

# Appendix: Aspects of data treatment for transverse $\mu$ SR

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## 1 Introduction

My main message is that in  $\mu$ SR experiments we are always fighting with poor counting statistics, so we must do nothing to our data which makes matters worse, and we should do whatever we can to extract the most from what we have. The approach is geared to the typical set-up encountered at the pulsed muon beams at ISIS, but is readily generalised to other situations.

### A typical ISIS $\mu$ SR data set.

A data set collected on the MuSR or EMU spectrometers at ISIS consists typically of 32 histograms containing between 1000 to 2000 time channels; the channel widths are 8 or 16ns. These widths are chosen to match the width of the muon pulse, which is of order 70ns (FWHM). As an example let us consider a data set of 1500 channels, with channel width 16ns. The total time window for data collection is then 0 to 24 $\mu$ s. As the muon lifetime  $\tau_\mu$  is 2.2 $\mu$ s, the end of the time window corresponds to 10.9 $\tau_\mu$ , by which time the initial decay count rate will have dropped by a factor  $\exp(-10.9) = 2 \times 10^{-5}$ ! Fortunately the background at ISIS is very low, so it is still possible to collect data out to these times, though the statistics will inevitably be poor.

To develop a feeling for counting statistics, let us consider a standard silver run, measured for one hour (this is a typical duration for a measurement), corresponding to  $2 \times 10^7$  events (20 "Mev"), summed over all 32 histograms. The counts in channel  $n$  of detector  $j$  are given by:

$$C_j(t_n) = N_j^0 \Delta t \exp(-t_n/\tau_\mu) [1 + A_j \cos(\omega_L t_n - \phi_j)] \quad (1)$$

where  $A_j$  is the asymmetry parameter (typically  $A_j = 0.23$  at ISIS),  $\phi_j$  is the phase,  $\Delta t$  is the channel width,  $N_j^0$  is the initial count rate,  $\omega_L = \gamma B$  is the muon Larmor precession

frequency for an applied field  $B$  and the gyromagnetic ratio  $\gamma/2\pi = 135.54\text{MHz/tesla}$ . Ignoring the oscillatory term in (1) for the moment, we can sum over all time channels, to estimate the total number of events per histogram:

$$\sum_n C_j(t_n) \approx \int_0^\infty N_j^0 \exp(-t/\tau_\mu) dt = C_j(0)\tau_\mu/\Delta t$$

Taking the total counts to be  $2 \times 10^7/32$ , then we find that  $C_j(0)$ , the counts at the start of each histogram, to be about 4500. The statistical error in this count is  $\sqrt{C_j(0)} = 67$ . Of all the events, we are only interested in that portion associated with the asymmetry,  $A_j C_j(0) = 0.2 \times 4500 = 900$  counts. It follows that the statistical error in the asymmetry, at the beginning of the histogram, where we have the highest count-rate, is only  $67/900 \equiv 7.4\%$ . This is not very impressive! And at longer times it will be worse. If we wanted, say, 1% statistics on the initial asymmetry we would need  $\sqrt{C}/(0.2C) = 0.01$ , corresponding to  $C_j(0) = 2.5 \times 10^5$  counts, or a total of  $10^9$  events in all 32 histograms! This would mean running for 55 hours on ISIS!

The moral is that in the average  $\mu\text{SR}$  experiment we are dealing with quite poor counting statistics. This is largely a consequence of (i) the signal being associated with only 20% of the total counts, and (ii) the short lifetime of the muon. Clearly it is essential, when analysing  $\mu\text{SR}$  data, to make every event count and to avoid any process which throws away information, e.g. grouping detectors with different phases together; this might be useful for summary purposes, or plotting data during an experiment, but it will reduce the effective asymmetry, and is therefore a bad thing for the ultimate analysis of  $\mu\text{SR}$  data.

## 2 Determination of instrumental parameters

### 2.1 Phases and start time

The time  $t_n$  in (1) is measured with respect to the start time  $t_0$ , when the muons arrive in the sample:  $t_n = n\Delta t + t_0$ . The effective phase of the oscillatory term is therefore  $\psi_j = \phi_j - \omega_L t_0 = \phi_j - \gamma B t_0$ . All detectors should have a common value of  $t_0$ . This can be determined by measuring silver spectra for several different transverse fields  $B$ , fitting the count-rate to (1) to determine the effective phases  $\psi_j$ , then plotting these as a function of  $B$ . The plots give straight lines which, when extrapolated to zero field, give the true phases  $\phi_j$ . The start time  $t_0$  can be extracted from the gradients. Alternatively the phases  $\psi_j$  can be determined for different assumed values of  $t_0$ , then plots of  $\psi_j(t_0)$  for different fields should intersect at the true value of  $t_0$ .

