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What are, and what are not, Inverse Laplace Transforms

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Abstract

Time-domain NMR, in one and higher dimensionalities, makes routine use of inversion algorithms to generate results called "T_2-distributions" or joint distributions in two (or higher) dimensions of other NMR parameters, T_1, diffusivity D, pore size a, etc. These are frequently referred to as "Inverse Laplace Transforms" although the standard inversion of the Laplace Transform long-established in many textbooks of mathematical physics does not perform (and cannot perform) the calculation of such distributions. The operations performed in the estimation of a "T_2-distribution" are the estimation of solutions to a Fredholm Integral Equation (of the First Kind), a different and more general object whose discretization results in a standard problem in linear algebra, albeit suffering from well-known problems of ill-conditioning and computational limits for large problem sizes. The Fredholm Integral Equation is not restricted to exponential kernels; the same solution algorithms can be used with kernels of completely different form. On the other hand, (true) Inverse Laplace Transforms, treated analytically, can be of real utility in solving the diffusion problems highly relevant in the subject of NMR in porous media.

Keywords: T_2-distribution, Laplace Transform, Inverse Laplace Transform, Fredholm Integral Equation

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1. Introduction

Low-resolution NMR (with limited spectral resolution) concentrates on relaxation parameters such as $T_{1,2}$ or diffusivity D_0. Such measurements are ubiquitous in the study of porous media, either for themselves or for derived parameters such as pore size a which may be based on measurements of the relaxation or diffusion parameters. In such applications, spectral resolution (along a frequency axis, for NMR chemical shift δ) is typically absent. In many systems on which such data are acquired, the inhomogeneity of the static field B_0 available may exceed the dispersion in chemical shift δ, and thus dominate any information in principle available from δ. The basic data acquired in a NMR experiment are almost always quadrature-detected transverse magnetization in the time domain:

$$S(t) = M_x(t) + \mathrm{i}M_y(t) + e_{\mathrm{noise}}(t) \tag{1}$$

where $e_{\mathrm{noise}}(t)$ represents a (complex) time-dependent noise process which can never be wholly disregarded. In chemical spectroscopy the use of the Fourier Transform to display information in the conjugate frequency domain is ubiquitous; a (complex) spectrum in (cyclic) frequency ν is obtained from signal $S_{\mathrm{F}}(t)$ (typically a Free Induction Decay) as

$$\mathcal{S}(\nu) = \int_{-\infty}^{\infty} S_{\mathrm{F}}(t)\, \mathrm{e}^{-2\pi\mathrm{i}\nu t}\, \mathrm{d}t \tag{2}$$

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Whether the forward or inverse Fourier Transform is used is (almost) immaterial because of the (near) symmetry between the forward and inverse transforms. The spectrum $\mathcal{S}(\nu)$ may be understood as the relative weights of individual complex sinusoids $\mathrm{e}^{+2\pi\mathrm{i}\nu t}$ in an expansion of the measured signal $S_{\mathrm{F}}(t)$:

$$S_{\mathrm{F}}(t) = \int_{-\infty}^{\infty} \mathcal{S}(\nu)\, \mathrm{e}^{+2\pi\mathrm{i}\nu t}\, \mathrm{d}\nu \tag{3}$$

Equations (2) and (3) are related by the Fourier Integral Theorem; $S_{\mathrm{F}}(t)$ and $\mathcal{S}(\nu)$ conveniently form a Fourier Transform pair. The use of cyclic frequency ν rather than angular frequency $\omega = 2\pi\nu$ conforms to experimental practice and conveniently results in unit normalization factors in both (2) and (3). Practical data processing uses the widely-available FFT algorithm. With quadrature detection (complex $S(t)$) a sense of rotation is distinguishable so negative frequencies are well-defined and the doubly-infinite integration range in (3) makes sense, even if experimental $S(t)$ is zero for $t < 0$ in (2).

