An Ornamental Garden of Field Distributions and Static ZF Muon Spin Relaxation Functions

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Abstract

A variety of static local field distributions and their associated static ZF Kubo-Toyabe μSR relaxation functions are derived by mathematical manipulation, often without reference to any particular physical model of any particular real material. The relation of such distributions and relaxation functions, not already in use, to μSR in the lab is not clear. However, the static Lorentzian Kubo-Toyabe function, which is in use, is well known to be pathological because the field distribution has infinite second moment, which causes the relaxation function to have a slope as $t \to 0$. Most of the distributions discussed do not have such a pathology.

1 Uemura's Site-Distribution Trick

1.1 Lorentzian from Gaussian

In publications on dilute spin glass moment dynamics probed by μSR, Uemura[1] modeled the Lorentzian field distribution at the muon site due to the dilute spins

$$P_L(B_i) = \frac{\gamma_\mu a}{\pi(a^2 + \gamma_\mu^2 B_i^2)}$$

as a Gaussian distribution of fields at each "class" of muon site

$$P_G(B_i) = \frac{\gamma_\mu}{\sqrt{2\pi}\Delta} \exp\left(-\frac{\gamma_\mu^2 B_i^2}{2\Delta^2}\right)$$

convoluted with a strange distribution of such classes of site (see Fig.1)

$$\rho(\Delta) = \sqrt{\frac{2}{\pi}} \frac{a}{\Delta^2} \exp\left(-\frac{a^2}{2\Delta^2}\right),$$

$$P_L(B_i) = \int_0^\infty \rho(\Delta) P_G(B_i) d\Delta.$$

This convolution also works to generate the distribution of magnitudes of field:

$$P_L(|\mathbf{B}|) = \int_0^\infty \rho(\Delta) P_G(|\mathbf{B}|) d\Delta,$$

where

$$P_L(|\mathbf{B}|) = \frac{4wB^2}{\pi\left(w^2 + B^2\right)^2}, \qquad w = \frac{a}{\gamma_\mu}$$

$$P_G(|\mathbf{B}|) = \sqrt{\frac{2}{\pi}} \frac{B^2}{\sigma^3} \exp\left(-\frac{B^2}{2\sigma^2}\right), \qquad \sigma = \frac{\Delta}{\gamma_\mu},$$

and to generate the static ZF Lorentzian Kubo-Toyabe relaxation function:

$$G_L(t) = \int_0^\infty \rho(\Delta) G_G(t) d\Delta,$$

where

$$G_L(t) = \tfrac{1}{3} + \tfrac{2}{3}\left(1 - at\right) e^{-at}$$

$$G_G(t) = \tfrac{1}{3} + \tfrac{2}{3}\left(1 - \Delta^2 t^2\right) \exp\left(-\tfrac{\Delta^2 t^2}{2}\right).$$

In spite of the apparent strangeness $\rho(\Delta)$, Uemura was able to use this to model moment dynamics (for a stationary muon) to produce dynamic muon spin relaxation functions $G(t)$ that decoupled properly in the fast fluctuation limit (direct "dynamicization" of the Lorentzian field distribution, equivalent muon diffusion in a the spin glass, does not result in fluctuation decoupling), and were consistent with observed μSR. So, this convolution does seem to bear some relation to reality.

1.2 Between Gaussian and Lorentzian

1.2.1 Pearson from Gaussian

Consider changing $\rho(\sigma)$, the distribution of classes, to

$$\rho_n(\sigma) = N\left(\frac{w^{n-1}}{\sigma^n}\right)\exp\left(-\frac{w^2}{2\sigma^2}\right), \qquad n > 1.$$

The normalization N is

$$N = \frac{1}{2^{(n-3)/2}\Gamma\left(\frac{n-1}{2}\right)}.$$

Convolution of this with the Gaussian distribution produces Pearson distributions[2]

$$P_{P,b}(B_i) = \frac{(norm)}{w\left(\frac{B_i^2}{w^2}+1\right)^b}, \qquad b = \frac{n}{2} > \frac{1}{2},$$

$$P_{P,b}(|\mathbf{B}|) = (norm)\frac{B^2}{w^3}\left(\frac{1}{\left(\frac{B^2}{w^2}+1\right)^{(b+1)}}\right).$$

This includes the Lorentzian as the b=1 special case, and the Gaussian as the $b \to \infty$ limit. While it is thus expected that the relaxation function $G_{P,b}(t)$ will evolve smoothly from Lorentzian KT to Gaussian KT as b increases, b=2 (n=4) is the only nontrivial case for which closed form $G(t)$ is known:

$$G_{P,2}(t) = \frac{1}{3} + \frac{2}{3}\left(1 + at - a^2t^2\right)e^{-at}.$$

1.2.2 A different way to go from Gaussian toward Lorentzian

Let

$$P_e(\sigma) = \left(\frac{\sigma_{\max}\sigma_{\min}}{\sigma_{\max} - \sigma_{\min}}\right)\frac{1}{\sigma^2}, \qquad \sigma_{\min} < \sigma < \sigma_{\max}.$$

