The Lorentz Integral Transform (LIT) method and its applications in nuclear physics

First proposed in
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Recent Topical Review:
V. D. Efros, W. Leidemann, G. Orlandini and N. Barnea
“The Lorentz Integral Transform (LIT) method and its applications to perturbation induced induced reactions”

The LIT method

- It is an *ab initio* method for calculations of reactions involving states in the (far) continuum.
- It is general enough to be applied to perturbative as well as non-perturbative reactions.
- The applications so far have been to electromagnetic and weak reactions on light nuclei (perturbative reactions).
Integral transform approaches

\[ \Phi (\tau) = \int d\omega \; K(\omega, \tau) \; S(\omega) \]
Integral transform approaches

\[ \Phi(\tau) = \int d\omega \ K(\omega, \tau) \ S(\omega) \]

There are many classes of problems that are difficult to solve in their original representations. An integral transform "maps" an equation from its original "domain" into another domain. Manipulating and solving the equation in the target domain is sometimes much easier than manipulation and solution in the original domain.
Integral transform approaches

There are many classes of problems that are difficult to solve in their original representations. An integral transform "maps" an equation from its original "domain" into another domain. Manipulating and solving the equation in the target domain is sometimes much easier than manipulation and solution in the original domain.

The solution is then mapped back to the original domain with the inverse of the integral transform.
In theoretical physics:

\[ \Phi(\tau) = \int <|\Theta^\dagger(\tau, x) \Theta(0, 0)|> d^3x \rightarrow \int e^{-\tau \omega} S(\omega) d\omega \]

\[ \tau = \text{it} \]

In Condensed Matter Physics:
- \( \Theta = \) Density Operator
- \( S(\omega) = \) Dynamical Structure Function
- \( \Phi(\tau) \) is obtained with Monte Carlo Methods

In Nuclear Physics:
- \( \Theta = \) Charge or current density operator
- \( S(\omega) = R(\omega) \) “Response” Function (to external perturbative probe)
- \( \Phi(\tau) \) is obtained with Monte Carlo Methods

In QCD:
- \( \Theta = \) quark or gluon creation operator
- \( S(\omega) = \) Hadronic Spectral Function
- \( \Phi(\tau) \) is obtained by OPE - QCD sum rules or Lattice
It is well known that the numerical inversion of the Laplace Transform is a (tremendous) ill-posed problem.
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It is well known that the numerical inversion of the **Laplace Transform** is a (tremendous) **ill-posed** problem.
a “good” Kernel has to satisfy two requirements

**N. 1)** one must be able to calculate the integral transform

**N. 2)** one must be able to invert the transform, minimizing instabilities
What would be the “perfect” Kernel?
What would be the “perfect” Kernel?

the delta-function!
What would be the “perfect” Kernel?

the delta-function!

in fact

\[ \Phi(\tau) = S(\tau) = \int \delta(\omega - \tau) S(\omega) \, d\omega \]
the LIT method is based on the idea to use one of the so-called “representations of the delta-function”:

it turns out that a very good Kernel is the Lorentzian function

\[ \Phi (\omega_0, \Gamma) = \int [\frac{1}{(\omega - \omega_0)^2 + \Gamma^2}]^{-1} S(\omega) \, d\omega \]
The Lorentz Kernel satisfies the two requirements!

N.1. one can calculate the integral transform

N.2 one is able to invert the transform, minimizing instabilities
Illustration of requirement N.1:
one can calculate the integral transform
Suppose we want an $R(\omega)$ defined as
(for example for perturbation induced inclusive reactions)

$$R(\omega) = \sum_n \left| \langle n | \Theta | 0 \rangle \right|^2 \delta(\omega - E_n + E_0)$$
choosing the **2-parameter** kernel $L(\omega, \omega_0, \Gamma)$ a theorem based on closure states that the **integral transform** $\Phi(\omega_0, \Gamma)$ is given by:

$$\Phi(\omega_0, \Gamma) = \left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle = \int R(\omega) L(\omega, \omega_0, \Gamma) d\omega$$

where

$$|\tilde{\Psi} > = \frac{1}{(H - E_0 - \omega_0 + i\Gamma) \Theta} |0 >$$
Proof of the theorem:

