PAUL SCHERRER INSTITUT

Memorandum

Datum:	December 23, 2008		
Von:	Andreas Suter	An:	
Telefon:	+41 (0)56 310 4238		
Raum:	WLGA / 119	cc:	
e-mail:	andreas.suter@psi.ch		

The Skewed Gaussian

Sometimes one is encountering skewed lineshapes in μSR experiments. This is obviously true for vortex lattices of superconductors. If there is a full theory present to describe the particular $p(B)$ associated with μSR lineshape that's fine and one should use the appropriate theory in that situation. However, there are sometimes situations where the lineshape is skewed and **no** theory is at hand, as for instance in the superlattice measurements I have performed. For this situation one would like to have a function with a minimal set of parameters which might fetch the situation. The **Skewed Gaussian** is such a minimal approach.
The skewed Gaussian is defined as

$$p_{\rm skg}(B) = \sqrt{\frac{2}{\pi}}\,\frac{\gamma}{(\sigma_+ + \sigma_-)} \begin{cases} \exp\left[-\frac{1}{2}\,\frac{(B-B_0)^2}{(\sigma_+/\gamma)^2}\right] & B \geq B_0 \\ \exp\left[-\frac{1}{2}\,\frac{(B-B_0)^2}{(\sigma_-/\gamma)^2}\right] & B < B_0 \end{cases} \tag{1}$$

This function is normalized, i.e. $\int_{-\infty}^{\infty} p_{\rm skg}(B) dB = 1$. The nice thing about the skewed Gaussian is that all for our purpose relevant properties can be calculated, i.e. the moments, and the Fourier transform.
Here a list of the calculated moments:

mean value

$$M_-^{(1)} = \int_{-\infty}^{B_0} B\, p_{\rm skg}(B)\, dB = \frac{\sigma_-}{\sigma_+ + \sigma_-}\left(B_0 - \sqrt{\frac{2}{\pi}}\sigma_-/\gamma\right) \tag{2}$$

$$M_+^{(1)} = \int_{B_0}^{\infty} B\, p_{\rm skg}(B)\, dB = \frac{\sigma_+}{\sigma_+ + \sigma_-}\left(B_0 + \sqrt{\frac{2}{\pi}}\sigma_+/\gamma\right) \tag{3}$$

and therefore

$$\langle B \rangle = M_1 = M_-^{(1)} + M_+^{(1)} = B_0 + \sqrt{\frac{2}{\pi}}\,(\sigma_+ - \sigma_-)/\gamma \tag{4}$$

second moment – variance

$$M_-^{(2)} = \int_{-\infty}^{B_0} (B - \langle B \rangle)^2\, p_{\rm skg}(B)\, dB = \frac{\sigma_-(2\sigma_+^2 + (\pi-2)\sigma_-^2)}{\pi\,\gamma^2\,(\sigma_- + \sigma_+)} \tag{5}$$

$$M_+^{(2)} = \int_{B_0}^{\infty} (B - \langle B \rangle)^2\, p_{\rm skg}(B)\, dB = \frac{\sigma_+(2\sigma_-^2 + (\pi-2)\sigma_+^2)}{\pi\,\gamma^2\,(\sigma_- + \sigma_+)} \tag{6}$$

and therefore

$$M_2 = M_-^{(2)} + M_+^{(2)} = \frac{1}{\pi}\,\frac{1}{\gamma^2}\left[(\pi-2)\sigma_-^2 - (\pi-4)\sigma_-\sigma_+ + (\pi-2)\sigma_+^2\right] \tag{7}$$

higher moments

$$M_-^{(n)} = \int_{-\infty}^{B_0} (B - \langle B\rangle)^n\, p_{\rm skg}(B)\, dB \tag{8}$$

$$M_+^{(n)} = \int_{B_0}^{\infty} (B - \langle B\rangle)^n\, p_{\rm skg}(B)\, dB \tag{9}$$

