On the ill-posed character of the Lorentz integral transform †

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Abstract

An exact inversion formula for the Lorentz integral transform (LIT) is provided together with the spectrum of the LIT kernel. The exponential increase of the inverse Fourier transform of the LIT kernel entering the inversion formula explains the ill-posed character of the LIT approach. Also the continuous spectrum of the LIT kernel, which approaches zero points necessarily to the same defect. A possible cure is discussed and numerically illustrated.

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I. INTRODUCTION

Integral transformations
\[
L(y) = \int_{-\infty}^{\infty} dx \kappa(y, x) R(x)
\] (1)
are widespread used in physics. According to Hadamard [1], the problem of finding the unknown function \( R \) for a given transform \( L \) is called “well-posed”, if the following conditions are fulfilled:

- The function \( R \) exists and is unique.
- The function \( R \) depends continuously on the input \( L \).

Otherwise, the problem (1) is called “ill-posed”. As example, let us consider the well-known Laplace transformation
\[
L(y) = \int_{0}^{\infty} dxe^{-xy} R(x)
\] (2)
which is widely used in physics and engineering. It turns out to be ill-posed. For illustration, consider the test function
\[
R(x) = \frac{\sin(\frac{\pi}{\epsilon} x)}{\frac{\pi}{\epsilon} x}
\] (3)
and its Laplace transform
\[
L(y) = \epsilon \arctan\left(\frac{1}{\epsilon y}\right). 
\] (4)

For \( \epsilon \to 0 \), the maximum norm of \( L \) goes to 0, whereas the maximum norm of \( R \) is 1 for any \( \epsilon \).

In this paper we study integral transforms, where the kernel \( \kappa \) in (1) has the form [7]
\[
\kappa(y, x) = K(z = y - x)
\] (5)
In detail, we will concentrate on the Lorentz integral transform (LIT) (\( \sigma_i > 0 \) fixed)
\[
K_{LIT}(z) = \frac{\sigma_i}{\pi} \frac{1}{z^2 + \sigma_i^2} 
\] (6)
which has recently been applied extensively in photo- and electronuclear physics [2].

In the LIT-approach, due to the choice \( \sigma_i \neq 0 \), the calculation of physical observables in the \( A \)-particle scattering problem can be traced back rigorously to the solution of an
appropriate bound state problem. This is of course a tremendous technical simplification and offers a unique possibility to carry out rigorous ab initio calculations on few-nucleon systems even beyond mass number $A = 4$\textsuperscript{2}. However, the LIT is known to be ill-posed as will be again outlined below.

In general, in order to obtain $R$ from a given ill-posed transform, an appropriate regularization scheme is essential. For example, in one class of inversion schemes for the LIT, the numerically gained Lorentz transform is expressed as a finite sum of appropriate basis functions whose inversion in explicitly known, i.e.

$$L(y) = \sum_{i=1}^{N} c_i \chi_i(y). \quad (7)$$

Due to the ill-posed character of the LIT, the upper value $N$ of basis functions must be limited for obtaining reliable results. Otherwise, the gained solution for $R$ may contain strong, unphysical oscillations. This reduction in the numerical resolution is nothing else as a regularization, see [3] for further details.

In this paper, we intend to tackle the inversion problem of any ill-posed integral transform of type (5) in a conceptually completely new manner, namely, without any use of regularization techniques. For that purpose, we present in section 2 a new inversion formula for kernels of the type (5) which will then be applied to the LIT. It turns out that this inversion formula directly exhibits the ill-posed character of the LIT. We further provide the spectrum of that LIT kernel, which also makes its ill-posed character evident.

Section 3 is devoted to a numerical case study for the LIT approach, which illustrates the very source for the ill-posed property. A possible reduction of that illness is proposed, i.e. a strategy will be developed to heal, at least under certain circumstances, the ill-posed character of the LIT. We end with a brief summary in section 4.

