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The Lorentz Integral Transform and its Inversion

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Abstract The Lorentz integral transform method is briefly reviewed. The issue of the inversion of the transform, and in particular its ill-posedness, is addressed. It is pointed out that the mathematical term *ill-posed* is misleading and merely due to a historical misconception. In this connection standard regularization procedures for the solution of the integral transform problem are presented. In particular a recent one is considered in detail and critical comments on it are provided. In addition a general remark concerning the concept of the Lorentz integral transform as a method with a *controlled resolution* is made.

1 Introduction

The Lorentz integral transform (LIT) method [1] allows the calculation of observables for reactions into the many-body continuum without an explicit use of a many-body continuum wave function. The LIT approach has had a wide application range in the field of electroweak reactions with few-nucleon systems. In fact calculations of inclusive inelastic reactions of nuclei with $A = 3$ (see e.g. [2; 3; 4; 5]), $A = 4$ (see e.g. [6; 7; 8; 9; 10; 11; 12]) and $A = 6,7$ [13; 14] have been carried out. In some cases also exclusive reactions have been considered [15; 16; 17]. Various successful comparisons to results of conventional calculations, with explicit continuum state wave functions, have been performed for the two- and three-body systems [1; 3; 18; 19; 20; 21]. A recent review of the LIT method is given in [20].

To illustrate the LIT approach we consider the following inelastic response function

$$R(\omega) = \sum\!\!\!\!\!\!\int df |\langle f|\Theta|0\rangle|^2 \delta(E_f - E_0 - \omega). \tag{1}$$

Here E_0 and $|0\rangle$ are ground state energy and wave function of the particle system under consideration, E_f and $|f\rangle$ denote final state energy and wave function of the final particle system, and Θ is the operator inducing the response function R. The LIT of the response R is given by

$$\mathscr{L}(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2}. \tag{2}$$

The key point of the method is that $\mathscr{L}$ can be calculated without any knowledge of the final state wave functions $|f\rangle$. In fact the transform is given by

$$\mathscr{L}(\sigma_R, \sigma_I) = \langle \tilde{\Psi}|\tilde{\Psi}\rangle \tag{3}$$

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and the Lorentz function $\tilde{\Psi}$ is obtained from

$$(H - E_0 - \sigma_R - i\sigma_I)|\tilde{\Psi}\rangle = \Theta|0\rangle. \tag{4}$$

The solution of Eq. (4) is unique and has an asymptotic boundary condition similar to a bound state and thus can be solved with bound-state methods. As final step, the response $R(\omega)$ is obtained by inverting Eq. (2). Such an inversion, however, represents a so called *ill-posed* problem. For non-experts in the field of ill-posed problems the question may arise if the ill-posedness does not lead to a serious drawback of the LIT approach. Therefore the aim of this paper is a clarification of the mathematical term *ill-posed* and to outline how ill-posed problems can be reliably solved.

2 Ill-Posed Problems

To illustrate the general situation regarding the ill-posed problems, let us first consider an example that shows how ill-posed problems are quite common. This is the problem of calculating the derivative $g(x)$ of a function $f(x)$ in accordance with the definition

$$g(x) = \mathscr{D}f(x); \qquad \mathscr{D}f(x) = \lim_{\delta\to 0}\frac{f(x+\delta) - f(x-\delta)}{2\delta}. \tag{5}$$

This very familiar problem is an ill-posed one, since it does not satisfy a requirement characteristic for a *well-posed problem* as defined by Hadamard in 1902s. In fact the function $g(x)$ does not depend continuously on the input $f(x)$. For example, consider $F(x) = f(x) + \Delta f(x)$, then $G(x) = g(x) + \Delta g(x)$. If $\Delta f(x) = \varepsilon \sin(\nu x)$, it is evident that for any small value of ε, ν values can be found that make $\Delta g(x) = \mathscr{D}\Delta f(x)$ large.

This means that the problem of the derivative of any function calculated numerically is ill-posed, since this function inevitably includes a random noise.

