The Lorentz Integral Transform (LIT) method and its connections with other approaches

First proposed in
V. D. Efros, W. Leidemann and G. Orlandini,
Phys. Lett. **B**338, 130 (1994)

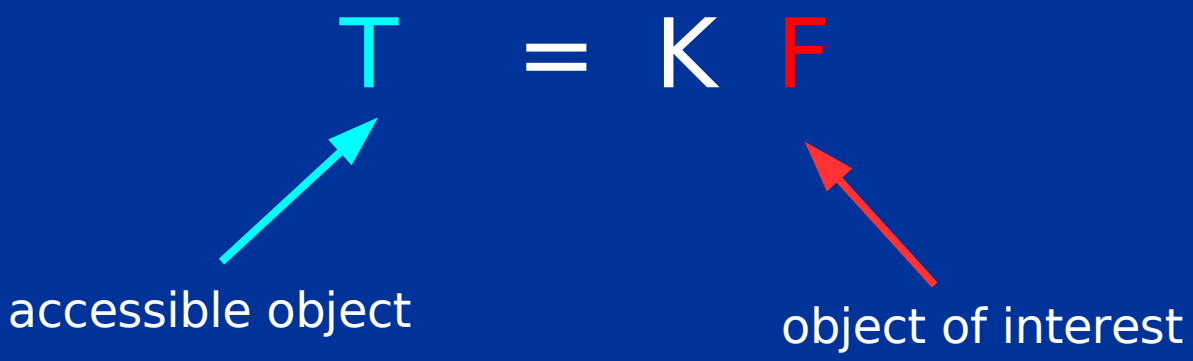
Recent Topical Review:
V. D. Efros, W. Leidemann, G. Orlandini and N. Barnea
"The Lorentz Integral Transform (LIT) method and its applications to perturbation induced reactions"
arXiv:0708.2803

The LIT method

- it is an ***ab initio*** method for **nuclear dynamics** calculations and in particular for **continuum** dynamics
- it is general enough to be applied to strong as well as electro-weak **reactions** of inclusive as well as exclusive nature
- the applications so far have been to electromagnetic and weak reactions on light nuclei.

Integral transform approaches

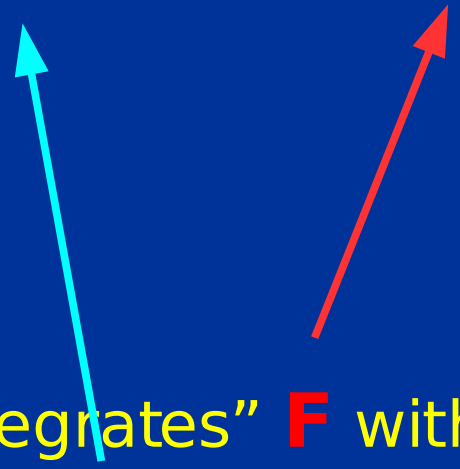
There are many examples in physics where one uses
“integral transform approaches”



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 **experimental physics** this is common in that one wants to extract information on the observable from the data which is obtained by means of the instrumentation.

$$T = K F$$



The instrument “integrates” **F** with the form of its “window” **K** and gives **T**

In theoretical physics:

Laplace Kernel

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

"Euclidean Correlation Function"

In Condensed Matter Physics:

Θ = Density Operator

$S(\omega)$ = Dynamical Structure Function

$\mathbf{\Phi}(\,\tau\,)$ is obtained with Monte Carlo Methods

In Nuclear Physics:

Θ= Charge or current density operator

$S(\omega) = \mathbf{R}(\omega)$ "Response" Function

(to e.w. excitation)

$\mathbf{\Phi}\,(\,\tau\,)$ is obtained with Monte Carlo Methods

In QCD

Θ = quark or gluon creation operator

$S(\omega)$ = Hadronic Spectral Function

τ = "Borel mass"

$\mathbf{\Phi}\,(\,\tau\,)$ is obtained by OPE - QCD sum rules or Lattice

$$\Phi(\tau) = \int d\omega \; K(\omega,\sigma)\, S(\omega)$$

One is able to calculate (or measure) $\Phi(\tau)$ but wants $S(\omega)$, which is the quantity of direct physical meaning.