II. MATHEMATICAL PROPERTIES OF KERNELS INCLUDING THE LIT

For kernels of the type (5), eq. (1) has the form

$$L(y) = \int_{0}^{\infty} dx K(y - x) R(x) \quad (8)$$

which Fourier transformed leads to

$$\tilde{L}(k) = \sqrt{2\pi} \tilde{K}(k) \tilde{R}(k) \quad (9)$$
with

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy e^{iky} f(y)$$  \hspace{1cm} (10)$$

for any function \(f\). Immediately, from (9), it follows the inversion in \textit{closed} form

$$R(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \frac{\tilde{L}(k)}{\tilde{K}(k)} e^{-ikx}$$  \hspace{1cm} (11)$$

Provided that the Fourier transform \(\tilde{K}(k)\) of the kernel is a continuous function and that the infinum of its absolute value has a lower bound larger zero, i.e.

$$C = \inf |K| > 0 \hspace{1cm} ,$$  \hspace{1cm} (12)$$

we obtain for the \(L_2\) norm

$$||R||^2 \equiv \int_{-\infty}^{\infty} dx |R(x)|^2 \leq \frac{1}{4\pi^2 C^2} ||L||^2 \hspace{1cm} .$$  \hspace{1cm} (13)$$

In consequence, we can formulate a very simple criterion to distinguish between ill-posed and well-posed integral kernels of the type (5). If \(C > 0\) is fulfilled, the integral transformation is well-posed. Otherwise, it turns out to be ill-posed, as it becomes obvious by studying the spectrum of integral kernels of the type (5). It is defined as

$$\int_{-\infty}^{\infty} dx K(y-x) \chi_{k_0}(x) = \mu(k_0) \chi_{k_0}(y) \hspace{1cm} ,$$  \hspace{1cm} (14)$$

or Fourier transformed as

$$\sqrt{2\pi} \tilde{K}(k) \tilde{\chi}_{k_0}(k) = \mu(k_0) \tilde{\chi}_{k_0}(k) \hspace{1cm} .$$  \hspace{1cm} (15)$$

This leads to

$$\tilde{\chi}_{k_0}(k) \sim \delta(k - k_0) \hspace{1cm} (16)$$

and

$$\mu(k_0) = \sqrt{2\pi} \tilde{K}(k_0) \hspace{1cm} .$$  \hspace{1cm} (17)$$

Therefore, the spectrum of any arbitrary integral kernel of the type (5) is given by its Fourier transform. If a kernel fulfills \(C = 0\) in (12), the spectrum is continuous and has zero as accumulation point. In consequence, the kernel is obviously ill-posed and an unprotected inversion cannot work.
In case of the LIT, $\tilde{K}(k)$ is given by

$$\tilde{K}_{\text{LIT}}(k) = \sqrt{\frac{1}{2\pi}} e^{-\sigma_i |k|}.$$  

(18)

It fulfills $C = 0$, its spectrum is continuous,

$$\mu_{\text{LIT}}(k_0) = e^{-\sigma_i |k_0|},$$  

(19)

and approaches zero for large $k_0$. Therefore, the LIT is ill-posed. Its eigen functions are given by

$$\chi_{k_0}(x) \sim e^{ik_0x}.$$  

(20)

### III. A NUMERICAL CASE STUDY FOR THE LIT

The application of the inversion formula (11) requires a reliable numerical treatment of Fourier transforms. In this work, this is performed with the help of Filon’s integration formula [4]. In order to check our numerical routines, we take a simple analytical test case for the function $R$:

$$R(x) = \sqrt{x} e^{-ax} \Theta(x),$$  

(21)

with $\Theta$ denoting the Heavyside step function, i.e. the threshold of this function is placed at $x = 0$. $a$ is a free parameter which we choose from now on as $a = 0.05 \text{ MeV}^{-1}$. Following the nomenclature in literature, we call $R$ from now the response function. Its Fourier transform is known analytically

$$\tilde{R}(k) = \sqrt{\frac{1}{8}} \left( \frac{1}{a^2 + k^2} \right)^{\frac{3}{4}} e^{\frac{3}{2} \tan^{-1}(\frac{k}{a})}$$  

(22)

so that the quality of our numerical routines for the Fourier transform can be tested straightforwardly. For that purpose, we cut at first the integrations bounds in (10) according to

$$\tilde{R}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{ikx} R(x) \longrightarrow \frac{1}{\sqrt{2\pi}} \int_{-x_{\text{max}}}^{x_{\text{max}}} dx e^{ikx} R(x)$$  

(23)

with $x_{\text{max}} = 3000 \text{ MeV}$. With respect to the strong exponential decrease of our test function (21), this upper value for $x_{\text{max}}$ is more than sufficient. The remaining integral in (23) is now evaluated with the help of Filon’s integration formula using $N$ equidistant grid points. It turns out that the numerical precision in calculating the Fourier transform
increases naturally with increasing $N$, but decreases strongly with increasing argument $k$ of the Fourier transform. For example, for $N = 20001$ mesh points the numerical error in the real part of the Fourier transform is of the order of about 1.7 percent for $k = 0.8\text{ MeV}^{-1}$, increasing to about 6.9 percent for $k = 2.0\text{ MeV}^{-1}$.