Then, convoluting with Gaussian,

$$P_e(B_i) = \frac{(norm)}{(B_i^2)}\left(\exp\left(-\frac{B_i^2}{2\sigma_{\max}^2}\right) - \exp\left(-\frac{B_i^2}{2\sigma_{\min}^2}\right)\right),$$

$$P_e(|\mathbf{B}|) = \frac{(norm)}{B^2}\left[\left(1+\frac{B^2}{2\sigma_{\max}^2}\right)\exp\left(-\frac{B^2}{2\sigma_{\max}^2}\right) - \left(1+\frac{B^2}{2\sigma_{\min}^2}\right)\exp\left(-\frac{B^2}{2\sigma_{\min}^2}\right)\right],$$

and

$$\begin{aligned} G_e(t) = \; & \tfrac{1}{3} + \tfrac{2}{3}\;\left(\tfrac{\sigma_{\max}}{\sigma_{\max}-\sigma_{\min}}\right)\exp\left(-\tfrac{1}{2}\sigma_{\min}^2 t^2\right) - \left(\tfrac{\sigma_{\min}}{\sigma_{\max}-\sigma_{\min}}\right)\exp\left(-\tfrac{1}{2}\sigma_{\max}^2 t^2\right) \\ & +\sqrt{2\pi}\left(\tfrac{\sigma_{\max}\sigma_{\min} t}{\sigma_{\max}-\sigma_{\min}}\right)\left(\mathrm{erfc}\left(\tfrac{\sigma_{\max} t}{\sqrt{2}}\right) - \mathrm{erfc}\left(\tfrac{\sigma_{\min} t}{\sqrt{2}}\right)\right) \; . \end{aligned}$$

$P_e(|\mathbf{B}|)$ is shown for a variety of $\sigma_{\max}$ values while keeping $\sigma_{\min}$ constant in Fig.2, and similarly $G_e(t)$ in Fig.3. As $\sigma_{\max} \to \sigma_{\min}$, $P_e(\sigma)$ becomes trivial, so all the distributions and the relaxation function tend to Gaussian in that limit. As $\sigma_{\max} \to \infty$ for finite nonzero $\sigma_{\min}$, the distributions and the relaxation function evolve in a Lorentzian-like direction, but even in the limit, they do not quite get there. The depth of the minimum of the limit relaxation function is significantly deeper than the minimum of the Lorentzian Kubo-Toyabe. At the limit, $\sigma_{\max} = \infty$, the "Lorentzian pathology" does develop: the second moments of the distributions diverge, and the relaxation function develops a slope at $t = 0$. Note that taking $\sigma_{\min} \to 0$ for any fixed value of $\sigma_{\max}$ makes the distributions' norms diverge, and drives $G(t) \to 1$.

1.3 (Gaussian)x(power) distribution of Gaussians

Consider the distribution of site classes:

$$\rho_{Gn}(\sigma) = \mathbf{N}\left(\frac{\sigma^n}{w^{n+1}}\right)\exp\left(-\frac{\sigma^2}{2w^2}\right), \qquad n > -1,$$

(n=0 is simply Gaussian) convoluted with a Gaussian field distribution for each class:

$$P_{GnG}(...) = \int_0^\infty \rho_{Gn}(\sigma) P_G(...) d\sigma.$$

Closed forms can be found for small odd integer n:

$$\begin{aligned} n=1: \;\; P_{G1G}(B_i) &= \tfrac{1}{w} e^{-B_i/w} \\ P_{G1G}(|\mathbf{B}|) &= (norm)\left(\tfrac{B}{w^2}\right) e^{-B/w} \\ n=3: \;\; P_{G3G}(B_i) &= \tfrac{(norm)}{w}\left(1+\tfrac{2B_i}{w}\right) e^{-B_i/w} \\ P_{G3G}(|\mathbf{B}|) &= (norm)\left(\tfrac{B^2}{w^3}\right) e^{-B/w} \end{aligned}$$

$$n=5: P_{G5G}(|\mathbf{B}|) = (norm)\frac{B^2}{w^3}\left(1+\frac{B}{w}\right) e^{-B/w},$$

and static ZF relaxation functions for all n:

$$G_{GnG}(t) = \frac{1}{3} + \frac{2\left(1 - na^2t^2\right)}{3\left(1 + a^2t^2\right)^{(n+3)/2}}, \qquad a = \frac{w}{\gamma_\mu}.$$

This is plotted for small n in Fig.4. Note that while $G_{GnG}(t)$ always has zero slope as $t \to 0$, as is proper for a static ZF relaxation function caused by a field distribution with finite second moment, for small values of n the minimum is shallower than for the static Lorentzian Kubo-Toyabe, and $G_{G0G}(t)$ has Pearson $b = 3/2$ shape, that is, monotonic relaxation with no minimum at all. This suggests that $P_{G0G}(|\mathbf{B}|)$ has its maximum value at $|\mathbf{B}| = 0$ and has no peak at finite field value (see below).