Problem:

The "inversion" of $\Phi(\tau)$ may be an "ill posed problem"

Definition of "**well-posed**" problems in making mathematical models of physical phenomena (by Hadamard).:

1. A solution exists **2.** The solution is unique

3. The solution depends continuously on the inputs in some reasonable topology .

Continuum problems must often be **discretized** in order to obtain a numerical solution. While in terms of functional analysis such problems are typically continuous, they may suffer from **numerical instability** when solved with finite precision i.e. a small error in the initial data can result in much larger errors in the answers i.e. they become "**ill-posed**" problems

They need to be re-formulated for numerical treatment. Typically this involves including additional assumptions, such as smoothness of solution. This process is known as **regularization.**

The regularization procedure may be unstable

It is well known that the numerical inversion of the **Laplace** Transform is a terribly **ill-posed** problem

a “good” Kernel has to satisfy two requirements

1) one must be able to calculate the integral transform

2) one must be able to invert the transform, minimizing instabilities

What is the perfect Kernel?

What is the perfect Kernel?

the delta-function!

What would be the “perfect” Kernel?

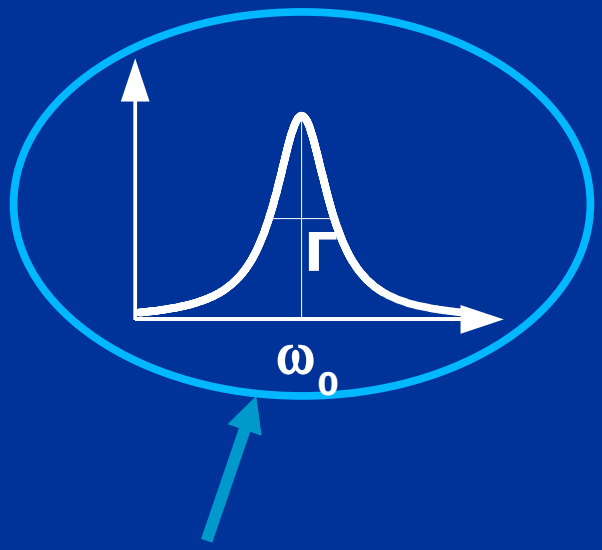
the delta-function!

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



$$\Phi(\omega, \Gamma) = \int [(\omega - \omega_0)^2 + \Gamma^2]^{-1} \, S(\omega) \, d\omega$$

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(ω)** defined as

(for example for perturbation induced inclusive reactions)

$$R(\omega) = \sum\!\!\!\!\!\!\int_n |\langle n|\Theta|0\rangle|^2 \, \delta(\omega - E_n + E_0)$$

Using the **Lorentz Kernel** one has the following theorem:

Closure = 1

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

$$= \int_{E_{th}^-}^{\infty} d\omega \sum dn \frac{|\langle n|\Theta|0\rangle|^2 \delta(\omega - E_n + E_0)}{(\omega-\omega_0-i\Gamma)(\omega-\omega_0+i\Gamma)}$$

$$= \sum dn < 0|\Theta^\dagger \frac{1}{(E_n - E_0 - \omega_0 - i\Gamma)}|n>$$

$$< n|\frac{1}{(E_n - E_0 - \omega_0 + i\Gamma)}\Theta|0>$$

$$= \sum dn < 0|\Theta^\dagger \frac{1}{(H - E_0 - \omega_0 - i\Gamma)}|n><n|$$

$$\frac{1}{(H - E_0 - \omega_0 + i\Gamma)}\Theta|0>$$

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

$$=<\tilde{\Psi}|\tilde{\Psi}>$$

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

Using the **Lorentz Kernel** one has the following theorem:

Closure = 1

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

$$= \int_{E_{th}^-}^{\infty} d\omega \sum dn \frac{|\langle n|\Theta|0\rangle|^2 \delta(\omega - E_n + E_0)}{(\omega-\omega_0-i\Gamma)(\omega-\omega_0+i\Gamma)}$$

