FirstPage

On "inverse Laplace transforms" as a mean of analyzing ^{8}Li spin-lattice relaxation

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Here we explore the use of inverse Laplace transforms (ILTs) as a means of analyzing spin-lattice relaxation (SLR) data obtained in ion-implanted ^{8}Li β-detected nuclear magnetic resonance (β-NMR) experiments. . . . The results are consistent with conclusions arrived at from a diligent "classical" analysis, but with significantly less effort and additional information. We anticipate this approach will be an indispensable complementary means of analyzing β-NMR SLR spectra, particularly in materials comprised of: multilayers, random disorder, or depth dependent properties.

I. INTRODUCTION sec:introduction

In the last few decades, ion-implanted β-detected nuclear magnetic resonance (β-NMR) has established itself as unique microscopic probe of condensed matter [1]. In many respects it is quite similar muon spin rotation/relaxation/resonance (μSR) [2, 3], with differences in the nuclear properties of the implanted probes making the two techniques complimentary rather than competitors [4].

The most common β-NMR probe ^{8}Li often exhibits multi-exponential relaxation, complicating analysis. Its high nuclear spin $I = 2$ is unique among (stable) nuclear magnetic resonance (NMR) nuclei, yielding fundamentally bi-exponential quadrupole relaxation [5–7]. In an experiment, especially in complex materials, it is not known beforehand if the multi-exponential polarization transients are due to: multiple ^{8}Li stopping sites with distinct T_1s; quadrupolar relaxation at a single site; a distribution of relaxation times; or combinations of the above possibilities. In such cases, extreme care is required during the analysis when selecting a model to describe the data. The same is especially true for the interpretation. Both may be tackled through due diligence and exhaustive testing, but the process is hardly expedient. It has therefore been desirable to have complementary means of addressing these uncertainties (e.g., what is the *distribution* of T_1). To this end, we explore the use of inverse Laplace transforms (ILTs) as an alternative approach to analyzing ^{8}Li β-NMR spin-lattice relaxation (SLR) data.

Recall that ILTs are useful when considering a signal that has the form:

$$y(t) = \int_0^\infty p(\lambda) \exp(-\lambda t)\, \mathrm{d}\lambda, \qquad (1)$$ eq:signal-integral

where λ is the relaxation rate and $p(\lambda)$ is its amplitude or probability density. The implicit goal of the analysis is to determine $p(\lambda)$, which can, in principle, be obtained by taking the ILT of the transient $y(t)$:

$$p(\lambda) = \frac{1}{2\pi\imath} \int_{c-\imath\infty}^{c+\imath\infty} y(t) \exp(\lambda t)\, \mathrm{d}t, \qquad (2)$$ eq:ilt

where c is a real constant.

Evaluating the integral in Equation (2), sometimes referred to as the Bromwich integral, is straightforward so long as $y(t)$ is known analytically; however, *this is almost never the case in experimental science*! **See review on exponential analysis for more details [8].** Pragmatically, $p(\lambda)$ can only be found through solving Equation (1). Note that Equation (1) is a member of the more general class of Fredholm integral equations of the first kind. These integrals are known to be "ill", "incorrectly", or "improperly" posed. That is, the solution $p(\lambda)$ obtained on solving Equation (1) may not be unique or even exist!

To deal with this **. . . more needed here!** At this juncture, it is worth mentioning that using the term "ILT" is somewhat inappropriate language, as discussed in detail elsewhere [9]. Nevertheless, we preserve the nomenclature for consistency with the NMR literature.

The use of ILTs is not uncommon in conventional NMR, particularly when investigating environments of inherent complexity (e.g., in porous materials or petroleum deposits).

The goal of this paper is to describe how to perform the ILT on discretized and reasonably noisy data. The SLR measurements produced by implanted-ion β-NMR serve as a good candidate for demonstrating the functionality of the method described here. The scatter in the data are largely statistical, and are typically well-described via Poisson statistics. That said, they are inhomogeneous in time, resulting from a necessary pulsing of the ion beam. The SLR is observed in the histogrammed arrival times of the betas emitted from the implanted ^{8}Li$^+$. The nuclear lifetime of the ^{8}Li determines how the signal statistics vary with time, which in turn fixes the observable window of the SLR to about 15 s. While this restricts the upper bound of the observable λ, the lower bound is set by the size of the histogram bins, typically chosen to be 10 ms (a factor of ∼120 smaller than the nuclear lifetime). In summary, the range of

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accessible λ is known; the errors represent a well-defined, but rather general case; and there are many β-NMR measurements in extremely well-studied classes of materials, for which the relaxation function is known.