At next, let us check the inversion formula (11) for our test response (21). For that purpose, we calculate at first numerically the LIT transform $L(y)$ of $R(x)$ and then its Fourier transformations $\tilde{L}(k)$ corresponding to (23) with $x_{\text{max}} = 3000$ and $N = 20001$ equidistant mesh points. Then, with the help of the known Fourier transform of the Lorentz kernel (18), we can perform the inversion (11) where we again, similar as in (23), have to cut the integration at the lower and upper limit, i.e.

$$R(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \frac{\tilde{L}(k)}{K_{\text{LIT}}(k)} e^{-ikx} \rightarrow \frac{1}{2\pi} \int_{-k_{\text{max}}}^{k_{\text{max}}} dk \frac{\tilde{L}(k)}{K_{\text{LIT}}(k)} e^{-ikx}. \quad (24)$$

This second Fourier integral is calculated with Filon, considering again $N = 20001$ equidistant mesh points in the interval $[-k_{\text{max}}, k_{\text{max}}]$.

In order to obtain in general a quantitative estimate for arising numerical uncertainties, we define in this context the quantity

$$\epsilon = \frac{||R_{\text{num}}(x) - R(x)||^2}{||R_{\text{num}}(x)||^2} \quad (25)$$

with $R_{\text{num}}$ denoting our numerical result for the real part of the response derived via the inversion formula (11). Concerning the norm $||$, we use (13), i.e. the $L_2$ norm.

In our first attempt, calculation $A$, we choose $k_{\text{max}} \equiv k_{\text{max}}^A = 0.8\text{ MeV}^{-1}$ in (24). The resulting response ($\epsilon = 2.2\times10^{-3}$, dashed curve in Fig. 1), using (24), turns out to be qualitatively correct beyond the threshold region, but unsatisfactory at threshold. The reason for this failure and a convenient improvement will be discussed below. Apart from that point, we can conclude that our new inversion formula (11) works, at least in principle for a LIT with arbitrarily high precision. In practical applications, however, the LIT $L(y)$ is not known perfectly well. In order to take this important fact into account in the present case study, we proceed as follows. We take, for a given value of $y$, the exact Lorentz transform of (21) (“exact” within the limits of the compiler precision) in the form $0.x_1x_2x_3x_4x_5\ldots 10^{-d}$ with $x_i, d$ integer numbers and $x_1 \neq 0$. Then, we substitute this number by hand according to

$$0.x_1x_2x_3x_4x_5x_6\ldots 10^{-d} \rightarrow 0.x_1x_2x_3 10^{-d}, \quad (26)$$
i.e. we cut all relevant digits beyond the first three ones. This ad hoc procedure simulates a numerical error in $L$ in the range $\sim 10^{-3} - 10^{-2}$ – a level which can, under favourable conditions, reached in state-of-the-art calculations in nuclear physics. This modified Lorentz transformation, used from now on in this work, can hardly be distinguished from the original one. However, the resulting response function, yielded by the application of (11), shows large oscillations ($\epsilon = 5 \times 10^{-2}$, dotted curve in Fig. 1). This calculation is denoted from now on as calculation B. This numerical fact shows insistently the well-known ill-posed character of the Lorentz integral transformation: a small change in $L$ (lhs. of (11)), generated in our test case by the modification (26), leads to large changes in the response $R$ (rhs. of equation (1)).

As a novel feature, our inversion procedure allows now to pin down precisely the source for the ill-posed character of the Lorentz transform. For that purpose, Fig. 2 shows for calculation A and B the real part of the corresponding Fourier transforms $\tilde{R}(k)$ yielded via (9), i.e.

$$\tilde{R}(k) = \frac{1}{\sqrt{2\pi}} \frac{\tilde{L}(k)}{K_{\text{LIT}}(k)} .$$

One obtains a remarkable fact. For arguments $k > 0.4 \text{ MeV}^{-1}$, the Fourier transform yielded in calculation B (dashed) differs considerably from the “exact” result A (full). This can be easily understood by the explicit form of $\tilde{K}_{\text{LIT}}(k)$ (18). Its inverse is growing exponentially so that in (27) even small errors in $\tilde{L}(k)$ are tremendously amplified. This fact also explains intuitively why for small arguments $k$ both Fourier transforms are almost identical. This important result can also be understood from a more rigorous point of view. For $k \to 0$, we have

$$\lim_{k \to 0} \sqrt{2\pi} \tilde{R}(k) = \int dx R(x) = \int dy L(y) ,$$

where the last equation follows from the structure of Lorentz kernel (6). In consequence, if the LIT $L$ contains only a small error, then the last integral in (28) will also contain only a small error. Therefore, the Fourier transform $\tilde{R}(k)$ can be determined with great precision for $k \to 0$ via (9) – despite that the LIT is ill-posed.