Fitting of (1) to a silver spectrum in order to determine the phases is straightforward: it can be implemented by a linear least squares method, since (1) can be written as:  $C_j^t = \alpha_j F_t + \beta_j G_t$ , with  $\alpha_j = \sin \phi_j$  and  $\beta_j = \cos \phi_j$ . Then following the usual approach

$$\chi^2 = \sum_t [C_j^t - \alpha_j F_t - \beta_j G_t]^2 / \sigma_{jt}^2$$

and the values of  $\alpha_j$  and  $\beta_j$  can be found by minimising  $\chi^2$  in the normal way.

## 2.2 Dead time corrections

The count-rate equation (1) assumes a linear detector response, *i.e.* that the number of detected events in a given time channel is simply proportional to the number of decay positrons at that time. In general this is a reasonable assumption for low count rates, but at high count-rates we have to correct for the "dead time" of the detector. This arises because the counting chain cannot respond to two events that come very close together: the counter is "dead" for a time  $\tau_d$  after the first positron is detected. Since for  $\mu$ SR data the count rate is initially high and then falls with time, the effect of the dead time will be biggest at early times, and will become negligible at later times. The corrections for dead time can be derived from a standard zero field silver run, preferably one with good statistics.

To see the effect of dead time, let us consider a simple case, where  $N(t)$  represents the ideal counting rate and  $M(t)$  is the recorded counting rate. In a single time channel of width  $\Delta t$  the detector will be dead for a time  $M(t)\Delta t\tau_d$ , so the measured count in this time channel will be  $M(t)\Delta t = N(t)\Delta t[1 - M(t)\tau_d]$ . It follows that the recorded count rate is

$$M(t) = \frac{N(t)}{1 + N(t)\tau_d}. \quad (2)$$

Clearly for  $N(t)$  small and  $N(t)\tau_d \ll 1$ , then  $M(t) \approx N(t)$ . However when the count-rate is very high, the measured counts tend to the limiting value  $M(t) = 1/\tau_d$ . To determine the dead times for each detector, the reciprocal of the measured counts in a zero field silver run can be plotted against the reciprocal of  $N(t)$  with  $N(t) = N_0 \exp(-t/\tau_\mu)$ . From (2) it can be seen that a straight line should result with intercept  $\tau_d$ :

$$\frac{1}{M(t)} = \frac{1}{N(t)} + \tau_d.$$

The value of the dead time can then be extracted from a least squares fit to the straight line. If only a transverse field silver run is available, the same procedure can be used, but in this case the ideal counts are as given in Equation (1). In practice for a typical ISIS count rate the dead time corrections at short times are about 5% or less.

## 3 Analysis of $\mu$ SR spectra

There are two perspectives for the interpretation of transverse field  $\mu$ SR spectra:

- **Case (a):** The muon spins precess at a unique frequency  $\omega_L$ , but their polarisation decays with time due to the muons' interaction with static or dynamic fluctuations in its environment. In metals the precession frequency  $\omega_L$  might be shifted slightly from the value  $\gamma B_{\text{ext}}$  (Knight shift), reflecting an enhanced susceptibility at the muon site in the sample.
- **Case (b):** The muons at different sites see a distribution of internal fields, and therefore precess at different rates. This is the case, for example, in the mixed state of superconductors.

We will consider these situations in turn in Sections 3.1 and 3.3, following. In both cases there are special techniques available which are useful for tackling data comprising multiple histograms.

### 3.1 Modelling the depolarisation in the time domain: case (a)

If the muons precess at a common frequency  $\omega_L$ , but their polarisation decays with time, the counts in the  $n$ -th time channel of the  $j$ -th detector can be written:

$$C_j(t_n) = N_j^0 \Delta t \exp(-t_n/\tau_\mu) [1 + A_j P_x(t_n) \cos(\omega_L t_n - \phi_j)]. \quad (3)$$

$P_x(t)$  describes the decay of the muon polarisation. The form of this decay depends on the physics of the muon's interaction with its environment. In the limit of fast temporal fluctuations of the local field or of rapid hopping of the muon from site to site it can be shown that  $P_x(t) = \exp(-\lambda t)$ : this is traditionally (and confusingly) called "Lorentzian damping" because this limit is identical to the limit of strong motional narrowing in NMR, where the line-shape (equivalent to the Fourier transform of  $P_x(t)$ ), is indeed a Lorentzian function. In the limit of slow temporal fluctuations, but where there is a Gaussian distribution local fields (inhomogeneous broadening) it is readily shown that  $P_x(t) = \exp(-\sigma^2 t^2)$ . Other functions in the literature, e.g. the Abragam function, are designed to describe circumstances between these two limiting cases. The point is that the shape of the envelope of the decaying polarisation gives information about the physics of the interaction at the muon site, which can be described by an analytical function with a few parameters (e.g.  $\lambda$  or  $\sigma$  in the above expressions). Analysis of the data is then a simple matter of least squares fitting the expression (3) to the data, with the appropriate form of  $P_x(t)$ . Following our dictum in Section 1, we should, if possible, fit all the histograms ( $j = 1, \dots, 32$ ) at the same time, without grouping them together, after making necessary corrections for dead times. In this case there will be three instrumental parameters for each histogram, namely  $N_j^0$ ,  $A_j$  and  $\phi_j$  as well as the parameters describing the polarisation  $P_x(t)$ . In practice it is best to predetermine the phases as described in Section 2.1, using a standard silver run, since the phases might not be well determined in a fit to the data, especially when the polarisation is rapidly damped. Fitting  $32 \times 1500$  time channels with 65 parameters might seem like a tall order, but computing power is cheap compared to the cost of doing  $\mu$ SR experiments. In the next section we show a way of combining multiple histograms without losing information, which reduces considerably the effort of fitting models to the data.