The rest of the paper is organized as follows: in Section II we outline the details of the "ILT" analysis, including some particulars to β-NMR SLR data; results from the approach are presented in Section III, followed by a discussion in Section IV. Finally, a concluding summary is given in Section V.

II. THEORY

A. β-NMR Relaxation

In a β-NMR experiment, the experimental observable is the β-decay asymmetry $A(t)$, measured by the normalized difference in counting rates between two opposing detectors N_i (see e.g., [1, 10]). Because of the parity violation in β-decay, $A(t)$ is proportional to nuclear spin-polarization $P(t)$ of the β-emitting probes. That is,

$$A(t) = A_0 P(t), \tag{3}$$

where the proportionality factor A_0 the depends on the details of the β-decay and the geometry of the experiment. The quantity of real interest is $P(t)$, whose temporal behaviour is connected with the fundamental properties of the host material.

In order to introduce the β-NMR probes in a host material of interest, they are ion-implanted using a direct current (DC) beam for a finite period of time Δ, typically on the order of few seconds. On arrival, each β-NMR probe interacts with electromagnetic fields inside the host and relaxes (i.e., re-orients); however, not all probes arrive at the same time, which must be accounted for. For probes arriving at time t' during a beam pulse of duration Δ and decaying at a later time t, the time dependence of $P(t)$ can be written as [11, 12]

$$P(t) = P_0 \frac{\int_0^{\xi} \exp\left[-(\xi - t')/\tau_\beta\right] R(t,t')\, \mathrm{d}t'}{\int_0^{\xi} \exp\left[-t'/\tau_\beta\right]\, \mathrm{d}t'}, \tag{4}$$

where $\xi = t$ if $t \leq \Delta$ and $\xi = \Delta$ otherwise, P_0 is the degree of polarization at $t = 0$, and $R(t,t')$ is the relaxation function.

The simplest form for $R(t,t')$ is a single decaying exponential:

$$R(t,t') = \exp\left[-\lambda (t - t')\right], \tag{5}$$

where $\lambda \equiv 1/T_1$ is the SLR rate. Quite generally, however, $R(t,t')$ can be written as a superposition of decaying exponentials, according to a distribution $p(\lambda)$ of the SLR rates. This is quite analogous to Equation (1). In practice, spectra are often well-described (at the level of phenomenology) by a stretched exponential:

$$R_{\mathrm{KWW}}(t,t') = \exp\left\{-\left[\lambda (t - t')\right]^{\beta}\right\}, \tag{6}$$

where $0 < \beta \leq 1$ is the stretching exponent. This form of $R(t,t')$ can arise when λ is distributed according to the Kohlrausch-Williams-Watts (KWW) distribution [13–17]. The special cases of $\beta = 1/2$ [18, 19] and $\beta = 1/3$ [20] originate from SLR that is inhomogenously averaged in the three-dimensional (3D) and two-dimensional (2D) limits respectively. The approach is often used in conventional solid-state NMR [21], though chiefly as an expedient simplification of the multi-exponential magnetization transients, particularly when quadrupolar interactions are present [22].

While the KWW distribution is successful at describing a great deal of relaxation phenomena, it is hardly the simplest distribution to work with. In fact, it may be a little *too* successful: the high degree of correlation between λ and β allows Equation (6) to do a good job in fitting relaxation spectra whose underlying $p(\lambda)$ may be much simpler (e.g., a biexponential). This ease of use may disguise the proper relaxation function and lead to an incorrect interpretation of the relaxation mechanism. It is clear that a method is needed to identify the nature of the SLR, and solve for the underlying distribution of relaxation functions.

B. Solving for the Distribution

We now describe how the ILT method may be used to determine $p(\lambda)$, revealing the underlying distribution of exponentials. To start, we discretize t and λ, choosing Equation (5) as the fundamental relaxation function, out of which we will construct superpositions:

$$R(t_i, t'; \lambda_j) = \exp\left[-\lambda_j (t_i - t')\right]. \tag{7}$$

The asymmetry $A(t)$ may be written in matrix form,

$$\mathbf{A} = K\mathbf{p}, \tag{8}$$

where $\mathbf{p}$ is a vector weighting each of the $R(t_i, t'; \lambda_j)$, and K is the kernel matrix composed of these functions:

$$K_{ij} = A_0 P(t_i; \lambda_j). \tag{9}$$

The solution of Equation (8) satisfies

$$\arg\min_{\mathbf{p}\geq 0} ||\Sigma (K\mathbf{p} - \mathbf{y})||^2, \tag{10}$$

where Σ is a diagonal matrix of the reciprocal uncertainties, and $\mathbf{y}$ is the measured asymmetry.