The distributions of site classes above in this section all peaked at zero: the most likely value of σ is zero. In a variation of the idea of this section, a Gaussian ($n = 0$) distribution of site classes peaked around a positive value σ_0 was convoluted with a Gaussian field distribution for each class to produce the "Gaussian-broadened Gaussian" relaxation function which applies to some highly-disordered magnetic materials.[3]

1.4 Lorentzian distribution of Lorentzians

As an example of a case where a field-magnitude distribution with no peak at finite $|\mathbf{B}|$ is generated by this kind of convolution, let

$$\rho_L(a) = \frac{\mathrm{w}}{2\pi}\left(\frac{1}{a^2 + \mathrm{w}^2}\right)$$

be convoluted with a Lorentzian distribution at each site:

$$P_{LL}(B_i) = \frac{(norm)\ln\left(\frac{B_i}{\mathrm{W}}\right)}{\mathrm{W}\left(\frac{B_i^2}{\mathrm{W}^2} - 1\right)}$$

$$P_{LL}(|\mathbf{B}|) = \frac{(norm)}{\mathrm{W}}\left[\frac{2\left(\frac{B^2}{\mathrm{W}^2}\right)\ln\left(\frac{B}{\mathrm{W}}\right)}{\left(\frac{B^2}{\mathrm{W}^2} - 1\right)^2} - \frac{1}{\left(\frac{B^2}{\mathrm{W}^2} - 1\right)}\right].$$

In spite of these expressions not being well defined when $B_i =$w or $B =$w, these distributions are smooth through those values. $P_{LL}(|\mathbf{B}|)$ is shown in Fig.5. Note that it is finite, nonzero at $B = 0$. The corresponding relaxation function is expressible in sine-integral and cosine-integral functions.

2 Monotonic-decreasing field-magnitude distributions

Monotonic decreasing distributions of magnitude of field are easy to write down (they may be hard to justify in a physical model of a material, and the corresponding component distributions are sometimes not easy to identify). For the exponential

$$P_E(|\mathbf{B}|) = \left(\frac{1}{W}\right) e^{-B_i/W}$$

by direct integration

$$G_E(t) = \frac{1}{3} + \frac{2}{3}\int_0^\infty P(|\mathbf{B}|)\cos(\gamma_\mu|\mathbf{B}|t)d|\mathbf{B}|,$$

$$\Longrightarrow G_E(t) = \frac{1}{3} + \frac{2}{3}\left(\frac{1}{1+(\gamma_\mu W t)^2}\right),$$

a monotonic Lorentzian relaxation shape.

If the standard Lorentzian field distribution, with width parameter w, is convoluted with a step function:

$$P_{step}(w) = \frac{1}{w_{\max}} = const., \qquad 0 < w < w_{\max},$$

then

$$P_{Lstep}(B_i) = \frac{1}{2\pi w_{\max}} \ln\left(1 + \frac{w_{\max}^2}{B_i^2}\right),$$

$$P_{Lstep}(|\mathbf{B}|) = \frac{2}{\pi}\left(\frac{w_{\max}}{B^2 + w_{\max}^2}\right).$$

This process creates a simple Lorentzian distribution for the magnitude of field, and reveals the corresponding component distribution. The Fourier transform of a simple Lorentzian is well known to be an exponential, so by direct integration:

$$G_{Lstep}(t) = \frac{1}{3} + \frac{2}{3}\exp\left(-\gamma_\mu w_{\max} t\right).$$

The convolution has preserved the Lorentzian pathology, the second moments diverge, and the initial slope of the relaxation is nonzero.