Where relaxation parameters are of primary interest, the universal practice is the estimation of a T_2-distribution i.e. the relative weightings of exponential decays of the form $\exp(-t/T_2^{(i)})$:

$$S_{\mathrm{C}}(t_n) = \int_{0}^{\infty} \mathcal{P}(T_2)\, \mathrm{e}^{-t_n/T_2}\, \mathrm{d}T_2 \tag{4}$$

Here several things are changed. Typically the signal $S_{\mathrm{C}}(t_n)$ is derived from the peaks of an echo train at discrete t_n; the actual echo shapes may retain some spectral information but in this archetype are not analysed. The data the integration range starts at $T_2 = 0$ because negative relaxation times are entirely unphysical; finally the kernel function has changed from a complex to a real exponential. The desired data representation is $\mathcal{P}(T_2)$, and clearly a solution to equation (4) is required. Because the Laplace Transform $F(s)$ of some function $f(x)$ is defined by the integral:

$$F(s) = \int_{0}^{\infty} f(x)\, \mathrm{e}^{-sx}\, \mathrm{d}x \tag{5}$$

to which equation (4) has a superficial similarity, many authors in the NMR of porous media describe the solution $\mathcal{P}(T_2)$ to equation (4) as an "Inverse Laplace Transform" (or "ILT") of $S(t)$ by analogy with the "(Inverse) Fourier Transform" of equation (2). The terminology has been widely followed in many research papers in the NMR of porous media, e.g. [1, 2] and authoritative texts [3]. However, although $S_{\mathrm{F}}(t)$ and $\mathcal{S}(\nu)$ are a (valid) Fourier Transform pair, we show below that $S_{\mathrm{C}}(t_n)$ and $\mathcal{P}(T_2)$ cannot similarly be treated as a Laplace Transform pair. Moreover, actual Inverse Laplace Transforms are of genuine use in the theory of diffusion (and elsewhere). We thus find, within the field of NMR in porous media, the same name used for two entirely different mathematical objects. This paper therefore offers some pointers as to what are, and what are not, Inverse Laplace Transforms.

2. Changes of variable

The near-universal practice of presenting results on a logarithmic T_2 axis is useful for systems where relaxation times may span several decades in size; however this is simply a change of variables. If $\mathcal{P}_{\mathrm{lin}}(T_2)\,\mathrm{d}T_2$ is the fraction of the total signal with relaxation times between T_2 and $T_2 + \mathrm{d}T_2$, and we define $y = \log_{10} T_2$, and $\mathcal{P}_{\mathrm{log}}(y)\,\mathrm{d}y$ as the fraction of total signal with $\log_{10} T_2$ between y and $y + \mathrm{d}y$, then clearly $\mathcal{P}_{\mathrm{lin}}(T_2)\,\mathrm{d}T_2 = \mathcal{P}_{\mathrm{log}}(y)\,\mathrm{d}y$, and thus

$$\mathcal{P}_{\mathrm{log}}(\log_{10} T_2) = T_2 \log_{\mathrm{e}} 10\, \mathcal{P}_{\mathrm{lin}}(T_2) \tag{6}$$

so the two distributions are simply related and one determines the other. Rarely performed, but useful for the discussion in this paper, is the related distribution $\mathcal{P}_{\mathrm{rate}}(R_2)$ of relaxation *rates* $R_2 = 1/T_2$. Similarly to the above, if $\mathcal{P}_{\mathrm{rate}}(R_2)\,\mathrm{d}R_2$ is the fraction of signal with $1/T_2$ between R_2 and $R_2 + \mathrm{d}R_2$, then $\mathcal{P}_{\mathrm{lin}}(T_2)\,\mathrm{d}T_2 = \mathcal{P}_{\mathrm{rate}}(R_2)\,\mathrm{d}R_2$ and so

$$\mathcal{P}_{\mathrm{rate}}(R_2) = -T_2^2 \mathcal{P}_{\mathrm{lin}}(T_2) \tag{7}$$

Hence $\mathcal{P}_{\text{rate}}(R_2)$, $\mathcal{P}_{\text{lin}}(T_2)$ and $\mathcal{P}_{\text{log}}(\log_{10} T_2)$ are all different representations of the same distribution, based on the same kernel $\exp(-t/T_2)$. We may thus write equation (4) as

$$S(t) = \int_0^\infty \mathcal{P}_{\text{rate}}(R_2)\, \mathrm{e}^{-R_2 t}\, \mathrm{d}R_2 \tag{8}$$

and if $\mathcal{P}_{\text{rate}}(R_2)$ is determined as a solution of equation (8), then $\mathcal{P}_{\text{lin}}(T_2)$ and $\mathcal{P}_{\text{log}}(x)$ are similarly determined by the appropriate change of variables. The lower limit should strictly be adjusted to reflect the physical fact that bulk relaxation processes impose a floor on relaxation *rate* at $R_{2\text{B}} = 1/T_{2\text{B}}$.

