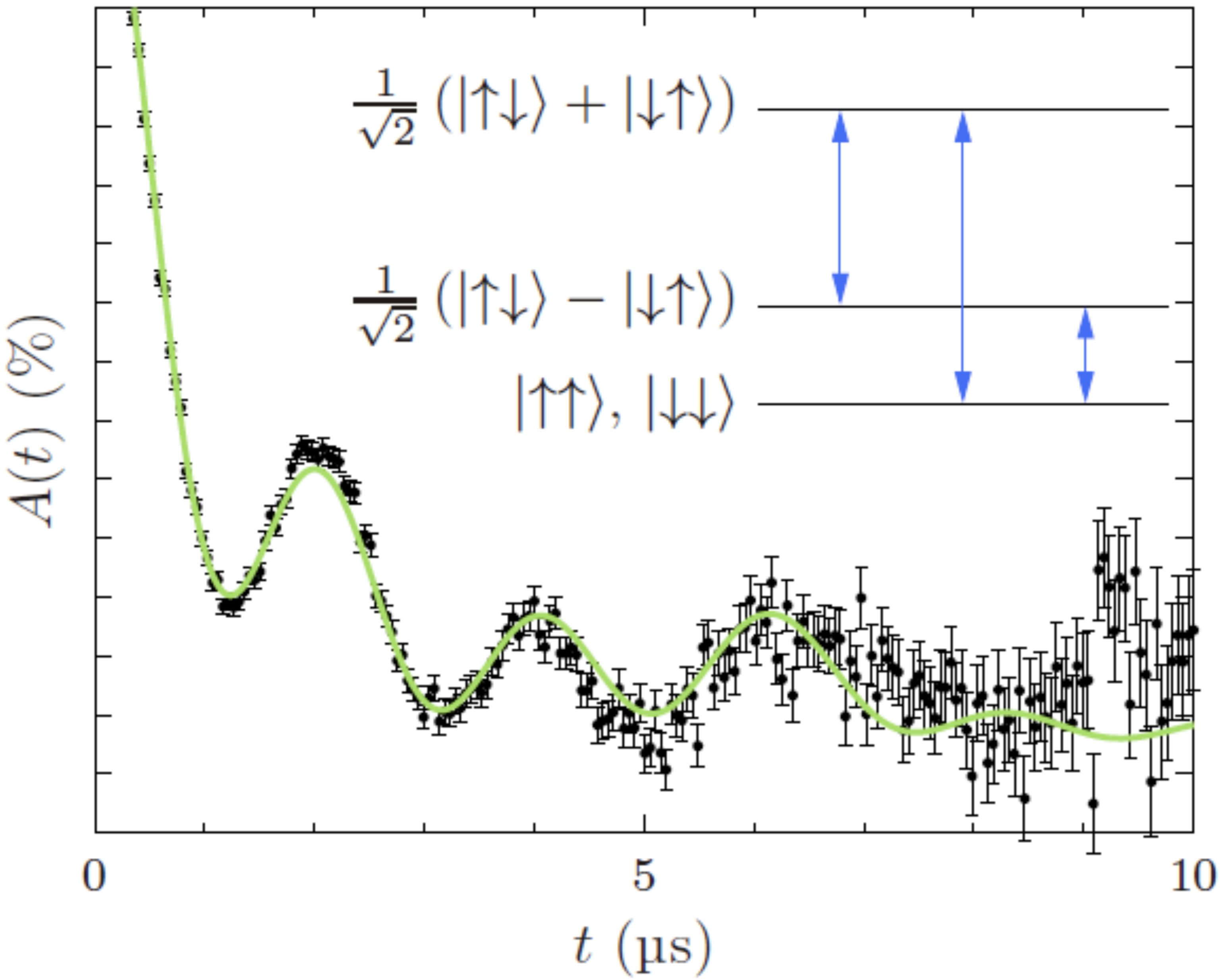
Hints of Quantum Coherence



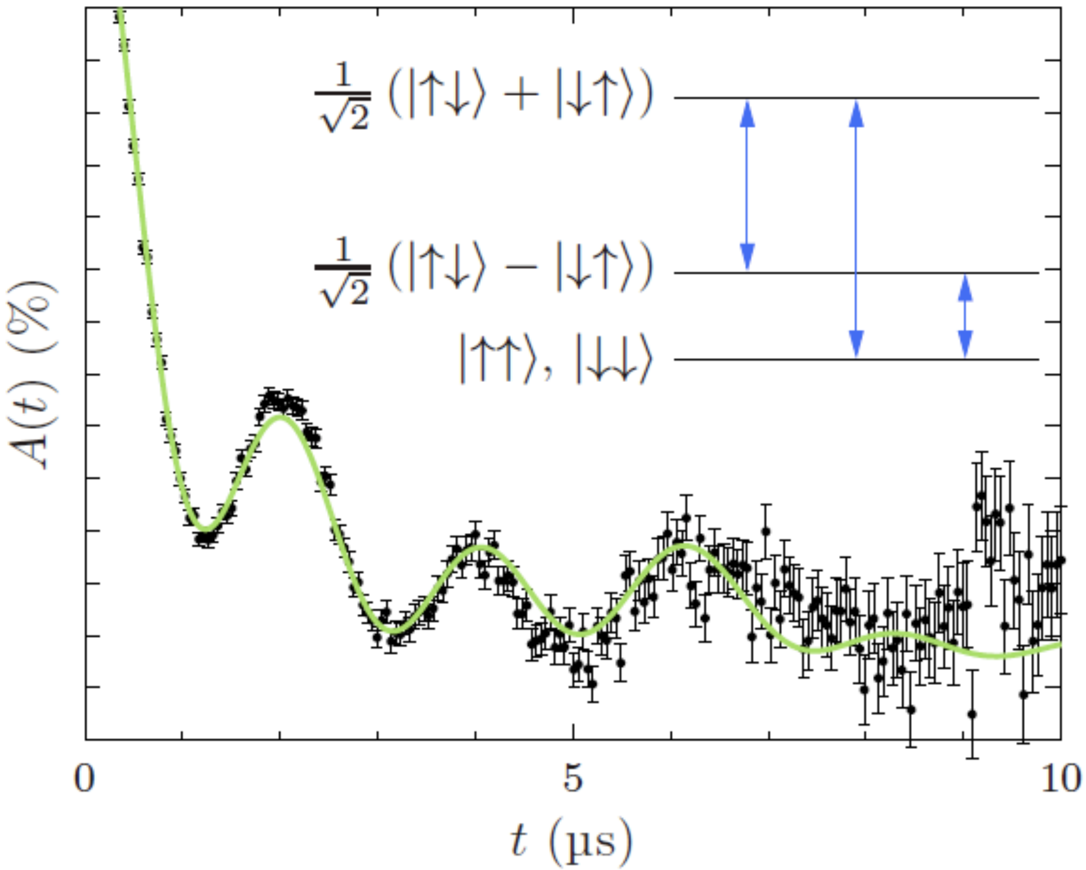
The F-μ-F State

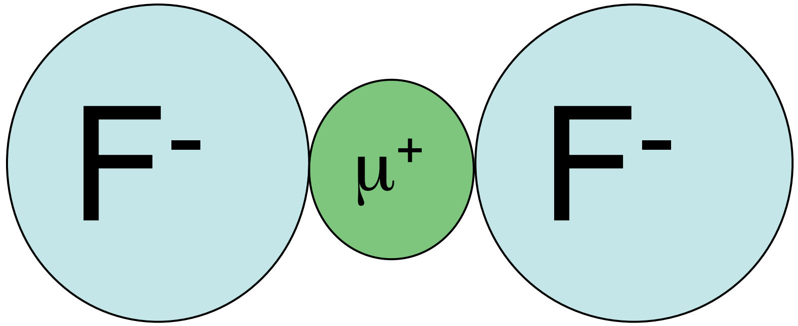


The F-μ-F State



The F-μ-F State





coherent oscillations arising from the magnetic dipolar interaction

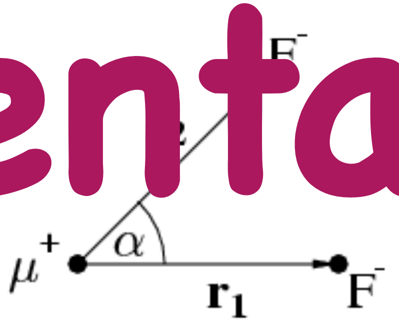
$$P_z(t) = \frac{1}{6}\left(3 + \cos\sqrt{3}\omega t + \left(1 - \frac{1}{\sqrt{3}}\right)\cos\left[\frac{3-\sqrt{3}}{2}\omega t\right] + \left(1 + \frac{1}{\sqrt{3}}\right)\cos\left[\frac{3+\sqrt{3}}{2}\omega t\right]\right)$$

