2012

Gaussians versus back-to-back exponentials: a numerical study

M. G. Humpherys

C. Donnelly

A. J. Greer

W. J. Kossler
William & Mary, kossler@physics.wm.edu

Recommended Citation

Humpherys, M. G., Donnelly, C., Greer, A. J., & Kossler, W. J. (2012). Gaussians versus back-to-back exponentials: a numerical study. Physics Procedia, 30, 26-29.

Available online at www.sciencedirect.com
SciVerse ScienceDirect
Physics Procedia 30 (2012) 26 – 29
Physics Procedia

12^{th} International Conference on Muon Spin Rotation, Relaxation, and Resonance

Gaussians versus back-to-back exponentials: a numerical study

M.G. Humpherys[a], C. Donnelly[a], A.J. Greer[a], W.J. Kossler[b]

[a]Physics Department, Gonzaga University, Spokane, WA 99258, USA
[b]Physics Department, College of William and Mary, Williamsburg, VA, 23187-8795, USA

Abstract

The underlying magnetic field distribution in many samples studied by the μSR technique is asymmetric. Despite this, quite often fit functions assuming symmetric (Gaussian) distributions are used. Here, a back-to-back exponential function, which can be made asymmetric with fit parameters, is studied numerically alongside a Gaussian function to see how well each fits symmetric and asymmetric simulated data. Both fit symmetric data well, but the back-to-back exponential is found to be superior for fitting asymmetric data.

Keywords: muSR, field distributions, moments, numerical simulation
PACS: 75.40.Mg

1. Motivation for this work

Many materials studied by μSR, like the high-T_c superconductors YBCO, many of the *La* series, and even the pnictides, yield asymmetry data that when Fourier transformed show an underlying asymmetric field distribution[1, 2, 3, 4, 5]. However, many of the functions used to fit the data have the following (Gaussian) form:

$$P(t) = a \cdot G(t) \cos(\omega t + \phi) \tag{1}$$

where $G(t)$ is the Gaussian relaxation function

$$G(t) = e^{-\frac{\sigma^2 t^2}{2}}, \tag{2}$$

a is the polarization asymmetry, ω is the average precession frequency, ϕ is the initial phase angle, and σ is the second moment of the assumed underlying Gaussian field distribution. Theoretical calculations for ideal, triangular magnetic flux line lattices in superconductors also show very asymmetric field distributions[6, 7, 8]. A function which can be asymmetric, and with fit parameters which determine its asymmetry, should give more meaningful results with such materials.

2. The back-to-back function

In this work we chose a back-to-back exponential function, which can be made asymmetric by varying decay parameters[6, 7, 9, 10]. Here, we have followed what was done in reference [9]. The frequency space representation

Email address: greera@gonzaga.edu (A.J. Greer)

doi:10.1016/j.phpro.2012.04.032

can be defined by the following

$$n(\omega) = \begin{cases} a\, e^{(\omega-\omega_p)\tau_L} & (\omega < \omega_p) \\ a\, e^{(\omega_p-\omega)\tau_R} & (\omega > \omega_p) \end{cases} \tag{3}$$

where ω_p is the the frequency of the peak of the distribution, a is a normalization constant, and τ_L and τ_R are decay parameters to the left and right of the peak, respectively. This function, once properly normalized, has an analytical Fourier transform which can be used to fit transverse field μSR asymmetry data in time space:

$$P(t) = A\left[(r_1(t) + r_2(t))\cos(\omega t + \phi) + t(r_1(t)/\tau_L - r_2(t)/\tau_R)\sin(\omega t + \phi)\right] \tag{4}$$

where

$$r_1(t) = \frac{\tau_R}{(\tau_L+\tau_R)(1+(t/\tau_L)^2)} \qquad r_2(t) = \frac{\tau_L}{(\tau_L+\tau_R)(1+(t/\tau_R)^2)} \tag{5}$$

Once values for τ_L and τ_R are found from a fit, we can calculate the second and third moments of the resulting distribution. These are

$$\sqrt{\langle(\Delta\omega)^2\rangle} = \frac{\sqrt{\tau_R^2+\tau_L^2}}{\tau_L\tau_R} \qquad \sqrt[3]{\langle(\Delta\omega)^3\rangle} = \frac{\sqrt[3]{2\tau_L^3-2\tau_R^3}}{\tau_L\tau_R} \tag{6}$$

3. The Plan

This function has been used to fit data previously[9], but in that work no direct comparison to Gaussian fits was made. So, it was determined that a numerical technique was in order to see how the back-to-back and Gaussian functions compared. With a numerical simulation we would know the underlying parameters used, and then be able to test unequivocally how well each function fit. Our aim here was to see if the back-to-back function could fit as well or better than the Gaussian, and how to interpret the results of such fits.