Writing $S(t)$ in the form of equation (8) makes as clear as possible the potential analogy between $S(t)$ and the Laplace Transform (5). We examine this further below.

3. Laplace Transforms and their relation to Fourier Transforms

The Laplace Transform $F(s)$ of a function $f(x)$ is generally defined by the integral in (5). In elementary texts (e.g. [4], Ch23 p449 Eq1), $F(s)$ may be regarded as a function of a real variable s, the typical application being the formal solution of differential equations.

In more advanced texts, e.g. [5–7], $F(s)$ is regarded as a function of a *complex* variable s, which reveals the relation between the Fourier and Laplace transforms. The Laplace transform is introduced in [6] as a means of accommodating functions whose Fourier Transforms do not exist, because the defining integral (2) diverges. Elementary examples cited are $f(x) = x^2$, and even $f(x) = \text{const}$. The defining integral is in principle defined on $(-\infty, +\infty)$ (the "bilateral" Laplace Transform) [8]; however for dynamical systems, where x is physical time, causality requires impulse or step responses to be zero for $x < 0$, restricting attention to functions of the form $f(x)H(x)$ where $H(x)$ is the Heaviside function. This results in the more familiar "unilateral" Laplace Transform (5) where divergent behaviour as $x \to -\infty$ does not prevent convergence of the integral. Divergences arising as $x \to +\infty$ are removed by introducing a "convergence factor" e^{-cx} for real $c > \alpha$, where α is some positive parameter, the only purpose of which is to ensure convergence. The function $f(x)\mathrm{e}^{-cx}H(x)$ then possesses a Fourier transform even if $f(x)$ does not:

$$\mathcal{F}(\omega) = \int_0^\infty f(x)\, \mathrm{e}^{-cx}\, \mathrm{e}^{-\mathrm{i}\omega x}\, \mathrm{d}x = \int_0^\infty f(x)\, \mathrm{e}^{-sx}\, \mathrm{d}x \tag{9}$$

defining the *complex* Laplace variable $s = c + \mathrm{i}\omega$. The Fourier Transform $\mathcal{F}(\omega; c > \alpha)$ of the modified function $f(x)H(x)\mathrm{e}^{-cx}$ is seen to be the Laplace Transform $F(s)$ of $f(x)$, as defined in (5), with s regarded as a complex variable.

The Fourier Integral Theorem can now be applied to derive the Inverse Laplace Transform:

$$f(x) = \frac{1}{2\pi\mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} F(s)\, \mathrm{e}^{+sx}\, \mathrm{d}s \tag{10}$$

with $f(x) = 0$ for $x < 0$. This is a contour integral of the complex function $F(s)\,\mathrm{e}^{sx}$, along any line $\Re(s) = c = \text{const}$ for $c > \alpha$, where α is a minimum "convergence factor" dependent on the nature of $f(x)$. This contour integral, of an analytic function $F(s)\mathrm{e}^{sx}$ of a complex variable s, is the (true) Inverse Laplace Transform as given in the standard texts e.g. [5–7].