### 3.2 Combining multiple histograms

We need a technique that allows us to condense a data set comprising multiple (e.g. 32) histograms without losing information. The following method is based on unpublished work by G J Daniell and has been implemented in a practical program for ISIS data by W R Dickson. Starting from the raw data, as described by (3) above, it is straightforward to extract the exponential decay term due to the muon lifetime and the uniform contribution. This yields the component of the signal that oscillates about zero:

$$d_j(t_n) = N_j^0 \Delta t A_j P_x(t_n) \cos(\omega_L t_n - \phi_j) = D_j(t) \cos(\omega_L t_n - \phi_j) \quad (4)$$



for each histogram,  $j = 1, \dots, J$  and time channel,  $n = 1, \dots, N$ . We also have the corresponding variances  $\sigma_j(t_n)$  in the  $d_j(t_n)$ . Now we can project all the data onto a given phase by taking a linear combination of all the histograms. Suppose we choose a value of zero for the phase: we can define a function  $X(t)$  such that

$$\begin{aligned} X(t_n) = D_j(t_n) \cos(\omega_L t_n) &= \sum_j x_j d_j(t_n) \\ &= \sum_j x_j D_j(t_n) \{ \cos(\omega_L t_n) \cos(\phi_j) - \sin(\omega_L t_n) \sin(\phi_j) \}. \end{aligned} \quad (5)$$

Obviously this identity is true if the weights  $x_j$  are chosen so that  $\sum_j x_j \cos \phi_j = 1$  and  $\sum_j x_j \sin \phi_j = 0$ . We can use these two conditions as constraints in a least-squares minimisation of the square of the variance of our new histogram  $X(t_n)$  by using Lagrange multipliers. We then have to minimise

$$\sum_j \sum_n x_j^2 \sigma_j^2(t_n) - \lambda \left[ \sum_j x_j \cos \phi_j - 1 \right] - \mu \sum_j x_j \sin \phi_j$$

with respect to the weights  $x_j$ , where  $\lambda$  and  $\mu$  are the Lagrange multipliers. This leads to the result:

$$x_j = \frac{\lambda \cos \phi_j + \mu \sin \phi_j}{2 \sum_n \sigma_j^2(t_n)} \quad (6)$$

We can now use the two constraints equations to determine  $\lambda$  and  $\mu$ . In order to simplify the resulting expression let us introduce the following notation for the sums involved:

$$\sum^{ss} = \sum_j \sin^2(\phi_j) / \Delta_j; \quad \sum^{sc} = \sum_j \sin(\phi_j) \cos(\phi_j) / \Delta_j; \quad \sum^{cc} = \sum_j \cos^2(\phi_j) / \Delta_j;$$

where

$$\Delta_j = 2 \sum_n \sigma_j^2(t_n).$$

The final result for the weights  $x_j$  is then:

$$x_j = \Delta_j^{-1} \left\{ \cos \phi_j - \sin \phi_j \frac{\sum^{sc}}{\sum^{ss}} \right\} / \left\{ \sum^{cc} - \left( \frac{\sum^{sc}}{\sum^{ss}} \right)^2 \right\} \quad (7)$$

We can now choose a second orthogonal value for the phase and define another function  $Y(t)$  such that:

$$Y(t_n) = D_j(t_n) \sin(\omega_L t_n) = \sum_j y_j d_j(t_n) \quad (8)$$

The weights  $y_j$  are now chosen so that  $\sum_j y_j \cos \phi_j = 0$  and  $\sum_j y_j \sin \phi_j = -1$ . Following the same method we find that the weights are given by:

$$y_j = \Delta_j^{-1} \left\{ -\sin \phi_j + \cos \phi_j \frac{\sum^{sc}}{\sum^{ss}} \right\} / \left\{ \sum^{cc} - \left( \frac{\sum^{sc}}{\sum^{ss}} \right)^2 \right\} \quad (9)$$

By combining all  $J$  histograms with the appropriate weights  $x_j$  and  $y_j$  we can project out two histograms with orthogonal phases. These contain all the original information

and the variance of each is of order  $1/J$  times that of a single histogram. These projections of the data are very convenient for displaying the "real" information content in the data and for modelling the form of the depolarisation, as discussed in section 3.1 above, since now there are only two amplitudes to be determined, besides the parameters describing the model for  $P_x(t)$ . It is also possible to combine the two histograms with orthogonal phases to give a signal proportional to  $P_x(t)$  directly, without any oscillating component.

