On the determination of response functions obtained from their Lorentz integral transforms

V.D. Efros and V.Y. Shalamova (MEPhI and Kurchatov Institute)

and W. Leidemann

UNIVERSITÀ DEGLI STUDI DI TRENTO

INFN

Outline

- Motivation
- Integral Transform Approach
- Inversion: can go wrong!

Motivation

Problem: Calculation of Reactions

involving the many-body continuum

- Integral transform methods: calculation of continuum wf can be avoided

- Nonetheless only few groups use this technique for nuclear reactions

  Probably most important reason: The necessary inversion of the integral transform

Motivation

Problem: Calculation of Reactions

involving the many-body continuum

- Integral transform methods: calculation of continuum wf can be avoided
- Nonetheless only few groups use this technique for nuclear reactions

  Probably most important reason: The necessary inversion of the integral transform

ILL-POSED

Integral transform approaches

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

$$\Phi \quad = \; K \; R$$

accessible object

object of interest

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.

KERNEL

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

One is able to calculate $\Phi(\sigma)$ but wants $R(\omega)$, which is the quantity of direct physical meaning.

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

One is able to calculate $\Phi(\sigma)$ but wants $R(\omega)$, which is the quantity of direct physical meaning.

Warning:

The “inversion” of $\Phi(\sigma)$ may be problematic (“**ill posed problem**”)

LIT method

The LIT of a function $R(E)$ is defined as follows

$$\Rightarrow \quad L(\sigma) = \int dE\, \mathcal{L}(E,\sigma)\, R(E)\,,$$

where the kernel $\mathcal{L}$ is a Lorentzian,

$$\Rightarrow \quad \mathcal{L}(E,\sigma) = \frac{1}{(E-\sigma_R)^2 + \sigma_I^2}$$

For inclusive reactions the LIT $L(\sigma)$ is calculated by solving an equation of the form

$$\boxed{(H-\sigma)\,\tilde{\Psi} = S\,,}$$

where H is the Hamiltonian of the system under consideration and S is an asymptotically vanishing source term related to the operator inducing the specific reaction.

The solution $\tilde{\Psi}$ is localized and the LIT is given by

$$\boxed{L(\sigma) = \langle \tilde{\Psi} | \tilde{\Psi} \rangle\,.}$$

Alternative way:

$$L(\sigma) = -\frac{1}{\sigma_I} Im(\langle S | \frac{1}{\sigma_R + i\sigma_I - H} | S \rangle)\,.$$

Inversion of the LIT

- LIT is calculated for a fixed σ_I in many σ_R points

- Express the searched response function formally on a basis set with M basis basis functions $f_m(E)$ and open coefficients c_m with correct threshold behaviour for the $f_m(E)$ (e.g., $f_m = f_{thr}(E) \exp(-\alpha E/m)$)

- Make a LIT transform of the basis functions and determine coefficents c_m by a fit to the calculated LIT

- Increase M up to the point that a sufficient convergence is obtained (uncontrolled oscillations should not be present)