\[ \Phi(\omega_0, \Gamma) = \int_{E_{th}^-}^{\infty} d\omega \frac{R(\omega)}{(\omega - \omega_0)^2 + \Gamma^2} \]

\[ = \int_{E_{th}^-}^{\infty} d\omega \left[ \sum_n |n \langle \Theta | 0 \rangle|^2 \delta(\omega - E_n + E_0) \right] \frac{1}{(\omega - \omega_0 - i\Gamma)(\omega - \omega_0 + i\Gamma)} \]

\[ = \sum \delta n \left< 0 | \Theta^\dagger \frac{1}{(E_n - E_0 - \omega_0 - i\Gamma)} \right| n > \]

\[ = \sum \delta n \left< 0 | \Theta^\dagger \frac{1}{(H - E_0 - \omega_0 - i\Gamma)} \right| n > < n | \Theta | 0 > \]

\[ = \left< 0 | \Theta^\dagger \frac{1}{(H - E_0 - \omega_0 - i\Gamma)} \frac{1}{(H - E_0 - \omega_0 + i\Gamma)} \Theta | 0 > \right> \]

\[ = \left< \tilde{\Psi} | \tilde{\Psi} > \right> \]

\[ | \tilde{\Psi} > = \frac{1}{(H - E_0 - \omega_0 + i\Gamma)} \Theta | 0 > \]
Closure = 1
The LIT in practice:

1. The state $|\tilde{\Psi}\rangle$ is found solving for fixed $\Gamma$ and many $\omega_0$:

$$|\tilde{\Psi}\rangle = \frac{1}{(H - E_0 - \omega_0 + i\Gamma)} \Theta |0\rangle$$

$$(H - E_0 - \omega_0 + i\Gamma) \tilde{\Psi} = \Theta |0\rangle$$
2. the overlap $\langle \tilde{\Psi} | \tilde{\Psi} \rangle$ is calculated

3. the transform is inverted

$\langle \tilde{\Psi} | \tilde{\Psi} \rangle = \int R(\omega) L(\omega, \omega_0, \Gamma) d\omega$
main point of the LIT:

Schrödinger-like equation with a source

\[(H - E_0 - \omega_0 + i\Gamma) \tilde{\Psi} = S\]

\[S = \Theta |0\rangle\]
The main point of the LIT:

Schrödinger-like equation with a source

\[(H - E_0 - \omega_0 + i\Gamma) \tilde{\Psi} = S\]

Theorem:

The solution is unique and has bound state asymptotic behavior

\[\langle \tilde{\Psi} | \tilde{\Psi} \rangle = \int \left[ \left( \omega - \omega_0 \right)^2 + \Gamma^2 \right]^{-1} S(\omega) \, d\omega < \infty\]
main point of the LIT:

Schrödinger-like equation with a source

\[(H - E_0 - \omega_0 + i\Gamma) \tilde{\Psi} = S\]

Theorem:

The solution is unique and has \textit{bound state} asymptotic behavior.

one can apply \textit{bound state methods}
The LIT method

- reduces the **continuum** problem to a **bound state** problem
- needs “**only**” a good method for **bound state** calculations (FY, HH, NCSM, ...???)
- has been **benchmarked** in systems (A=2,3) where one can solve the Schroedinger equation in the **continuum**
A= 4 AB INITIO BOUND STATE CALCULATIONS

BE of $^4$He

from H.Kamada et al. (18 authors 7 groups) PRC 64 (2001) 044001
A very good method to solve bound states:

the Effective Interaction in Hyperspherical Harmonics method (EIHH)


- **HH basis** (generalization to many-body of the spherical harmonics, satisfies translational invariance)
- Use of Effective Interaction (use of Lee – Suzuki unitary transformation)
- fast convergence
- can be applied to A>3 (up to now ----> A=7)
Practical calculation of $\Phi (\omega_0, \Gamma)$

1. Eigenvalue method:

$\tilde{\Psi}$ is expanded on localized functions

$$\sum_n | \phi_n > < \phi_n | = 1$$

$H$ is represented in this basis $\rightarrow H_{mn}$

$H_{mn}$ is diagonalized $\rightarrow | \phi_v > \epsilon_v$
Practical calculation of $\Phi (\omega_0, \Gamma )$

1. Eigenvalue method:

$\tilde{\Psi}$ is expanded on localized functions (now it is legitimate no discretization of the continuum !!!)