with

$$M_n = M_-^{(n)} + M_+^{(n)} \tag{10}$$

skewness

If we, instead of using σ_- and σ_+, define new variables

$$\sigma := \sigma_+ \tag{11}$$

$$\zeta := \sigma_-/\sigma_+ \tag{12}$$

The previous moments can be written as

$$\langle B\rangle = B_0 - \frac{\sigma}{\gamma}\sqrt{\frac{2}{\pi}}\,(\zeta-1) \tag{13}$$

$$M_2 = \left(\frac{\sigma}{\gamma}\right)^2 \frac{1}{\pi}\left[\pi(1-\zeta+\zeta^2) - 2(\zeta-1)^2\right] \tag{14}$$

$$M_3 = \left(\frac{\sigma}{\gamma}\right)^3 \sqrt{\frac{2}{\pi^3}}\,(\zeta-1)\left[\pi(1-3\zeta+\zeta^2) - 4(\zeta-1)^2\right] \tag{15}$$

$$M_4 = \left(\frac{\sigma}{\gamma}\right)^4 \frac{1}{\pi^2}\left[3\pi^2(1-\zeta+\zeta^2-\zeta^3+\zeta^4) - 4\pi(\zeta-1)^2(1+3\zeta+\zeta^2) - 12(\zeta-1)^4\right] \tag{16}$$

$$M_5 = \left(\frac{\sigma}{\gamma}\right)^5 \sqrt{\frac{2}{\pi^5}}(\zeta-1)\left[\pi^2(7-15\zeta+7\zeta^2-15\zeta^3+7\zeta^4)\right. \tag{17}$$

$$\left. -20\pi(\zeta-1)^2(1+\zeta+\zeta^2) - 16(\zeta-1)^4\right] \tag{18}$$

for $\zeta = 1$, it is immediately clear from the above table that all odd moments vanish (as they should), and that $\langle B\rangle = B_0$, $M_2 = (\sigma/\gamma)^2$, and $M_4 = 3\,(\sigma/\gamma)^4$.
Typically not ζ, as defined here, is used as the skewness but

$$\alpha := \frac{M_3^{1/3}}{M_2^{1/2}} \tag{19}$$

see Fig.1

The Fourier Transform of the Skewed Gaussian

The polarization $P(t)$ is the cosine Fourier transform of $p_{\rm skg}(B)$, namely

$$P(t) = \int_0^{\infty} p_{\rm skg}(B)\, \cos(\gamma B t)\, dB, \tag{20}$$

however, what will be given below is the following Fourier transform

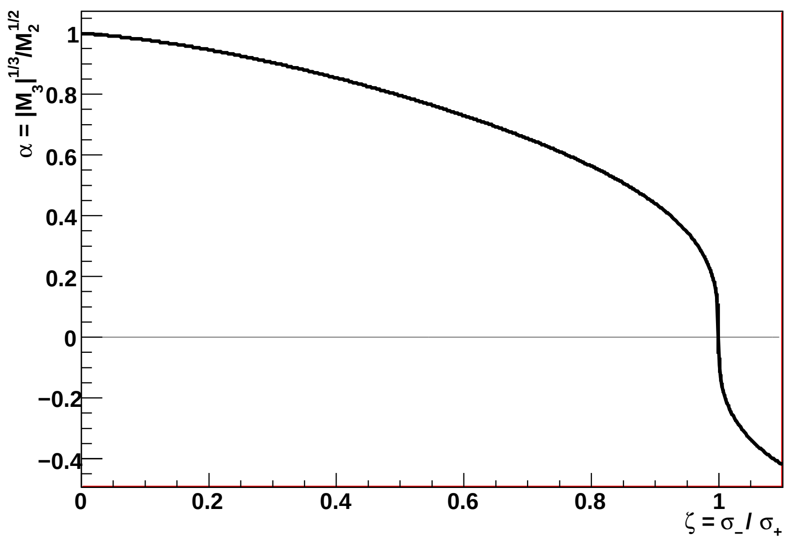

Figure 1: Skewness α versus ζ.