4. Evaluating Inverse Laplace Transforms

The result (10) is not of use unless the integral can be evaluated. Closed contours enable an appeal to Cauchy's Theorem, so theoretical approaches generally close the contour by a large semicircle in the region $\Re(s) < 0$ and allowing the radius R to proceed to $R \to \infty$. This is often called the "Bromwich contour" after its introduction in [9]. Completion of the contour in $\Re(s) < 0$ is necessary for $x > 0$, so that e^{sx} vanishes as $R \to \infty$; the contribution of the completion semicircle to (10) also then vanishes. But $F(s)$ is only defined by (5) for $\Re(s) = c > \alpha$. However the process of "analytic continuation" allows us to extend the domain of definition of a function of a complex variable by means of power series in contiguous or overlapping circles of convergence, except possibly at *singularities* of the function $F(s)\mathrm{e}^{sx}$. The "calculus of residues" then evaluates the ILT if the residues of all poles or isolated essential singularities of $F(s)\mathrm{e}^{sx}$ can be evaluated. Such methods are described in texts on complex analysis e.g. [10], and depend on $F(s)$ being known analytically in the complex plane. For the common case where $F(s) = g(s)/h(s)$ with $g(s)$ analytic and non-zero at all singularities s_n, the singularities of $F(s)\mathrm{e}^{sx}$ are poles corresponding to the zeroes of the denominator $h(s)$. The residue theorem yields the Inverse Laplace Transform as

$$f(x) = \sum_n \mathrm{e}^{s_n t} \frac{g(s_n)}{h'(s_n)} \tag{11}$$

where $h'(s) = \mathrm{d}h/\,\mathrm{d}s$. In diffusion problems, the singularities typically occur for s_n real and negative. The ILT then yields a discrete set of real exponential decays, with amplitudes found by a simple differentiation, after locating the singularities, where $h(s_n) = 0$. A specific example is given later.

Where $F(s)$ is known numerically along some line $\Re(s) = c$, then the relationship of $F(s)$ to the Fourier Transform can be exploited:

$$f(x) = \frac{\mathrm{e}^{cx}}{2\pi} \int_{-\infty}^{+\infty} F(c + \mathrm{i}\omega)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}\omega \tag{12}$$

which is seen to be an Inverse *Fourier* Transform amenable to numerical evaluation by the FFT algorithm.

Remarkably, knowledge of $F(s)$ for complex s is not always necessary. Several algorithms are known for estimation of $f(x)$, given knowledge of $F(s)$ along the positive real axis only. A popular method is the Stehfest algorithm [11, 12] which estimates $f(x)$ at $x = X$ by

$$f(X) \simeq \frac{\log_\mathrm{e} 2}{X} \sum_{n=1}^{N} V_n F(s_n) \tag{13}$$

where $F(s)$ is known at N discrete points s_n along the real s axis:

$$s_n = \frac{\log_\mathrm{e} 2}{X} n \qquad n = 1, \ldots N \text{ (even)} \tag{14}$$

and the coefficients V_n are given by

$$V_n = (-1)^{N/2+n} \sum_{k=[(n+1)/2]}^{\min(n,N/2)} \frac{k^{N/2}(2k)!}{(N/2-k)!k!(k-1)!(n-k)!(2k-n)!} \tag{15}$$

Note that each value of $x = X$ requires a different sampling of s_n along the real axis. The relationship between (13) and the general contour formula (10) is entirely non-trivial; an outline is found in [13] and [11]. The Stehfest algorithm is powerful for estimating $f(x)$ numerically when $F(s)$ is known to arbitrary precision for real s; in practice this means an analytical expression for $F(s)$. It is not useful when the estimates of $F(s)$ at the discrete points $s_n = n \log 2/X$ are contaminated by noise, or large rounding or truncation errors.

The above methods cover (a) wholly analytical evaluation of $f(x)$ (for $x > 0$), where $F(s)$ is known analytically in the complex plane (b) numerical evaluation of $f(x)$ from numerical data for $F(s)$ along lines $\Re(s) = \text{const}$, and (c) numerical evaluation of $f(x)$ given an analytical expression for $F(s)$ for real s ($\Im(s) = 0$). Relevant regions of the complex plane are shown in Figure 1.