What is done in this case is to replace Eq. (5) with its analogue, but with a finite δ (denoted by d):

$$G(x,d) = \hat{D}(d)f(x); \qquad \hat{D}(d)f(x) = \frac{f(x+d) - f(x-d)}{2d}. \tag{6}$$

The quantity $G(x,d)$ is called a regularized solution to the problem, and d is called a regularization parameter. In contrast to $g(x)$ from Eq. (5), $G(x,d)$ depends continuously on $f(x)$. Thus, for sufficiently small increments $\Delta f(x)$ the increments $\Delta g = \hat{D}(d)\Delta f$ will also be small. At the same time, one can find d values such that the right-hand side of Eq. (6) with the true, noiseless, $f(x)$ differs from the true derivative $g(x) = \mathscr{D}f(x)$ by an arbitrarily small amount. As a result, if one considers a sequence of noise increments $\Delta f(x)$ with amplitudes tending to zero one can choose a sequence of corresponding d parameters in a way that the arising sequence of regularized solutions $G(x,d)$ will tend to the true solution $g(x)$.

It is easy to obtain that, at a given noise increment $\Delta f(x), d$ values of about $[2\Delta f(x)/f''(x)]^{1/2}$ in $G(x,d)$ provide an optimal approximation to the true derivative $\mathscr{D}f(x)$. At such d values, the error in $\mathscr{D}f(x)$ is about $[2f''(x)\Delta f(x)]^{1/2}$. When $\Delta f(x)$ tends to zero this error tends to zero as well. From what has been said above one can infer that the d dependence of $G(x,d)$ at a given x value should include a plateau at an appropriate level of accuracy, and any value of d belonging to this plateau can be adopted for representing $\mathscr{D}f(x)$.

The situation is quite similar when one deals with the problem of finding a solution to the integral equation of the first kind (Eq. (2) is a specific example)

$$L(y) = \int_0^\infty K(y,x)R(x)dx, \tag{7}$$

or, in short, $L = \hat{K}R$. The case when there exists a unique solution is considered. The role of the operator $\mathscr{D}$ from Eq. (5) is played here by the operator $\hat{K}^{-1}$. We also assume that either a) $\int_0^\infty |K(y,x)|dx$ is convergent or b)
$\int_0^a |K(y,x)|dx$ is convergent at any finite a and $K(y,x) \to 0$ monotonically at $x \to \infty$. The solution R does not depend continuously on the input L. Indeed, let us replace L with $L + \Delta L$ and suppose that an increment $\Delta L(y)$ is such that it causes a given increment $\Delta R = A\sin(kx)$ to the solution R. When $|k|$ is sufficiently large

the required ΔL is arbitrarily small, see e.g. [22]. Therefore, Eq. (7) poses an ill-posed problem.[1] One may note that this property is a very general one so that a special explanation of the ill-posedness of the transform when the kernel is a Lorentzian function is superfluous.

Similar to the example of the derivative mentioned above, Eq. (7) can be solved by a regularization method. The regularization suppresses the unphysical high-frequency components that might arise in an approximate solution. The problem (7) is replaced with a well-posed problem that includes a *regularization parameter* "r". The solution $R(x,r)$ of this *well-posed* problem depends on $L(y)$ continuously and thus sufficiently small increments in $L(y)$ lead to only small increments in $R(x,r)$. At the same time, with the true $L(y)$, the solution $R(x,r)$ is arbitrarily close to $R(x)$ at a proper choice of r. If a sequence of inputs $L(y)$ with increasing accuracy is considered, then choosing r in a proper way one has a sequence of solutions $R(x,r)$ tending in the limit to the true $R(x)$. The corresponding r values may be found using estimates of magnitudes of uncertainties in $L(y)$ and estimates on how close $R(x,r)$ is to $R(x)$ at a given r. This can also be done without such estimates, relying on stability of $R(x,r)$ when r varies.

For a number of regularization methods the mentioned convergence of $R(x,r)$ to $R(x)$ is proven, and in spite of the unfortunate term *ill posed*, which sounds negative, the approach is *well-founded* (see e.g. [23; 24; 25]). The origin of this term lies merely in the history and has by no means a relation to the accuracy of the results obtained by the outlined approach. The term was introduced about hundred years ago by the mathematician Hadamard who suggested that such problems cannot have a physical relevance. As we know nowadays, this was definitely a mistake as it is claimed by modern authors. For example at p. 2 of [24], the authors write "It turned out that the opinion of Hadamard regarding the Cauchy problem for the Laplace equation and a number of other problems of the same type was erroneous".

