Relaxation functions

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Outline

Introduction: Larmor equation and polarisation functions

Static polarisation functions from a field distribution approach
  Transverse-field polarisation function
  Longitudinal-field polarisation function
  Effect of external field

Computation of the field distribution
  Nature of the field at the muon site
  Zero-field polarisation function in magnets
  Uncorrelated moments

Dynamical polarisation functions
  Stochastic approach: the weak and strong collision models
  Quantum approach
  Spin correlation functions

Correlations or not correlations

Stretched exponential function

Summary
Foreword

- Polarisation function vs relaxation function
- Statistics, probability and stochastic processes theory
- Most methodologies apply to transverse and longitudinal polarisation functions
- Background for the lecture is in the framework of magnetism or sometimes the diffusion of a light interstitial in a crystal
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Summary
The evolution of the muon spin $S_\mu(t)$

The Larmor equation

Basic principle of mechanics:
The time derivative of angular momentum is equal to the sum of the torques:

$$\frac{d\hbar S_\mu(t)}{dt} = m_\mu(t) \times B_{loc}(t).$$

Since

$$m_\mu = \gamma_\mu \hbar S_\mu,$$

by definition of the gyromagnetic ratio, we have

$$\frac{dS_\mu(t)}{dt} = \gamma_\mu S_\mu(t) \times B_{loc}(t).$$

$\gamma_\mu = 851.6 \text{ Mrad s}^{-1} \text{ T}^{-1}$. 
Basics of motion properties deriving from the Larmor equation

From

\[ \frac{dS_\mu(t)}{dt} = \gamma_\mu S_\mu(t) \times B_{\text{loc}}(t) \]

we deduce:

- \( \frac{dS_\mu(t)}{dt} \cdot S_\mu(t) = 0 \):
  \( S_\mu(t) \) is a constant of the motion, i.e. \( S_\mu(t) = S_\mu(0) \)

- \( \frac{dS_\mu(t)}{dt} \cdot B_{\text{loc}}(t) = 0 \):
  this implies \( \frac{dS_\mu(t)}{dt} \) is perpendicular to \( B_{\text{loc}}(t) \).
The transverse and longitudinal polarisation functions

- The polarisation function $P_\alpha(t)$ is the evolution of the projection of the muon ensemble polarisation along axis $\alpha$:

$$P_\alpha(t) = \left\langle \frac{S_{\mu,\alpha}(t)}{S_\mu} \right\rangle.$$ 

- $S_\mu \equiv S_\mu(t = 0)$: initial muon beam polarisation

### Transverse-field geometry

- $S_\mu \parallel X \rightarrow P_X(t)$ or $P_Y(t)$.

### Longitudinal- or zero-field geometry

- $S_\mu \parallel Z \rightarrow P_Z(t)$.

Convention for the axes: $B_{\text{ext}}$ is always parallel to $Z$. 

- in transverse field experiment: $S_\mu \parallel X \rightarrow P_X(t)$ or $P_Y(t)$.
- in zero-field and longitudinal-field experiment: $S_\mu \parallel Z \rightarrow P_Z(t)$. 

The muon spin evolution in a static field

Recall the Larmor equation,

\[ \frac{dS_\mu(t)}{dt} = \gamma_\mu S_\mu(t) \times B_{\text{loc}}(t). \]

Assuming \( B_{\text{loc}}(t) = B_{\text{loc}} \), the solution is a precession motion:

\[ S_\mu(t) = S_{\parallel\mu}(0) \mathbf{u} + S_{\perp\mu}(0)[\cos(\omega_\mu t) \mathbf{v} - \sin(\omega_\mu t) \mathbf{w}], \]

with \( \omega_\mu = \gamma_\mu B_{\text{loc}} \).

The precession frequency only depends on \( B_{\text{loc}} \), not on the angle between \( S_\mu \) and \( B_{\text{loc}} \)!
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Summary
Transverse-field polarisation function

Per definition, $S_{\mu} \equiv S_{\mu}(t = 0) \parallel \mathbf{X}$.

From the solution of the Larmor equation,

$$S_{\mu}^X(t) = S_{\mu} \left\{ \left( \frac{B_{\text{loc}}^X}{B_{\text{loc}}} \right)^2 + 1 - \left( \frac{B_{\text{loc}}^X}{B_{\text{loc}}} \right)^2 \right\} \cos(\omega_{\mu} t),$$

$$S_{\mu}^X(t) = S_{\mu} \left\{ \cos^2 \theta + \sin^2 \theta \cos(\omega_{\mu} t) \right\},$$

with $B_{\text{loc}}^2 = (B_{\text{loc}}^X)^2 + (B_{\text{loc}}^Y)^2 + (B_{\text{loc}}^Z)^2$, and $\omega_{\mu} = \gamma_{\mu} B_{\text{loc}}$.

Let $D_{\nu}(B_{\text{loc}})$ be the distribution of static fields probed by the muons,

$$P_{\mu}^{\text{stat}}(t) = \left\langle \frac{S_{\mu}^X(t)}{S_{\mu}} \right\rangle = \int \left[ \cos^2 \theta + \sin^2 \theta \cos(\omega_{\mu} t) \right] D_{\nu}(B_{\text{loc}}) \, d^3 B_{\text{loc}}.$$
Transverse-field polarisation function

Example: single field

Recall,

\[ P_{\chi}^{\text{stat}}(t) = \int \left[ \cos^2 \theta + \sin^2 \theta \cos(\omega_\mu t) \right] D_v(B_{\text{loc}}) d^3B_{\text{loc}}. \]

Assume all the muons to be submitted to \( B_{\text{loc}} = B_0 \parallel Z \), i.e. \( \theta = \pi/2 \),

\[ P_{\chi}^{\text{stat}}(t) = \cos(\omega_0 t) \]

with \( \omega_0 = \gamma_\mu B_0 \).
Transverse-field polarisation function

Large transverse field

Recall,

\[ P^{stat}_{X}(t) = \int [\cos^2 \theta + \sin^2 \theta \cos(\omega_\mu t)] D_v(B_{loc}) \, d^3B_{loc}. \]

Suppose \( B_{loc} \) to be dominated by \( B_{ext} \), i.e. \( \theta \approx \pi/2 \),

\[ B_{loc} \approx |B^Z_{loc}|, \]

\[ P^{stat}_{X}(t) = \int \cos(\omega_\mu t) D_c(B^Z_{loc}) \, dB^Z_{loc}, \]

\[ = \left[ \int D^{sh}_c(x) \cos(\gamma_\mu tx) \, dx \right] \cos(\gamma_\mu B_{ext} t). \]

The last line is obtained after the substitution \( B^Z_{loc} = B_{ext} + x \).