Let us summarize this important result again: The LIT is an ill-posed integral transform. However, this ill-posed character does not affect at all the numerical stability of the obtained Fourier transform $\tilde{R}(k)$ of the resulting response for sufficiently small arguments $k$. Only for moderate and large arguments $k$, numerical instabilities arise which can be traced back
to the ill-posed character of the LIT.

In consequence: If it were possible to determine, from general principles, the asymptotic
behaviour of the Fourier transform \( \hat{R}(k) \), one could hope to circumvent, or at least to reduce
significantly, any arising numerical instability problems due to the ill-posed character of the
LIT. From a certain point of view, the ill-posed character of the LIT could be “healed”.

For our case study, we proceed now as follows. At first, we have to fix the value \( k_{\text{thres}} \) up
to which the ill-posed character is irrelevant for the determination of \( \hat{R}(k) \) via (27). Unlike
as in our case study, the exact Fourier transform \( \hat{R}(k) \) is of course not known in general.
In practice, one could help oneself by repeating the calculation for a slightly different value
\( \sigma_i \). In an ideal calculation, without any numerical errors, the resulting Fourier transform
\( \hat{R}(k) \) should of course be independent from the chosen value \( \sigma_i \). In Fig. 2 the real part
of \( \hat{R}(k) \) can be compared for our standard value \( \sigma_i = 10 \text{ MeV} \) (dashed) to the one for
\( \sigma_i = 11 \text{ MeV} \) (dotted). Till about \( k = 0.25 \text{ MeV}^{-1} \), both Fourier transforms are almost
identical, however, especially for arguments larger than about \( k = 0.4 \text{ MeV}^{-1} \) substantial
differences arise. Therefore, we could trust our results only till about \( k_{\text{thres}} = 0.25 \text{ MeV}^{-1} \).
For \( k > 0.25 \text{ MeV}^{-1} \) we have to substitute the unphysical result obtained in calculation B
by a more reasonable one. For that purpose, we exploit general theorems on the asymptotic
behaviour of Fourier transforms [5, 6]. It turns out that quite in general the latter is
unambiguously fixed by the knowledge of the threshold behaviour of the response function
\( R \). Now, the threshold behaviour of \( R \) is, for a given reaction, in general known from basic
physical principles. Without any considerable loss of generality, we can therefore assume
that we know not only in our case study, but quite in general the threshold behaviour of our
unknown response (21), i.e.

\[
R(x) \sim \sqrt{x}.
\]

(29)

Due to [6], its Fourier transform must therefore behave asymptotically as

\[
\hat{R}(k) \sim \frac{1}{\sqrt{k}},
\]

(30)
in agreement with the exact analytical result [22].

Now, it is almost straightforward how to proceed. Only for \( k < k_{\text{thres}} \) we use in (24)
numerical results for \( \hat{L}(k) \). For \( k > k_{\text{thres}} \), we use instead the asymptotic ansatz (compare
with (29))

\[
\hat{L}_{\text{asy}}(k) = \sqrt{2\pi K(k)} \hat{R}_{\text{asy}}(k)
\]

(31)
with
\[ \tilde{R}_{\text{asy}}(k) = \frac{c}{\sqrt{k^3}}. \] (32)
The complex parameter \( c \) is chosen to guarantee a continuous integrand at \( k = \pm k_{\text{thres}} \) in (24). By this prescription, it is of course easily possible to extend the limit \( k_{\text{max}} \) in (24) to arbitrarily large values without any arising numerical errors. In the resulting calculation \( \mathbf{C} \), we choose \( k_{\text{max}} = 10 \text{ MeV}^{-1} \) with again \( N = 20001 \) equidistant mesh points in the region \([-k_{\text{max}}, k_{\text{max}}]\). The resulting response is depicted as the dashed curve in Fig. 3 \((\epsilon = 4.2 \times 10^{-4})\).

One readily realizes two very important improvements: (i) The heavy oscillations found in calculation \( \mathbf{B} \) have vanished, (ii) the threshold behaviour is considerably improved compared to calculation \( \mathbf{A} \). Both features can be traced back to the improved treatment of \( \tilde{L}(k) \) by exploiting the known asymptotic behaviour of \( \tilde{R}(k) \). Since we assume that we know the threshold behaviour of the response, the still arising problem of a small, but nonvanishing numerical result for \( R(x) \) below threshold is irrelevant in practice.