The F-μ-F State

Fluorine: small, high nuclear moment abundant species

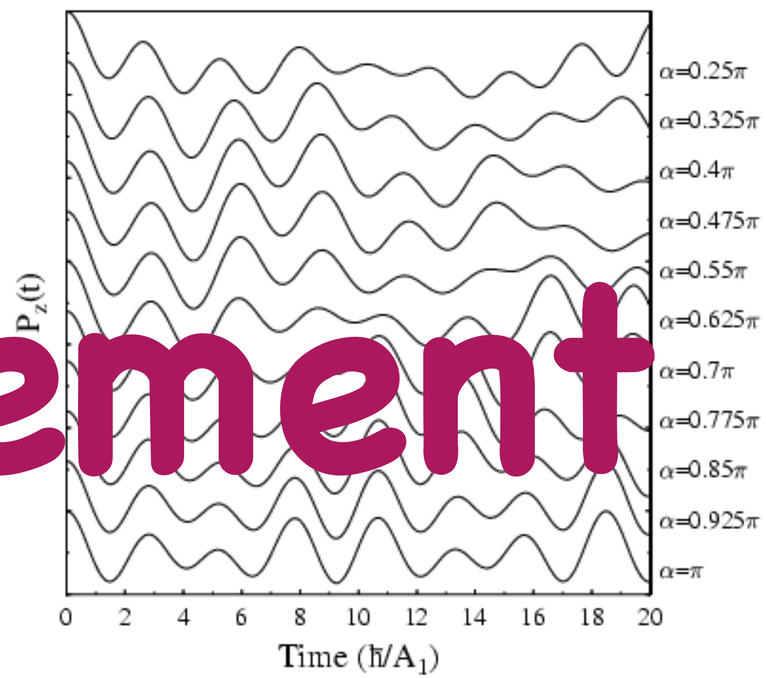
Anion	Abundance	Spin	Ionic radius (pm)	Magnetic moment (μ_N)
^{19}F	100%	1/2	119	2.6
^{35}Cl	~ 75%	3/2	167	0.82
^{37}Cl	~ 25%	3/2	167	0.68
^{79}Br	~ 50%	3/2	182	2.1
^{81}Br	~ 50%	3/2	182	2.3
^{127}I	100%	5/2	206	2.8
^{17}O	0.04%	5/2	126	-1.9
^{33}S	0.76%	3/2	170	0.64
^{77}Se	7.6%	1/2	184	0.53
^{123}Te	0.89%	1/2	207	-0.73
^{125}Te	7.1%	1/2	207	-0.89