A regularization method is needed for the inversion

ILL-POSED

ILL-POSED

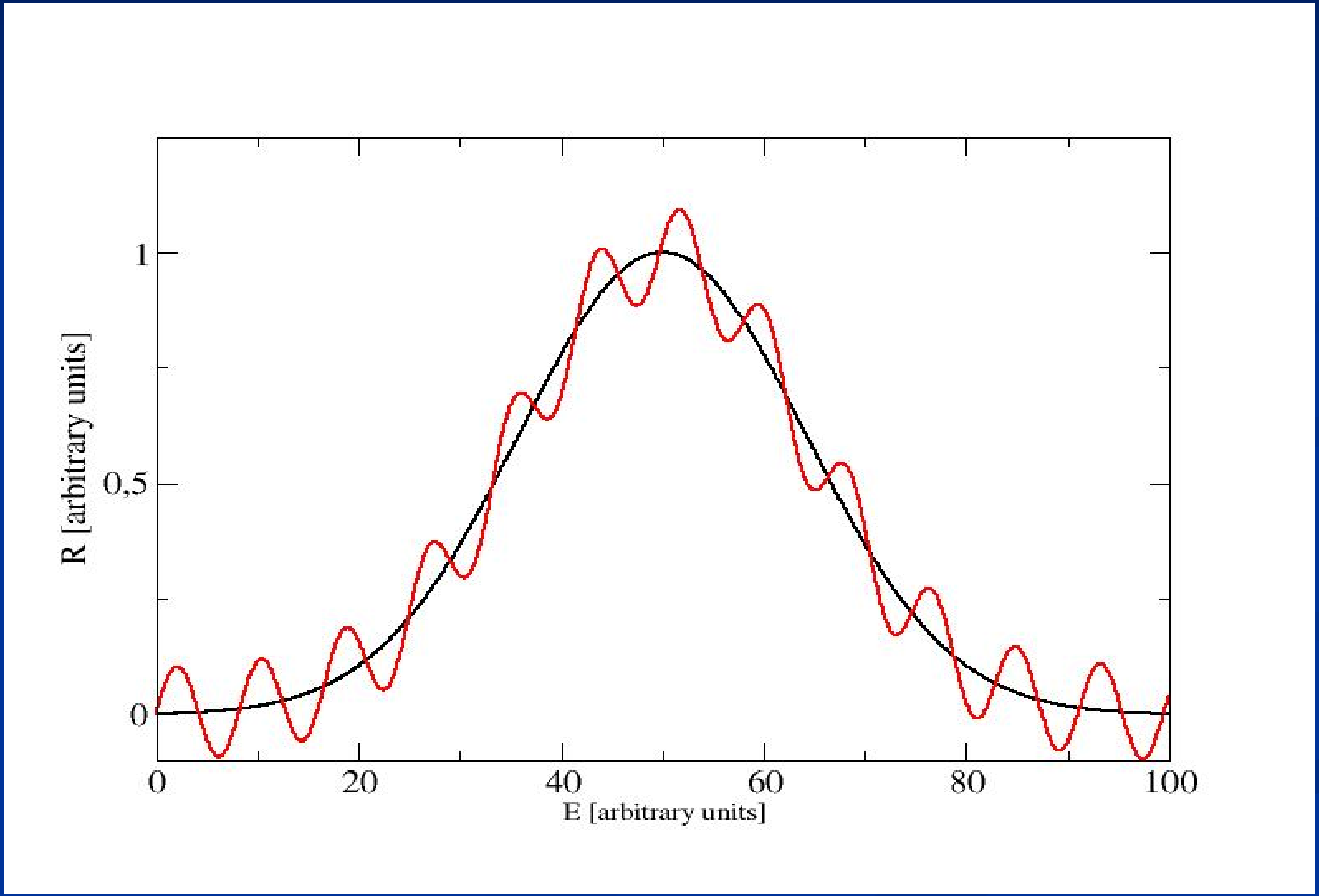
What does it mean?