\( D^{sh}_c(x) \) is assumed to be an even function, otherwise a phase shift is present.
Transverse-field polarisation function

Example: typical distributions and associated polarisation functions

Gaussian distribution:

\[ D_{\text{c} \text{sh}}^{\text{sh}}(B) = \frac{1}{\sqrt{2\pi}\Delta_G} \exp\left(\frac{-B^2}{2\Delta_G^2}\right) \]

\[ P_{X \text{stat}}^\text{stat}(t) = \exp\left(\frac{-\gamma_{\mu}^2\Delta_G^2 t^2}{2}\right) \times \cos(\gamma_{\mu} B_{\text{ext}} t) \]

Example: nuclear dipoles

Lorentzian distribution:

\[ D_{\text{c} \text{sh}}^{\text{sh}}(B) = \frac{1}{\pi} \frac{\Delta_L}{\Delta_L^2 + B^2} \]

\[ P_{X \text{stat}}^\text{stat}(t) = \exp \left( -\gamma_{\mu} \Delta_L t \right) \times \cos(\gamma_{\mu} B_{\text{ext}} t) \]

Example: diluted magnetic systems
Transverse-field polarisation function
Example: Mixed phase of superconductors

Type II superconductors submitted to a magnetic field:

Field (deviation) profile in the flux-line lattice phase.

Associated field distribution.
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Summary
Zero- or longitudinal-field polarisation function

Per definition, $S_\mu \equiv S_\mu (t = 0) \parallel Z$. From the solution of the Larmor equation,

$$S^Z_\mu (t) = S_\mu \left\{ \left( \frac{B^Z_{\text{loc}}}{B_{\text{loc}}} \right)^2 + 1 - \left( \frac{B^Z_{\text{loc}}}{B_{\text{loc}}} \right)^2 \right\} \cos(\omega_\mu t),$$

$$S^Z_\mu (t) = S_\mu \left[ \cos^2 \theta + \sin^2 \theta \cos(\omega_\mu t) \right],$$

with $B^2_{\text{loc}} = (B^X_{\text{loc}})^2 + (B^Y_{\text{loc}})^2 + (B^Z_{\text{loc}})^2$ and $\omega_\mu = \gamma_\mu B_{\text{loc}}$.

Let $D_\nu (B_{\text{loc}})$ be the distribution of static fields probed by the muons,

$$P^\text{stat}_Z (t) = \left\langle \frac{S^Z_\mu (t)}{S_\mu} \right\rangle = \int [\cos^2 \theta + \sin^2 \theta \cos(\omega_\mu t)] D_\nu (B_{\text{loc}}) d^3 B_{\text{loc}}.$$
Zero-field polarisation function

Case of isotropic distribution

Recall

\[ P_{Z}^{\text{stat}}(t) = \int [\cos^2 \theta + \sin^2 \theta \cos(\omega_{\mu} t)] D_v(B_{\text{loc}}) \, d^3 B_{\text{loc}}. \]

Assume \( D_v(B_{\text{loc}}) \, d^3 B_{\text{loc}} = D_v(B_{\text{loc}}) B_{\text{loc}}^2 \, dB_{\text{loc}} \sin \theta \, d\theta \, d\varphi, \)

\[ P_{Z}^{\text{stat}}(t) = \frac{1}{3} + \frac{2}{3} \int 4\pi D_v(B_{\text{loc}}) B_{\text{loc}}^2 \cos(\omega_{\mu} t) \, dB_{\text{loc}}, \]

with \( \omega_{\mu} = \gamma_{\mu} B_{\text{loc}}. \)

Example: \( 4\pi D_v(B_{\text{loc}}) B_{\text{loc}}^2 = \delta(B_{\text{loc}} - B_0) \)

ideal magnetic polycrystal

\[ P_{Z}^{\text{stat}}(t) = \frac{1}{3} + \frac{2}{3} \cos(\gamma_{\mu} B_0 t) \]
Zero-field polarisation function

Example: Maxwell-Boltzmann distribution for $B_{\text{loc}}$

For isotropic Gaussian distributed $B^\alpha$ with rms $\Delta_G$,

$$D_v(B) \, d^3B = \left( \frac{1}{\sqrt{2\pi}\Delta_G} \right)^3 \exp \left( \frac{-B^2}{2\Delta_G^2} \right) B^2 \, dB \sin \theta \, d\theta \, d\varphi,$$

$$D_m(B) = 4\pi D_v(B) B^2,$$

$$P_{\text{stat}}^Z(t) = P_{\text{KT}}(t) = \frac{1}{3} + \frac{2}{3}(1 - \gamma^2 \Delta_G^2 t^2) \exp \left( -\frac{\gamma^2 \Delta_G^2 t^2}{2} \right),$$

which is the so-called **Kubo-Toyabe function**.

**Component distribution**

**Modulus distribution**

**Kubo-Toyabe function.**

Minimum at $t = \sqrt{3}/\gamma \mu \Delta_G$
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Summary
Effect of external field

Case of transverse $B_{\text{ext}}$

If $B_{\text{ext}}$ is strong enough, recall

$$P_{X}^{\text{stat}}(t) = \left[ \int D_{c}^{\text{sh}}(x) \cos(\gamma_{\mu}tx) \, dx \right] \cos(\gamma_{\mu}B_{\text{ext}}t).$$

Trivial effect of $B_{\text{ext}}$ on oscillation frequency.

If width of distribution is non-negligible compared to $B_{\text{ext}}$, resort to general formula

$$P_{X}^{\text{stat}}(t) = \int \left[ \cos^{2} \theta + \sin^{2} \theta \cos(\omega_{\mu}t) \right] D_{v}(B_{\text{loc}}) \, d^{3}B_{\text{loc}}.$$

Example: Gaussian field distribution

Towards the Kubo-Toyabe function
Effect of external field

Case of longitudinal $B_{\text{ext}}$

Recall,

$$P_{Z}^{\text{stat}}(t) = \int [\cos^2 \theta + \sin^2 \theta \cos(\omega \mu t)] D_v(B) \, d^3 B,$$

and the former isotropic Gaussian distribution.