very sensitive to r_1/r_2 and α



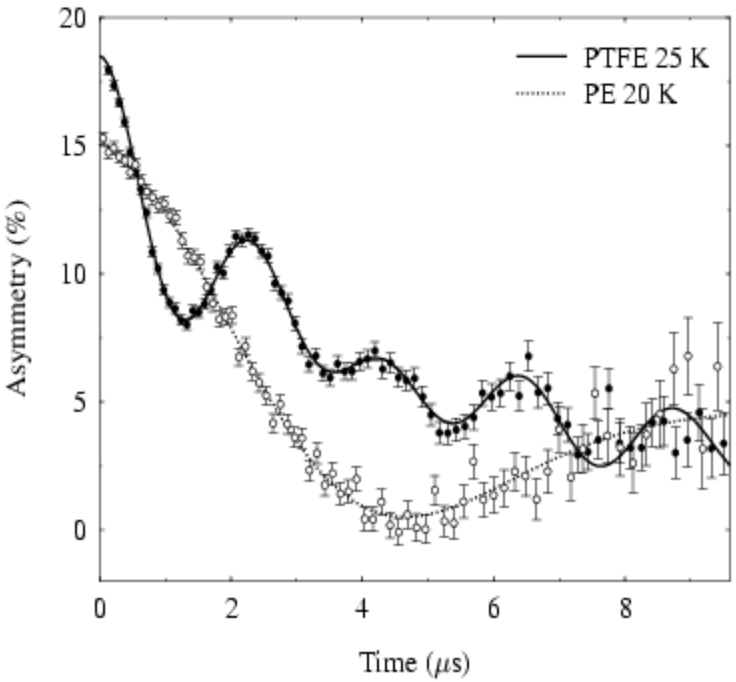
entanglement

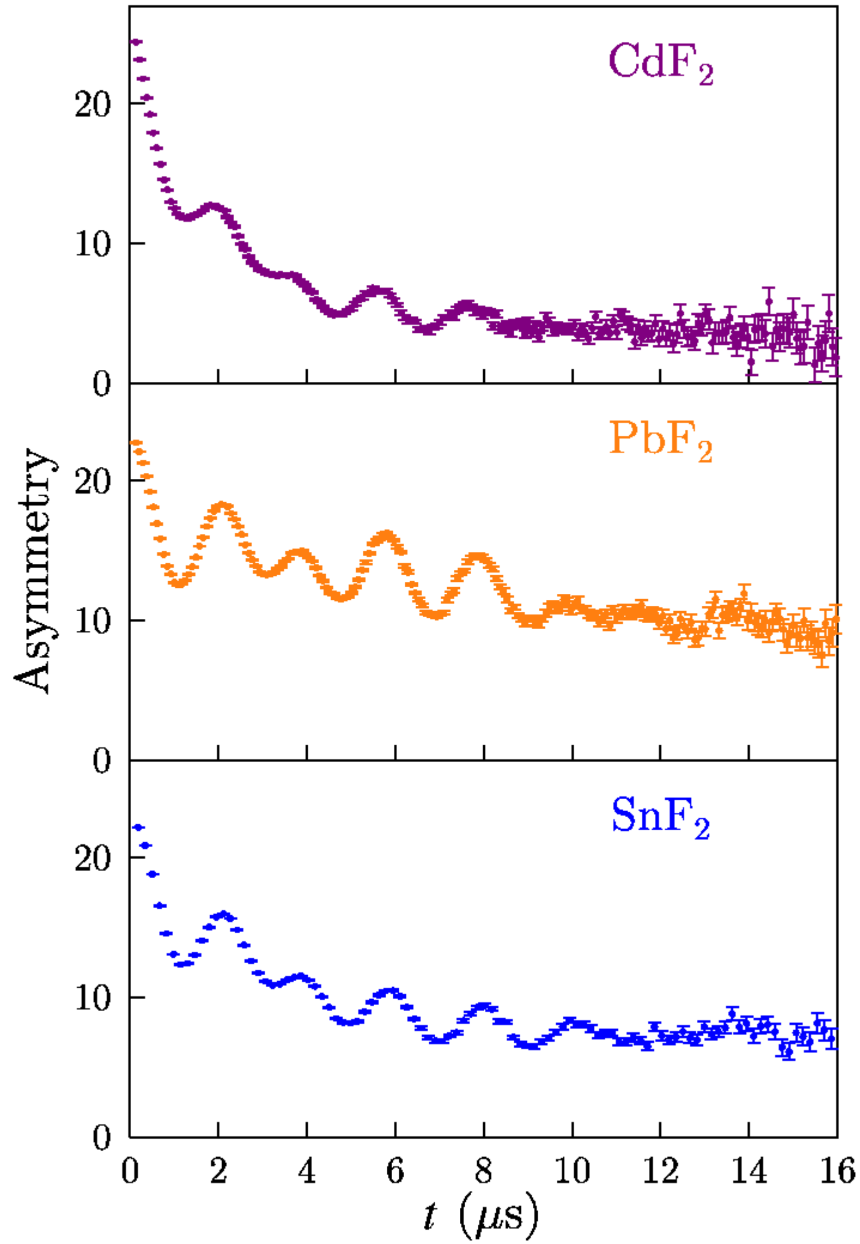
Muon Polarisation for variable α



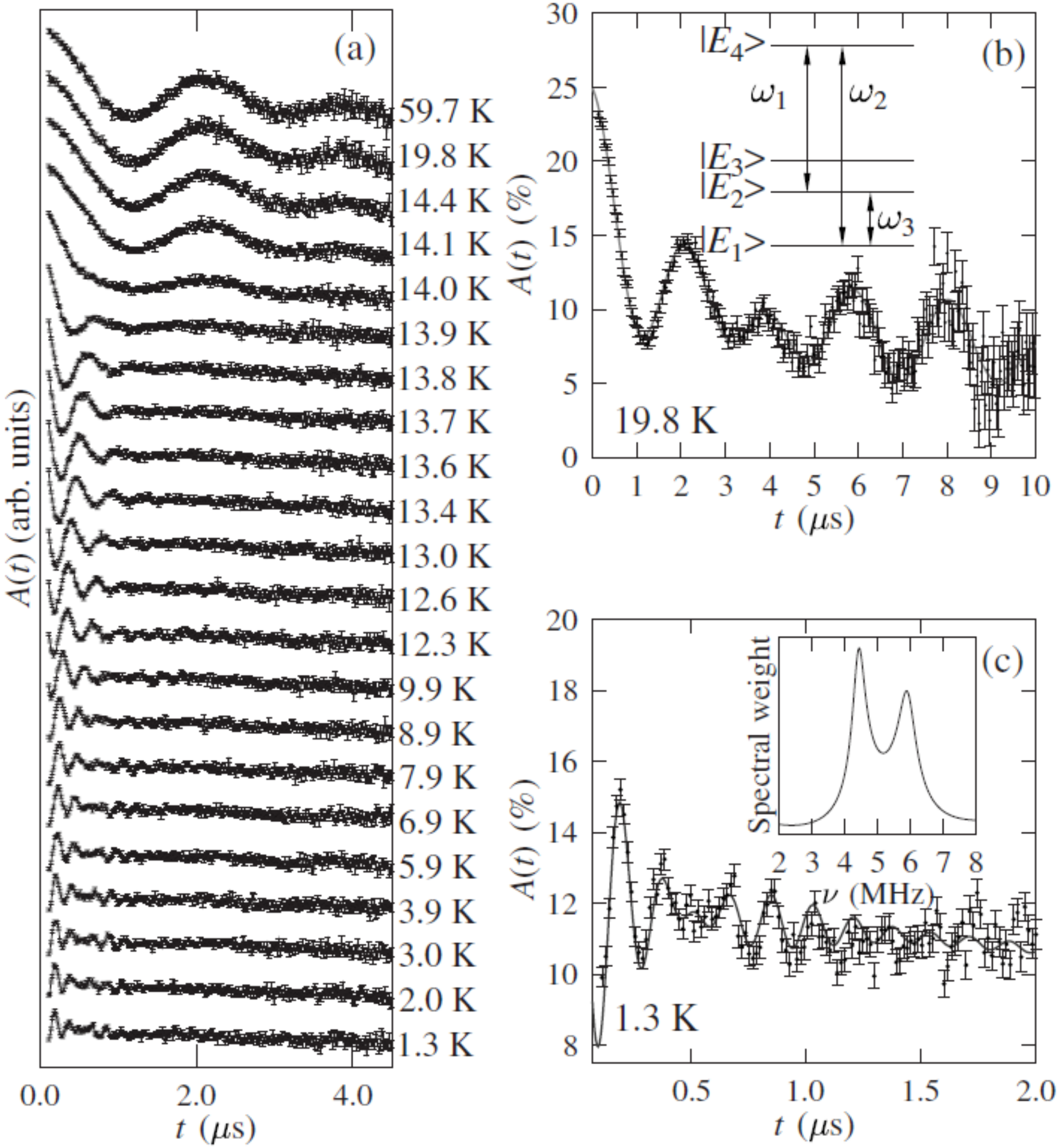
The F-μ-F State

state found in many ionic fluorides, and also teflon (PTFE)





The F-μ-F State



Cs_2AgF_4

$\omega_d = 2\pi \times 0.211(1)$ MHz

F-μ separation 1.19(1) Å.