ILL-POSED

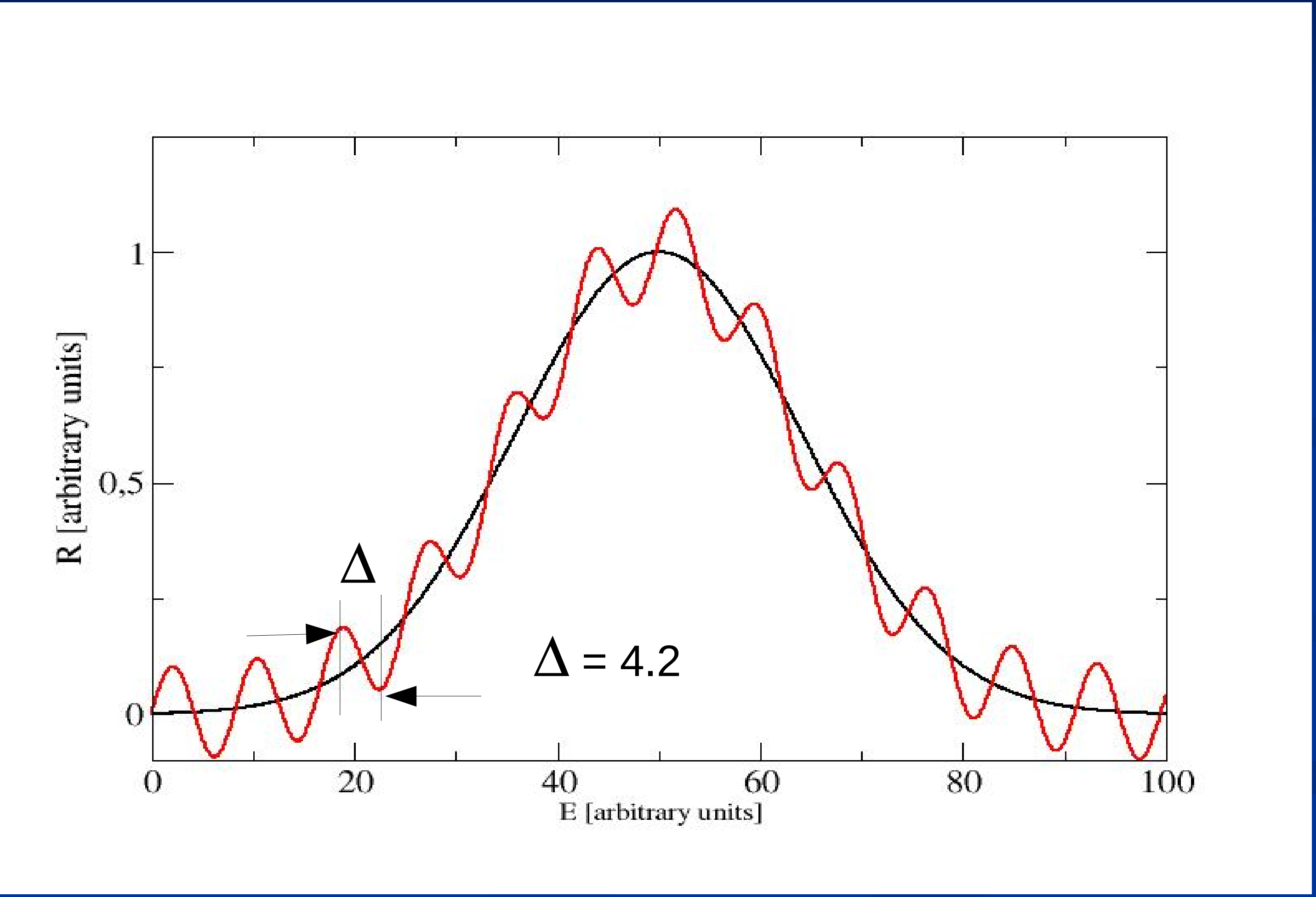
What does it mean?