We developed a plan to pit the Gaussian fit function versus the back-to-back function. Data of varying statistics were generated with $P(t)$ being both Gaussian (equation 1) and back-to-back (equation 4), keeping other parameters the same for both. Noise was introduced to the data by using a Poisson deviate routine [11], thus better approximating real data[8, 12]. This noisy data was multiplied by e^{t/τ_μ} and the average value subtracted off. Fits were then done to the data using both Gaussian fit functions and back-to-back functions. We hoped to try to answer the following questions: 1.) How well does a back-to-back function fit data derived from a Gaussian distribution, and how do statistics affect this? 2.) How well does a Gaussian function fit data derived from a symmetric back-to-back distribution, and how do statistics affect this? 3.) How well does a Gaussian function fit data derived from an asymmetric back-to-back function, and how do statistics affect this? 4.) At what level of asymmetry does the Gaussian fit fail to give reliable results, and how do statistics affect this?

4. Results

For data derived from a Gaussian distribution results are shown in figure 1 on the left panel as a function of total events in the histogram. It can be seen here that both fit functions mimic each other almost exactly point by point, but there is a clear separation between fits, with the back-to-back results always being greater than the corresponding Gaussian values. This is due to the nature of the underlying functions, as shown in the right panel of the figure. Here, a frequency space Gaussian of second moment $0.25\,\mu s^{-1}$ has been generated and a frequency space back-to-back function has been fit to it. The back-to-back (symmetric) fit yields a second moment value of $0.36(1)\,\mu s^{-1}$. This is due to the tails of the back-to-back function (which are truncated in the figure). The separation between the two second moments varies as a function of the second moment value, and the two values become indistinguishable by $\simeq 0.05\,\mu s^{-1}$.

A second investigation was to generate data from a symmetric back-to-back function and then to fit this data with both Gaussian and back-to-back functions. Results of this are shown in figure 2. The left panel is fits to data with a second moment of $0.20\,\mu s^{-1}$, and the behavior is almost identical to that in the left panel of figure 1. We believe this is for the same reason. The right panel shows fits to data that had a second moment of $0.04\,\mu s^{-1}$. Here we see that the

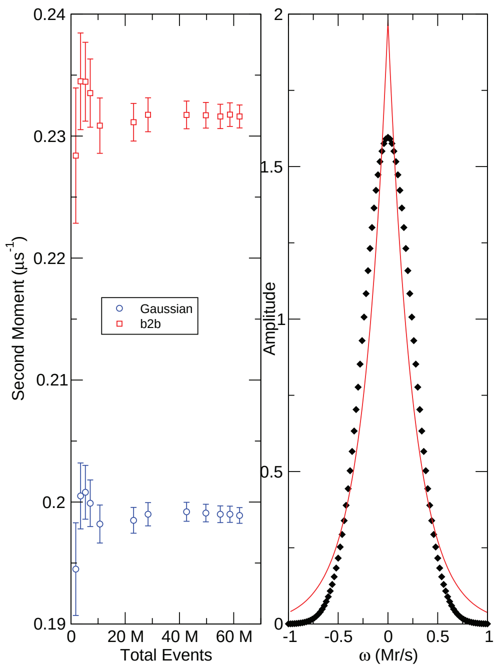

Figure 1. The left panel is results from fitting both Gaussian and back-to-back exponentials to data derived from a Gaussian line shape. The back-to-back results mimic the Gaussian data exactly, but are displaced vertically. The right hand panel shows a frequency space Gaussian function (points) that has been fit with a back-to-back function (curve). The second moments of each are given in the text.

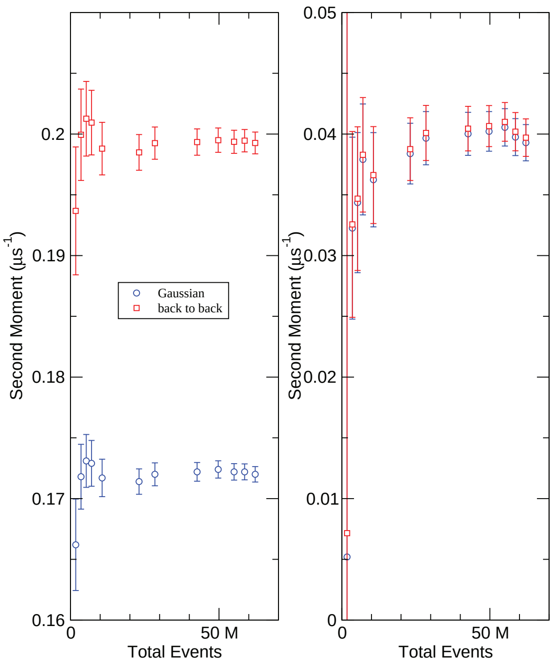

Figure 2. Fit results for both Gaussian and back-to-back functions whe applied to data generated from a symmetric back-to-back function. Fc the left panel, the second moment was $0.20\,\mu s^{-1}$ and for the right panel was $0.04\,\mu s^{-1}$.

data are almost indistinguishable, and this is interpreted as resulting from the fact that the Gaussian and back-to-back frequency representations, for such small widths, are essentially identical.