T_c=13.95(3) K

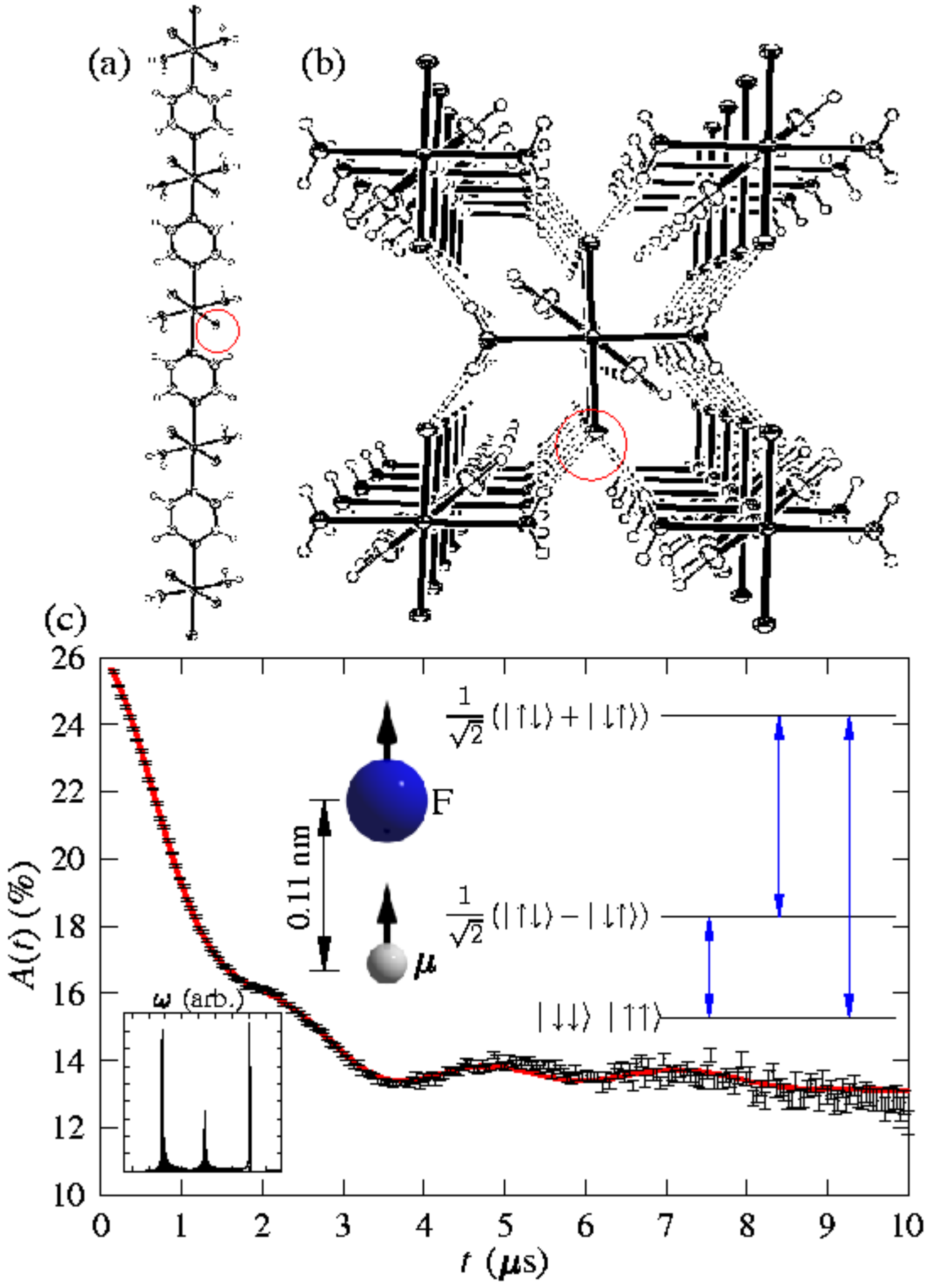
T. Lancaster, S. J. Blundell, et al.

Phys. Rev. B **75**, R220408 (2007)