### 3.3 Transforming data into the frequency domain: case (b)

If the muon sees a distribution of internal fields the counts in each detector will be:

$$C_j(t_n) = N_j^0 \Delta t \exp(-t_n/\tau_\mu) [1 + A_j F_j(t_n)] \quad (10)$$

where

$$F_j(t_n) = \int_0^\infty F(\omega) \cos(\omega t_n - \phi_j) d\omega.$$

The function  $F(\omega)$  gives the distribution of precession frequencies, which maps directly onto the distribution of internal fields through the gyromagnetic ratio:  $\omega = \gamma B$ . The problem is how to extract  $F(\omega)$  from the data. This is clearly a Fourier transform problem, but standard Fourier methods have some drawbacks, in particular:

1. The poor statistical accuracy of the  $\mu$ SR data at long times leads to very noisy transforms. Of course there are standard techniques for coping with this, for example use of window functions ("apodisation"). There is a large literature on how to choose the optimum window function, however whichever one is chosen, they all involve throwing away data, and some deterioration of the frequency resolution.
2. We have a problem of how to derive a unique frequency spectrum  $F(\omega)$  from 32 separate histograms, with different phases  $\phi$ .

Recently this problem has been tackled by Rainford and Daniell (1994) using the Maximum Entropy method. This technique has been widely used to deal with a range of inverse problems in fields such as radio astronomy, geophysics and image reconstruction (including processing images from the Hubble telescope to correct for the aberrations in the mirror) etc. Applied to the present problem it has many advantages:

- It uses all the data available, but allows a unique frequency spectrum to be determined from multiple histograms.
- The frequency spectrum derived is necessarily positive.
- There are no prior assumptions about the form of  $F(\omega)$ .
- It gives the most uniform (N.B. not smoothest) distribution consistent with the data.
- It is possible to include convolution with the muon pulse shape.
- The ultimate frequency resolution can be achieved.

Details  
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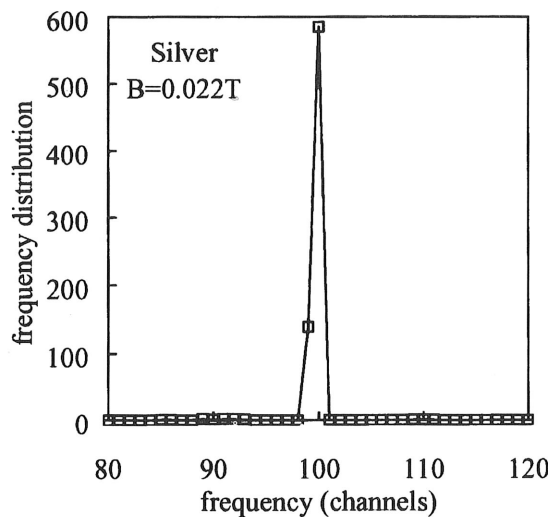
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Details of the method will not be given here, since they are discussed in Lee (1993). Briefly the entropy  $S$  is defined in the information theoretic sense as

$$S = - \sum_k (p_k/b_k) \log(p_k/b_k)$$

where the  $\{p_k\}$  represent the heights of the bins in the histogram representing the frequency spectrum. The  $b_k$  represent the default values which give a scale to the magnitudes of the  $p_k$ . In practice the default is taken to be a flat level, independent of  $k$ . Starting from this featureless default level, the ME algorithm searches for a solution which maximises  $S - \lambda \chi^2$  where  $\lambda$  is a Lagrange multiplier. Initially  $\lambda$  is chosen so that the algorithm puts most effort into minimising  $\chi^2$ , with the aim of reducing its value to be equal to the number of data points. In the later stages the value of  $\lambda$  is altered to concentrate on maximising the entropy. The advantage of the technique is that it tackles the forward problem, *i.e.* generates a frequency spectrum which is then transformed, as in (10), to give the measured counts in each histogram, which are then compared to the measured values. This facilitates the incorporation of any transformation between the frequency domain and the time domain, *e.g.* convolution with the pulse shape of the muon bursts. The resulting frequency spectra produced by the method are impressive. For example Figure 1 shows the frequency spectrum for silver, which is very close to a delta function, as we might expect. This technique has been widely used by a number of groups (Lee et al 1993) to study the mixed state of superconductors. The distribution of internal fields in this case is highly asymmetric, with a high field tail extending up to  $B_{c2}$ , resulting from the flux lattice structure. The asymmetry of the  $\mu$ SR frequency distribution can therefore be used as an indicator of a well ordered flux lattice.



**Figure 1.** Frequency spectrum from a Maxent analysis of a silver data set with  $B_{ext} = 220$  gauss. The width of one frequency channel corresponds to 30.5kHz or 2.25 gauss. The small feature to the left of the main peak near channel 92 is due to muons stopping in the end of a collimator.