Now the $Z$ component of $D_v(B)$ is shifted:

$$D_v(B) \, d^3 B = \left( \frac{1}{\sqrt{2\pi} \Delta G} \right)^3 \exp \left( \frac{-B_X^2 - B_Y^2}{2\Delta_G^2} \right) \exp \left( \frac{-(B_Z - B_{\text{ext}})^2}{2\Delta_G^2} \right) \, dB_X \, dB_Y \, dB_Z.$$

► at large field: muon spin decoupling
► oscillations at $\gamma \mu B_{\text{ext}}$
► field dependence serves to ascertain the model
► sensitivity in the range $\Delta_G/5 \lesssim B_{\text{ext}} \lesssim 5\Delta_G$
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Summary
Origin of field at the muon site

- **nuclei**
  - high concentration of magnetic moments
  - quasi-static on $\tau_\mu$ scale
  - disordered and no correlation

- **electrons**
  - high concentration of magnetic moments/structural order
    $\rightarrow$ magnetically ordered phase
    $\rightarrow$ paramagnetic phase (dynamical on $\tau_\mu$ scale)
  - low concentration of magnetic moments/structural disorder (spin-glass)
    $\rightarrow$ frozen state
    $\rightarrow$ paramagnetic state (dynamical on $\tau_\mu$ scale)

Muon life time $\tau_\mu = 2.2 \, \mu s$
The magnetic field at the muon site

Dipolar and Fermi contact fields

The dipolar field arising from localized spins $J_j$ with Landé factors $g$ is

$$ B_{dip} = -\frac{\mu_0}{4\pi} g \mu_B \sum_j \left[ -\frac{J_j}{r_j^3} + 3\frac{(J_j \cdot r_j)r_j}{r_j^5} \right]. $$

$r_j$ is the vector distance from the spin to the muon.

When a polarised electron density is present at the muon, an additional contribution is present, the Fermi contact field:

$$ B_{con} = -\frac{\mu_0}{4\pi} g \mu_B \sum_{j \in NN} H_j J_j. $$

Only the muon nearest neighbors (NN) usually contribute to $B_{con}$.

When both $B_{dip}$ and $B_{con}$ contribute to $B_{loc}$ (i.e. in metals) they generally have the same order of magnitude.
The magnetic field at the muon site
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The magnetic field at the muon site

Reciprocal space

\( B_{\text{dip}} \) and \( B_{\text{con}} \) linearly depending on \( J_j \),

\[
B_{\text{loc}} = B_{\text{dip}} + B_{\text{con}} = -\frac{\mu_0}{4\pi} \frac{g\mu_B}{v_c} \sum_j G_j J_j.
\]

\( G_j \) is the muon-spin \( j \) coupling tensor.

It is often a good idea to introduce the Fourier space quantities:

\[
G_q = \sum_j G_j \exp(iq \cdot r_j),
\]

\[
J_q = \frac{1}{\sqrt{n_c}} \sum_j J_j \exp(-iq \cdot j).
\]

Then,

\[
B_{\text{loc}} = -\frac{\mu_0}{4\pi} \frac{g\mu_B}{\sqrt{n_c} v_c} \sum_q \exp(-iq \cdot r_0) G_q J_q.
\]
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Summary
Zero-field polarisation function in magnets

Reminder:

- \( J_q = \frac{1}{\sqrt{n_c}} \sum_j \exp(-i \mathbf{q} \cdot \mathbf{j}) J_j \), \( J_j = \frac{1}{\sqrt{n_c}} \sum_q \exp(i \mathbf{q} \cdot \mathbf{j}) J_q \)

- **Ferromagnet:** \( J_q = 0 \) (\( J_q \neq 0 = 0 \))

- **Antiferromagnet:** \( J_q \) is finite only for \( \mathbf{q} = \pm \mathbf{k} \), where \( \mathbf{k} \) is the propagation wavevector of the magnetic structure.

In a \( \mu \)SR experiment several millions muons are implanted: they randomly localise in different unit cells of the crystal structure.
Zero-field polarisation function in magnets

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Zero-field polarisation function in magnets

Commensurate magnets

Recall,

\[ B_{\text{loc}} = -\frac{\mu_0 G\mu_B}{4\pi \sqrt{n_c v_c}} \sum_{q=0 \text{ or } q=\pm k} \exp(-i\mathbf{q} \cdot \mathbf{r}_0) G_q J_q. \]

An antiferromagnetic structure is commensurate if \( k = rQ \) where \( Q \) is a reciprocal lattice vector and \( r \) is a rational number.

\( \exp(-i\mathbf{q} \cdot \mathbf{r}_0) \) takes a finite number of values, so \( B_{\text{loc}} \) does.

Obviously, this is also true for a ferromagnet in which \( q = k = 0 \).

\( \exp(-i\mathbf{q} \cdot \mathbf{r}_0) \) takes a finite number of values, so \( B_{\text{loc}} \) does.

One (or more) muon spin precession frequency(ies).

\( \mu \text{SR} \) cannot directly tell whether a system is a ferro- or an antiferromagnet.
Zero-field polarisation function in magnets

Incommensurate magnets — spin density wave

Recall,
\[
B_{\text{loc}} = -\frac{\mu_0}{4\pi} \frac{g\mu_B}{\sqrt{n_c n_v}} \sum_{q=\pm k} \exp(-iq \cdot r_0) G_q J_q.
\]

For an incommensurate magnetic structure, \( k = sQ \) where \( s \) is an irrational number.
\( \rightarrow \) \( \exp(-iq \cdot r_0) \) takes an infinite number of values,
\( \rightarrow \) a continuous distribution of \( B_{\text{loc}} \) is expected.
Zero-field polarisation function in magnets
Spin density wave, simple case (1)

Recall,

\[ B_{\text{loc}} = -\frac{\mu_0}{4\pi} \frac{g\mu_B}{\sqrt{n_c v_c}} \sum_{q=\pm k} \exp(-i\mathbf{q} \cdot \mathbf{r}_0) G_q \mathbf{J}_q. \]

Assume that the vectors \( B_{\text{loc}} \) remain collinear when \( \mathbf{q} \cdot \mathbf{r}_0 \) spans the interval \([0, 2\pi]\), then

\[ B_{\text{loc}} = \cos \alpha B_{\text{max}}, \quad \text{with } \alpha \in [0, 2\pi]. \]
Zero-field polarisation function in magnets

Spin density wave, simple case (2)
Assume for simplicity $\mathbf{B}_{\text{max}} \parallel \mathbf{X}$,

$$D_c(B_X) = \int \delta(B_X - B_{\text{loc},X}) dB_{\text{loc},X} = \frac{\int_0^{2\pi} \delta(B_X - B_{\text{max}} \cos \alpha) \, d\alpha}{\int_0^{2\pi} d\alpha} = \frac{1}{\pi} \frac{1}{\sqrt{B_{\text{max}}^2 - B_X^2}},$$

$$P^{\text{stat}}_Z(t) = \int_{-B_{\text{max}}}^{B_{\text{max}}} D_c(B_X) \cos(\gamma \mu B_X t) \, dB_X = J_0(\gamma \mu B_{\text{max}} t)$$

$J_0(x)$: zeroth-order Bessel function of the first kind.