$$\sum_n | \phi_n \rangle \langle \phi_n | = 1$$

$H$ is represented in this basis $\Rightarrow H_{mn}$

$H_{mn}$ is diagonalized $\Rightarrow | \phi_v \rangle \ $ $\epsilon_v$
Practical calculation of $\Phi(\omega_0, \Gamma)$

1. Eigenvalue method: \( \tilde{\Psi} \) can be expanded on localized functions \( |\varphi_\nu \rangle \) with \( \epsilon_\nu \) as:

\[
\Phi(\omega_0, \Gamma) = \langle S | \frac{1}{(\hat{H} - E_0 - \omega_0 + i\Gamma)} \frac{1}{(\hat{H} - E_0 - \omega_0 - i\Gamma)} | S \rangle \\
|\tilde{\Psi}\rangle = \sum_\nu^N \frac{\langle \varphi_\nu^N | S \rangle}{\epsilon_\nu^N - E_0 - \omega_0 + i\Gamma} |\varphi_\nu^N \rangle ,
\]

\[
\Phi(\omega_0, \Gamma) = \sum_\nu \frac{|\langle \varphi_\nu^N | S \rangle|^2}{(\epsilon_\nu^N - E_0 - \omega_0)^2 + \Gamma^2} .
\]
Practical calculation of $\Phi(\omega_0, \Gamma)$

1. Eigenvalue method: The wave function $\Psi$ can be expanded on localized functions $|\varphi_\nu\rangle$: $\epsilon_\nu$

$$
\Phi(\omega_0, \Gamma) = \langle S | \frac{1}{(\hat{H} - E_0 - \omega_0 + i\Gamma)} \frac{1}{(\hat{H} - E_0 - \omega_0 - i\Gamma)} | S \rangle \\
|\Psi\rangle = \sum_{\nu}^{N} \frac{\langle \varphi^N_\nu | S \rangle}{\epsilon^N_\nu - E_0 - \omega_0 + i\Gamma} |\varphi^N_\nu\rangle,
$$

sum of Lorentzians around $\epsilon^N_\nu$. 

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Practical calculation of $\Phi(\omega_0, \Gamma)$

2. Lanczos method

\[
\Phi(\omega_0, \Gamma) = \langle S \rvert \frac{1}{(\hat{H} - E_0 - \omega_0 + i\Gamma)} \frac{1}{(\hat{H} - E_0 - \omega_0 - i\Gamma)} \lvert S \rangle, 
\]

\[
\Phi(\omega_0, \Gamma) = -\frac{1}{\Gamma} \text{Im} \left\{ \langle S \rvert \frac{1}{\omega_0 + i\Gamma + E_0 - \hat{H}} \lvert S \rangle \right\}. 
\]

\[
\Phi(\omega_0, \Gamma) = -\frac{1}{\Gamma} \text{Im} \left\{ \frac{\langle S \rvert S \rangle}{z - a_0 - \frac{b_1^2}{z - a_1 - \frac{b_2^2}{z - a_2 - \frac{b_3^2}{...}}}} \right\}. 
\]
Illustration of requirement N.2:

one can invert the integral transform minimizing instabilities
test on the Deuteron:

$R(\omega)$ is the longitudinal $(e,e')$ response function

$R^l(\omega)$ [MeV$^{-1}$]

$q = 2.3$ fm$^{-1}$

$\omega$ [MeV]

test on the Triton:

$R(\omega)$ is the Dipole Photoabsorption Cross Section
Inversion of the LIT: the **regularization** method

\[
R(\omega) = \sum_{n=1}^{N_{\text{max}}} c_n \chi_n(\omega, \alpha_i)
\]

The \( \chi_n \) are given functions with nonlinear parameters \( \alpha_i \). A basis set frequently used for LIT inversions is

\[
\chi_n(\omega, \alpha_i) = \omega^{\alpha_1} \exp\left(-\frac{\alpha_2 \omega}{n}\right).
\]

Substituting such an expansion in the integral equation

\[
\Phi(\omega_0, \Gamma) = \sum_{n=1}^{N_{\text{max}}} c_n \tilde{\chi}_n(\omega_0, \alpha_i),
\]

where

\[
\tilde{\chi}_n(\omega_0, \alpha_i) = \int_0^\infty d\omega \frac{\chi_n(\omega, \alpha_i)}{(\omega - \omega_0)^2 + \Gamma^2}.
\]

For given \( \alpha_i \) the linear parameters \( c_n \) are determined from a least–square best fit to the calculated \( \Phi(\omega_0, \Gamma) \) for a number of \( \omega_0 \) points much larger than \( N_{\text{max}} \).