$$= \sum dn < 0|\Theta^\dagger \frac{1}{(E_n - E_0 - \omega_0 - i\Gamma)}|n>$$

$$< n|\frac{1}{(E_n - E_0 - \omega_0 + i\Gamma)}\Theta|0>$$

$$= \sum dn < 0|\Theta^\dagger \frac{1}{(H - E_0 - \omega_0 - i\Gamma)}|n>< n|$$

$$\frac{1}{(H - E_0 - \omega_0 + i\Gamma)}\Theta|0>$$

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

$$= < \tilde{\Psi}|\tilde{\Psi}>$$

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

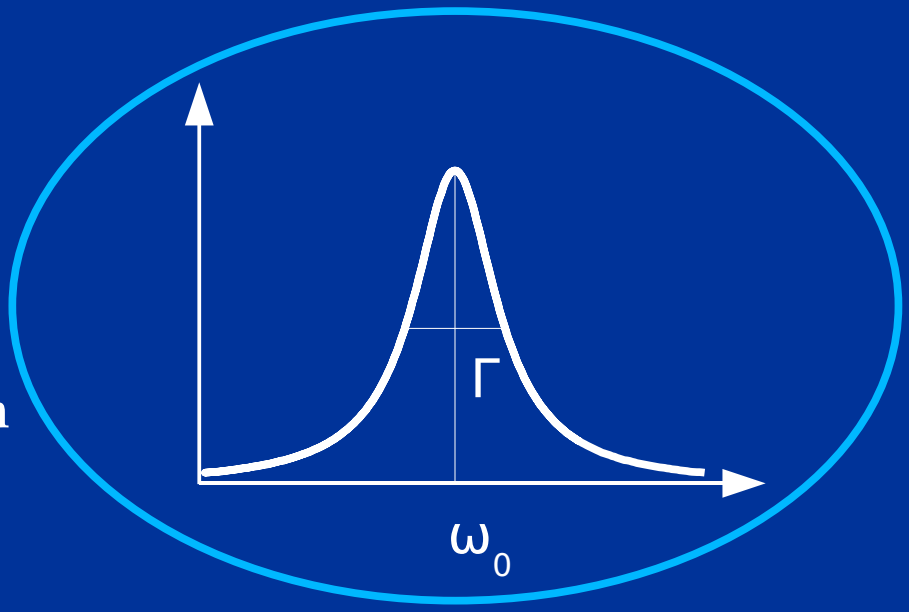
Summarizing:

choosing the 2-parameter kernel

$L(\omega,\omega_0,\Gamma)$ the 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

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

The LIT in practice:

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

is found solving for fixed Γ and many ω_0

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

2. the overlap $\left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle$ is calculated

3. the transform is inverted

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

main point of the LIT :

Schrödinger-like equation with a source

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

$S = \Theta\,|0\rangle$

main point of the LIT :

Schrödinger-like equation with a source

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

Theorem:

The $\tilde{\Psi}$ solution is unique and has ***bound state*** asymptotic behavior

main point of the LIT :

Schrödinger-like equation with a source

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

Theorem:

The $\tilde{\Psi}$ solution is unique and has ***bound state*** asymptotic behavior

→ one can apply ***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, ...???)
- applies both to inclusive reactions (straightforward!) and to exclusive ones
- has been benchmarked in “directly solvable” systems (A=2,3)

A very good method to solve bound states:

the Effective Interaction in Hyperspherical Harmonics method (EIHH)

N.Barnea, W.Leidemann, G.O.
PRC61(2000)054001

- similar idea as for the No Core Shell Model method i.e. use of Effective Interaction
- applied to H.H. instead of H.O.
- avoids the $\Omega_{H.O.}$ parameter dependence
- fast convergence
- can be applied to A>3

Benchmarks:

- with R(ω) calculated with traditional differential equation algorithm in A=2 [V.D.Efros et al. Phys. Lett. **B**338, 130 (1994)]

- with R(ω) calculated with Faddeev solutions in the continuum in A=3 [J.Golak et al. [Nucl. Phys. A707 (2002) 365]

For A>3 no other benchmark is possible!
NO viable solution of the scattering problem beyond the 3-body break up threshold for A=4 and larger.

The LIT approach is at present the only viable one!

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

1. Eigenvalue method: $\tilde{\Psi}$ **can** be expanded on localized functions

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

$$|\tilde{\Psi}\rangle = \sum_{\nu}^{N} \frac{\langle \varphi_\nu^N | S\rangle}{\epsilon_\nu^N - E_0 - \omega_0 + i\Gamma} |\varphi_\nu^N\rangle \,,$$

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

sum of Lorentzians around $\varepsilon_{\upsilon}^{N}$

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

2. Lanczos method

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

$$\Phi(\omega_0,\Gamma) = -\frac{1}{\Gamma}\mathrm{Im}\left\{ \langle S| \frac{1}{\omega_0 + i\Gamma + E_0 - \hat{H}} |S\rangle \right\}$$

$$\Phi(\omega_0,\Gamma) = -\frac{1}{\Gamma}\mathrm{Im}\left\{ \frac{\langle S|S\rangle}{z - a_0 - \dfrac{b_1^2}{z - a_1 - \dfrac{b_2^2}{z - a_2 - b_3^2 \ldots}}} \right\} .$$