- For $x \ll 1$, $J_0(x) \rightarrow 1 - x^2/4$
- For $x \rightarrow \infty$, $J_0(x) \rightarrow \sqrt{2/\pi x} \cos(x - \pi/4)$: $\pi/4$ dephasing of oscillations
Zero-field polarisation function in magnets
Spin density wave, general case

\[ B_{\text{loc}} = \cos \alpha B_{\text{max}} + \sin \alpha B_{\text{min}}, \text{ with } B_{\text{max}} \perp B_{\text{min}}. \]

The ellipse follows from the anisotropy of the dipolar interaction.

\[ D_m(B) = \frac{2B}{\pi \sqrt{B_{\text{max}}^2 - B^2} \sqrt{B^2 - B_{\text{min}}^2}}. \]

\[ D_m(B) \text{ and } P_Z(t) \text{ in the case } \]
\[ B_{\text{max}} = 2B_{\text{min}} \]
\[ \text{and} \]
\[ B_{\text{max}}, B_{\text{min}} \perp Z \]

Real life case of MnSi
(helical spin density wave):
\[ \begin{align*}
  &\triangleright B_{\text{max}} \text{ and } B_{\text{min}} \text{ not } \perp Z, \\
  &\triangleright \text{four magnetic muon sites,} \\
  &\triangleright \text{four magnetic domains.}
\end{align*} \]
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  - Transverse-field polarisation function
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Summary
Consider magnetic impurities randomly distributed in a matrix of non-magnetic sites. With the notations

- $j$ for a site among a total of $N$,
- $c_{\text{imp}}$ for the occupation probability of an impurity (possibly $c_{\text{imp}} = 1$),
- $B_{Z,j}$ for the $Z$ component of the field at the muon arising from atom at site $j$,
- $w_j(B_{Z,j})$ for the distribution of field $B_{Z,j}$ produced at the muon by impurity at site $j$,

\[
D_{\text{sh}}(B_Z) = \int \cdots \int \delta \left( B_Z - \sum_{j=1}^{N} B_{Z,j} \right) \prod_{j=1}^{N} \left[ (1 - c_{\text{imp}}) \delta(B_{Z,j}) + c_{\text{imp}} w_j(B_{Z,j}) \right] dB_{Z,1} \cdots dB_{Z,N}.
\]

The distributions due to the impurities are assumed to be independent, hence $\prod_{j=1}^{N}$. We will take $B_{Z,j} = -\frac{\mu_0}{4\pi} J_{Z,j} \frac{g_i \mu_B}{r_j^3} (3 \cos^2 \theta_j - 1)$, i.e. the impurity dipole field.
Computation of field distributions
Uncorrelated moments, high-transverse field case, extreme dilution limit ($c_{\text{imp}} \ll 1$)

Computation of the characteristic function

$$G_{\text{TF}}(t) = \int \exp(i\gamma \mu B_Z t) D_c^{\text{sh}}(B_Z) \, dB_Z,$$

for $c_{\text{imp}} \ll 1$, i.e. the large dilution limit:

$$G_{\text{TF}}(t) = \exp(-\gamma \mu \Delta L |t|),$$

with $\Delta L = K_L \frac{\mu_0}{4\pi} \rho_{\text{vol}} c_{\text{imp}} g \mu_B \langle |m| \rangle$, where $\rho_{\text{vol}}$ is number of sites per unit volume, the $m$’s are the eigenvalues of $J_Z$ and $K_L \approx 2.5325$ (case where each impurity has its own quantisation axis).

From an inverse Fourier transform of $G_{\text{TF}}(t)$,

$$D_c^{\text{sh}}(B_Z) = \frac{1}{\pi} \frac{\Delta L}{\Delta_L^2 + B_Z^2}$$

i.e. a Lorentzian or Cauchy distribution.
Computation of field distributions
Uncorrelated moments, high-transverse field case, $c_{\text{imp}} = 1$

The characteristic function is

$$G_{TF}(t) \approx \exp \left( -\frac{\gamma \mu \Delta^2_G t^2}{2} \right),$$

in the short-time limit, with $\Delta^2_G = \frac{1}{3} \left( \frac{\mu_0}{4\pi} \right)^2 \sum_{j=1}^{N} \frac{g^2 \mu_B^2}{r_j^6} \langle J^2_Z \rangle (1 - 3 \cos^2 \theta_j)^2$.

Extremely fast convergence of the sum, due to the $r_j^{-6}$ factor.

Case of nuclear dipoles: the $2J + 1$ Zeeman levels of $J_Z$ are equipopulated, hence $\langle J^2_Z \rangle = J(J + 1)/3$. The initial $1/3$ factor drops when all the nuclei have the same quantisation axis.

From an inverse Fourier transform of $G_{TF}(t)$,

$$D_{c}^{\text{sh}}(B_Z) = \frac{1}{\sqrt{2\pi \Delta_G}} \exp \left( -\frac{B_Z^2}{2\Delta^2_G} \right),$$

i.e. a Gaussian distribution.
Computation of field distributions
Uncorrelated moments, zero-field case, $c_{\text{imp}} \ll 1$

Procedure similar to the high transverse field case:

$$D_v(B) = \int \cdots \int \delta \left(B - \sum_{i=1}^{N} B_i \right) \prod_{i=1}^{N} \left[(1 - c_{\text{imp}})\delta(B_i) + c_{\text{imp}}w_i(B_i)\right] dB_1 \ldots dB_N.$$ 

For $c_{\text{imp}} \ll 1$,

$$G_{ZF}(t) = \exp(-\gamma \mu \Delta_L t),$$

with $\Delta_L = K_L \mu_0 \rho_{\text{vol}} c_{\text{imp}} g \mu_B \langle |m| \rangle$, where $K_L \approx 4.5406$.

Since $G_{ZF}(t)$ only depends on $t$, $D_v(B)$ is isotropic with

$$D_v(B) = D_v(B) = \frac{1}{\pi^2} \frac{\Delta_L}{\left( \Delta_L^2 + B^2 \right)^2}.$$
Recap on the static polarisation functions

- Computation of $P_{\chi,Z}^{\text{stat}}(t)$ assuming a field distribution
- Nature of field at the muon site (dipole and Fermi contact)
- Derivation of $D_c(B_Z)$ and $D_v(B)$ for usual physical situations
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Summary
The Larmor equation

\[ \frac{dS_\mu(t)}{dt} = \gamma_\mu S_\mu(t) \times B_{\text{loc}}(t), \]

is still valid.

However it is difficult to solve it when \( B_{\text{loc}}(t) \) is a stochastic variable.
Stochastic account of dynamics

We compute $P_\alpha(t)$ for two different models.

Hypothesis for both models:
- $B_{\text{loc}}(t)$ follows a stationary Gaussian-Markovian process, i.e.
  - independent of origin of time
  - $B^\alpha_{\text{loc}}(t)$ belongs to a Gaussian distribution
  - $B_{\text{loc}}(t)$ evolves in jumps, with a hopping probability which does not depend on the system state before the jump.

