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

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Abstract

Data were numerically generated which simulated that taken in an actual muon spin rotation (μSR) experiment. Two different mathematical functions were used in the generation of the data: Gaussian and back-to-back exponentials. This clean data was then given statistical noise as per a Poisson deviate algorithm to simulate the effects of actual experimental noise (statistics). Fits to this now noisy data were done with both Gaussian and back-to-back fitting functions in an effort to see if the fitting functions could distinguish between the underlying generating functions, and at what level of statistics such a distinction could occur. Our results show that for data derived from symmetric functions both Gaussian and back-to-back fits mimic each other, but are separated by a constant amount. For asymmetrically derived data, however, the Gaussian fits do not do well except for fairly small asymmetry, whereas the back-to-back function fits well. Using back-to-back fitting functions may, therefore, give more reliable second moments for real data with asymmetric line shapes.

1. Gaussian

THE standard Gaussian fit function is:

$$A_s(t) = a e^{-\frac{\sigma^2 t^2}{2}} \cos(\omega t + \phi) \quad (1)$$

where 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. However, not all samples have Gaussian-like field distributions, and in some cases a direct Fourier transform of the asymmetry data can show very asymmetric field distributions[1, 2, 3, 4]. Theoretical calculations for ideal, triangular magnetic flux line lattices also show very asymmetric field distributions[5, 6, 8]. This suggests that using a Gaussian function for time-space fits (reflecting an underlying Gaussian field distribution via a Fourier transform) may not be the best approach.

2. Alternative approach

INSTEAD of using a Gaussian function, it has been suggested that exponential functions, of appropriate forms, may be a good alternative[5, 6, 7]. Here, we have followed what was done in reference [7] in what was called a back-to-back exponential function. The frequency space representation can be defined by the following

$$n(\omega) = \begin{cases} a\, e^{(\omega-\omega_p)\tau_L} & (\omega < \omega_p) \\ a\, e^{(\omega_p-\omega)\tau_R} & (\omega > \omega_p) \end{cases} \quad (2)$$

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 constants to the left and right of the peak, respectively. This function, once properly normalized, has an analytical Fourier transform which is:

$$G(t) = A\left[\begin{matrix}(r_1(t)+r_2(t))\cos(\omega t+\phi)+ \\ t(r_1(t)/\tau_L - r_2(t)/\tau_R)\sin(\omega t+\phi)\end{matrix}\right] \quad (3)$$

where

$$r_1(t) = \frac{\tau_R}{(\tau_L+\tau_R)(1+(t/\tau_L)^2)} \qquad r_2(t) = \frac{\tau_L}{(\tau_L+\tau_R)(1+(t/\tau_R)^2)} \quad (4)$$

This equation can then be used to fit asymmetry μSR data. Further, 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

$$\sqrt{\langle(\Delta\omega)^2\rangle} = \frac{\sqrt{\tau_R^2+\tau_L^2}}{\tau_L\tau_R} \quad (5)$$

and

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

3. The Plan

- Generate single histo simulated data of Gaussian, symmetric b2b, and asymmetric b2b
- Vary statistics, and send to Poisson deviate routine for noise
- Create asymmetry representation of noisy data
- Fit data with Gaussian, symmetric b2b and/or asymmetric b2b function

4. Results

FITS to simulated data of Gaussian origin:

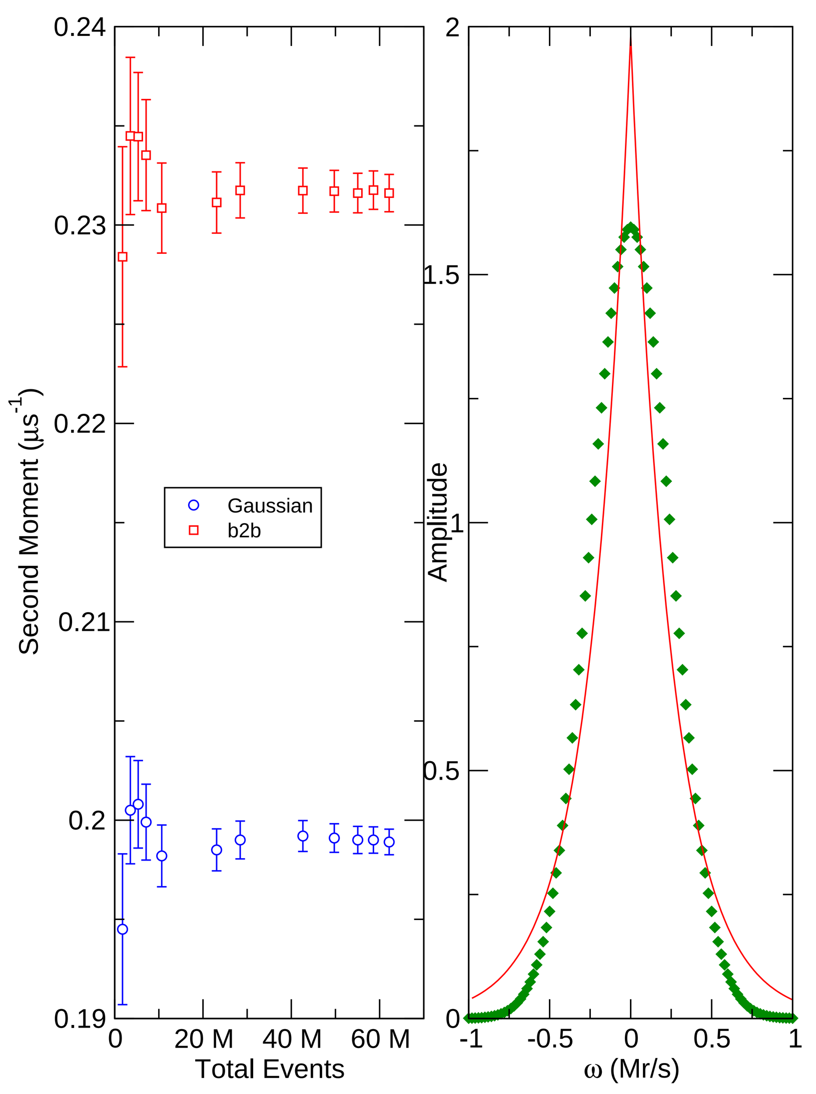

Figure 1: *Left panel: results from fitting Gaussian and back-to-back exponentials to data derived from a Gaussian line shape. Right panel: a Gaussian function (points) that has been fit with a back-to-back function (curve). The Gaussian has second moment of $0.25\,\mu s^{-1}$ and the back-to-back fit gives $0.36(1)\,\mu s^{-1}$. The two become nearly indistinguishable by $\simeq 0.05\,\mu s^{-1}$.*

FITS to simulated data of symmetric back-to-back origin:

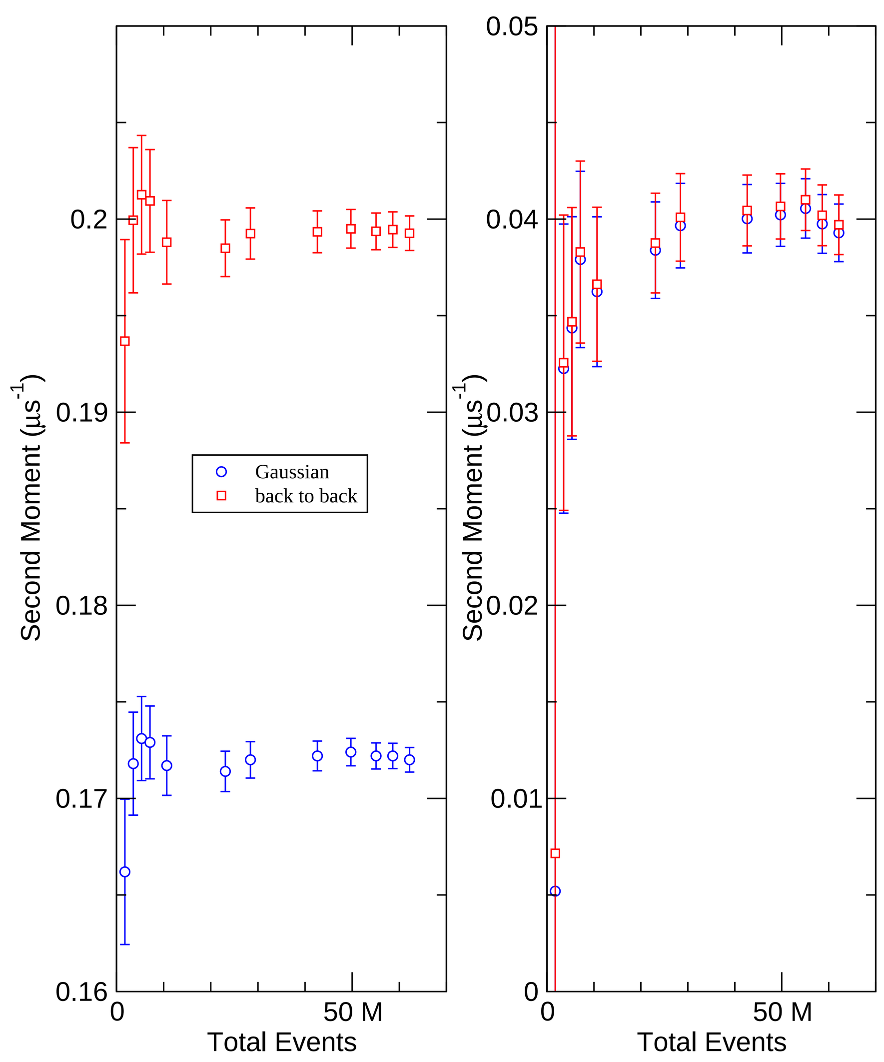

Figure 2: *Fit results for both Gaussian and back-to-back functions when applied to data generated from a symmetric back-to-back function. For the left panel, the second moment was $0.20\,\mu s^{-1}$ and for the right panel it was $0.04\,\mu s^{-1}$.*