Illustration of requirement N.2: one can invert the integral transform minimizing instabilities

Inversion of the LIT: the **regularization** method

$$R(\omega) = \sum_{n=1}^{N_{max}} c_n \chi_n(\omega, \alpha_i) \qquad (1)$$

The χ_n are given functions with nonlinear parameters α_i. A basis set frequently used for LIT inversions is

$$\chi_n(\omega, \alpha_i) = \omega^{\alpha_1} \exp(-\frac{\alpha_2 \omega}{n}) \,. \qquad (2)$$

Substituting such an expansion in the integral equation

$$\Phi(\omega_0, \Gamma) = \sum_{n=1}^{N_{max}} c_n \tilde{\chi}_n(\omega_0, \alpha_i) \,, \qquad (3)$$

where

$$\tilde{\chi}_n(\omega_0, \alpha_i) = \int_0^\infty d\omega \frac{\chi_n(\omega, \alpha_i)}{(\omega - \omega_0)^2 + \Gamma^2} \,. \qquad (4)$$

For given α_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 ω_0 points much larger than N_{max}.

Inversion of the LIT: the **regularization** method

$$R(\omega) = \sum_{n=1}^{N_{max}} c_n \chi_n(\omega, \alpha_i) \qquad (1)$$

The χ_n are given functions with nonlinear parameters α_i. A basis set frequently used for LIT inversions is

$$\chi_n(\omega, \alpha_i) = \omega^{n_1} \exp(-\frac{\alpha_2 \omega}{n}) \,. \qquad (2)$$

Substituting such an expansion in the integral equation

$$\Phi(\omega_0, \Gamma) = \sum_{n=1}^{N_{max}} c_n \tilde{\chi}_n(\omega_0, \alpha_i) \,, \qquad (3)$$

where

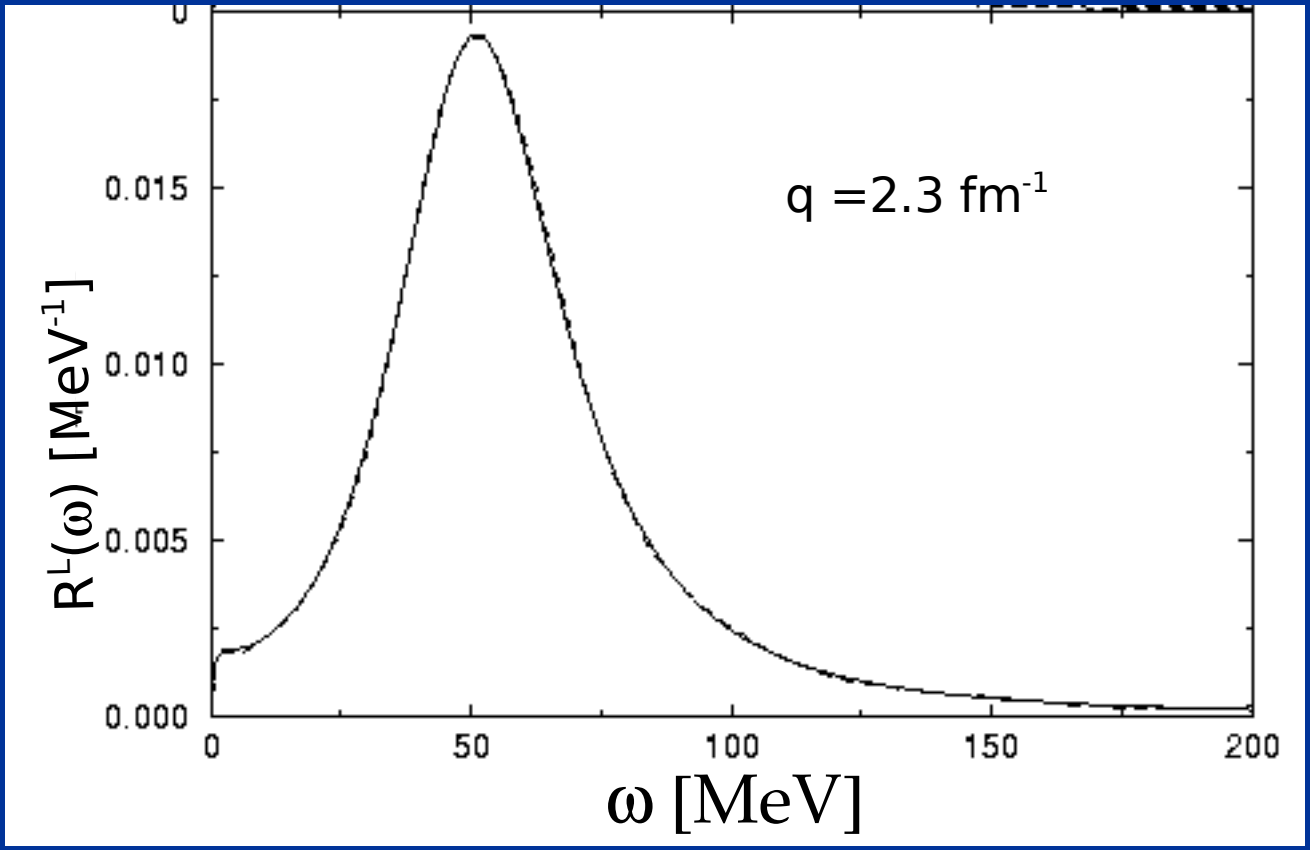
$$\tilde{\chi}_n(\omega_0, \alpha_i) = \int_0^\infty d\omega \frac{\chi_n(\omega, \alpha_i)}{(\omega - \omega_0)^2 + \Gamma^2} \,. \qquad (4)$$