Doob’s theorem (1942):

$$\langle B_{\text{loc}}^{\alpha}(t_0)B_{\text{loc}}^{\alpha}(t_0 + t) \rangle = \langle (B_{\text{loc}}^{\alpha})^2 \rangle \exp (-\nu_c |t|)$$

where $\nu_c^{-1} = \tau_c$ is the field correlation time.
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Summary
The weak collision model (1)

Computation of $P_X(t)$

Recall, for a single static field $B_{\text{loc}}^Z = B_0$,

$$P_X^{\text{stat}}(t) = \cos(\omega_0 t)$$

with $\omega_0 = \gamma \mu B_0$.

For $B_{\text{loc}}^Z(t)$, the phase at time $t$ is

$$\gamma \mu B_{\text{loc}}^Z(t_0) (t_1 - t_0) + \ldots + \gamma \mu B_{\text{loc}}^Z(t_{n-1}) (t_n - t_{n-1}) = \int_0^t \gamma \mu B_{\text{loc}}^Z(t') dt'.$$

After averaging over the muon ensemble

$$P_X(t) = \mathcal{R}e \left\{ \left< \exp \left[ i \int_0^t \gamma \mu B_{\text{loc}}^Z(t') dt' \right] \right> \right\}.$$
The weak collision model (2)

Computation of $P_X(t)$

Now, for a stationary Gaussian process,

$$
\left\langle \exp \left[ i \int_0^t \gamma_\mu \delta B_{1 loc}^Z (t') dt' \right] \right\rangle = \exp \left[ - \int_0^t dt' \int_0^t \gamma_\mu^2 \left\langle \delta B_{1 loc}^Z \delta B_{1 loc}^Z (t' - t'') \right\rangle dt'' \right],
$$

where $\delta B_{1 loc}^Z (t') = B_{1 loc}^Z (t') - \langle B_{1 loc}^Z \rangle$. Using Doob's theorem and the relation

$$
\int_0^t dt' \int_0^t f(t' - t'') dt'' = 2 \int_0^t (t - \tau)f(\tau)d\tau
$$

where $f(t)$ is an even function, we get

$$
P_X(t) = \exp \left\{ - \frac{\gamma_\mu^2 \Delta_G^2}{\nu_c^2} \left[ \exp(-\nu_c t) - 1 + \nu_c t \right] \right\} \cos \left( \gamma_\mu \langle B_{1 loc}^Z \rangle t \right),
$$

with $\Delta_G^2 = \left\langle \left( \delta B_{1 loc}^Z \right)^2 \right\rangle$.

This is the so-called Abragam formula (Anderson, 1954).
The weak collision model (2)

Computation of $P_X(t)$

Now, for a stationary Gaussian process,

$$\langle \exp \left[ i \int_0^t \gamma \mu \delta B_{\text{loc}}^Z(t') dt' \right] \rangle = \exp \left[ - \int_0^t dt' \int_0^t \gamma \mu^2 \langle \delta B_{\text{loc}}^Z \delta B_{\text{loc}}^Z (t' - t'') \rangle dt'' \right],$$

where $\delta B_{\text{loc}}^Z(t') = B_{\text{loc}}^Z(t') - \langle B_{\text{loc}}^Z \rangle$. Using Doob's theorem and the relation

$$\int_0^t dt' \int_0^t f(t' - t'') dt'' = 2 \int_0^t (t - \tau)f(\tau)d\tau$$

where $f(t)$ is an even function, we get

$$P_X(t) = \exp \left\{ - \gamma \mu^2 \Delta_G^2 \frac{\nu_c^2}{\nu_c^2} \left[ \exp(-\nu_c t) - 1 + \nu_c t \right] \right\} \cos \left( \gamma \mu \langle B_{\text{loc}}^Z \rangle t \right),$$

with $\Delta_G^2 = \langle \left( \delta B_{\text{loc}}^Z \right)^2 \rangle$.

This is the so-called Abragam formula (Anderson, 1954).
The Abragam function

\[ P_X(t) = \exp \left\{ -\frac{\gamma^2 \Delta_G^2}{\nu_c^2} \left[ \exp(-\nu_c t) - 1 + \nu_c t \right] \right\} \cos \left( \gamma \mu \langle B^Z_{\text{loc}} \rangle t \right) \]

- For \( \nu_c \ll \gamma \mu \Delta_G \),
  \[ P_X(t) = \exp \left( -\frac{\gamma^2 \Delta_G^2}{\nu_c^2} t^2 / 2 \right) \cos \left( \gamma \mu \langle B^Z_{\text{loc}} \rangle t \right). \]

- For \( \nu_c \gg \gamma \mu \Delta_G \),
  \[ P_X(t) = \exp(-\lambda_X t) \cos \left( \gamma \mu \langle B^Z_{\text{loc}} \rangle t \right), \]

with \( \lambda_X = \frac{\gamma^2 \Delta_G^2}{\nu_c} = \frac{\gamma^2 \Delta_G^2 \tau_c}{\nu_c} \).

This is the so-called extreme motional narrowing limit (NMR language).
The strong collision model (1)

Computation of $P_Z(t)$

Let $\ell$ be the number of changes for $B_{\text{loc}}(t)$ during the muon life time,

$$P_Z(t) = \sum_{\ell=0}^{+\infty} R_{\ell}(t),$$

where $R_{\ell}(t)$ is the contribution to $P_Z(t)$ of muons which have experienced $\ell$ field changes between 0 and $t$.

Now,

$$R_0(t) = P^\text{stat}_Z(t) \exp(-\nu_c t),$$

since the probability for $B_{\text{loc}}(t)$ to be unchanged between 0 and $t$ is $\exp(-\nu_c t)$. 
The strong collision model (2)

Computation of $P_Z(t)$

- For $\ell = 1$ field change and since the process is Gaussian-Markovian,

$$R_1(t) = \left\langle \int_0^t \frac{S^Z_{\mu,j}(t - t')}{{S_\mu}} \exp[-\nu_c(t - t')] \nu_c \frac{S^Z_{\mu,i}(t')}{{S_\mu}} \exp(-\nu_c t') dt' \right\rangle_{ij}$$

$$= \nu_c \int_0^t R_0(t - t') R_0(t') dt'.$$

- Recursion relation:

$$R_{\ell+1}(t) = \nu_c \int_0^t R_\ell(t - t') R_0(t') dt'.$$

- From the previous relation and the definition $P_Z(t) = \sum_{\ell=0}^{+\infty} R_\ell(t)$,

$$\sum_{\ell=0}^{+\infty} R_{\ell+1}(t) = \nu_c \int_0^t P_Z(t - t') R_0(t') dt' = P_Z(t) - R_0(t),$$

...
The strong collision model (3)