## 4 Limitations to the transverse $\mu$ SR method

### 4.1 Effect of finite muon lifetime

Clearly  $\mu$ SR would not work if the muon did not decay! However the finite lifetime of the muon means that we can only collect useful data for, perhaps, five muon lifetimes (data at longer times are useful if we are prepared to count for a long time to improve the statistics). This immediately implies a limit to the frequency resolution of the transverse  $\mu$ SR technique. To see this consider the standard approach from the theory of discrete Fourier transforms (DFT): in a DFT of data comprising  $n$  channels with channel width  $\Delta t$  the frequency resolution  $\Delta f$  is simply  $1/n\Delta t = 1/T$ , *i.e.* the reciprocal of the total time for which data has been collected. If we take  $T = 5\tau_\mu = 11\mu\text{sec}$ , then  $\Delta f \approx 90\text{kHz}$ . Transforming this from frequency to magnetic field, using the gyromagnetic ratio of the muon, the resolution in magnetic field is about 0.7mT or 7 gauss. Note that this is a fundamental restriction, no matter how good our instrumentation or data analysis.

### 4.2 Effect of finite pulse width

The time structure of the muon beam at ISIS reflects that of the proton pulses at the production target, *i.e.* two pulses of width 70ns (FWHM) with a separation of 340ns. The repetition rate is 50Hz. The pulses are further smeared by the 26ns lifetime of the parent pions. The first of the double pulses is split between the two  $\mu$ SR instruments EMU and DEVA, while the second pulse passes on to the MuSR instrument. It follows that the time dependent count-rate (3) or (10) should be convoluted with the pulse shape of the incident muon beam. This will have a significant effect only when there are variations in the count-rate on a time scale comparable to the pulse width. There are two particular cases where this might be important: (i) when the Larmor precession frequency is high, and (ii) where there is rapid decay of the muon polarisation. Let us consider these in turn.

#### Upper limit to the external field

Suppose that we take the muon pulse shape to be a gaussian:  $W(t) = \exp(-t^2/\tau_w^2)$ . This is not strictly correct: a better approximation at ISIS is an inverted parabola, describing the proton pulse, convoluted with a decaying exponential, in order to account for the pion lifetime component. However a simple gaussian simplifies the result greatly. If we are studying a material like silver which is weakly damped, the resulting signal would be the convolution of the "ideal" signal  $[1 + A \cos(\omega_L t)]$  with  $W(t)$ . Here  $A$  is the ideal asymmetry and  $\omega_L$  is the Larmor precession frequency, as usual. It is straightforward to show that the effect of the convolution is to reduce the asymmetry to a value  $A \exp[-(\omega_L \tau)^2/4]$ . The reduction in the asymmetry with applied field is shown in Figure 2 for different values of the pulse width  $\tau_w$ . It follows that the asymmetry falls to  $1/e$  of its ideal value at an applied field  $B$  given by  $(\omega_L/2) = (\gamma/2)B_{1/e} = 1/\tau_w$ . For a pulse width of 70ns (FWHM) the value of  $\tau_w \approx 42\text{ns}$ , and the corresponding field  $B_{1/e}$  is 560 gauss. The reduced asymmetry resulting from high Larmor precession rates degrades the signal to noise, as is clear from the discussion in Section 1 above.

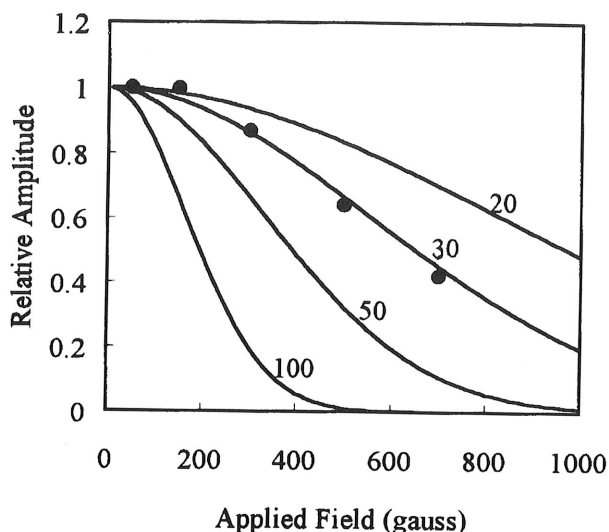
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**Figure 2.** Variation of the asymmetry with external field due to the finite width of the muon pulses, after Nagamine and Yamakazi. The numbers on the curves give the value of  $\tau_w$  in nanoseconds.

#### Upper limit to damping rate

If the damping rate were very high then the muon polarisation  $P_x(t)$  would fall to a small value within one Larmor precession period, or in the extreme case, within the muon pulse width. In the latter case, Lorentzian damping would only be visible for values of the damping rate smaller than  $\lambda_{\max}$  given by, say,  $\exp(-\lambda_{\max}\tau_w) \approx e^{-1}$ , that is we suppose that the muon polarisation decays by  $1/e$  over the duration of the muon pulse. Using the above value  $\tau_w = 42\text{ns}$  gives a value for  $\lambda_{\max} \approx 24\mu\text{s}^{-1}$ . However to extract such a value from real data would require a very accurate knowledge of the pulse shape and the start times for each histogram, and a careful deconvolution procedure. Notice that the situation at ISIS for measuring heavily damped signals is very much improved now that single pulses are used: with the same criterion as above for a double pulse of muons separated by  $320\text{ns}$  we find a value of  $\lambda_{\max}$  of only  $2.9\mu\text{s}^{-1}$ . In practice deconvolution of the pulse shape is necessary to extract reliable values of  $\lambda$  for damping rates greater than  $3\text{--}5\mu\text{s}^{-1}$ , but the extra data analysis effort required is well justified.