For given α_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 ω_0 points much larger than N_{max}.

works quite well with bell-shaped kernels!

test on the Deuteron:

R(ω) is the longitudinal (e,e') response function



Phys Lett. B338 (1994) 130

Importance of the regularization:

Remember the practical calculation of $\Phi(\omega, \Gamma)$

the eigenvalue method implies that

$\Phi(\omega, \Gamma)$ is a sum of Lorentzians around $\varepsilon_{\upsilon}^{N}$

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

$$|\tilde{\Psi}\rangle = \sum_{\nu}^{N}\frac{\langle\varphi_\nu^N|S\rangle}{\epsilon_\nu^N-E_0-\omega_0+i\Gamma}|\varphi_\nu^N\rangle\,,$$

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

Remember the practical calculation of $\Phi(\omega, \Gamma)$

the eigenvalue method implies that

$\Phi(\omega, \Gamma)$ is a sum of Lorentzians around $\varepsilon_{\upsilon}^{N}$

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

$$|\tilde{\Psi}\rangle = \sum_{\nu}^{N}\frac{\langle\varphi_\nu^N|S\rangle}{\epsilon_\nu^N-E_0-\omega_0+i\Gamma}|\varphi_\nu^N\rangle\,,$$

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

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

$$R(\omega) = \lim_{\Gamma\to 0} R_\Gamma(\omega),$$

The extrapolation would give

$$R(\omega) = \sum_{n=1}^{N} r_n\delta(E_n-\omega).$$

Remember the practical calculation of $\Phi(\omega, \Gamma)$

the eigenvalue method implies that

$\Phi(\omega, \Gamma)$ is a sum of Lorentzians around $\varepsilon_{\upsilon}^{N}$

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

$$|\tilde{\Psi}\rangle = \sum_{\nu}^{N}\frac{\langle\varphi_\nu^N|S\rangle}{\epsilon_\nu^N-E_0-\omega_0+i\Gamma}|\varphi_\nu^N\rangle ,$$