$$P(t) = \int_{-\infty}^{B_0} p_{\rm skg}(B)\,\cos(\gamma B t)\,dB + \int_{B_0}^{\infty} p_{\rm skg}(B)\,\cos(\gamma B t)\,dB \tag{21}$$

which means that B_0 has to be sufficiently high so that $p_{\rm skg}(B=0) \approx 0$.
The polarization is given by the following expression

$$\begin{aligned} P(t) &= \frac{\sigma_-}{\sigma_- + \sigma_+}\exp\left[-\frac{1}{2}(\sigma_- t)^2\right]\left\{\cos(\gamma B_0 t) + \sin(\gamma B_0 t)\,\mathrm{Erfi}\left(\frac{\sigma_- t}{\sqrt{2}}\right)\right\} + \\ &\quad \frac{\sigma_+}{\sigma_- + \sigma_+}\exp\left[-\frac{1}{2}(\sigma_+ t)^2\right]\left\{\cos(\gamma B_0 t) - \sin(\gamma B_0 t)\,\mathrm{Erfi}\left(\frac{\sigma_+ t}{\sqrt{2}}\right)\right\} \end{aligned} \tag{22}$$

where $\mathrm{Erfi}(x)$ is the imaginary error function (see also `http://functions.wolfram.com/GammaBetaErf/Erfi/`) with the following properties

$$\mathrm{Erfi}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{t^2}\,dx = \frac{2}{\sqrt{\pi}}\sum_{k=0}^{\infty}\frac{x^{2k+1}}{k!(2k+1)} = \frac{2x}{\sqrt{\pi}}\,{}_1\mathrm{F}_1\left(\frac{1}{2};\frac{3}{2};x^2\right) \tag{23}$$

where ${}_1\mathrm{F}_1(m;n;x)$ is the so called Kummer confluent hypergeometric function. This function is mentioned here because it is implemented in most numerical packages as for instance in the GSL (see `http://www.gnu.org/software/gsl/`).

How does this look like compared to an ordinary Gaussian? Fig.2 shows such a comparison. The Gaussian, i.e. $P(t) = \exp\left[-1/2(\sigma t)^2\right]\,\cos(\gamma \hat{B} t)$, where $\hat{B} = \langle B \rangle$ [see Eq.(13)] in order that the two functions have about the same frequency. The most obvious difference is the longer decay time of a skewed Gaussian.

Implementation and Tests

At the moment the skewed Gaussian is only implemented in my forthcoming WKM replacement. The plan is to implement it in WKM before end of the shutdown 2008.

In order to check the robustness of this function I have performed some testing. I have generated a set of fake data. For this I generated $p(B)$'s and than calculated $N_i(t)$ (μSR spectra) with and without TF background. $N_i(t)$ were generated including Poisson noise and a flat static background. A typical statistics of $\approx 1.2 \cdot 10^6$ per histogram was used. To be more precise