While easily identified as a simple weighted least-squares problem, the number of degrees of freedom present in $\mathbf{p}$ make the problem ill-defined: with only a small amount of random error in $\mathbf{y}$, the matrix inversion is unstable, and many choices of $\mathbf{p}$ provide good candidates for the minimization of Equation (10). *Regularization* is often introduced to increase the stability of the inversion. This can done through the addition of a penalty term with a scale factor α. With this modification, Equation (10) becomes

$$\arg\min_{\mathbf{p}\geq 0} ||\Sigma(K\mathbf{p}_\alpha - \mathbf{y})||^2 + \alpha^2 ||\mathbf{p}_\alpha||^2. \tag{11}$$

Equation (11) is commonly known as Tikhonov regularization [23] or ridge regression. Effectively, the added term $\alpha^2||\mathbf{p}_\alpha||^2$ seeks to prevent the coefficients in $\mathbf{p}_\alpha$ from adopting large values without incurring a penalty. Pragmatically, this has the effect that, when $\alpha = 0$, $\mathbf{p}$ is likely to contain elements that are either very large or zero, such that the solution resembles a collection of delta functions. Conversely, when $\alpha = \infty$, it forces the elements of $\mathbf{p}$ to zero, as $\alpha^2||\mathbf{p}_\alpha||^2$ is the dominant contribution to Equation (11). As α grows, it tends to broaden the peaks present in $\mathbf{p}_\alpha(\lambda)$, smoothing the distribution. Therefore, the solution depends greatly on the choice of α, which is not known a priori and must be determined for a meaningful result. An "optimum" regularization parameter $0 \leq \alpha_{\text{opt}}$ exists which balances the degree of error introduced by the smoothing of $\mathbf{p}_\alpha(\lambda)$, with the scatter present in $\mathbf{y}$. Once an optimal value of α has been chosen, Equation (11) can be solved straightforwardly using a non-negative least squares (NNLS) optimization [24].

C. Optimizing Regularization

There are many approaches to find α_{opt} [25, 26]. In this section we briefly highlight three of the most common, neglecting the Butler-Reeds-Dawson [27] and the "the discrepancy principle" [28]. These methods rely on an estimation of the global random error in the data, a task made extraordinarily difficult the intrinsically inhomogeneous statistical errors of β-NMR SLR. **Is this the same as the "the discrepancy principle" [28]? It is possible this approach may work? See Eqs. (7.9)–(7.10) on pp. 180–181 in [29].** BRD seems to be the same as DP.. but I'm a little unclear. The approach in 29 seems to be the save as GCV. This is in contrast to, for example, an inversion-recovery NMR experiment, where the level of noise can be determined, in principle, by turning off the RF amplifier. Because of this, we will limit the discussion to methods independent of an a priori estimation of the error: the "S-curve" method, the "L-curve" method, and generalized cross validation (GCV). In general, the goal of all three can be simplified as finding the largest value of α, thereby producing the most smoothing, while maintaining a high fitting quality.

The S-curve method is perhaps the simplest and most intuitive of the three. Define the residual norm as

$$\chi(\alpha) = ||\Sigma\,(K\mathbf{p}_\alpha - \mathbf{y})\,||_2. \tag{12}$$ {eq:chi}

Generally, χ is relatively insensitive to small values of α; therefore, a good choice of α may be when χ starts to increase rapidly. Choosing some tolerance beforehand, a small χ can be maintained by choosing the minimum α which satisfies

$$\left.\frac{\mathrm{d}\log\chi}{\mathrm{d}\log\alpha}\right|_{\alpha_{\min}} > \text{tol}, \tag{13}$$ {eq:L-opt}

where $0 < \text{tol} < 1$ [30]. A reasonable choice of the tolerance for β-NMR is ~0.1.

The L-curve analysis aims to find a balance between the solution norm ($\eta(\alpha) = ||\mathbf{p}_\alpha||_2$) and the residual norm (Equation (12)). This balance between the smoothing and fit quality, and therefore α_{opt}, is found in the "corner" of the L-curve. Numerically, one can reasonably estimate the position the corner by using the point of greatest curvature:

$$\max_{\alpha\geq 0}\kappa(\alpha) = \frac{\eta'\chi'' - \chi'\eta''}{(\eta'^2 + \chi'^2)^{3/2}}, \tag{14}$$

where the derivatives are taken with respect to α. However if the curvature is slight, then the curvature method tends to find values of α for which χ is too large. To resolve this the following "balanced" method reproduces the corner for highly curved L-curves, as well as for cases when the curvature is small:

$$\min_{\alpha\geq 0}\chi^2\eta, \tag{15}$$

where the exponent is empirically determined.