5. Are T_2-distributions ILTs ?

Are any of the above methods of evaluation of ILTs of value in evaluating T_2-distributions ? Comparison between (8) and (5) reveals a problem: although the kernel function $\mathrm{e}^{-R_2 t}$ is of the required form, integration

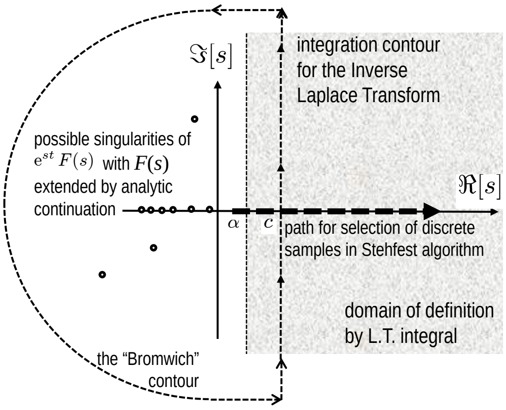

Figure 1: Domain of definition for Laplace Transforms, and contours for Inversion.

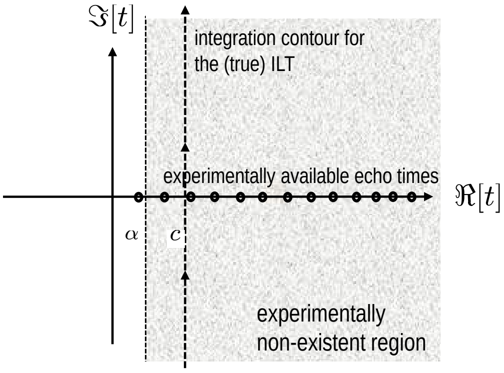

Figure 2: Experimental echo times nt_e where $S(t)$ is regarded as a (forward) Laplace Transform.

is over R_2, not t. Thus experimental time t in (8) corresponds to the Laplace variable s in (5), not to the independent variable x. Treating s as experimental time t creates a contradiction: s is required in general to be complex, but “complex time” has no physical meaning. There is no possibility of measuring $S(t)$ for other than real t.

We thus see that methods (a) and (b) above are out of the question for evaluation of $\mathcal{P}(R_2)$ as an ILT; the necessary data for “complex time” t can never exist. This is illustrated in Figure 2.

Nevertheless, given experimental echoes $S_\mathrm{C}(t)$ at times $t = n_\mathrm{e}t_\mathrm{e}$, is it possible to use methods of type (c), such as the Stehfest algorithm, for evaluating $\mathcal{P}(R_2)$? This requires knowledge of $F(s)$ only for $\Re(s) > \alpha$. There are several problems: (i) the required sampling points s_n do not necessarily correspond to the experimental points $n_\mathrm{e}t_\mathrm{e}$; (ii) different sampling of $F(s_n)$ is required for different values of X; hence interpolation of the experimental $S_\mathrm{C}(n_\mathrm{e}t_\mathrm{e})$ is always required. Finally, (iii) $S_\mathrm{C}(t)$ is never known to arbitrary accuracy because of the presence of measurement noise $e_\mathrm{n}(t)$, as in (1). Conditions for application of the Stehfest algorithm are not satisfied. Moreover its relationship with (10) remains unclear if $S_\mathrm{C}(t)$ is undefined except for real t; there is no “ϵ-neighbourhood” within which to define an analytic function S, of complex t, for any point on the real t axis.

We conclude that none of $\mathcal{P}_\mathrm{rate}(R_2)$, $\mathcal{P}_\mathrm{lin}(T_2)$, nor $\mathcal{P}_\mathrm{log}(\log_{10} T_2)$, can be regarded as ILTs of $S_\mathrm{C}(n_\mathrm{e}t_\mathrm{e})$.

6. Fredholm Integral Equations

Many books discuss the most general *linear* integral equation in an unknown $f(x)$:

$$\lambda \int_a^b K(x,y) f(y)\,\mathrm{d}y + g(x) = h(x) f(x) \tag{16}$$

where λ is a parameter, $g(x)$ and $h(x)$ are given functions, and the function $K(x,y)$ is known as the *kernel* (or in older texts [14], the *“nucleus”*). “Volterra” equations have $K(x,y) = 0$ for $y > x$ and are usually convertible to ODE’s. “Fredholm” equations have general $K(x,y)$. “First Kind” equations have $h(x) \equiv 0$; “Second Kind” equations have $h(x) \equiv 1$. A “Fredholm integral equation of the First Kind” is therefore a *linear* integral equation in $f(x)$ of the general form:

$$\lambda \int_a^b K(x,y) f(y)\,\mathrm{d}y + g(x) = 0 \tag{17}$$

Hence (4) is seen to be a Fredholm integral equation of the First Kind, making the correspondences $(x,y) \to (t, \log_{10} T_2)$, with the kernel function

$$K(x,y) = \mathrm{e}^{-t/T_2} \tag{18}$$

and the unknown $f(y)$ corresponding to the distribution $\mathcal{P}_{\log}(\log_{10} T_2)$. The experimental data $S(t)$ correspond to the source term $-g(x)/\lambda$.

Because there is no limitation on the form of $K(x,y)$, the integral equation terminology applies immediately to related distributions of relaxation parameters, e.g. of T_1, or D, determined by various experimental methods, where the kernel function $K(x,y)$ is no longer a simple exponential decay as in (18). The integral equation framework is also generalizable immediately [15] to the multi-dimensional distributions in (T_1, T_2), (D, T_2) *etc*, which abound in studies of NMR in porous media.

With the functions $f(y)$ discretized as vectors f_j for practical computation, the first kind Fredholm equation becomes a matrix equation

$$\lambda K_{nm} f_m + g_m = 0 \tag{19}$$

where the index m runs over discretized values of T_2 (or $\log_{10} T_2$) and the index n runs over experimental echo times nt_e. All the apparatus of linear algebra is then available to guide the solution of (19). In general *Second* Kind equations tend to be more stable in numerical solution than First Kind equations because of the presence of f outside of the integral: $\lambda K f = f - g$. The "First Kind" qualifier is therefore relevant, because of the well-known ill-conditioned behaviour of solutions of (4) with exponential kernels. What is meant by ill-conditioned in this context is that the vectors $k_n(y) = K(t_n, \log_{10} T_2)$ are "almost linearly dependent" such that the matrix

$$G_{nm} = \int_{y_a}^{y_b} k_n(y) k_m(y)\, \mathrm{d}y \quad n, m = 1, \ldots N \tag{20}$$

of dimension N^2 over N data points, is "almost" singular.

7. Evaluating T_2-distributions, and other Integral Equations

Irrespective of terminology, the principal difficulty in practical solution is the ill-conditioned nature of the numerical task. The usual strategy is regularization, discussed in many sources e.g. [15–17], the review [17] outlining other strategies also. Similar problems of course occur in many fields other than NMR and general texts on regularisation include [18–20]. Regularization is available even when the problem is generalized to multi-dimensional distributions of T_1–T_2, or D–T_2 [15].

Such methods and algorithms are entirely free from any requirement that the kernel be of the form (18). In [21], and elsewhere e.g. [22], they are used for the estimation of distributions of internal field gradients g_int, relaxivity-independent pore sizes a, and susceptibility contrasts $\Delta\chi$. In [23], we employ essentially the same methods to invert experimental data over recovery times t_1 and echo times nt_e for correlation times τ_c and quadrupolar coupling constants `QCC`, using a complicated kernel given in [23]. Such applications are all processed by algorithms reviewed in [17]. However they have lost even a passing resemblance to inversion of a Laplace Transform.

8. Inverse Laplace Transforms in the theory of diffusion

Theoretical work on diffusion in restricted geometries e.g. [24], [25] makes use of Laplace Transform methods, with actual Inverse Laplace Transforms to derive real time-dependent solutions. We illustrate this by a simple case taken from [26], one of the foundation papers for NMR in porous media. A slot-like pore geometry of size a is defined over position x in $[0, a]$, with one relaxing surface at $x = a$ (with relaxivity ρ), and a reflecting surface at $x = 0$. The governing equation for magnetization M is the diffusion equation $\partial M/\partial t = D\partial^2 M/\partial x^2$ subject to uniform initial conditions $M(x, 0) = M_0$ and boundary conditions $-D\partial M/\partial x = \rho M$ at $x = a$ and $\partial M/\partial x = 0$ at $x = 0$. Solving for $m(t) = M(t) - M_0$ involves homogeneous initial conditions (convenient for the forward Laplace Transform of time derivatives). With overbar denoting Laplace transforms with respect to time t and primes denoting $\mathrm{d}/\mathrm{d}x$, the transformed problem becomes the ODE