A third investigation was to generate data from an asymmetric back-to-back function and then to fit this data with Gaussians and back-to-back functions. Data again look quite similar to that shown above when in that representation. However, we feel a more useful representation for this is as shown in figure 3. The dashed (dotted) line shows the actual values for the second (third) moment calculated from the τ_L and τ_R used to generate the data. It can be seen that the Gaussian fits give incorrect second moment values everywhere, but that the discrepancy is worse as the asymmetry grows. The value $1/\tau_R = 0.2\,\mu s^{-1}$ corresponds to a symmetric back-to-back situation, and so the separation at this point is essentially what was seen in the earlier figures. It can also be seen in the inset that the two curves are beginning to diverge as the origin is approached. This indicates the frequency space function moving away from a symmetric situation in the other direction, and one can see the third moment going negative below the value $1/\tau_R = 0.2\,\mu s^{-1}$.

These results strongly suggest that Gaussian fitting functions can give misleading results for any data whose Fourier transform shows an asymmetric field distribution. Even for a second moment as small as $0.1\,\mu s^{-1}$ the difference between the two is $0.04\,\mu s^{-1}$. Typical Gaussian-fit second moments for YBCO at low T are in the 1 to $3\,\mu s^{-1}$ range, and the pnictides come in around $0.25\,\mu s^{-1}$. These results suggest that a back-to-back function can better fit the underlying asymmetry, yield more reliable second moments, and also give third moments.

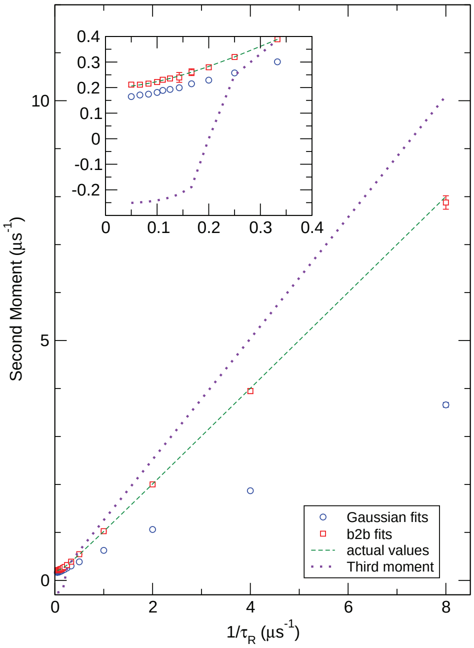

Figure 3. Fit results for both Gaussian and back-to-back functions when applied to data generated from an asymmetric back-to-back function. The parameter τ_L was held fixed at $5.0\,\mu s$ and τ_R was varied. There were $\sim 7 \times 10^6$ events for each histogram. The inset is a magnified view near the origin. The figure is discussed in the text.

5. Conclusion

We have discussed a numerical study comparing a back-to-back exponential fitting function in time space to the more standard Gaussian fitting function for transverse field μSR data analysis. It was shown, using simulated noisy data, that both functions' results mimic each other, but are separated vertically, for symmetric data derived from either. However, for asymmetric data the Gaussian fits do not well represent the underlying asymmetric line shape, whereas the back-to-back function fits quite well for all asymmetries and yields both second and third moment information.

References

[1] R.F. Kiefl et al., *Hyperfine Interactions* **86** (1994) 537.
[2] J.E. Sonier et al., *Phys. Rev. B* **55** (1997) 11789.
[3] J.E. Sonier et al., *Rev. Mod. Phys.* **72** (2000) 769.
[4] C.M. Aegerter et al., *Phys. Rev. B* **57** (1998) 1253.
[5] R. Kasanov et al., *Phys Rev Lett.* **98** (2007) 057007.
[6] D.R. Harshman et al., *Phys. Rev. B* **39** (1989) 851.
[7] D.R. Harshman et al., *Phys. Rev. Lett.* **66** (1991) 3313.
[8] A.J. Greer and W.J. Kossler, *Low Magnetic Fields in Anisotropic Superconductors*, no 30 in m, Springer, Heidelberg, Germany, 1995.
[9] A.J. Greer et al., *Physica C* **400** (2003) 59.
[10] Others (starting at S.L. Lee *et al.*, Phys. Rev. Lett. **71**, 3862(1993) and subsequent publications) have analyzed μSR data using second and third moments, but their approach was to first convert the data to a freqency space representation and analyze the line shape.
[11] W.H. Press et al., *Numerical Recipes in C++*, 2^{nd} Edition, Cambridge University Press, Cambridge, UK, 1999, Ch 7.
[12] A.J. Greer, *Low internal magnetic fields in anisotropic superconductors*, PhD thesis, The College of William and Mary in Virginia, Williamsburg, VA 23187-8795, 1994.