The GCV approach attempts to find the α which produces the best regularized pseudo-inverse kernel matrix, as defined by $\mathbf{p}_\alpha = K^\#\mathbf{y}$ [31]. The quality of $K^\#$ increases with α, and therefore must be tempered with the residual norm, such that α_{opt} satisfies:

$$\min_{\alpha\geq 0} G(\alpha) = \frac{\chi^2}{\text{Tr}\left[I - KK^\#\right]}. \tag{16}$$ {eq:gcv}

For the case of Tikhonov regularization, as considered here, $K^\# = \left(K^TK + \alpha^2 I\right)^{-1}K^T$ [30]. We note the existence of an alternative method for cases when K is large [32]. Finding α_{opt} using this method can be difficult as $G(\alpha)$ is generally quite flat.

III. RESULTS {sec:results}

We apply the procedure outlined in the previous section to both real β-NMR data, and to data generated by Monte Carlo (MC) simulation.

IV. DISCUSSION {sec:discussion}

V. CONCLUSION {sec:conclusion}

We have shown . . . We feel this method of analysis will be particularly useful when studying materials of inherent complexity, such as: heterostructures and multilayers; glassy and disordered systems; or any sample with depth-dependent properties.

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Appendix A: Miscellaneous

sec:miscellaneous

discussion of pitfalls [33].
L-curve regularization [34, 35]. An earlier example [36]?
Nice high-level article [37].
bridge vs. lasso regularization methods [38].
[39].
Review of ILTs in noisy NMR data [40].
Discussion of what exactly are ILTs [9].
(see e.g., the classic textbook on the subject [24]).
see also fairly recent multiexponential analysis review [8] and numerical recipes [41].
A recent, long review on regularization methods [42].
Triangle method for finding the corner of the L-curve [43].
Example of using weights like we do [44].
Some papers mention application to muons [45].
People are still writing theses on regularization (see e.g., [46]).
Paper with explicit re-casting of the equations being solved [47] — good to check against our implementation.
Another book by an authority on the topic [29].

Appendix B: Implementation

sec:implementation

The NNLS algorithm solves equations of the form $L\mathbf{p} = \mathbf{z}$. The minimization Equation (11) is accomplished using the following transformation of variables:

$$L = \begin{pmatrix} \Sigma K \\ \Gamma \end{pmatrix} \qquad \mathbf{z} = \begin{pmatrix} \Sigma \mathbf{y} \\ \mathbf{0} \end{pmatrix}, \tag{B1}$$

where K is defined by Equation (9), Σ is the diagonal matrix of reciprocal uncertainties, and Γ is the regularization matrix. In general, the choice of Γ is general, however in this work we define $\Gamma \equiv \alpha I$. It is trivial to then show that

$$||\mathbf{z} - L\mathbf{p}||^2 = ||\Sigma(\mathbf{y} - K\mathbf{p})||^2 + ||\Gamma\mathbf{p}||^2. \tag{B2}$$

The NNLS optimization was performed via widely used Fortran subroutines [24], as implemented in Python, with the aid of the common scientific computing packages NumPy [48], SciPy [49], Matplotlib [50], and Pandas [51].

Appendix C: β-NMR Data Simulation

sec:datasim

MC simulation was used to generate data sets where the underlying polarization function is fully known and absent of any distortion or artifacts due to technical considerations. Differences in detector geometry and placement, implantation rate, polarization effectiveness, and helicity all may be sources of distortion in the data. The probability that an electron is emitted at angle θ from the forward direction given by[52]

$$W(t, \theta) = 1 + \frac{v}{c} A P(t) \cos(\theta) \tag{C1}$$

eq:decay_direction

where v is the velocity of the emitted electron, c is the speed of light, $P(t)$ is the single particle polarization at time t after implantation, and A is the intrinsic beta-decay asymmetry unique to the nuclear species. For ^{8}Li, $A = -1/3$[53].

The implantation energies are uniformly distributed from 0 to Δ, as defined in Equation (4). The decay times are exponentially distributed and the sum of the two is the beta detection time. The electron velocity arises from the distribution of decay energies [54]. Thus, Equation (C1) can be used to calculate the decay direction, and if $3\pi/2 < \theta$ or $\theta < \pi/2$ then the particle is said to be detected by the forward detector, and otherwise it interacts with the backward detector. In this sense, the detectors "work" with perfect efficiency and coverage. The MC simulation is implemented using C++ and ROOT [55], and the permuted congruential generator (PCG) random number generator.

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