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

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

$$R(\omega) = \lim_{\Gamma\to 0} R_\Gamma(\omega),$$

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

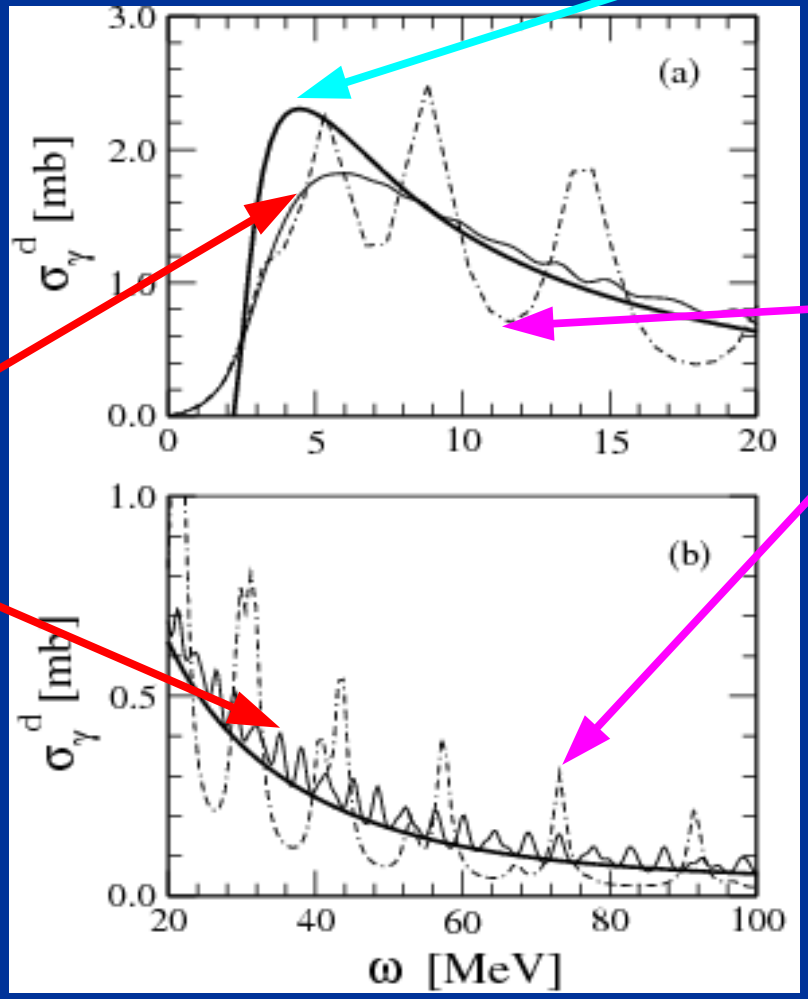
h.o. basis:

fixed Γ=1 MeV

N_{ho}=2400

"true"

N_{ho}=150



test on deuteron photodisintegration

"true"

