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Memorandum

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1 Rotating Reference Frame Fits

High transverse field μSR (HTF-μSR) experiments will typically lead to rather large data sets since it is necessary to follow the high frequencies present in the positron decay histograms. Currently the HAL-9500 instrument at PSI [1] is operated with 2 positron detector, with a typical number of $\sim 4 \times 10^5$ histogram bins. To analyze HTF-μSR data on rather slugish computer hardware is a challenge. In the last millennium the people invented the rotating reference frame transformation (RRF) [4] to reduce to data sets to be handled.

Here I will shortly describe the ways how it is implemented in MUSRFIT, and why it should be avoided to be used altogether. The starting point of all is given by the positron decay spectrum which formally takes the form

$$N^{(j)}(t) = N_0^{(j)} \exp(-t/\tau_\mu) \left[1 + A^{(j)}(t)\right] + N_{\rm bkg}^{(j)}, \tag{1}$$

where (j) is the index of the positron counter, N_0 gives the scale of recorded positrons, τ_μ is the muon lifetime, $A(t)$ the asymmetry, and $N_{\rm bkg}$ describes the background due to uncorrelated events.

The idea behind the RRF is twofolded: (i) try to extract $A(t)$, and (ii) shift the high frequency data set $A(t)$ to lower frequencies such that the number of necessary bins needed can be reduced (packing / rebinning), and hence the overall number of bins is much smaller.

As I will try to explain, this is not for free, and there are problems arising from this kind of data treatment.

1.1 Single Histogram RRF Implementation

In a first step the asymmetry needs to be determined. This is done the following way:

1. Determine the background, $N_{\rm bkg}$, at times before t_0 (t_0 is the time of the muon implantation). Hopefully the background before and after t_0 is equal, which is not always the case.

2. Multiple the background corrected histogram with $\exp(+t/\tau_\mu)$, this is leading to

$$M(t) \equiv [N(t) - N_{\rm bkg}] \exp(+t/\tau_\mu) = N_0 [1 + A(t)] \,. \tag{2}$$

3. In order to extract $A(t)$ from $M(t)$, N_0 needs to be determined, which is almost the most tricky part here. The idea is simple: since $A(t)$ is dominated by high frequency signals, proper averaging over $M(t)$ should allow to determine N_0, assuming that $\langle A(t) \rangle = 0$. Is this assumption always true? *No!* For instance it is *not* true if the averaging is preformed over incomplete periodes of a single assumed signal. Another case where it will fail is if multiple signals with too far apart frequencies is present, as *e.g.* in the case of muonium. Said all this, let's come back and try to determine N_0:

$$N_0 = \sum_{k=0}^{N_{\rm avg}} w_k M(t_k), \tag{3}$$

where $N_{\rm avg}$ is determined such that $N_{\rm avg}\Delta t \simeq 1\mu$s ($\Delta t$ being the time resolution. 1μs means averaging over many cyles). In order to get a good estimate for $N_{\rm avg}$, $N(t)$ is Fourier transformed, and from this power spectrum the frequency with the largest amplitude is determined, ν_0. From ν_0, Δt, the number of cycles fitting into 1μs can be determined, and from this and the time resolution $N_{\rm avg}$ can be calculated. The weight w_k is given by:

$$w_k = \frac{[\Delta M(t_k)]^{-2}}{\sum_{j=0}^{N_{\rm avg}} [\Delta M(t_j)]^{-2}}, \tag{4}$$

where

$$\Delta M(t) = \left[\left(\frac{\partial M}{\partial N} \Delta N \right)^2 + \left(\frac{\partial M}{\partial N_{\rm bkg}} \Delta N_{\rm bkg} \right)^2 \right]^{1/2} \simeq \exp(+t/\tau_\mu)\sqrt{N(t)}. \tag{5}$$

The error estimate on N_0 is then

$$\Delta N_0 = \sigma_{N_0} = \sqrt{\sum_k w_k^2 \Delta M(t_k)^2}. \tag{6}$$

Having estimated N_0, the asymmetry can be extracted as:

$$A(t) = M(t)/N_0 - 1. \tag{7}$$

4. Now the actual RRF transformation can take place: $A_{\rm rrf}(t) = 2 \times A(t)\cos(\omega_{\rm rrf} t + \phi_{\rm rrf})$. The factor of 2 is introduced to conserve the asymmetry amplitude. The idea is the following: Fourier transform theory tells as that

$$\mathcal{F}\{2 \times A(t)\cos(\omega_{\rm rrf} t + \phi_{\rm rrf})\} = \mathcal{F}\{A(t)\}(\omega - \omega_{\rm rrf}) + \mathcal{F}\{A(t)\}(\omega + \omega_{\rm rrf}), \tag{8}$$

i.e. that the Fourier spectrum of $A(t)$ is shifted down and up by $\omega - \omega_{\rm rrf}$ and $\omega + \omega_{\rm rrf}$, respectively. In order to get rid of the high frequency part ($\mathcal{F}\{A(t)\}(\omega + \omega_{\rm rrf})$), $A_{\rm rrf}(t)$ will be heavily over-binned, *i.e.*