The F-μ-F State

$CuF_2(H_2O)_2(pyz)$

1. Interaction with a single fluorine ion

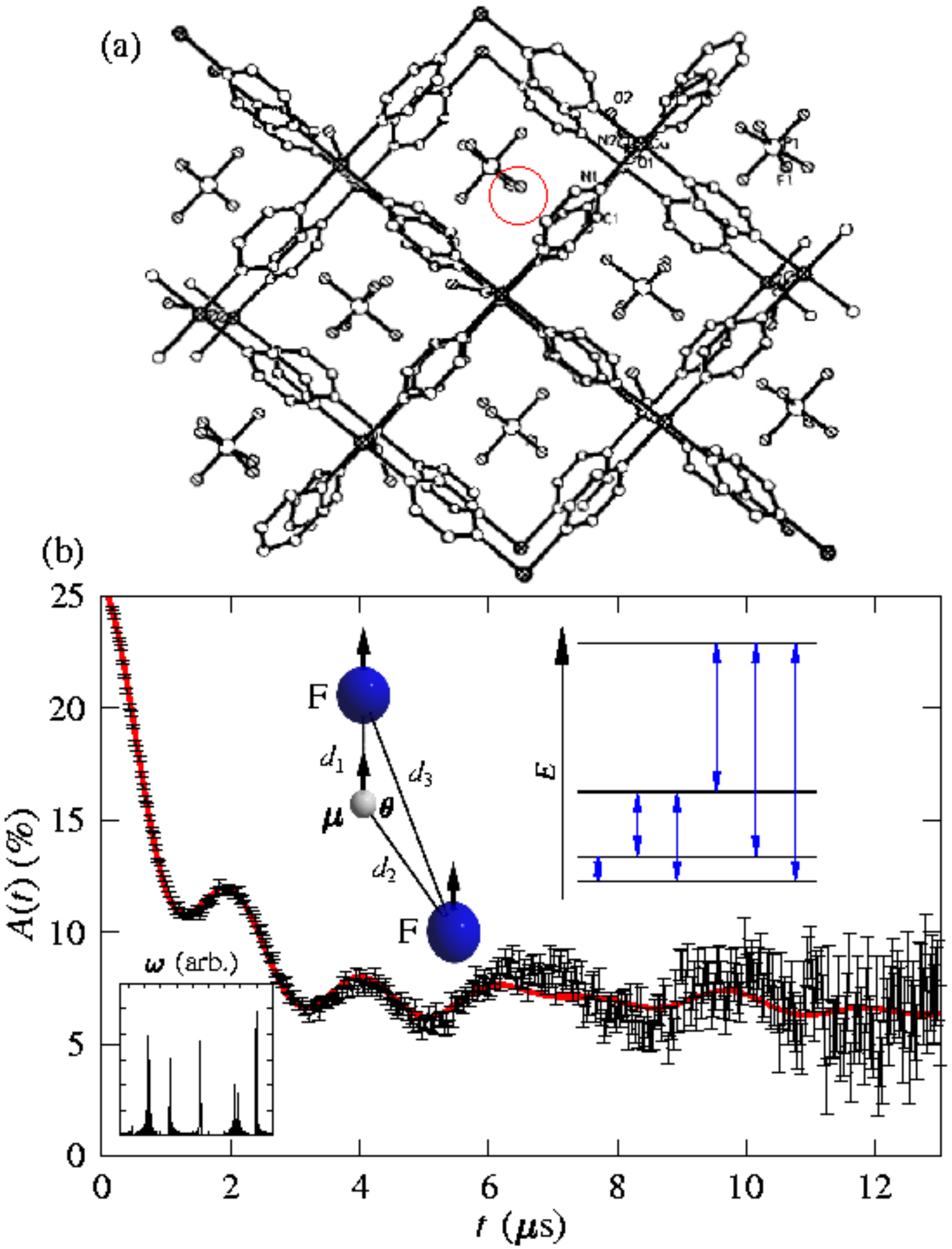


Phys. Rev. Lett. **99**, 267601 (2007)

The F-μ-F State

$[CuNO_3(pyz)_2]PF_6$

2. Crooked FμF bond close to a PF_6 ion

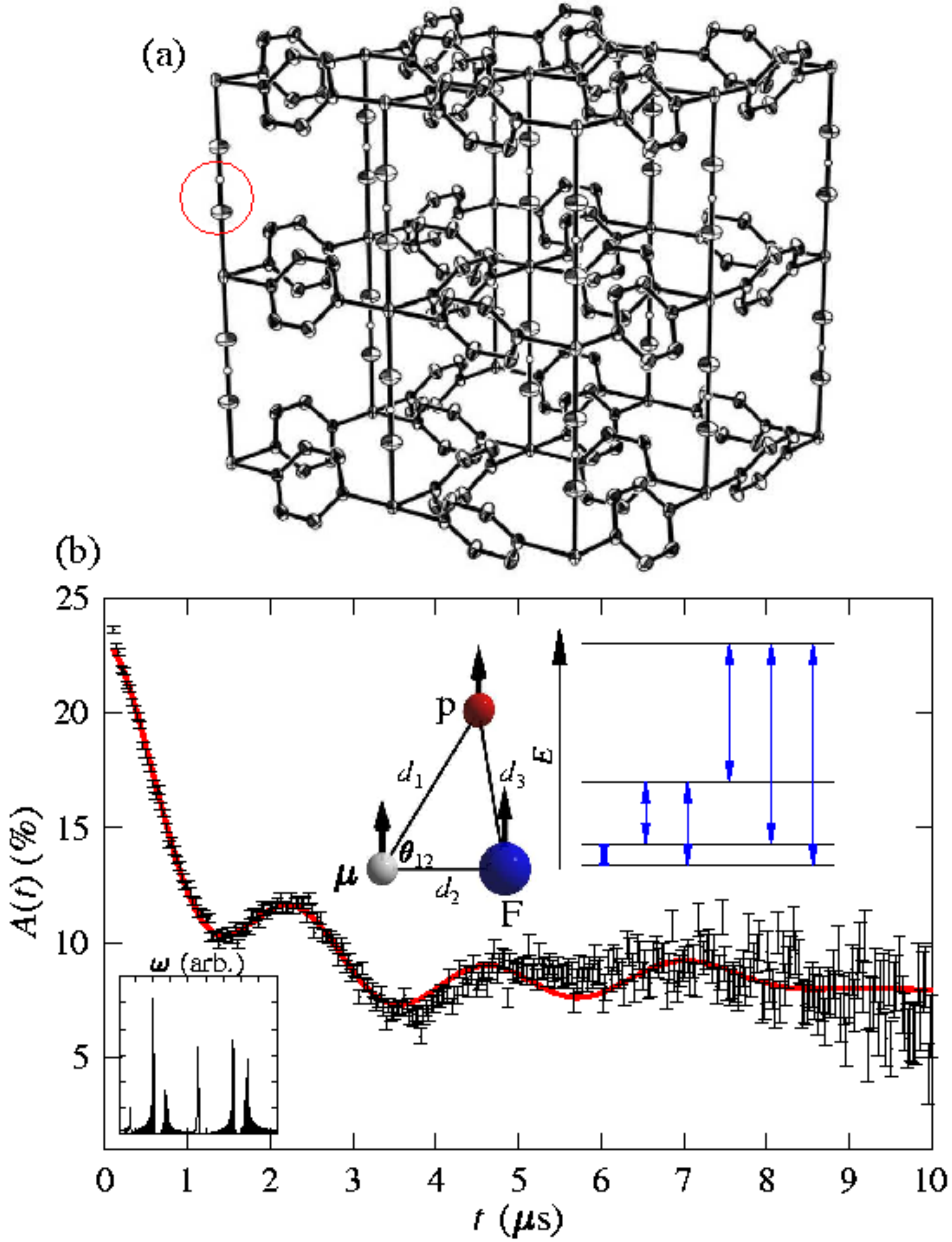


Phys. Rev. Lett. **99**, 267601 (2007)