*Works well with bell shaped kernels (and not too narrow resonances)*
Realistic interactions?

NN=AV18 + NNN=UIX

$^4\text{He}$
SURPRISE:
LARGE EFFECT OF 3-BODY FORCE AT LOW Q

NO MEASUREMENTS AT LOW q !!!

S.Bacca et al., PRL 102 (2009) 162501
\[ R_L \left[ 10^{-3} \text{ MeV}^{-1} \right] \]

\[ q = 50 \text{ MeV/c} \]

\[ \omega [\text{MeV}] \]

**Graph (d)**

- AV18
- AV18+UIX
- AV18+TM'
Final State Interaction (FSI) in “quasi elastic” processes

$^4\text{He}$
\[ R(\omega) = \sum_n |\langle n|\Theta|0\rangle|^2 \delta(\omega - E_n + E_0) \]

\[ \Theta = \rho \left( q \right) = \sum_i e_i \exp\{ i \cdot \mathbf{q} \cdot \mathbf{r}_i \} \]
Role of 3-body force

S. Bacca et al.,
PRL 102 (2009) 162501
Collective motions ???

N ----> 6
Dipole excitation

\[ ^4\text{He} \]

\[
\sigma_\gamma [\text{mb}] \quad \omega_\gamma [\text{MeV}]
\]

- AV18+UX
- Arkov et al. ('79)
- Shima et al. ('05)
- Nilsson et al. ('05)
- Berman ('80) + Feldman ('90)
6-Body total photodisintegration

Bacca et al. PRL89(2002)052502
7-Body total photodisintegration

S. Bacca et al.
PLB 603(2004) 159
Contact with other methods
(used in condensed matter)
Remember the practical calculation of $\Phi (\omega, \Gamma)$
Remember the practical calculation of $\Phi(\omega, \Gamma)$

1. Eigenvalue method:

\[ \tilde{\Psi} \text{ can be expanded on localized functions} \]

\[ \Phi(\omega_0, \Gamma) = \langle S | \frac{1}{(\hat{H} - E_0 - \omega_0 + i\Gamma)} \frac{1}{(\hat{H} - E_0 - \omega_0 - i\Gamma)} | S \rangle \]

\[ |\tilde{\Psi}\rangle = \sum_{\nu}^{N} \frac{\langle \varphi^N_\nu | S \rangle}{\epsilon^N_\nu - E_0 - \omega_0 + i\Gamma} |\varphi^N_\nu \rangle, \]

\[ \Phi(\omega_0, \Gamma) = \sum_{\nu} \frac{\langle \varphi^N_\nu | S \rangle^2}{(\epsilon^N_\nu - E_0 - \omega_0)^2 + \Gamma^2} \]

sum of Lorentzians around $\epsilon^N_\nu$
Since the Lorentzian function is a representation of the delta function

\[ \delta(\omega - \omega_0) = \lim_{\Gamma \to 0} \frac{\Gamma}{\pi} \frac{1}{(\omega - \omega_0)^2 + \Gamma^2}, \]

one could think of calculating \( R(\omega) \) as follows

\[ R(\omega) = \lim_{\Gamma \to 0} \Phi(\omega, \Gamma), \]

The extrapolation would give

\[ R(\omega) = \sum_{n=1}^{N} r_n \delta(E_n - \omega). \]
However, here comes the problem of the Continuum!