$$D\bar{m}'' - s\bar{m} = 0 \tag{21}$$

subject to $\bar{m}' = 0$ at $x = 0$ and $-D\bar{m}' = \rho\,(\bar{m} + M_0/s)$ at $x = a$. The solution satisfying these conditions is

$$\bar{m}(s) = \frac{-M_0 \beta \cosh qx}{s\,[\beta \cosh qa + qa \sinh qa]} \tag{22}$$

where $q = \sqrt{s/D}$ and $\beta = \rho a/D$ which is small in the "fast-diffusion" limit of [26]. This solution remains however in the s (transform) domain; a (true) Inverse Laplace Transform is required to convert back to the t (time) domain. This can be done using the calculus of residues as in equation (11) above. The even symmetry of the denominator in (22) ensures that there are no branch points. The singularities of $\bar{m}(s)$ occur at $s = 0$, and the zeroes of the denominator, i.e. the solutions s_n to

$$qa \tanh qa = -\beta \tag{23}$$

This has no solutions for s real and positive (real q), but for s real and negative (imaginary $qa = \mathrm{i}p$) the condition reduces to

$$p \tan p = +\beta \tag{24}$$

having roots $\pm p_n$. These correspond to the required singularities $s_n = -p_n^2 D/a^2$ of $\bar{m}(s)$. The ILT is then given by (11). Differentiating and evaluating the denominator at s_n we obtain the (true) ILT as:

$$\frac{M(t)}{M_0} = \sum_{n=1}^{\infty} \frac{2\cos(p_n x/a)}{\cos p_n + p_n/\sin p_n} \exp\left(-\frac{p_n^2 D}{a^2} t\right) \tag{25}$$

where we revert from $m(t)$ to $M(t)$ (the offset $-M_0$ cancels the residue of the pole at $s = 0$). Spatial averages over the eigenfunctions $\cos(p_n x/a)$ are $\sin p_n/p_n$, yielding the modal intensities

$$I_n = \frac{4\sin^2 p_n}{p_n\,[2p_n + \sin(2p_n)]} \tag{26}$$

The characteristic equation (24), the relaxation times $1/s_n$, and the intensities I_n are identical to those given in [26] (equations 13a–d), by the quite different method of separation of variables.

The Laplace Transform method has the advantage of avoiding potentially complicated quadratures needed in [26]. The (true) ILT in (25) requires only root-finding and a differentiation for a complete solution. Beyond this simple example, the LT method is powerful for exploration of the eigenvalue structure of the much more complicated problems discussed in [24, 25].

9. Conclusions

This paper reports no original research, and apart from the example in Sec. 8, rehearses only theory readily available in the standard texts. We show however that the terminology of "Inverse Laplace Transform", or "ILT", for the calculation of T_2 distributions, and their analogues and generalizations, cannot be rigorously sustained. Acquired NMR data $S_\mathrm{F}(t)$ and the spectrum $\mathcal{S}(\nu)$ do form a valid Fourier Transform pair; however $S_\mathrm{C}(t)$ and the T_2-distribution $\mathcal{P}(T_2)$ do not form a Laplace Transform pair. In the subject of NMR applications to porous media, "ILT" is nevertheless widespread for what is actually the regularized solution of a First Kind Fredholm integral equation. Moreover, the algorithms used in practice are applicable to a much wider class of integral equations than the exponential kernel case. Finally, true ILT's are powerful in the theory of bounded diffusion, as we illustrate by a simple re-derivation of basic results from a foundation paper [26].

Humpty Dumpty [27] held that a word "means just what I choose it to mean", so we fully expect the terminology "ILT" to remain widely used for the estimation of $\mathcal{P}(T_2)$ and its relatives. However Alice then questioned "whether you *can* make words mean so many different things", and this becomes harder to answer when actual ILT's are employed in the theory of bounded diffusion, similarly central to the subject of NMR in porous media. Using the same name ("ILT") for two entirely different things in the same subject cannot be conducive to clarity. We suggest that where brevity is required, a "numerical inversion" of equation (4) is non-specific as to method but avoids any misdirection.