Similarly, convoluting $P_{step}(\sigma)$ with the standard Gaussian field distribution results in:

$$P_{Gstep}(B_i) = \frac{-1}{2\sqrt{2\pi}\sigma_{\max}} Ei\left(\frac{-B_i^2}{2\sigma_{\max}^2}\right),$$

where $Ei(x)$ is the exponential-integral function as defined by Gradshteyn and Ryzhik,[4]

$$P_{Gstep}(|\mathbf{B}|) = \sqrt{\frac{2}{\pi}}\left(\frac{1}{\sigma_{\max}}\right)\exp\left(\frac{-B^2}{2\sigma_{\max}^2}\right),$$

$$G_{Gstep}(t) = \frac{1}{3} + \frac{2}{3}\exp\left(\frac{-\Delta_{\max}^2 t^2}{2}\right),$$

where $\Delta_{\max} = \gamma_\mu \sigma_{\max}$. Again the convolution with the step function has turned the magnitude distribution into the functional form normally associated with the component distribution, and also generated its component distribution. In both cases, the component distribution diverges logarithmically as $B_i \to 0$.

3 Incommensurate Magnetic Ordering

Long-range magnetic ordering incommensurate with the lattice is generally expected to generate broad field distributions at each crystallographic muon site in the material. In theory, this can still result in quite distinctive muon spin relaxation functions, even though real-world observation of μSR in incommensurate magnets has generally been disappointing. Generally, for an interstitial muon site in a lattice with local moments in a long range ordered state, there should be a strict upper-limit cutoff field magnitude, so in some sense the broadest possible field-magnitude distribution is $P_c(|\mathbf{B}|) = const.$, for $0 < |\mathbf{B}| < B_{\max}$. In spite of the broadness, this distribution causes a static ZF μSR relaxation function with clear oscillations. By direct integration

$$G_c(t) = \frac{1}{3} + \frac{2\sin(\gamma_\mu B_{\max} t)}{3(\gamma_\mu B_{\max} t)}.$$

Note that the fequency seen is not representative of some average of the fields in the distribution, but of the highest field involved in the distribution.

For a simple amplitude-modulation spin density wave (SDW) magnetic ordering, if the local field is assumed to be proportional to the local amplitude of the SDW, $|\mathbf{B}| = B_{\max}|\cos(\phi)|$, with all values of ϕ equally likely.

$$P(|\mathbf{B}|) = \frac{P(\phi)}{\left(\frac{dB}{d\phi}\right)},$$

$$\Longrightarrow P_{SDW}(|\mathbf{B}|) = \frac{2}{\pi\sqrt{B_{\max}^2 - B^2}}\;, \qquad 0 < B < B_{\max}.$$

Peretto *et al.*,[5] considering perturbed angular correlation (PAC) in chromium metal, call this the "Overhauser" distribution, and discuss PAC relaxation functions (slightly different than for μSR) in terms of J_0, the zero-order Bessel function. The static ZF μSR function is

$$G_{SDW}(t) = \frac{1}{3} + \frac{2}{3}J_0(\gamma_\mu B_{\max} t).$$

After some initial relaxation, this also settles down to oscillation at the maximum field frequency of the distribution.

To model μSR in a helical incommensurate magnetic ordered state, consider a single host moment to be closest to the muon site, and let the orientation of that moment point anywhere in a plane containing both the host moment and the muon positions, for fixed muon polarization direction. If there is only dipole coupling between host moment and muon spin,

$$|\mathbf{B}| = \frac{m}{r^3}\sqrt{1 + 3\cos^2\theta},$$

where, in a simple case, m and $\mathbf{r}$ are fixed, and all values of θ are equally probable. In this case $|\mathbf{B}|$ ranges between $B_{\min} = m/r^3$ and $B_{\max} = 2m/r^3$. If the plane of host moment orientation does not contain the muon, $B_{\max}$ is reduced. In the simplest "lone dipole" case, then,

$$P_{LD}(|\mathbf{B}|) = \frac{2}{\pi\sqrt{\left(B^2 - \left(\frac{m}{r^3}\right)^2\right)\left(\left(\frac{2m}{r^3}\right)^2 - B^2\right)}}, \qquad \frac{m}{r^3} < B < \frac{2m}{r^3}.$$

This distribution diverges as B goes to either $B_{\min}$ or $B_{\max}$. Numerical simulations[6] indicate that for muons dipole coupled to all the host moments in an incommensurate ordering in which the moments point anywhere in a plane the local field distribution has this form except that $B_{\min}$ and $B_{\max}$ are essentially independent parameters, and in particular, $B_{\min}$ can also be less than $B_{\max}/2$. This suggests that a generic incommensurate antiferromagnet muon-site field distribution might be

$$P_I(|\mathbf{B}|) = \frac{2}{\pi\sqrt{\left(B^2 - B_{\min}^2\right)\left(B_{\max}^2 - B^2\right)}}, \qquad B_{\min} < B < B_{\max}.$$

Note that $P_{SDW}(|\mathbf{B}|)$ is the $B_{\min} \to 0$ limit of $P_I(|\mathbf{B}|)$. This distribution is likely to generate a static ZF relaxation function with 2 frequencies, corresponding to the upper and lower limits of the distribution.

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