PSI

Memorandum

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Dynamic Gaussian-Lorentzian LF

For details about the Gaussian-, and Lorentzian dynamics in LF see [1, 2, 3, 4, 5].

Here, the focus is only on the strong collision model, where the local dynamics is given by a Gaussian distribution. The system, however, is dilute so that the overall distribution is Lorentzian. This has been discussed the first time in the context of spin-glasses [2], where a Laplace approach has been followed. This approach is unfavorable numerically. Here I follow the approach given in [5], Chapter 6.4.

The measured macroscopic longitudinal polarization function is given as

$$P_Z^{\mathrm{L}}(t, \Delta_{\mathrm{L,ZF}}, B, \nu) = \int_0^\infty P_Z^{\mathrm{G}}(t, \underbrace{r \cdot \Delta_{\mathrm{L,ZF}}}_{\Delta_{\mathrm{G,ZF}}}, B, \nu) \cdot \underbrace{\sqrt{\frac{2}{\pi}} \frac{1}{r^2} \exp\left(-\frac{1}{2r^2}\right)}_{=:f(r)} dr, \tag{1}$$

where $P_Z^{\mathrm{G}}(t, \Delta_{\mathrm{G,ZF}}, B, \nu)$ is the "local" Gaussian dynamic LF function, B the applied LF-field, ν the hopping frequency, and

$$r = \frac{\Delta_{\mathrm{G,ZF}}}{\Delta_{\mathrm{L,ZF}}}.$$

The function $P_Z^{\mathrm{L}}(t, \Delta_{\mathrm{L,ZF}}, B = 0, \nu = 0)$ can exactly be calculated and the resulting ZF function is

$$P_Z^{\mathrm{L}}(t, \Delta_{\mathrm{L,ZF}}, B = 0, \nu = 0) = \frac{1}{3} + \frac{2}{3}\left(1 - \gamma_\mu \Delta_{\mathrm{L,ZF}} \cdot t\right) \cdot \exp(-\gamma_\mu \Delta_{\mathrm{L,ZF}} \cdot t), \tag{2}$$

whereas $P_Z^{\mathrm{G}}(t, \Delta_{\mathrm{L,ZF}}, B = 0, \nu = 0)$ is

$$P_Z^{\mathrm{G}}(t, \Delta_{\mathrm{G,ZF}}, B = 0, \nu = 0) = \frac{1}{3} + \frac{2}{3}\left(1 - \left[\gamma_\mu \Delta_{\mathrm{G,ZF}} \cdot t\right]^2\right) \cdot \exp(-1/2\,(\gamma_\mu \Delta_{\mathrm{G,ZF}} \cdot t)^2). \tag{3}$$

In its general form $P_Z^{\mathrm{G}}(t, \Delta_{\mathrm{G,ZF}}, B, \nu)$ cannot be calculated analytically. The numerical evaluation used in `musrfit` is following the time domain approach as given in [3]
Eq.(1) can be written as a generalized Riemann sum as

$$P_Z^{\mathrm{L}}(t, \Delta_{\mathrm{L,ZF}}, B, \nu) \simeq \sum_k P_Z^{\mathrm{G}}(t, r_k \cdot \Delta_{\mathrm{L,ZF}}, B, \nu) \cdot \sqrt{\frac{2}{\pi}} \frac{1}{r_k^2} \exp\left(-\frac{1}{2r_k^2}\right) \Delta r_k, \tag{4}$$

where Δr_k are *non*-equidistant sampling intervals. r_k are values somewhere within a sampling interval Δr_k.
To understand the following it is useful to have a look at $f(r)$ (see Eq.(1) and Fig.(1)).

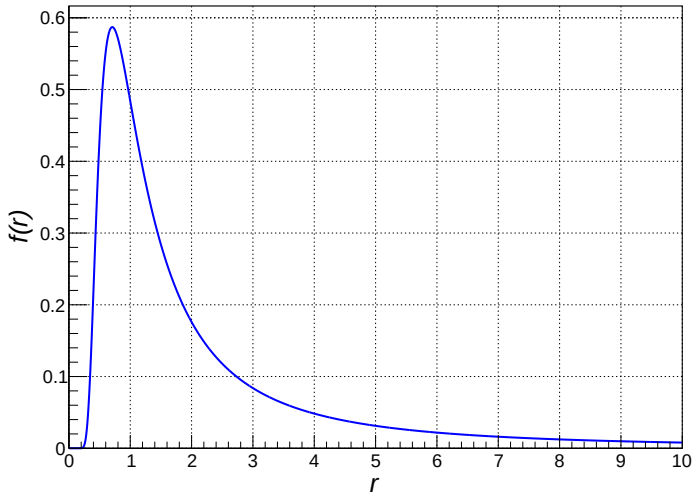


Figure 1:

This shows, that it will be important to have narrow enough r-intervals in the region from 0.2 and 5.0. The chosen sampling is given by the r-points

$$\begin{aligned}\vec{r} \;=\; & (0.0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.25, 1.5, 1.75, 2.0, 2.5, 3.0, 4.0, 5.0, 7.5, 10.0,\\ & 12.8125, 15.625, 18.4375, 21.25, 26.875, 32.5, 43.75, 55.0, 77.5, 100.0).\end{aligned}$$

The intervals are given by

$$\Delta r_k = \vec{r}(k+1) - \vec{r}(k).$$

The calculation of $P_Z^{\mathrm{G}}(t, r \cdot \Delta_{\mathrm{L,ZF}}, B, \nu)$ is quite costly, and hence the following approach has been chosen. Within an Δr_k-Interval we approximate Eq.(4) by

$$\begin{aligned}P_Z^{\mathrm{L}}(t, \Delta_{\mathrm{L,ZF}}, B, \nu) \;&\simeq\; \sum_k P_Z^{\mathrm{G}}(t, r_k \cdot \Delta_{\mathrm{L,ZF}}, B, \nu) \cdot \sqrt{\frac{2}{\pi}} \int_{\vec{r}(k)}^{\vec{r}(k+1)} \frac{1}{r^2} \exp\left(-\frac{1}{2r^2}\right) dr \\ &=\; \sum_k P_Z^{\mathrm{G}}(t, r_k \cdot \Delta_{\mathrm{L,ZF}}, B, \nu) \cdot \left[\mathrm{erf}\left(\frac{1}{\sqrt{2}\,\vec{r}(k)}\right) - \mathrm{erf}\left(\frac{1}{\sqrt{2}\,\vec{r}(k+1)}\right)\right] \quad (5)\end{aligned}$$

where $\mathrm{erf}(\cdot)$ is the Gaussian error function.

References

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