3 Solutions of Ill-Posed Problems: The Regularization Procedures

Among the number of regularization schemes for solving Eq. (9) that are known, the one that has been applied in conjunction with few-body calculations of the Lorentz transform allows reliable estimates of uncertainties of the results and keeps the uncertainties at a sufficiently low level. In all those applications the solution has been represented as the sum of the first N functions of a complete set $\{\phi_i(x)\}$,

$$R(x,N) = \sum_{i=1}^{N} c_i \phi_i(x). \tag{8}$$

Here the value N plays the role of the regularization parameter. The coefficients c_i are found from fitting $L(y)$ (for more detail see [20]). As pointed out in the introduction accurate solutions have been obtained using this procedure. On the one hand the accuracy is shown by the existence of a range of N values where the solution is stable, and on the other hand by the already mentioned various benchmark calculations.

In particular we would like to mention that with this regularization procedure it is very easy to implement the small x behaviour of $R(x)$, allowing the inclusion of the Coulomb case and the amplification of the role of the threshold region in the fitting procedure. The discussed regularization approach of Eq. (8) is well suited to describe responses $R(x)$ with a single-peak structure. Different methods might be advantageous in other cases (see also [26]).

One may also note that in this regularization scheme input values of $L(y)$ from a limited range of y is sufficient. This range is comparable to the range of x values of interest in $R(x)$. In addition one can easily work with different LIT resolution parameters σ_I in different y ranges (see e.g. [27]).

In conclusion, the regularization procedure used in few-body calculations allows reliable estimates of uncertainties of the results as well as keeping the uncertainties at a sufficiently low level.

In this context it is interesting that in a recent paper the claim is made that the inversion problem of any ill-posed integral transform of type

$$L(y) = \int_0^\infty K(y-x)R(x)dx. \tag{9}$$

[1] This consideration implies use of the metrics C in the space of $R(x)$ and the metrics C or the metrics L_2 in the space of $L(y)$.

can be tackled in a conceptually completely new manner, namely without any use of regularization techniques [28]. Since from a conceptual point of view this would be a very remarkable result, leading to an alternative method to invert the LIT, we will consider the proposed method in the following.

First of all we note that as a matter of fact the "novel inversion method" in [28] is in principle known, see e.g. [23]. It goes as follows. Equation (9) is solved via application of the Fourier transformation. This gives

$$\tilde{R}(k) = (2\pi)^{-1/2}\tilde{L}(k)/\tilde{K}(k), \tag{10}$$

where the Fourier transform of a function $f(x)$ is denoted by $\tilde{f}(k)$. In this way, the problem turns to the problem of numerical inversion of the Fourier transform $\tilde{R}(k)$. When calculated numerically this includes an admixture of errors whose relative magnitude increases at high frequencies. This happens because at large $|k|$ values $\tilde{K} \to 0$ and the errors in the input $\tilde{L}$ are amplified. Therefore the contribution of large $|k|$ to the integrand when inverting the Fourier transform should be suppressed in some way.

We note in passing that the criterion of *well-posedness* mentioned in [28] for the case of kernels which are functions of a difference, like those in Eq. (9), can never be satisfied. In fact the authors claim that only when $inf|\tilde{K}(k)| > 0, \tilde{K}$ being the Fourier transform of the kernel, the problem is well-posed. However that condition can never be fulfilled for kernels that satisfy the natural conditions for existence of their Fourier transform [22], i.e. either a) $\int_{-\infty}^{\infty}|K(s)|ds$ is convergent or b) such an integral over any finite interval is convergent and $K(s) \to 0$ monotonically at $s \to \pm\infty$. Indeed, when these conditions are satisfied one always has $\tilde{K}(k) \to 0$ at $k \to \pm\infty$.