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References

[1] P. Berman, O. Levi, Y. Parmet, M. Saunders, Z. Wiseman, Laplace inversion of low resolution NMR relaxometry data using sparse representation methods, Concepts in Magnetic Resonance A 42 (2013) 72–88.

[2] V. Bortolotti, R. J. S. Brown, P. Fantazzini, G. Landi, F. Zama, Uniform penalty inversion of two-dimensional NMR relaxation data, Inverse Problems 33 (1) (2016) 19.

[3] P. T. Callaghan, Translational dynamics and magnetic resonance, OUP, 2011.

[4] G. Stephenson, Mathematical methods for science students, Longman, 2nd edn., 1973.

[5] H. Jeffreys, B. S. Jeffreys, Methods of mathematical physics, CUP, 1956.

[6] J. Matthews, R. L. Walker, Mathematical methods of physics, Benjamin, 1970.

[7] G. Arfken, Mathematical methods for physicists, Academic Press, 1970.

[8] E. A. Faulkner, Introduction to the theory of linear systems, Chapman and Hall, 1st edn., 1969.

[9] T. J. I. Bromwich, Normal co-ordinates in dynamical systems, Proc. London Math. Soc. 2 (15) (1916) 401–448.

[10] E. C. Titchmarsh, Theory of functions, O.U.P., 1939.

[11] H. Stehfest, Numerical invesrion of Laplace transforms, Comm. ACM 13 (1) (1970) 47–49.

[12] H. Stehfest, Remark on Algorithm 368, Comm. ACM 13 (10) (1970) 624.

[13] D. P. Gaver, Observing stochastic processes, and approximate transform inversion, Operations Research 14 (3) (1966) 444–459.

[14] E. T. Whittaker, G. N. Watson, A course of modern analysis, C.U.P., 3rd edn., 1920.

[15] L. Venkataramanan, Y.-Q. Song, M. Hürlimann, Solving Fredholm Integrals of the First Kind with tensor product structure in 2 and 2.5 dimensions, IEEE Transactions on Signal Processing 50 (5) (2002) 1017–1026.

[16] E. J. Fordham, A. Sezginer, L. D. Hall, Imaging multi-exponential relaxation in the $(y, \log T_1)$ plane, with application to clay filtration in rock cores, Journal of Magnetic Resonance Series A 113 (1995) 139–150.

[17] J. Mitchell, T. C. Chandrasekera, L. F. Gladden, Numerical estimation of relaxation and diffusion distributions in two dimensions, Progress in Nuclear Magnetic Resonance Spectroscopy 62 (2012) 34–50.

[18] H. W. Engl, M. Hanke, A. Neubauer, Regularization of inverse problems, vol. 375 of *Mathematics and its Applications*, Kluwer, 1996.

[19] M. Bertero, P. Boccacci, Introduction to inverse problems in imaging, IOP Publishing, 1998.

[20] C. R. Vogel, Computational methdos for inverse problems, SIAM, 2002.

[21] M. D. Hürlimann, Effective gradients in porous media due to susceptibility differences, J. Magn. Reson. 131.

[22] R. T. Lewis, J. G. Seland, A multi-dimensional experiment for characterization of pore structure heterogeneity using NMR, J. Magn. Reson. 263 (2016) 19–32.

[23] J. Mitchell, E. Fordham, Sodium-23 NMR in porous media, Microporous and Mesoporous Materials (2017) In press.

[24] D. S. Grebenkov, NMR survey of reflected Brownian motion, Rev. Mod. Phys. 79 (2007) 1077–1135.

[25] S. D. Stoller, W. Happer, F. J. Dyson, Transverse spin relaxation in inhomogeneous magnetic fields, Phys. Rev. A 44 (11) (1991) 7459–7477.

[26] K. R. Brownstein, C. E. Tarr, Importance of classical diffusion in NMR studies of water in biological cells, Phys. Rev. A 19 (1979) 2446–2453.

[27] L. Carroll, Through the looking-glass, and what Alice found there, 1872.