#### References

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# Index

- Abragam formula, 100
- ac-Josephson effect, 414
- accelerators, 17
- amorphous semiconductors, 258
- anisotropic nuclear coupling, 189
- anisotropic superconductors, 155
- anomalous muonium, 257
- antiferromagnets, 124, 86
- avoided level crossing (ALC), 184, 249
  - comparison with transverse  $\mu$ SR, 187
  - in longitudinal  $\mu$ SR, 186
  - Zeeman state mixing, 185
  - $\mu$ SR line shapes, 189
- $\beta$ -Mn, 124, 130
- band structures, 116
- BCS theory 222
- binary collision, 369
- Bloch equations, 215, 218
- Bohr radius, 409
- bond centre, 257
- Bose-Einstein condensation, 167
- BPP relaxation, 270
- Breit-Rabi diagram, 202, 241, 278
- Breit-Rabi formula, 440
- Brillouin function, 268
- Brownian motion, 97
- $C_{60}$ , 247, 248, 281
- cage centre, 257
- charge exchange, 263, 276
- chemical shift, 51, 249
- classical hopping, 296
- coexistence of domains, 68
- coherent tunnelling, 287
- collision processes, 369, 390
- conduction electrons, 40, 43
- conformational preference, 179
- contact hyperfine fields, 86
- contact interactions, 57, 240
- continuous muon source, 273
- correlation time, 270, 273
- cosmic muons, 419
- counting statistics, 463
- CPT theorem, 410
- critical exponent, 228
- critical fluctuations, 232
- cross relaxation, 265
- cryocrystals, 308
- cuprous halides, 242
- Curie temperature, 213
- de Haas van Alphen effect, 43
- dead time, 465, 466
- decay asymmetry, 420
- decay beam, 18, 21
- decoupling, 258
- decoupling in LF, 90
- degraders, 4, 344
- delayed muon formation, 305
- demagnetisation in superconductors, 154
- density matrix, 218
- DEVA, 25
- diamagnetism, 40
- diamond, 253, 257
- diffusion, influence of zero point energy, 174
- dilute spin systems, 86
- dilute spin-glass, 90
- dipolar interaction, 86
- double resonance, 103
- $dt/\mu$  formation mechanism, 327
- dynamic range, 273
- dynamic relaxation functions, 97
- dynamic relaxation, Lorentzian fields, 104
- dynamical susceptibility, 40
- Edwards-Anderson order parameter, 107
- effective field, 213
- eigenenergies, 174
- electric field gradient, 212, 218
- electron mediation, 199
- electron nuclear double resonance, 204
- electron transfer in proteins, 332
- electron transport, 304
- electron-positron collider, 406
- electrostatic kicker, 24
- EMU, 25, 26
- endohedral muonium, 225, 243
- energy distribution, 345
- energy loss straggling, 391
- energy production, 327
- energy transfer in collisions, 370, 373

epithermal muons, 355, 359, 365  
 ESS, 33  
 ethylene, 245  
 exotic vortex behaviour, 158  
  
 Fermi contact interaction, 48, 240  
 Fermi temperature, 167  
 Fermi's Golden Rule, 219, 221, 270  
 Fermi-Teller law, 315  
 ferromagnets, 86  
 fine structure, 429  
 finite size of nucleus, 315  
 flip-flop transitions, 249, 280  
 fluctuational preparation of a barrier, 294  
 fluctuations, 97, 270  
 four-level system, 278  
 fourier transform, 468  
 free induction decay, 215  
 free radical, 245  
 frustration, 127  
 fullerene, 247, 281  
  
 GaAs, GaP, Ge, 255  
 gas phase, 280  
 Gaussian distribution, 86, 275  
 Ginzburg-Landau equations, 154  
 glass, 137  
 grand unification theories, 406  
 graphite, 253  
 Guggenheim plot, 228  
 gyromagnetic ratio, 266, 281  
  
 Hahn echo, 217  
 Hebel-Slichter peak, 222  
 Heisenberg spin exchange, ALC, 193  
 hop rate, 271  
 hydrogen bond, 250  
 hydrogen hyperfine structure, 408  
 hydrogen in metals, 251  
 hyperfine interactions, 46, 188, 240-243, 433  
  
 ice, 250  
 implantation depths, 343  
 incoherent tunnelling, 287  
 inequivalent magnetic ions and local  $\chi$ , 61  
 inhomogeneous quantum diffusion, 300  
 InP, 264  
 integral counting, 282  
 interaction representation, 218  
 inversion recovery, 217  
 ionisation of thermal muonium, 347  
 ISIS, 20, 22, 23, 463, 470

isotope effects on encaged D/H/Mu, 181  
 itinerant c.f. local moment magnet, 103  
 itinerant magnetism, 101, 115  
  