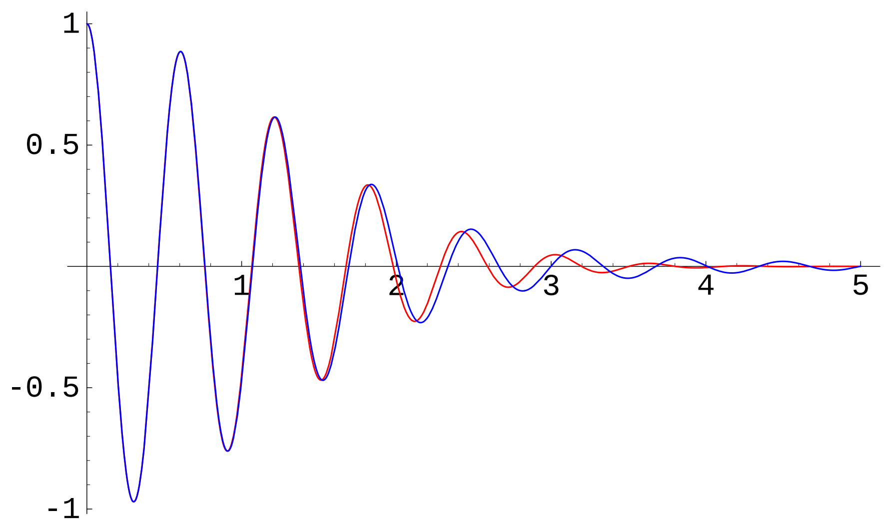

Figure 2: Skewed Gaussian $P(t)$ (blue), and Gaussian TF (red), for the following parameters: (i) skewed Gaussian (blue): $\gamma B_0 = 10$, $\sigma_+ = 1$, $\sigma_-/\sigma_+ = 0.6$; (ii) Gaussian (red): $\gamma B_0 = \langle B \rangle = 10.3192$ [see Eq.(13)], $\sigma = \sqrt{M_2} = 0.811259$. The horizontal axis is plotted in units $1/\gamma$.

$$\begin{aligned} N_i(t) &= N_0^{(i)}\, e^{-t/\tau} \left\{1 + A \left\langle w\, G_{\rm skg}(B_0, \sigma_-, \sigma_+, \phi_i, t) \right.\right. \\ &\quad \left.\left. +(1-w)\, \exp[-1/2(\sigma_{\rm ext} t)^2] \cos(\gamma B_{\rm ext} t + \phi_i) \right\rangle \right\} + \mathrm{Bkg}. \end{aligned} \tag{24}$$

where $G_{\rm skg}(B_0, \sigma_-, \sigma_+, \phi_i, t) = P(t)$ of Eq.(22).
The following data sets where generated and tested (each with 4 histograms and the phases $\phi_{\rm L} = 0, \phi_{\rm T} = 90, \phi_{\rm R} = 180, \phi_{\rm B} = 270$):

no	A	B_0 (G)	σ_- (G)	σ_+ (G)	w	$B_{\rm ext}$ (G)	$\sigma_{\rm ext}$ (G)
1	0.26	100.0	8.0	10.0	1.0	-	-
2	0.26	100.0	10.0	8.0	1.0	-	-
3	0.26	100.0	9.0	9.0	1.0	-	-
4	0.26	100.0	6.0	10.0	1.0	-	-
5	0.26	100.0	10.0	6.0	1.0	-	-
6	0.26	100.0	4.0	5.0	1.0	-	-
7	0.26	100.0	5.5	4.5	1.0	-	-
8	0.26	100.0	5.0	4.0	1.0	-	-
9	0.26	100.0	8.0	10.0	0.9	110.0	1.2
10	0.26	100.0	10.0	8.0	0.9	110.0	1.2
11	0.26	100.0	9.0	9.0	0.9	110.0	1.2
12	0.26	100.0	6.0	10.0	0.9	110.0	1.2
13	0.26	100.0	10.0	6.0	0.9	110.0	1.2
14	0.26	100.0	4.0	5.0	0.9	110.0	1.2
15	0.26	100.0	5.5	4.5	0.9	110.0	1.2
16	0.26	100.0	5.0	4.0	0.9	110.0	1.2

Table 1: Simulated data sets. First column is the label for the data set, the following parameters are defined via Eq.(24).