Computation of $P_Z(t)$

which can be rewritten as the integral equation

$$P_Z(t) = P_Z^{\text{stat}}(t) \exp(-\nu_c t) + \nu_c \int_0^t P_Z(t - t') P_Z^{\text{stat}}(t') \exp(-\nu_c t') \, dt',$$

or in terms of Laplace transforms ($f(s) = \int_0^{+\infty} f(t) \exp(-st) \, dt$),

$$P_Z(s) = \frac{P_Z^{\text{stat}}(s + \nu_c)}{1 - \nu_c P_Z^{\text{stat}}(s + \nu_c)}.$$

- Laplace transforms useful for studying analytical behaviour of $P_Z(t)$
- For numerical purposes, solving numerically the integral equation is efficient
Dynamical polarisation functions

$P_Z(t)$ in zero external field for an isotropic Gaussian distribution

Recall

$$P_Z^\text{stat}(t) = P_{KT}(t) = \frac{1}{3} + \frac{2}{3}(1 - \gamma^2 \Delta^2_G t^2) \exp\left(- \frac{\gamma^2 \Delta^2_G t^2}{2}\right),$$

- For $\nu_c \ll \gamma \mu \Delta_G$,

  $$P_Z(t) \simeq \frac{1}{3} \exp\left(- \frac{2}{3} \nu_c t\right) + \frac{2}{3}(1 - \gamma^2 \Delta^2_G t^2) \exp\left(- \frac{\gamma^2 \Delta^2_G t^2}{2}\right).$$

  High sensitivity to slow dynamics.

- For $\nu_c \gtrsim \gamma \mu \Delta_G$,

  $$P_Z(t) = \exp\left\{-2 \frac{\gamma^2 \Delta^2_G}{\nu^2_c} \left[\exp(-\nu_c t) - 1 + \nu_c t\right]\right\}. $$

- For $\nu_c \gg \gamma \mu \Delta_G$,

  $$P_Z(t) = \exp(-\lambda_Z t),$$

  with $$\lambda_Z = 2\frac{\gamma^2 \Delta^2_G}{\nu_c}.$$ (extreme motional narrowing limit).
Dynamical polarisation functions

$P_Z(t)$ in a longitudinal field for an isotropic Gaussian distribution

For $\nu_c \gg \gamma_\mu \Delta_G$, 

$$P_Z(t) = \exp(-\lambda_Z t),$$

with 

$$\lambda_Z = \frac{2\gamma_\mu^2 \Delta_G^2 \nu_c}{\nu_c^2 + \omega_\mu^2}$$

(Redfield formula) and $\omega_\mu = \gamma_\mu B_{\text{ext}}$.

Determination of $\nu_c$ from $\lambda_Z(B_{\text{ext}})$

$$P_Z(t) \text{ for } B_{\text{ext}} = 3\Delta_G.$$
Dynamical polarisation functions

The case of dilute spin glasses (1)

Recall

\[ D_{c}^{sh}(B_{Z}) = \frac{1}{\pi} \frac{\Delta L}{\Delta L^2 + B_{Z}^2}, \]

\[ D_{v}(B) = \frac{1}{\pi^2} \frac{\Delta L}{(\Delta L^2 + B^2)^2}, \]

Muons far from any magnetic site have no chance to experience a large field \( \rightarrow \) Gaussian-Markovian hypothesis breaks.
Dynamical polarisation functions
The case of dilute spin glasses (2)

To cope with the breakdown, we compute the dynamical polarisation function for muons at a given position and perform the spatial average in a second step.

We write

$$P_{Z \text{stat}}(t) = \int P_{KT}(t) \rho_{\Delta_L}(\Delta_G) d\Delta_G,$$

such that

$$P_{Z \text{stat}}(t) = \frac{1}{3} + \frac{2}{3} (1 - \gamma \mu \Delta_L t) \exp(-\gamma \mu \Delta_L t),$$

is the static function for muons in a dilute magnetic system.

The function

$$\rho_{\Delta_L}(\Delta_G) = \sqrt{\frac{2}{\pi} \frac{\Delta_L}{\Delta_G^2}} \exp\left(-\frac{\Delta_L^2}{2\Delta_G^2}\right),$$

fulfils the requirement. Then

$$P_Z(t) = \int P_{DKT}(t) \rho_{\Delta_L}(\Delta_G) d\Delta_G.$$
Dynamical polarisation functions

The case of dilute spin glasses (3)

For $\nu_c \ll \gamma_\mu \Delta_L$,

$$P_Z(t) \simeq \frac{1}{3} \exp \left( -\frac{2}{3} \nu_c t \right) + \frac{2}{3} (1 - \gamma_\mu \Delta_L t) \exp (-\gamma_\mu \Delta_L t).$$

High sensitivity to slow dynamics.

For $\nu_c \gtrsim \gamma_\mu \Delta_L$,

$$P_Z(t) = \exp \left\{ -\sqrt{\frac{4\gamma_\mu^2 \Delta_L^2}{\nu_c^2}} \left[ \exp(-\nu_c t) - 1 + \nu_c t \right] \right\}.$$

For $\nu_c \gg \gamma_\mu \Delta_L$,

$$P_Z(t) = \exp \left( -\sqrt{\frac{4\gamma_\mu^2 \Delta_L^2 t}{\nu_c}} \right).$$
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Summary
The polarisation functions from a quantum approach
A flavour for zero- and longitudinal-field experiments

Consider the Zeeman states of the muon spin (spin 1/2),

\[ \hbar \omega_{\mu} \]

At thermodynamical equilibrium, the populations of the two states are equal since

\[ \hbar \omega_{\mu} \ll k_B T. \]

Indeed, for \( B_{\text{loc}} = 1 \) T, \( \hbar \omega_{\mu} = 0.56 \) \( \mu \text{eV} \) (\( = k_B T \) for \( T = 6.5 \) mK).
The polarisation functions from a quantum approach

Derivation of $P_Z(t)$ (1)

Recall Stephen Blundell’s lecture,

\[
P_Z(t) = 2 \text{Tr} \left[ \rho_s S^Z_\mu S^Z_\mu (t) \right]
\]

with

\[
S^Z_\mu (t) = \exp \left( i \frac{\mathcal{H} t}{\hbar} \right) S^Z_\mu \exp \left( -i \frac{\mathcal{H} t}{\hbar} \right)
\]

where $\rho_s$ is the density operator and $\mathcal{H}$ is the Hamiltonian for the muon-system ensemble.
The polarisation functions from a quantum approach

Derivation of $P_Z(t)$ (2)

After some computation,

$$P_Z(t) \simeq \exp[-\psi_Z(t)]$$

with

$$\psi_Z(t) = 2\pi \gamma^2 \mu \int_0^t (t - \tau) \cos(\omega_\mu \tau) \left[ \Phi^{XX}(\tau) + \Phi^{YY}(\tau) \right] d\tau.$$

where $\Phi^{\alpha\beta}(\tau) = \frac{1}{4\pi} \left[ \langle \delta B^\alpha_\text{loc}(\tau) \delta B^{\beta}_\text{loc} \rangle + \langle \delta B^{\beta}_\text{loc} \delta B^\alpha_\text{loc}(\tau) \rangle \right]$ is the field correlation function and $\omega_\mu = \gamma_\mu B_{\text{ext}}$. 
The polarisation functions from a quantum approach

Derivation of $P_Z(t)$ (3)

Assuming $\Phi^{\alpha\beta}(\tau)$ to decay rapidly on the $\mu$SR time $t$ scale, we get $\psi_Z(t) = \lambda_Z t$ with

$$\lambda_Z = \pi \gamma^2 \mu \left[ \Phi^{XX}(\omega) + \Phi^{YY}(\omega) \right].$$

$\Phi^{\alpha\beta}(\omega)$ is the time Fourier transform of $\Phi^{\alpha\beta}(\tau)$.