5. Do the rrf packing: $A_{\rm rrf}(t) \to \langle A_{\rm rrf}(t) \rangle_p$. Packing itself is a filtering of data! Especially this kind of filter is dispersive [3], *i.e.* that it potentially is leading to line shape distortions. For symmetric, rather narrow lines, this is unlikely to be a problem. However, this might be quite different for complex line shapes as in the case of vortex lattices.

The property $\langle A_{\rm rrf}(t) \rangle_p$ is what is fitted. The error on this property is estimated the following way: (i) the unpacked error of $A(t)$ is:

$$\Delta A(t) \simeq \frac{\exp(+t/\tau_\mu)}{N_0} \left[N(t) + \left(\frac{N(t) - N_{\rm bkg}}{N_0} \right)^2 \Delta N_0^2 \right]^{1/2}, \tag{9}$$

and form this the packed $A_{\rm rrf}(t)$ error can be calculated.

1.2 Asymmetry RRF Implementation

1. In order to circumvent the difficulties to estimate N_0 the asymmetry of the starting positron histograms is formed. For details see [2]. For this, positron detectors geometrically under 180° are used. However, due the the spiraling of the positron in sufficiently high magnetic fields, and the uncertainties of the t_0's, the geometrical phase might *not* correspond to the positron signal phase! At $B = 9$T the uncertainty in t_0 by one channel leads to a phase shift of $\gamma_\mu B \Delta t \cdot (180/\pi) = 1.7°$. Fig.1 shows the t_0-region of a typical HAL-9500 spectrum. It shows that it is very hard to get the absolut value of t_0 right.

2. Carry out the RRF transformation $A_{\rm rrf}(t) = 2 \times A(t) \cos(\omega_{\rm rrf} t + \phi_{\rm rrf})$.

3. Do the rrf packing.

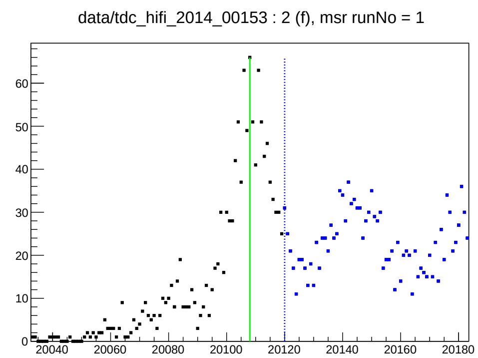

Figure 1: The t_0 region of a typical HAL-9500 spectrum. The broad black hump with the green line, is the "prompt" peak. It is *not* straight forward how to define t_0.

2 Discussion

Both RRF transformation sketched above have weak points which makes it hard to estimate systematic errors. Both methods will fail at too low fields of $\lesssim 1$T. The only and single purpose of the RRF transformation is slughish computer power! We developed GPU based fitting which overcomes *all* this uncontrolled weaknesses and henceforth RRF could be omitted altogether. I still added it for the time being, since strong GPU/CPU hardware is still a bit costly and therefore not affordable to everyone.

In order to give a feeling about what might go "wrong" with the RRF, I was running a couple of test cases. The chosen asymmetry is

$$A^{(j)}(t) = A_0^{(j)} \sum_{k=1}^{3} f_k \exp\left[-0.5 \cdot (\sigma_k t)^2\right] \cos(\gamma_\mu B_k t + \phi^{(j)}), \tag{10}$$

with values found in Tab.1. For the simulation 4 positron detector signals were generated with $A_0^{(j)} = \{0.2554, 0.2574, 0.2576, 0.2566\}$. The further ingredients were: $N_0^{(j)} = \{27.0, 25.3, 25.6, 26.9\}$, $N_{\rm bkg}^{(j)} = \{0.055, 0.060, 0.069, 0.064\}$, and $\phi^{(j)} = \{5.0, 95.0, 185.0, 275.0\}$.

k	f_k	σ_k ($1/\mu$s)	B_k (T)
1	0.5	7	1 or 9
2	0.2	0.75	1.02 or 9.02
3	0.3	0.25	1.06 or 9.06

Table 1: Parameters used in Eq.(10).