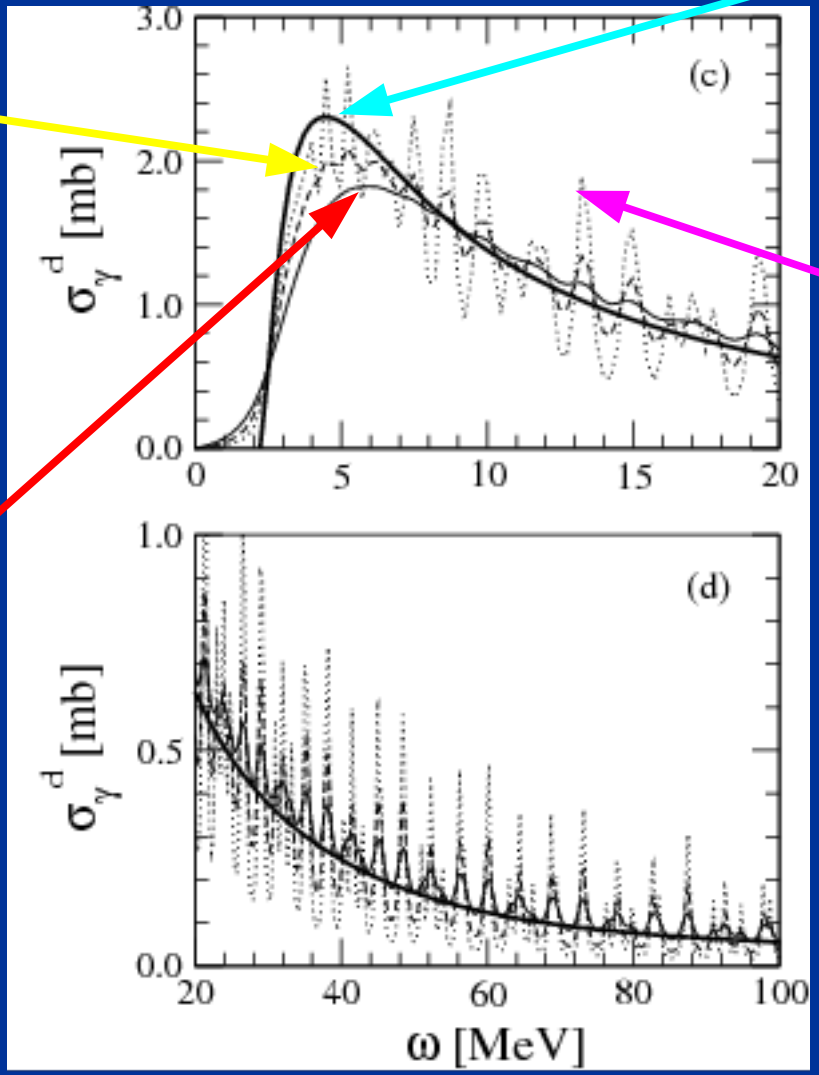
Γ= 0.5 MeV

h.o. basis:

fixed $N_{\eta o}$=2400

Γ=1 MeV

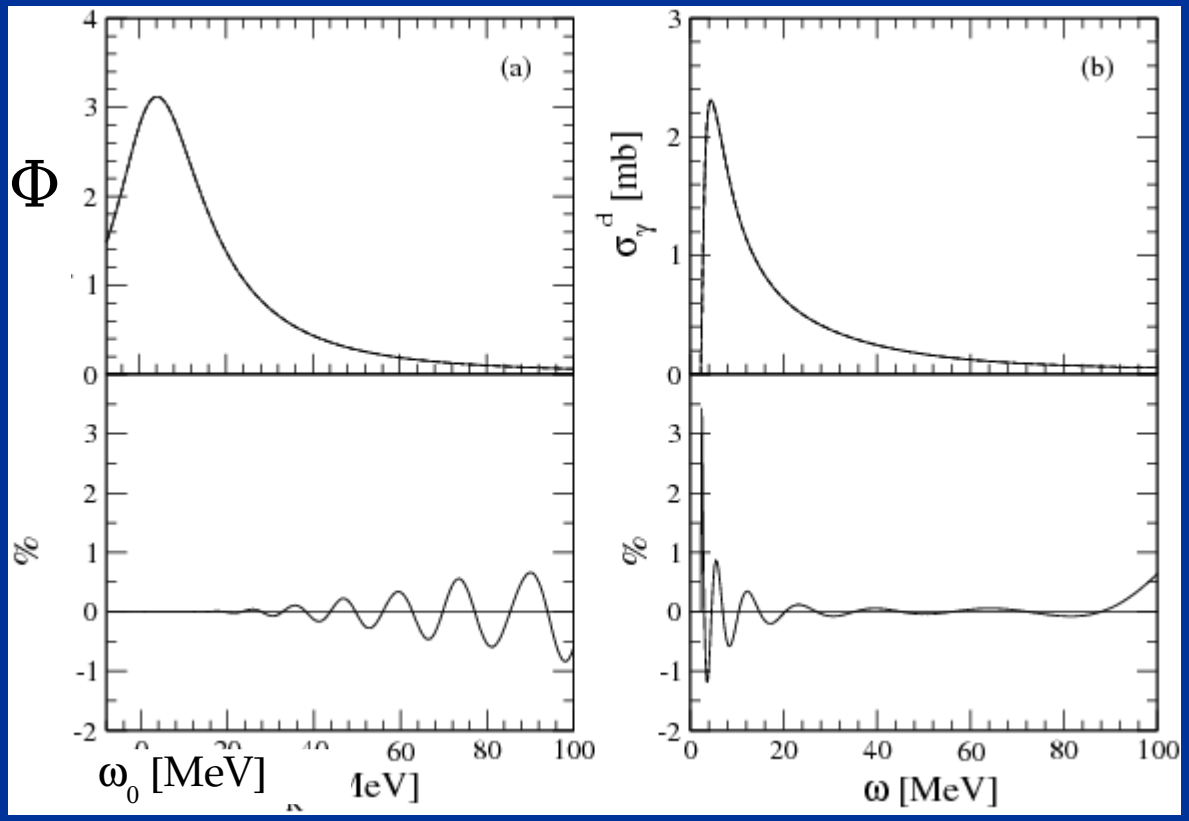
Γ=0.25 MeV



Γ=10 MeV
+ inversion / regularization

N_{ho}=150

N_{ho}=2400



N_{ho}=150 is enough for accuracies at the % level!!

Conclusions

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

ab initio NUCLEAR STRUCTURE

ab initio NUCLEAR REACTIONS

also for **A>3** (see Bacca's talk)

- 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.