In order to diminish the above mentioned faulty contribution to the inversion of $\tilde{R}(k)$ at large $|k|$, in [23] it is recommended to insert a damping factor $f(k,k_0)$ in the integrand where k_0 is a regularization parameter. The simplest possibility is to cut the integrand at some $|k| = k_{\max}$ getting, see e.g. [29],

$$R(x,k_{\max}) = \frac{1}{2\pi}\int_{-k_{\max}}^{k_{\max}} \frac{\tilde{L}(k)}{\tilde{K}(k)} e^{-ikx}dx. \tag{11}$$

In [28] a modification of this procedure is used, where in addition $\tilde{R}(k)$ with $|k| > k_{\max}$ is taken into account approximately. This is achieved by representing $\tilde{R}(k)$ in the high $|k|$ region with its leading asymptotics matched to the above $\tilde{R}(k)$ at $k = \pm k_{\max}$. The leading asymptotics are obtained from the known small x asymptotics of $R(x)$ (if $R(x) \sim x^{\lambda}$ at $x \to 0$ then $\tilde{R}(k) \sim |k|^{-(1+\lambda)}$ at $|k| \to \infty$, see e.g. [30]). In fact, in general the small x behaviour of a physically relevant R is known, and is, as already pointed out before, always implemented in the inversions of the above mentioned few-body applications. The criterion in [28] to choose the $k_{\max}$ value could probably be improved by considering the stability of $R(x,k_{\max})$ with respect to variations in $k_{\max}$.

If the error-admixture amplitude in $\tilde{R}(k)$ is sufficiently small then the contribution of this admixture to the approximate solution (11), or to such a quantity with the asymptotics contributions added, is also small. At the same time, in the absence of an admixture of errors, the corresponding approximate solution $R(x,k_{\max})$ of the form (11) tends to the true $R(x)$ when $k_{\max}$ tends to infinity. Thus, this is nothing else but a usual regularization procedure. Just as such, it is presented e.g. in [23; 29]. The said is, of course, true irrespective to whether one adds the approximate leading asymptotics contribution, or not.

The inversion method put forward in [28] can be be added to the list of already existing inversion techniques (see [26]). However, the method has not been applied in [28] to a realistic test case, therefore one does not know its quality. In particular it might be problematic to rely on the assumption that the threshold behaviour of the response function dominates the high $|k|$ behaviour of $\tilde{R}(k)$ obtained numerically. In fact if the high $|k|$ region is dominated by numerical errors then the matching procedure will fail. Such an undesirable behaviour has been found applying just this inversion technique, for example, to the ^{4}He photodisintegration LIT (E. Liverts and N. Barnea, private communication). In this realistic case the range of x values dominated by the asymptotics turns out to be too narrow. Consequently, the true $\tilde{R}(k)$ falls off quite fast and the $|k|$ values where its asymptotics start are higher.

Another possible drawback of this method could be the fact that in order to calculate $\tilde{L}(k)$ the input $L(y)$ is required in a very wide range of y. This is a disadvantage since the precision of the calculation of the LIT $L(y)$ is correlated with y. In particular at a fixed relative precision it is much more expensive to obtain $L(y)$ for large y.

Finally, we would like to make an additional remark concerning the general philosophy of the LIT also in relation to its ill-posed character. The LIT method has to be understood as an approach with a *controlled*

resolution. If one expects that R has structures of a width Δ then the LIT resolution parameter σ_I should be similar in size. Then it is sufficient to determine the corresponding LIT with a moderately high precision. If in reality no structures with a width smaller than Δ are present the inversion will lead to reliable results for $R(x)$. If, however, there is a reason to believe that $R(x)$ exhibits such smaller structures one should reduce σ_I accordingly and perform again a calculation of $L(y)$ with the same relative precision as before. Such a calculation is of course more expensive than the previous one with larger σ_I, but in principle one can reduce the LIT resolution parameter σ_I more and more. It is worth noticing that LIT procedure is similar to what is done in a conventional continuum calculation. In this case one calculates $R(x)$ for a finite number of x points which are then connected, e.g., by a spline interpolation. In doing so, also here one assumes that there is no structure between two neighbouring grid points. If, however, there is reason to believe that $R(x)$ exhibits such structures the density of the grid points has to be increased (normally easier in a conventional calculation).

The advantage of the LIT approach as compared with a conventional approach is evident. In the LIT case the finite resolution makes the calculations feasible, also when a conventional calculation which corresponds to an infinite resolution ($\sigma_I \to 0$) is not feasible any more.

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