The F-μ-F State

$[Cu(HF_2)(pyz)_2]X$

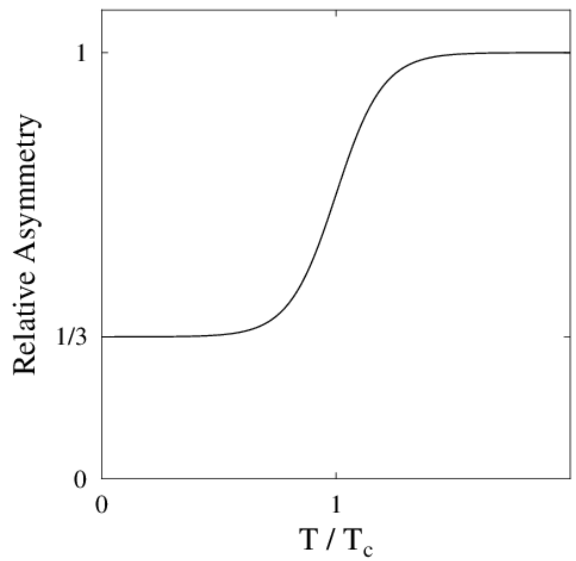
3. Interaction with a HF_2^- ion



Phys. Rev. Lett. **99**, 267601 (2007)

Analysing Asymmetry : Magnets

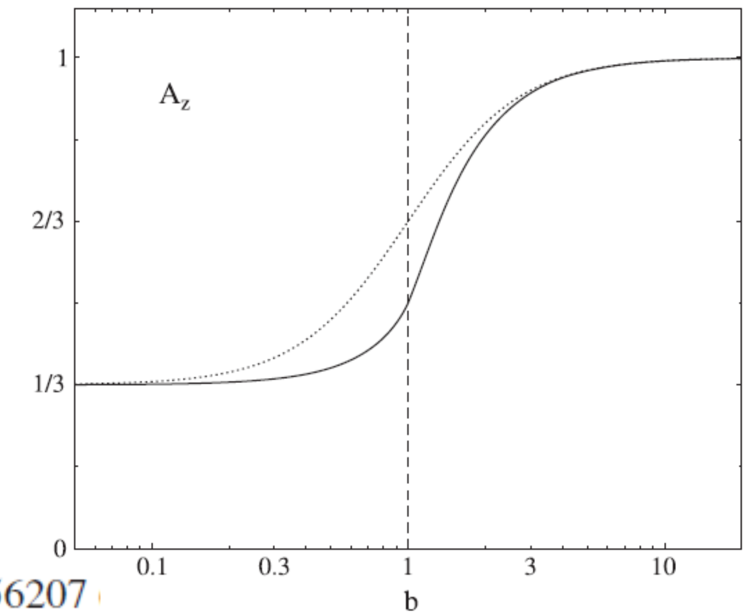
Polycrystalline samples



LF decoupling below T_c

$$A_z(b) = \frac{3}{4} - \frac{1}{4b^2} + \frac{(b^2-1)^2}{8b^3}\log\left|\frac{b+1}{b-1}\right|$$

$b = B / B_0$



F. L. Pratt J. Phys.: Condens. Matter **19** (2007) 456207

Analysing Asymmetry : Muonium-like States

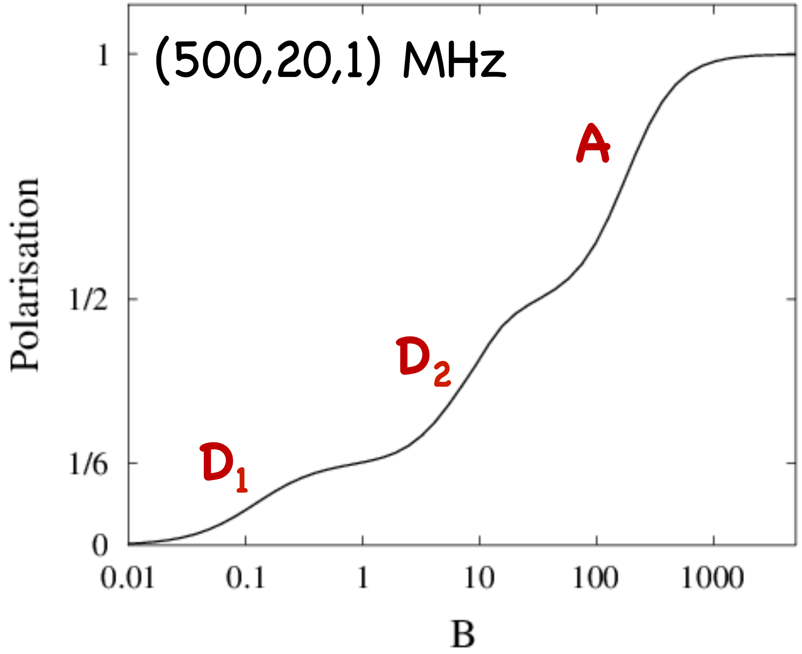
LF decoupling
or 'repolarisation'

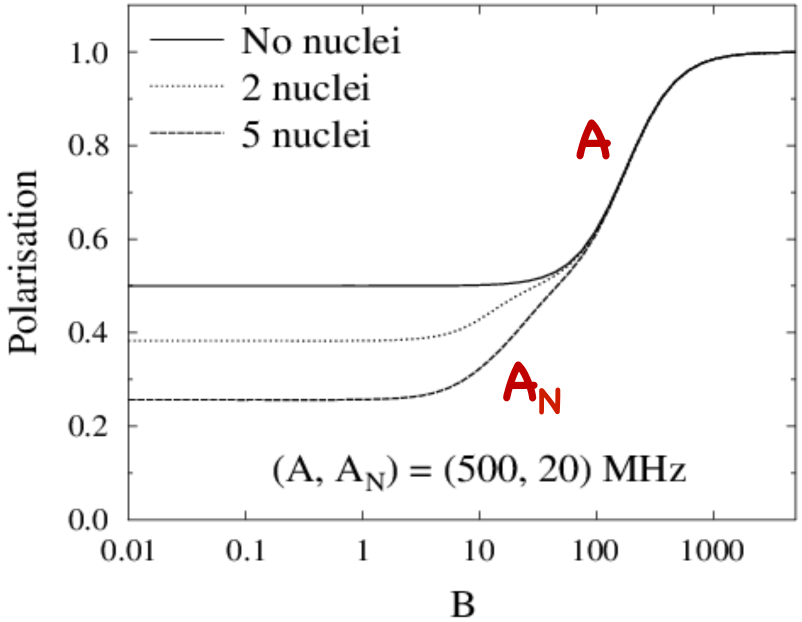
Hyperfine tensor (A, D_1, D_2)