The following figures show the fit results. The corresponding χ^2's are found in Tabs.2.

no	σ_-/σ_+ (G)/(G)	χ^2_{skg}/NDF	χ^2_{sg}/NDF
1	8/10	1970.6/2042	1993.3/2043
2	10/8	2002.2/2042	2034.9/2043
3	9/9	1964.9/2042	1965.2/2043
4	6/10	1997.3/2042	2121.3/2043
5	10/6	2000.1/2042	2143.2/2043
6	4/5	1984.8/2042	1998.7/2043
7	4.5/4.5	2017.9/2042	2018.0/2043
8	5/4	2031.9/2042	2052.8/2043

Table 2: χ^2's of the fits for skewed Gaussian (χ^2_{skg}) and purly Gaussian (χ^2_{sg}) *without* TF background. Data set according to Tab.1.

no	σ_-/σ_+ (G)/(G)	χ^2_{skg}/NDF	χ^2_{sg}/NDF
9	8/10	2047.1/2040	2059.2/2041
10	10/8	1986.1/2040	2010.8/2041
11	9/9	2032.7/2040	2033.1/2041
12	6/10	1992.2/2040	2063.4/2041
13	10/6	2104.1/2040	2167.1/2041
14	4/5	1971.2/2040	1973.0/2041
15	4.5/4.5	2010.7/2040	2010.8/2041
16	5/4	2073.0/2040	2373.1/2041

Table 3: χ^2's of the fits for skewed Gaussian (χ^2_{skg}) and purly Gaussian (χ^2_{sg}) *with* TF background. Data set according to Tab.1.

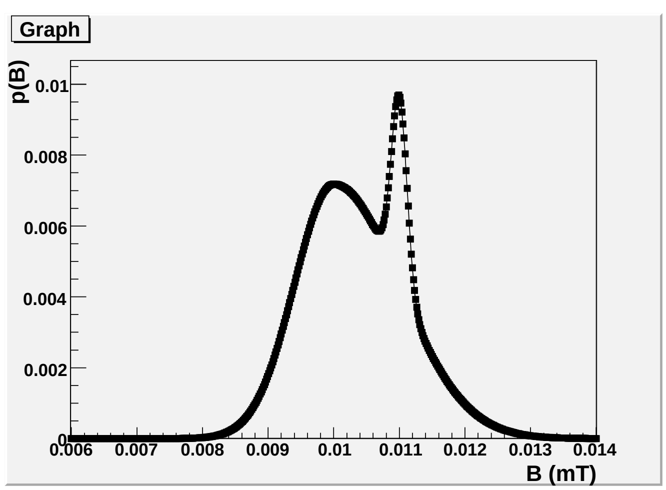

Figure 3: Example $p(B)$ no 12 of Tab.1.

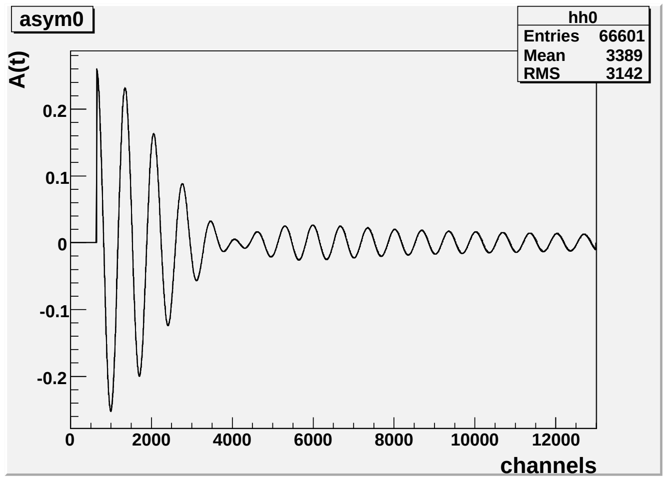

Figure 4: Example $A(t)$ no 12 of Tab.1, $\phi_0 = 0.0$.