 Japanese Hadron Facility, 32, 33  
  
 kinetic isotope effects, 181  
 Knight shift, 46, 49, 57, 58, 221, 273  
 Kondo effect, 58, 78  
 Korringa relation, 221, 273  
 Kubo-Toyabe function, 80, 89, 272  
  
 Lamb shift, 409, 430, 445  
 Larmor frequency, 249  
 level-crossing resonance (LCR), 242, 249, 282  
 LE beam intensity, 384  
 LE muon production, role of bandgap, 371  
 LE muon, energy range, 383  
 LE muons, stopping distances, 386-387  
 lepton number conservation, 422  
 linear response approximation, 40  
 local moments, 40  
 local susceptibility, muon modification, 63  
 London limit, 153  
 long-range magnetic order, 86  
 Lorentzian distribution, 80, 86  
 low energy muon beam, 382  
  
 $\mu \rightarrow \gamma$  decay, 424  
 $\mu \rightarrow e$  conversion, 425  
 $\mu$ CF neutron source, 329  
 $\mu^+e^- \rightarrow \mu^-e^+$  conversion, 426  
 Mössbauer effect, 109  
 magnetic anomaly of the muon, 414  
 magnetic structure, 70  
 magnetogyric ratio, 266  
 maximum entropy, 468  
 meta-stability, 242  
 metals, 251  
 methyl radical, 247  
 mixed state of superconductors, 149  
 MnSi, 119, 123  
 moderated muons, characteristics, 350  
 moderation efficiency, 361, 375  
 moderation in a molecular solid, 377  
 moderator target, 350  
 moderators degradation, 367  
 molecular field approximation, 41  
 motional narrowing, 272, 466  
 Mu\* state, 201, 255  
 muon catalysed fusion ( $\mu$ CF), 313, 315  
 muon decay, 413, 419, 420

muon molecule, 324  
 muon slowing down, 409  
 muon spin rotation, 409  
 muon transfer, 323  
 muon transport, 378  
 muonated radicals, 245  
 muonic atoms, 314  
 muonic H and He, 409  
 muonic X-ray studies, 409  
 muonium, 239, 407, 409  
 muonium diffusion, 280  
 muonium formation in  
 muonium hyperfine spin  
 Muonium isotope effects  
 muonium, microwave  
 muonium, two phases  
 muonium-antimuonium  
 MuSR, 25, 26  
  
 nanoclusters, 398  
 negative work function  
 neutron scattering and  
 neutron spin echo, 109  
 nickel borocarbide, 177  
 nitrogen, 243, 250  
 NMR, 211  
 non-Markovian processes  
 normal muonium, 254  
 nuclear dipolar fields, 86  
 nuclear fusion, 313  
 nuclear moments, 109  
 nuclear quadrupole moment  
  
 one-phonon quantum diffusion  
 ortho-muonium, 254  
 oxygen, 250  
  
 para-muonium, 254  
 paramagnetism, 40  
 parity violation, 409, 410  
 Pauli spin susceptibility  
 perturbation theory, 109  
 phase space compression  
 phase space steering  
 pinning of vortex lines  
 pionic hydrogen, 409  
 plastic crystals, 267  
 polarisation, 267  
 polarisation of spin  
 polarons, 277, 284, 285  
 polymers, 277