Let us check an example

Example: black and red responses

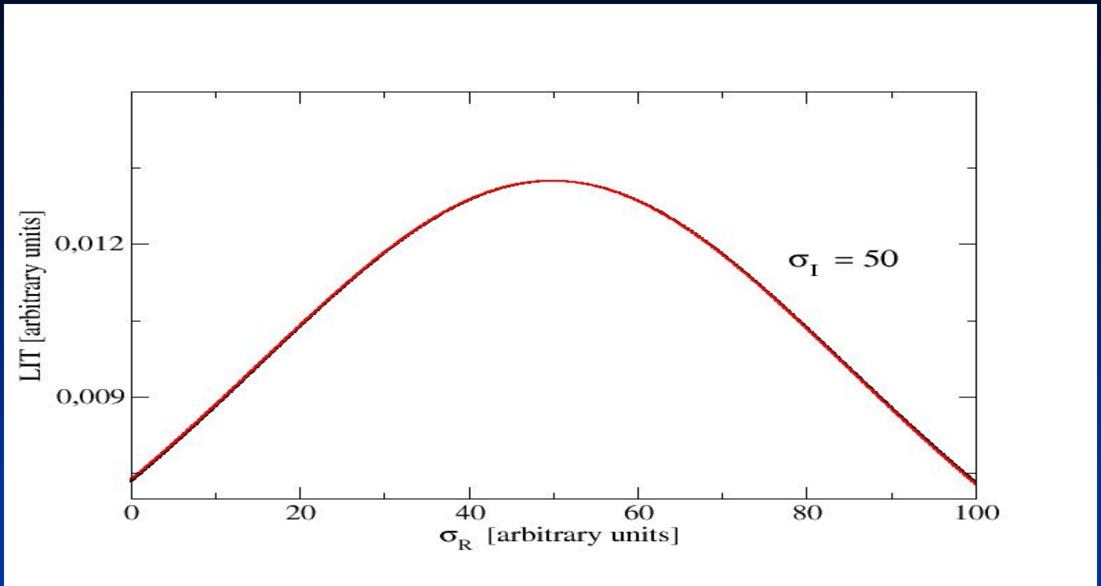


Example: black and red responses

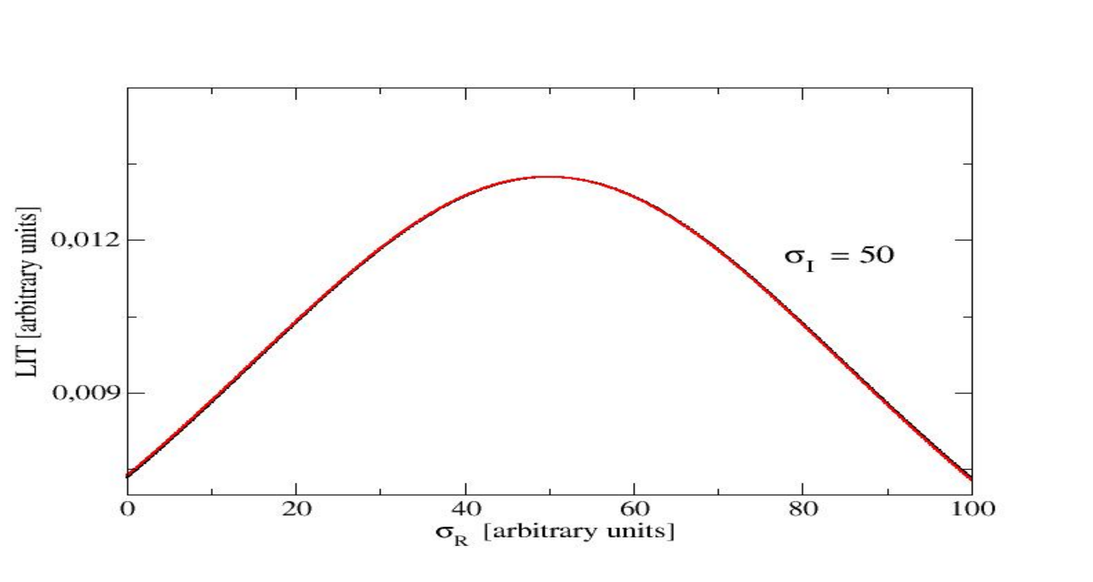