A regularization is needed!
TEST on deuteron photodisintegration

\[ \omega [\text{MeV}] \]

\[ \sigma_\gamma^d [\text{mb}] \]
TEST on deuteron photodisintegration

fixed $\Gamma=1$ MeV

increase size of the h.o. basis

$N_{ho}=150$
TEST on deuteron photodisintegration

fixed $\Gamma = 1$ MeV

$N_{ho} = 2400$

$\omega$ [MeV]

fix width

increase size of the h.o. basis
Test on deuteron photodisintegration

h.o. basis fixed
$N_{ho} = 2400$

$\Gamma = 1 \text{ MeV}$

fix size of the h.o. basis
decrease width

$\omega [\text{MeV}]$

$\sigma_y^d [\text{mb}]$

“true”
Test on deuteron photodisintegration

$$\Gamma = 0.5 \text{ MeV}$$

h.o. basis fixed

$$N_{\text{ho}} = 2400$$

fix size of the h.o. basis
decrease width
Test on deuteron photodisintegration

$h.o. \text{ basis fixed}$

$N_{h.o} = 2400$

$\Gamma = 0.25 \text{ MeV}$

fix size of the h.o. basis
decrease width
At $\Gamma=10$ very fast convergence of $\Phi$: two curves ($N_{ho}=150$ and $N_{ho}=2400$) on top of each other !!!

$N_{ho}=150$ is enough for accuracies at the % level!!!
At $\Gamma=10$ very fast convergence of $\Phi$: two curves ($N_{ho}=150$ and $N_{ho}=2400$) on top of each other!!!
More about the inversion of the transform and the “ill posed problem”
Definition of “well-posed” problems in making mathematical models of physical phenomena (by Jacques Hadamard 1865-1963):

1. Equations have solutions (existence)
2. The solution is unique
3. The solution depends continuously on the inputs in some reasonable topology.

When continuum problems are solved numerically errors are introduced. It may happen that a small error in the input may imply much larger errors in the output i.e. they become “ill-posed” problems.

A typical example: the “derivative”:

\[ g(x) = Df(x) = \lim_{\delta \to 0} \frac{f(x + \delta) - f(x - \delta)}{2\delta} \]

Suppose

\[ f(x) \longrightarrow F(x) = f(x) + \Delta f(x) = f(x) + \varepsilon \sin \omega x \]
\[ G(x) \longrightarrow G(x) = g(x) + \Delta g(x) = g(x) + \varepsilon \omega \cos \omega x \]

and \[ \Delta g(x) = \varepsilon \omega \cos \omega x \] may be LARGE !!!

i.e. g does not depend continuously on f
They need to be re-formulated for numerical treatment. Typically this involves including additional assumptions, such as smoothness of the solution. This process is known as regularization. The regularization can reduce the condition number (a measure of the degree of instability) to acceptable levels.

e.g. in the case of the “derivative” we perform a “regularization”

\[ G(x) \rightarrow G(h, x) = D(h, x) = \frac{f(x + h) - f(x - h)}{2h} \]

with \( h \) smaller and smaller till “some convergence” is reached

Now \( g \) does depend continuously on \( f \)
They need to be re-formulated for numerical treatment. Typically this involves including additional assumptions, such as smoothness of the solution. This process is known as regularization. The regularization can reduce the condition number (a measure of the degree of instability) to acceptable levels.

e.g. in the case of the “derivative” we perform a “regularization”

$$G(x) \rightarrow G(h, x) = D(h, x) = \frac{F(x + h) - F(x - h)}{2h}$$

with $h$ smaller and smaller till “some convergence” is reached

$$G(h, x) = \frac{f(x + h) - f(x - h)}{2h} + \epsilon \frac{\sin \omega (x + h) - \sin \omega (x - h)}{2h}$$

i.e. we let $\Delta G(h, x)$ remain SMALL !!!
Importance of the regularization!
Conclusions

- the **LIT** represents an accurate viable method on the way from

  \[ \text{\textit{ab initio}} \text{ NUCLEAR STRUCTURE} \]

  \[ \text{\textit{ab initio}} \text{ NUCLEAR REACTIONS} \]

  also for \( A>3 \)

- it allows to calculate reactions to the “far” continuum where the many-body scattering problem (all channels!) is not solvable

- only **bound state** technique is needed
Conclusions

- there is no discretization of the continuum: the LIT equation is bound-state like
- since the LIT is calculated numerically a regularization procedure is demanded to solve the integral equation (inversion of the LIT)
- the bell shaped kernel makes the regularization procedure “inexpensive”, and allows to control instabilities.
Future work

ab initio, small $A$
($A < 8$)

understand the only input
( nuclear interaction )

understand some “physics”

= 

( translate into languages we are used to in many-body theory )

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Future work

Apply LIT to larger systems with other bound state methods (NCSM, CC, MC ???)

The LIT in fields other than Nuclear Physics (small dots...???)