Figure.2 shows the averaged Fourier power spectra for the simulated data sets at 1T. Both RRF transformation are showing ghost lines, even for optimally chosen RRF rebinning. At higher fields this is less pronounced. The ghost lines have various origins such as aliasing effects due to the RRF packing not prefectly suppressing the high frequency part of $A_{\rm rrf}(t)$, leakage of the RRF frequency for not sufficently precise known N_0 (see Eq.(6)) for single histogram RRF fits, etc.

Fits of simulated data as described above (see Eq.(10), with fields 0.5, 1.0, 3.0, 5.0, 7.0, and 9.0T) show that above about 1T the model parameters of the RRF fits are acceptable, but the error bars are typically about a factor 3 larger compared to single histogram fits.

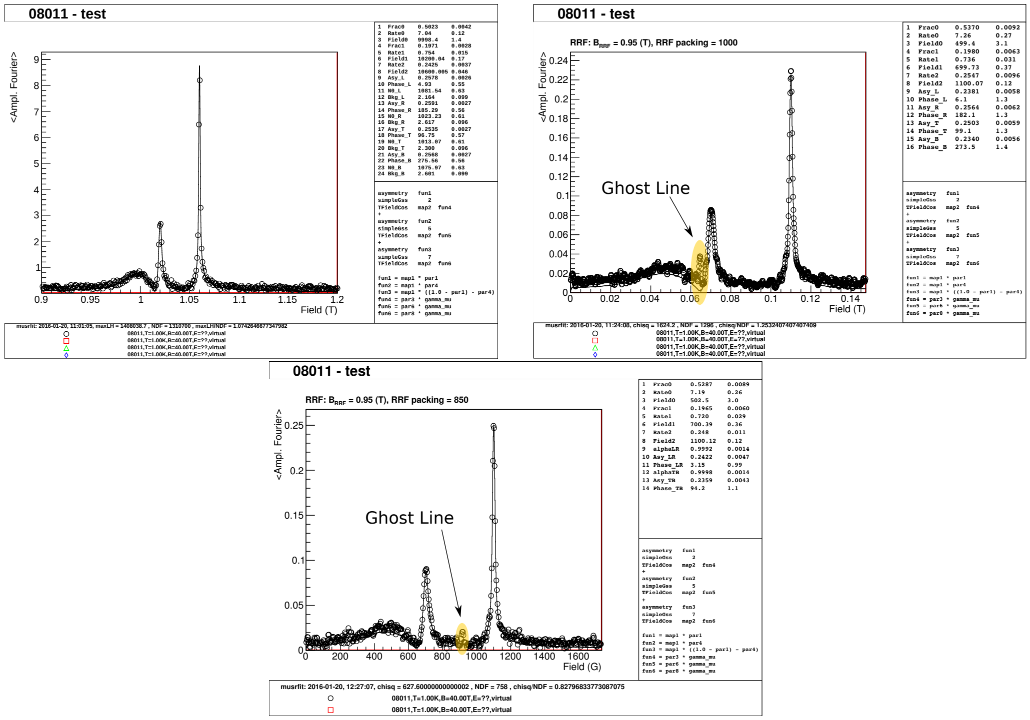

Figure 2: Averaged Fourier power spectra. Top left: from single histogram fit for the 1T data set. Top right: from single histogram RRF fit. Bottom: from asymmetry RRF fit. Both RRF sets show ghost lines.

The asymmetries of the RRF fits are "substantially" too small. The χ^2 values are close to meaningless for the RRF fits, since they are strongly depending on the RRF packing, time interval chosen, etc.

To summaries: RRF fits can be used for online analysis if no GPU accelerator is available, but *must not* be used for any final analysis!

References

[1] *HAL-9500*, `https://www.psi.ch/smus/hal-9500`

[2] *Musrfit User Guide*, `https://intranet.psi.ch/MUSR/MusrFit#A_5.3_Asymmetry_Fit`

[3] R. King, M. Ahmadi, R. Gorgui-Naguib, A. Kwabwe, and M. Azimi-Sajadi, *Digital filtering in one and two dimensions*, 1st ed., Plenum Press, New York, 1989.

[4] T. M. Riseman and J. H. Brewer, *The Rotating Reference Frame Transformation in μSR*, Hyperfine Interact. **65** (1990), 1107.