F. L. Pratt, Phil. Mag. Lett. 75, 371 (1997)

Nuclear couplings A_N

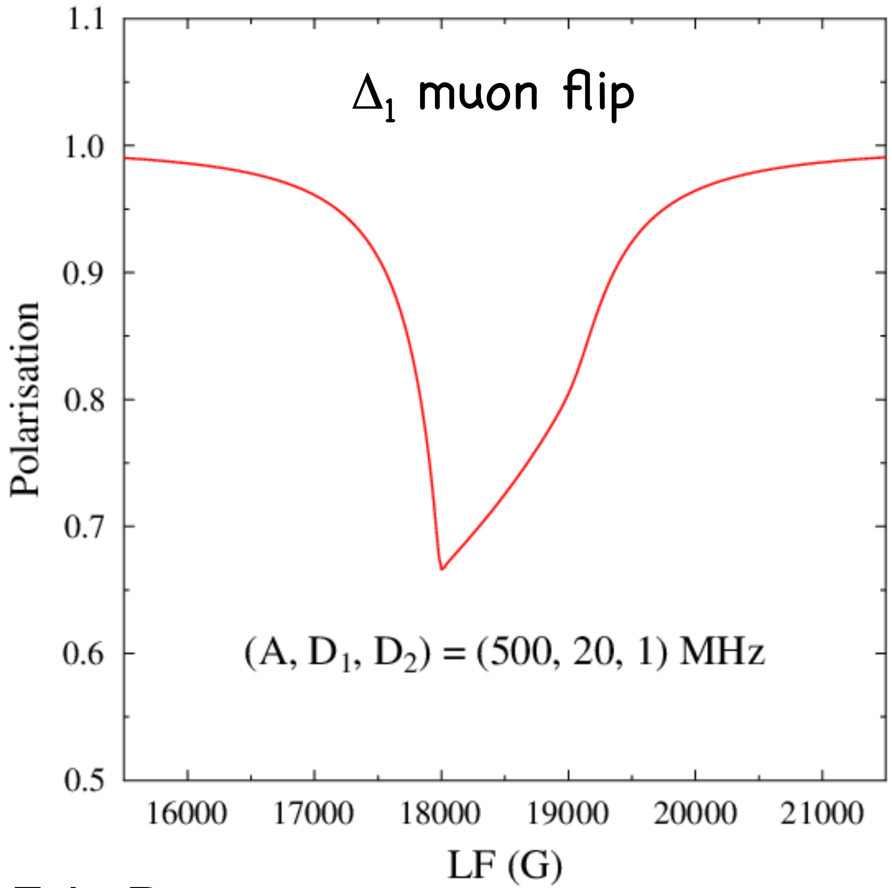
Z. Phys. B 22, 109 (1975)