If $\Phi^{\alpha\alpha}(\tau) = \frac{1}{2\pi} \langle (\delta B_{\text{loc}}^\alpha)^2 \rangle \exp(-\nu_c |\tau|)$

- $B_{\text{ext}} = 0$,

  $$\lambda_Z = \gamma^2 \mu \left( \langle (\delta B_{\text{loc}}^X)^2 \rangle + \langle (\delta B_{\text{loc}}^Y)^2 \rangle \right) / \nu_c,$$

  which can be identified to

  $$\lambda_Z = 2\gamma^2 \mu \Delta_G^2 / \nu_c.$$

- for any $B_{\text{ext}}$, assuming $\Phi^{\alpha\alpha}(\tau)$ independent of $B_{\text{ext}}$,

  $$\lambda_Z = \frac{2\gamma^2 \mu \Delta_G^2 \nu_c}{\nu_c^2 + \omega^2_\mu}.$$

This is again Redfield's formula.
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Summary
The magnetic field at the muon site

The dipolar field arising from localized spins $J_j$ with Landé factors $g$ is

$$B_{\text{dip}} = -\frac{\mu_0}{4\pi} g \mu_B \sum_j \left[ -\frac{J_j}{r_j^3} + 3\frac{(J_j \cdot r_j) r_j}{r_j^5} \right].$$

$r_j$ is the vector distance from the spin to the muon.

When a polarised electron density is present at the muon, an additional contribution is present, the Fermi contact field:

$$B_{\text{con}} = -\frac{\mu_0}{4\pi} g \mu_B \sum_{j \in \text{NN}} H_j J_j.$$

Only the muon nearest neighbors (NN) usually contribute to $B_{\text{con}}$. When both $B_{\text{dip}}$ and $B_{\text{con}}$ contribute to $B_{\text{loc}}$ (i.e. in metals) they generally have the same order of magnitude.

Altogether

$$B_{\text{loc}} = B_{\text{con}} + B_{\text{con}} = -\frac{\mu_0}{4\pi} \frac{g \mu_B \nu_c}{\nu} \sum_j G_j J_j.$$

$G$ is the muon-spin $j$ coupling tensor.
Spin-lattice relaxation rate $\lambda_Z$ and spin-correlation function

From

$$\lambda_Z = \pi \gamma_\mu^2 \left[ \Phi^{XX}(\omega_\mu) + \Phi^{YY}(\omega_\mu) \right],$$

introducing the space Fourier transform,

$$J(q) = \frac{1}{\sqrt{n_c}} \sum_j J_j \exp(-i q \cdot j),$$

we get

$$\lambda_Z = \frac{D}{2} \int \sum_{\alpha \beta} A^{\alpha \beta}(q) \Lambda^{\alpha \beta}(q, \omega_\mu) \frac{d^3q}{(2\pi)^3}.$$ 

$$\Lambda^{\alpha \beta}(q, \omega) = \frac{1}{2} \left[ \langle \delta J^\alpha(q, \omega) \delta J^\beta(-q) \rangle + \langle \delta J^\beta(-q) \delta J^\alpha(q, \omega) \rangle \right]$$

is the spin correlation tensor,

$$A^{\alpha \beta}(q) = G^{X\alpha}(q)G^{X\beta}(q) + G^{Y\alpha}(q)G^{Y\beta}(q)$$

is the muon-system coupling factor, and

$$D = \left( \frac{\mu_0}{4\pi} \right)^2 \gamma_\mu^2 (g \mu_B)^2 / \nu_c.$$
Spin-lattice relaxation rate $\lambda_Z$ and spin-correlation function

Recall

$$\lambda_Z = \frac{D}{2} \int \sum_{\alpha\beta} A^{\alpha\beta}(q) \Lambda^{\alpha\beta}(q, \omega_{\mu}) \frac{d^3q}{(2\pi)^3}. \quad (1)$$

$\lambda_Z$ is an integral of the spin-correlation function taken near 0 energy (neV to $\mu$eV range) over the Brillouin zone with a weighting factor depending on the muon site.
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Summary
Superposition of uncorrelated field distributions

The distribution resulting from independent distributions is the convolution product of each of the distributions.

- **High transverse field case**
  - The evaluation of $P^\text{stat}_X(t)$ is trivial since its envelope is the inverse Fourier transform of $D^\text{sh}_c(B_Z)$
  - Example: a dilute spin glass in a matrix of atoms with nuclear moments
    \[
    P^\text{stat}_X(t) = \exp \left( \frac{-\gamma^2 \Delta^2 t^2}{2} \right) \exp (-\gamma \mu \Delta_L t) \cos(\gamma \mu B_{ext} t)
    \]

- **Zero-field case**
  - Trivial case of Gaussian distributions, since the convolution of Gaussians is a Gaussian
  - Much trickier situation in the other cases, since $P^\text{stat}_Z(t)$ is not expressed as an inverse Fourier transform
  - Beware that the so-called Kubo golden formula is not of general validity
Occasionally, ZF spectra in quasi-static magnetic systems are found similar to the Kubo-Toyabe function but with a minimum less pronounced than predicted.