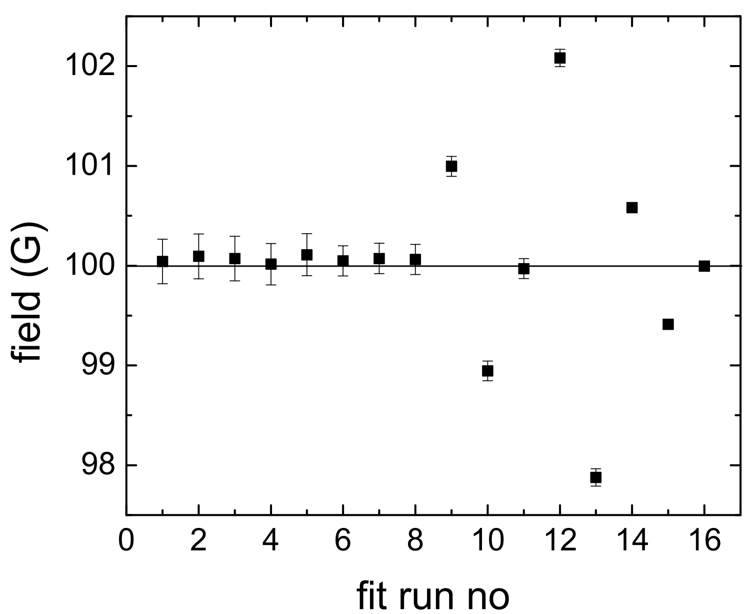

Figure 5: Fit results for the field B_0 of the fake data test *without* TF background. The fit run no $1 \dots 8$ correspond to a skewed Gaussian fit of the data set no $1 \dots 8$ of Tab.1. The fit run no $9 \dots 16$ are the results of a purly Gaussian fit to the same data set.

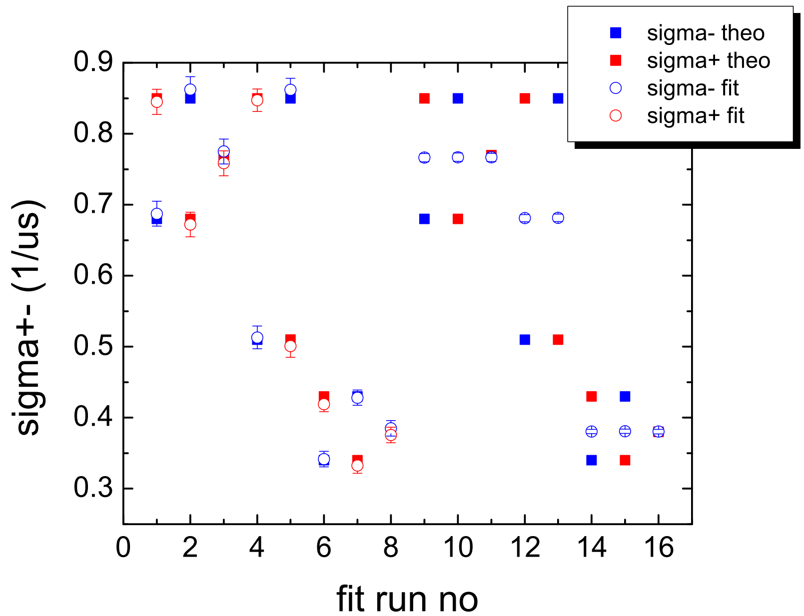

Figure 6: Fit results for σ_-/σ_+ of the fake data test *without* TF background. The fit run no $1\ldots 8$ correspond to a skewed Gaussian fit of the data set no $1\ldots 8$ of Tab.1. The fit run no $9\ldots 16$ are the results of a purly Gaussian fit to the same data set. The open symbols are the fit results, whereas the full symbols show the theoretical values.