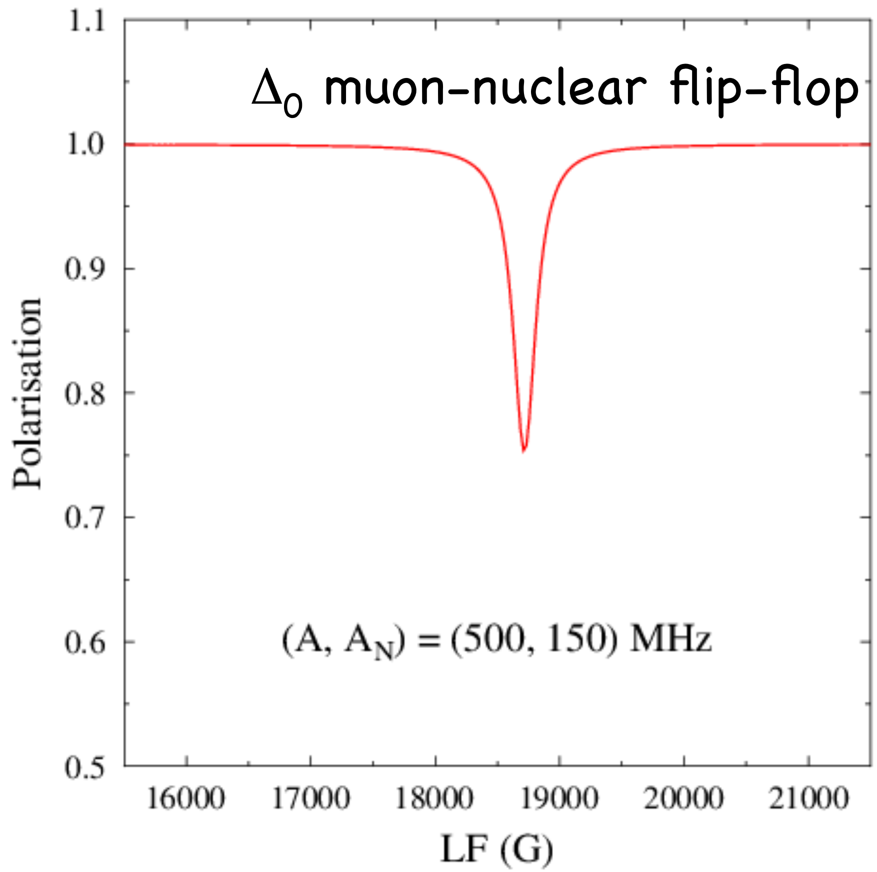




Analysing Asymmetry : Muonium-like States

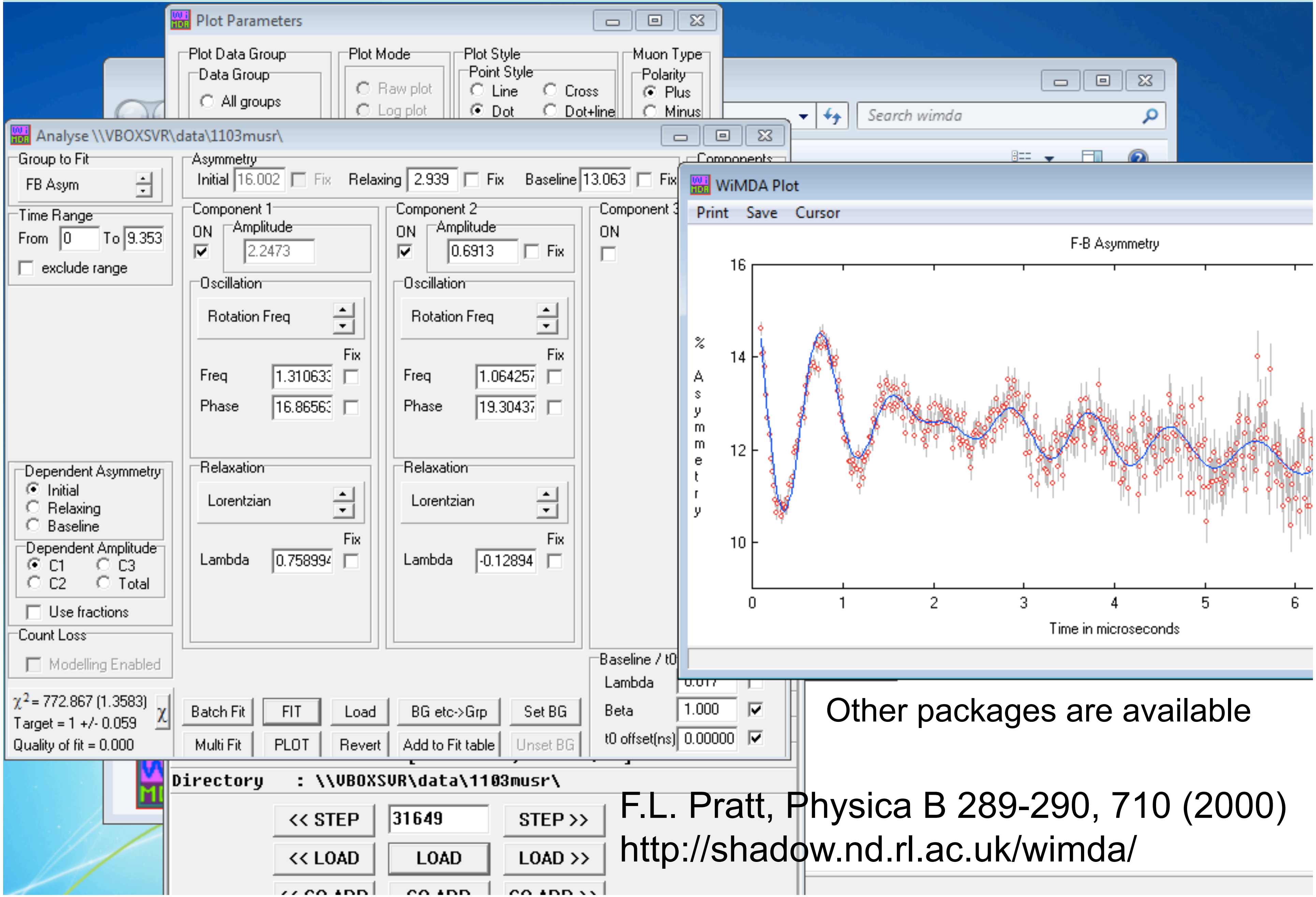
Avoided level-crossing resonances:





F. L. Pratt

All these functions available in Wimda



Other packages are available

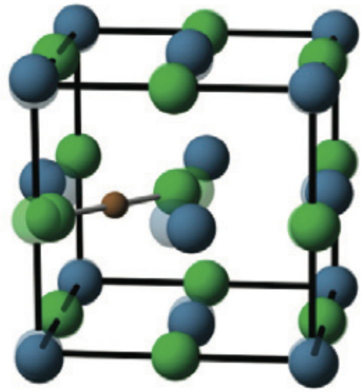
F.L. Pratt, Physica B 289-290, 710 (2000)
http://shadow.nd.rl.ac.uk/wimda/

DFT+μ

DFT+μ = (**density functional theory +μ**)

- numerically solve (lattice) structures
- determine muon site
- quantify perturbations

DFT+μ began with two papers (Oxford + Parma groups) studying **fluorides**:
J.S. Möller *et al.*, Phys. Rev. B **87**, 121108(R) (2013).
F. Bernadini, *et al.*, Phys. Rev. B **87**, 115148 (2013).



This work has been extended to many other systems, see e.g
S.J. Blundell *et al*, Phys. Rev. B **88**, 064423 (2013).
J.S. Möller *et al.*, Phys. Scr. **88**, 068510 (2013).
F. Xiao *et al.*, Phys. Rev. B **91**, 144417 (2015).
P. Bonfà *et al.*, J. Phys. Chem. C 119, 4278 (2015).
F. Lang *et al.*, Phys. Rev. B **94**, 020407(R) (2016).
P. Bonfà *et al.*, J. Phys. Soc. Jpn. **85**, 091014 (2016)

DFT+μ

DFT+μ = (**density functional theory +μ**)

- numerically solve (lattice) structures
- determine muon site
- quantify perturbations

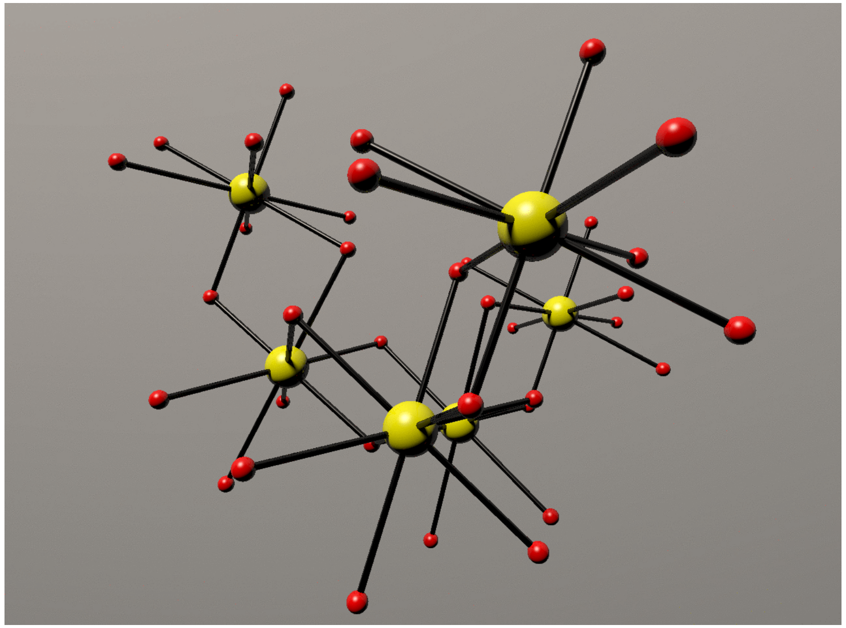
DFT+μ can not only assess the **muon site**, but also any **muon-induced distortion**. A ***worst-case scenario*** is where magnetism arises from a **non-Kramers ground state**. This leads to our study of **quantum spin ice**.
F. R. Foronda *et al.*, Phys. Rev. Lett. **114**, 017602 (2015).

Challenges for pyrochlores:

- 88 atoms per unit cell
- 4f valence electrons
- ~102-104 cpu hours per calculation

Results:

- typical O-H like bond with length 1 Å
- 4f electrons influence negligible
- $r_{4f} \approx 2 \times r_{5s} \approx 5 \times$(Pr-μ distance)



After all those relaxation functions…..

…it's now time for some relaxation!