FITS to simulated data of asymmetric back-to-back origin:

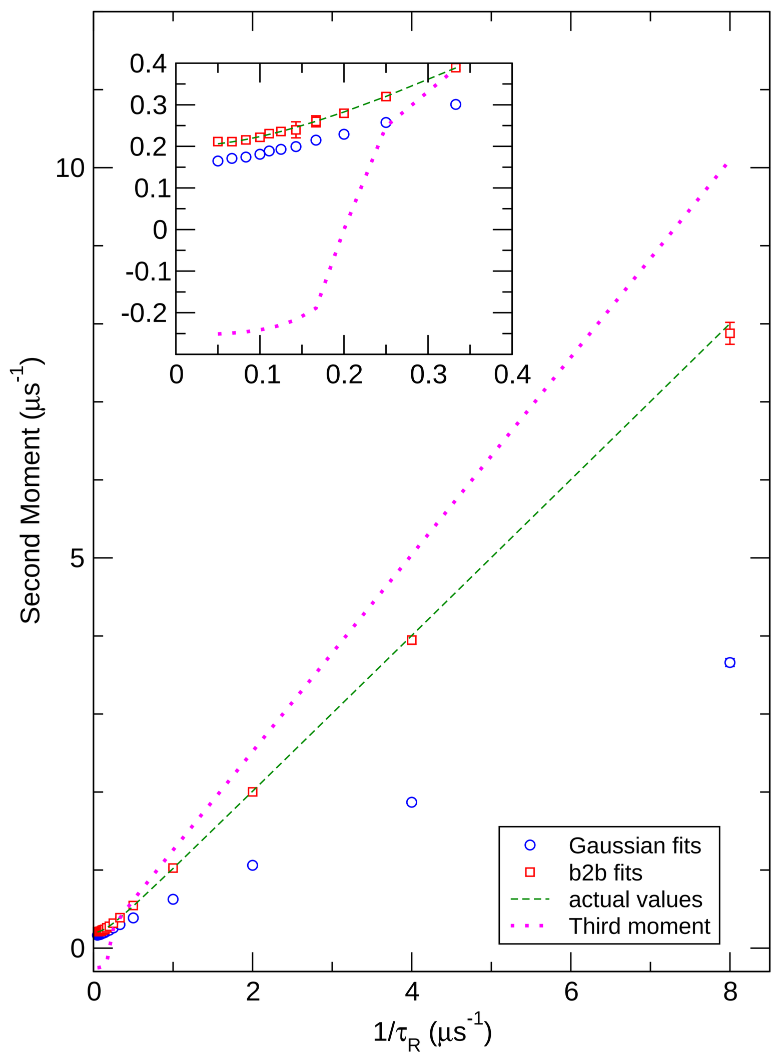

Figure 3: *The parameter τ_L was held fixed at $5.0\,\mu s$ and τ_R was varied. There were $\sim 7\times10^6$ events for each histogram. The value $1/\tau_R = 0.2\,\mu s^{-1}$ corresponds to a symmetric back-to-back situation, and so the separation at this point is essentially what was seen in the earlier figures. The dotted line is the actual value of the third moment calculated from the parameter values used initially to generate the data.*

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 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. For asymmetric data (derived from the back-to-back function), the Gaussian fits do not well represent the underlying asymmetric line shape except for slight asymmetry, whereas the back-to-back function does quite well.

References

[1] R.F. Kiefl *et al. Hyp. Int.*, **86**, 537 (1994).
[2] J.E. Sonier *et al. Phys. Rev. B*, **57**, 11789 (1997).
[3] J.E. Sonier *et al. Rev. Mod Phys.*, **72**, 769 (2000).
[4] C.M. Aegerter *et al. Phys. Rev. B*, **57**, 1253 (1998).
[5] D.R. Harshman *et al. Phys. Rev. B*, **39**,851 (1989).
[6] D.R. Harshman *et al. Phys. Rev. Lett.*, **66**,3313 (1991).
[7] A.J. Greer *et al. Physica C*, **400**,59 (2003).
[8] A.J. Greer and W.J. Kossler *Low Magnetic Fields in Anisotropic Superconductors*, Number 30 in series m. Springer, Heidelberg, Germany, 1995.