- muon molecule, 324
- muon slowing down, 440
- muon spin rotation, 165
- muon transfer, 323
- muon transport, 378
- muonated radicals, 200, 280
- muonic atoms, 314
- muonic H and He, 409–410
- muonic X-ray studies, 337
- muonium, 239, 407, 429
- muonium diffusion, 280
- muonium formation in gases, 440
- muonium hyperfine splitting, 447
- Muonium isotope effects, 173, 176, 178
- muonium, microwave spectroscopy, 439
- muonium, two photon spectroscopy, 449
- muonium-antimuonium conversion, 438
- MuSR, 25, 26
- nanoclusters, 398
- negative work function, 348
- neutron scattering and  $\mu$ -spectroscopy, 73
- neutron spin echo, 109
- nickel borocarbides, 171
- nitrogen, 248, 250
- NMR, 211
- non-Markovian processes, 110
- normal muonium, 256
- nuclear dipolar fields, 86
- nuclear fusion, 313
- nuclear moments, 199
- nuclear quadrupole resonance, 212, 213
- one-phonon quantum diffusion, 294, 297
- ortho-muonium, 358
- oxygen, 250
- para-muonium, 358
- paramagnetism, 40
- parity violation, 406, 419
- Pauli spin susceptibility, 43
- perturbation theory, 184
- phase space compression, 346
- phase space steering, 346
- pinning of vortex lines, 154
- pionic hydrogen, 411
- plastic crystals, 281
- polarisation, 267
- polarisation of epithermal muons, 357
- polarons, 277, 288, 295, 332
- polymers, 277
- positron emission, 420
- positron moderation, 349
- power spectrum, 270
- protonation, 248
- protonium, 411
- pulsed muon source, 273
- $q_{1s}$  problem, 324
- QED, 412, 444
- quadrupolar interaction, 200, 212, 218, 249
- quantum diffusion, 263, 280, 287
- quantum Hall effect, 414
- quantum tunnelling, 175, 176, 287
- quarks, 405
- quartz, 255
- quenching, 92, 258
- radicals, 245, 280
- random moments, 86
- rate equations (for level populations), 279
- reaction rates for  $\mu$ CF, 320
- reentrant systems, 141
- relaxation functions, 87, 92, 269
- relaxation matrix, 279
- relaxation rates, 100, 269
- reorientation, 192, 281
- repolarisation, 258
- Risch-Kehr function, 277
- RIKEN-RAL, 30
- RKKY, 45
- rotating reference frame, 213, 216–218
- screened-proton state, 251
- selection rules for ALC, 187
- self consistent theory, 102, 118
- semiconductors, 275
- Si, 255
- simulations, 138
- site determination, 51
- slow  $\mu^-$  source, 329
- slow muons, 29, 329, 344–351
- slow relaxation, 138
- slowing-down processes, 323
- small polaron, 294
- solitons, 277, 332
- solvent friction, 184
- spectral density function, 219, 270
- spin density, 241
- spin density waves, 94
- spin exchange, 263, 275
- spin fluctuations, 116–124, 130, 169

- spin glass, 86, 109, 132, 137, 275
- spin Peirls transition, 95
- spin rotation interaction (molecular), 280
- spin-lattice relaxation, 191, 265
- spin-orbit coupling, 281
- spin-spin relaxation, 265
- standard model, 405
- start time, 464
- static relaxation functions, 85
- sticking probability, 316
- stochastic cooling, 346
- stochastic fluctuations, 192
- Stoner criterion, 116, 118
- stretched exponential, 106, 129, 139, 275
- stretched exponential relaxation, 110
- strong collision approximation, 97
- structure factor of fluctuations, 234
- super-hyperfine interaction, 241
- superconducting coherence length, 150
- superconducting effective mass tensor, 156
- superconducting films, 392
- superconducting penetration, 150–161
- superconducting vortex, 150
- superconductivity, 45, 58, 59, 165
- superconductors, 149, 150
- superparamagnetism, 398
- surface muon, 18
- surface muons, 17, 267
- susceptibility, 115–118, 123–126, 129
- susceptibility tensor, 40
  
- T site, 256
- $T_1$ -minima, 271
- $T_1$ , 269
- time integrated mode, 186
- transition probability, 270
- trapping, 302
- trigger signal, 382
- triplet muonium, 241
- tunnel splitting, 178
  
- Uemura plot, 167
- ultra small magnetic moments, 78
- unconventional superconductors, 165
- universal scaling in superconductors, 165
  
- vacuum polarisation, 315
- valence transitions, 66
- Van der Waals solids, 368
- Van Vleck paramagnetism, 42
- vibrationally adiabatic barrier, 183
  
- vortex fluctuations, 160
- vortex lattice, 151
- vortex lattice melting, 160
- vortex systems, 149
  
- water, 248
- weak interaction, 435
  
- yields of epithermal muons, 363
- $\text{YMn}_2$ , 124
  
- Zeeman energy, 249, 266
- zero point energy, 174

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Muons in Physics, Chemistry and Materials

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51st Scottish Universities Summer School in Physics

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The Scottish Universities Summer Schools in Physics have been held every year since 1960. The purpose of these schools is to contribute to the dissemination of advanced knowledge and the formation of contacts among scientists from different countries.

The lecturers at these schools are all international experts in their subject. Their brief is to present an up-to-date survey of current research in their own field in the form of a coherent series of lectures at a level suitable for students who are normally in their second or third postgraduate year.

Muon science is rapidly assuming a central role in scientific and technological studies of the solid state within the disciplines of physics, chemistry and materials science. This book is a collection of lectures delivered at SUSSP 51, the aim of which is to formalize and publicize recent key developments in both theoretical and experimental aspects of muon spin relaxation, rotation and resonance. The contributors are internationally renowned experts in muon instrumentation and applications of muon science, who cover topics which include: muon production; beamlines and instrumentation; muonium chemistry; muon catalysed fusion; fundamental muon physics; ultra-cold muons; magnetism; superconductivity; diffusion; semiconductors; simulations and data analysis. The book, which is aimed primarily at a graduate audience, assumes no prior expertise in muon science, and takes the reader through from introductory material to the latest developments in the field. Consistent notation and nomenclature are maintained throughout, with cross-referencing and continuity between the contributions. The book provides an excellent introduction to both new and experienced muon beam scientists wishing to develop their knowledge and understanding of the subject.

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