In general, for an unknown response, it is of course not clear whether the asymptotic form is already working for \( k = k_{\text{thres}} \) where the Fourier transforms \( \tilde{R}(k) \) start to diverge from each other for different choices of \( \sigma_i \). The present case, considers, from that point of view, even an “almost” worst case scenario, since the Fourier transform is decreasing rather slowly, \( \tilde{R}(k) \sim \frac{1}{\sqrt{k}} \). It turns out that for \( k = 0.8 \text{ MeV}^{-1} \), the asymptotic form and the exact form of the real part of the Fourier transform, (32) vs. (22), differ by not less than about 40 percent. Nevertheless, even this quite reduced precision in the knowledge of \( \tilde{R}(k) \) for \( k \) at quite moderate values beyond \( k_{\text{thres}} \) is absolutely sufficient to obtain reasonable results in the inversion of the LIT. If the Fourier transform decreases stronger, e.g. exponentially, one can expect even more reliable results within our proposed inversion technique.

IV. SUMMARY

We illuminated the ill-posed character of the LIT approach by providing an exact inversion formula and giving the spectrum of the LIT kernel. The exact inversion formula requires the Fourier transform of the LIT transformed response, which has to be obtained numerically, whereas the Fourier transform of the LIT kernel is analytically known. Since \( \tilde{K}^{-1}(k) \) occurs in the inversion formula, even small numerical errors in \( \tilde{L}(k) \) at large \( k \)-values are drastically enhanced which lead to violent oscillations of \( R(x) \) in the inverse Fourier trans-
formation. We illustrated that situation in a numerical test case. Evaluating $L(y)$ and its FT very precisely and using the inversion formula we recovered the model response $R(x)$ with satisfactory precision, at least beyond the threshold region. However, truncating $L(y)$ to about three digits revealed very drastically the ill-posed character of LIT, namely leading to wild oscillations in $R(x)$ evaluated by the inversion formula. It is not the behaviour of $\tilde{L}(k)$ for small $k$-values which causes the oscillations but the behaviour for the large $k$-values. This is clearly demonstrated by putting $\tilde{L}(k)$ to its known asymptotic behaviour for $k$ larger a certain $k_{\text{thres}}$. The resulting $R(x)$ gained through the inversion formula is close to the exact one, without oscillations. In this framework, also the threshold behaviour of $R(x)$ can be reproduced satisfactorily.

As not outlined in this work, we verified in addition that for a more structured model response with two peaks, like the one used in [3], that inversion formula works equally well, provided one corrects again the asymptotic behavior of $\tilde{L}(k)$.

In the applications of LIT to electro weak processes in nuclear physics, $L(y)$ can be determined in various manners, see [2] for further details. Using our inversion formula, the Fourier transformed $\tilde{L}(k)$ of a numerically gained LIT is required. We conjecture that our results lead to the requirement to determine $L(y)$ with such a high precision that its Fourier transform is well under control for small and intermediate arguments, but not necessarily for large arguments. If this is guaranteed, and if the threshold behaviour of the response is known, the proposed method allows to heal the ill-posed character of the LIT without any use of regularization techniques. From a conceptual point of view, this a very remarkably result.

Since our proposed ansatz is quite general, provided the integral kernel is given in the form (5), one can apply the techniques developed in this work to a variety of different other ill-posed problems in physics and engineering.

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FIG. 1: Full curve: Exact Response function (21), dashed curve: Response function yielded by inversion formula (11) (calculation A) with \( k_{\text{max}} = 0.8 \, \text{MeV}^{-1} \). Dotted curve: result for response in calculation B with \( k_{\text{max}} = 0.8 \, \text{MeV}^{-1} \). In all curves, \( \sigma_i = 10 \, \text{MeV} \) has been used.

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[7] Please note that in the usual definition, no factor \( \frac{\sigma_i}{\pi} \) occurs in (6).
FIG. 2: Real part of $\tilde{R}(k)$ in calculation B for $\sigma_i = 10$ MeV (dashed) and $\sigma_i = 11$ MeV (dotted). The full curve corresponds to the result for calculation A with $\sigma_i = 10$ MeV.
FIG. 3: Full curve: exact response function (21), dashed curve: response yielded in calculation C with $\sigma_i = 10$ MeV.