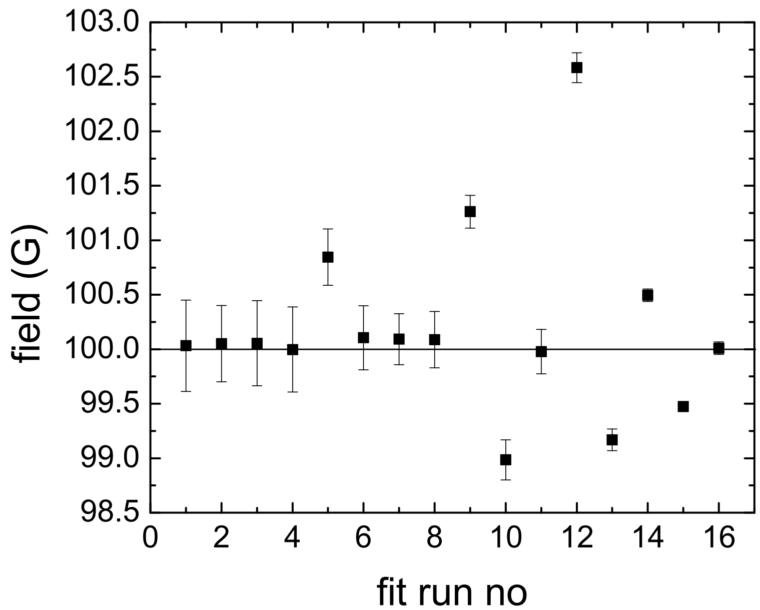

Figure 7: Fit results for the field B_0 of the fake data test *with* TF background. The fit run no $1\ldots 8$ correspond to a skewed Gaussian fit of the data set no $9\ldots 16$ of Tab.1. The fit run no $9\ldots 16$ are the results of a purly Gaussian (including the TF background) fit to the same data set.

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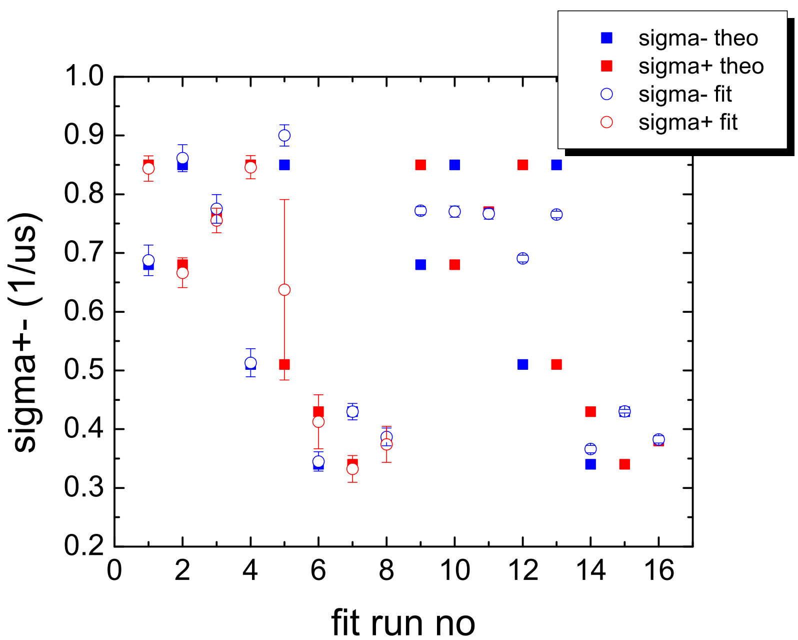

Figure 8: Fit results for σ_-/σ_+ of the fake data test *with* TF background. The fit run no $1 \ldots 8$ correspond to a skewed Gaussian fit of the data set no $9 \ldots 16$ of Tab.1. The fit run no $9 \ldots 16$ are the results of a purly Gaussian fit (including the TF background) to the same data set. The open symbols are the fit results, whereas the full symbols show the theoretical values.

Some Conclusions and Warnings

1. **WARNING:** if σ is rather small $\sigma \lesssim 0.15\,(\mu\mathrm{s}^{-1})$, minuit tends to have problems to converge. In all cases where minuit does not converge nicely, use another fit function!

2. The skewed Gaussian is a robust fit function, i.e. if converging, the fit is always finding the correct parameter values for all the tests performed so far.

3. If one wants to find the peak field B_{peak} of a Meissner profile measurement, the skewed Gaussian should be the better fit curve than a pure Gaussian.

Missing Tests

- Comparison between skewed Gaussian and mutiple Gaussian fits.