Taking the average of Kubo-Toyabe polarisation functions with Gaussian-distributed field widths,

\[ P_{GbG}(t) = \frac{1}{\sqrt{2\pi} \Delta_{GbG}} \int_{-\infty}^{\infty} P_{KT}(\Delta, t) \exp \left( -\frac{(\Delta - \Delta_0)^2}{2\Delta_{GbG}^2} \right) \, d\Delta, \]

provides the required spectral shape. This is the so-called Gaussian-broadened-Gaussian function (Noakes and Kalvius, 1997).

\[ P_{GbG}^{\text{GbG}}(t) \text{ as a function of } R \equiv \Delta_{GbG}/\Delta_0, \]

\[ \text{with } \Delta_{\text{eff}}^2 \equiv \Delta_0^2 + \Delta_{GbG}^2. \]
Presence of short-range correlations in the field distribution

Zero-field case (2)

- Monte Carlo simulations suggest the presence of short-range correlations to be responsible for the weak dip (Noakes, 1999)
- The spectral shape close to the Kubo-Toyabe lineshape suggests the field distribution to be close to a Gaussian
- Therefore, \( D_c(B_Z) \propto \exp \left( \frac{-B_Z^2}{2\Delta^2} \right) \rightarrow D_c(B_Z) \propto \exp \left[ -g \left( \frac{B_Z}{\delta} \right) \right] \) with \( g(x) = \frac{1}{2}x^2 + \frac{1}{3}(\eta_3x)^3 + \frac{1}{4}(\eta_4x)^4 \).

Example of \( \text{Yb}_2\text{Ti}_2\text{O}_7 \), a geometrically frustrated magnet with \( T_c \approx 0.25 \text{ K} \).

**Fits with the new distribution (full line) and the Kubo-Toyabe function (dotted line)**

**New distribution compared to Gaussian distribution**

\( \rightarrow \) Presence of short-range correlations in the magnetically ordered state (Yaouanc et al., 2013)
Outline

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Static polarisation functions from a field distribution approach
  Transverse-field polarisation function
  Longitudinal-field polarisation function
  Effect of external field

Computation of the field distribution
  Nature of the field at the muon site
  Zero-field polarisation function in magnets
  Uncorrelated moments

Dynamical polarisation functions
  Stochastic approach: the weak and strong collision models
  Quantum approach
  Spin correlation functions

Correlations or not correlations

**Stretched exponential function**

Summary
The stretched exponential function

The function

\[ P_Z(t) = \exp \left[ - (\lambda_Z t)^\beta \right], \]

with \(0 < \beta \leq 1\) is often used for the interpretation of \(\mu\)SR data. Sometimes, \(\beta > 1\) is even allowed (compressed exponential function).

It was introduced by Kohlrausch (1854), and can be understood as resulting from a collection of exponential functions \(\exp(-\lambda t)\) with a distribution \(P(s, \beta)\) of relaxation rates,

\[ \exp \left[ - (\lambda_Z t)^\beta \right] = \int_0^{\infty} P(s, \beta) \exp(-s\lambda_Z t) \, ds, \]

where \(s \equiv \lambda/\lambda_Z\) is a dimensionless relaxation rate.
The stretched exponential function

- It is rarely physically justified except in the case of dilute spin glasses, where \( \beta = 1/2 \) in the extreme motional narrowing limit. Recall
  \[
  P_Z(t) = \exp \left( -\sqrt{\frac{4\gamma^2 \Delta^2}{\mu \nu_c} t} \right).
  \]

- Sometimes a physically sound model approaches very well the stretched exponential function. Example of \( \text{Nd}_2\text{Sn}_2\text{O}_7 \), a geometrically frustrated magnet with \( T_N = 0.91 \) K.

\[\text{Nd}_2\text{Sn}_2\text{O}_7\]

\[\text{zero-field} \quad 2.1 \text{ K}\]

\[\text{Asymmetry: } a_{\text{norm}}(t)\]

\[0, 2, 4, 6\] Time \( t \) (\( \mu \)s)

\[0.25, 0.20, 0.15, 0.10\]

- Full line: stretched exponential with \( \beta = 0.70 \) (3).
- Dotted line: exponential.

\[\rightarrow\] Presence of quasi-static correlations in the paramagnetic phase
(Dalmas de Réotier et al, 2017)

\[A \text{ set of LF spectra fitted to the dynamical Kubo-Toyabe model.}\]
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Stretched exponential function

Summary
Summary

- Computation of $P_{X,Z}(t)$ in a static $B_{loc}$, for different field distributions
- Origin and nature of the field at the muon site
- Derivation of the form of the field distribution in selected cases
- Computation of $P_{X,Z}(t)$ when $B_{loc}$ is dynamical
- Effect of spatial correlations
Bibliography

▶ Books

▶ Introductory articles

▶ Relevant review articles
Zero-field polarisation function in magnets

Commensurate magnets: examples

**Ferromagnetic transition at** $T_C = 74.5 \, \text{K}$.

*Powder sample.*

**Antiferromagnetic transition at** $T_N = 57 \, \text{K}$.

*Axial magnet, single crystal*

$\mu$SR cannot directly tell whether a system is a ferro- or an antiferromagnet.
Computation of the field distribution width

Alternative approach, case of nuclear moments (1)

Start from

\[ P_X(t) = \frac{1}{2} \text{Tr}\{\rho_{\text{sys}} \sigma^X(t) \} \]

with

\[ \sigma^X(t) = \exp \left( i \frac{\mathcal{H}_{\text{tot}}}{\hbar} t \right) \sigma^X \exp \left( -i \frac{\mathcal{H}_{\text{tot}}}{\hbar} t \right), \]

and \( \mathcal{H}_{\text{tot}} = \mathcal{H}_{Z,\mu} + \mathcal{H}_{Z,\text{sys}} + \mathcal{H}_{\text{dip}} \).

The field distribution arises from \( \mathcal{H}_{\text{dip}} \), truncated to (high field and secular approximations)

\[ \tilde{\mathcal{H}}_{\text{dip,||}} = \sum_j \frac{\mu_0}{4\pi} \frac{\gamma_\mu \gamma_j \hbar^2}{2r_j^3} (1 - 3 \cos^2 \theta_j) \sigma^Z I^Z_j. \]

\( I_j \): nuclear spin at site \( j \) (distance \( r_j \) and polar angle \( \theta_j \) to the muon).
Computation of the field distribution width

Alternative approach, case of nuclear moments (2)

Expanding $P_X(t)$ up to second order in $t$, we recover the formula

$$\Delta^2_G = \left(\frac{\mu_0}{4\pi}\right)^2 \sum_j \gamma_j^2 \hbar^2 \frac{J_j(J_j + 1)}{r_j^6} \left(1 - 3 \cos^2 \theta_j\right)^2,$$

already given.

Outlook:

- The method allows the electric field gradient acting on the nuclei to be accounted for in the computation of $\Delta^2_G$.
- The above method is equivalent to the Van Vleck formula (1948)
  $$\Delta^2_G \propto -\frac{1}{2\gamma^2 \mu \hbar^2} \text{Tr}\{[\tilde{H}_{\text{dip},\|}, \sigma^X]^2\},$$
- Similar method for computation of the ZF field width
  $$\Delta^2_G \propto -\frac{1}{2\gamma^2 \mu \hbar^2} \text{Tr}\{[\mathcal{H}_{\text{dip},\perp}, \sigma^Z]^2\}.$$