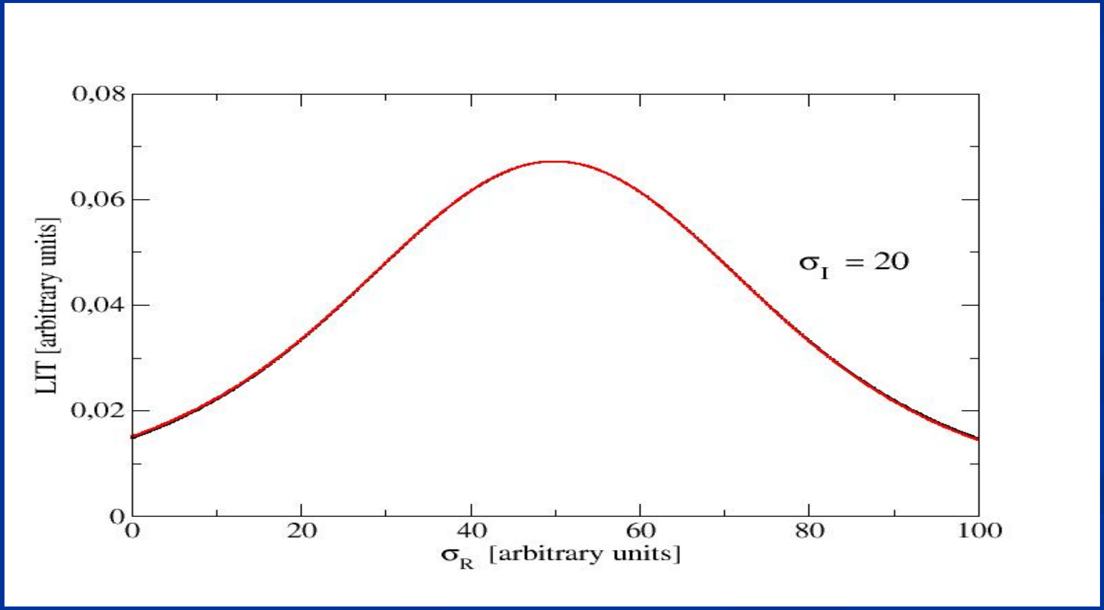
Now follows a series of LITs with various σ_I values

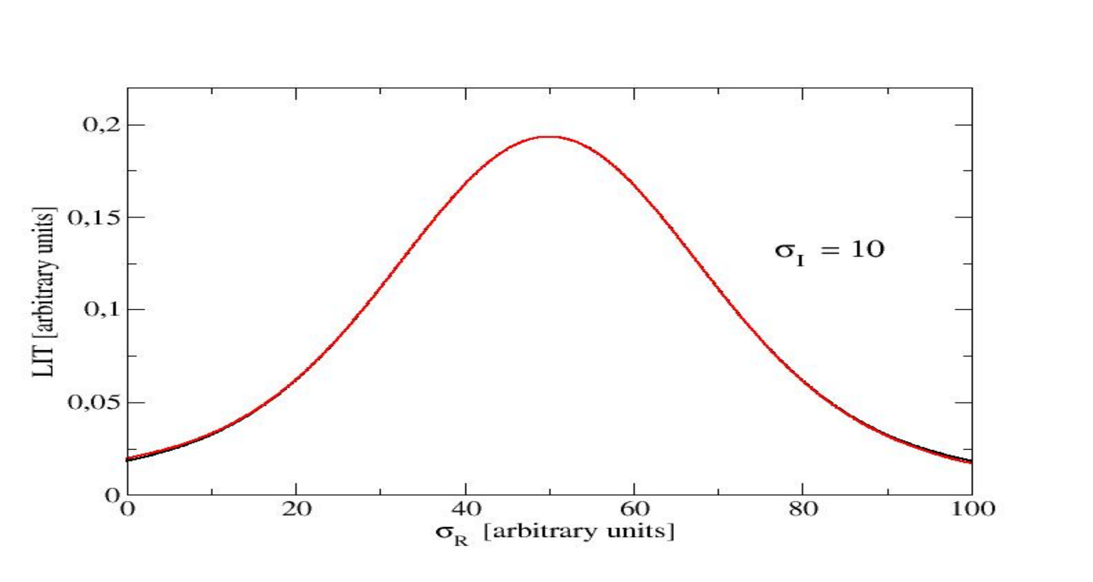
σ_I : 50 → 1 [arbitrary units]

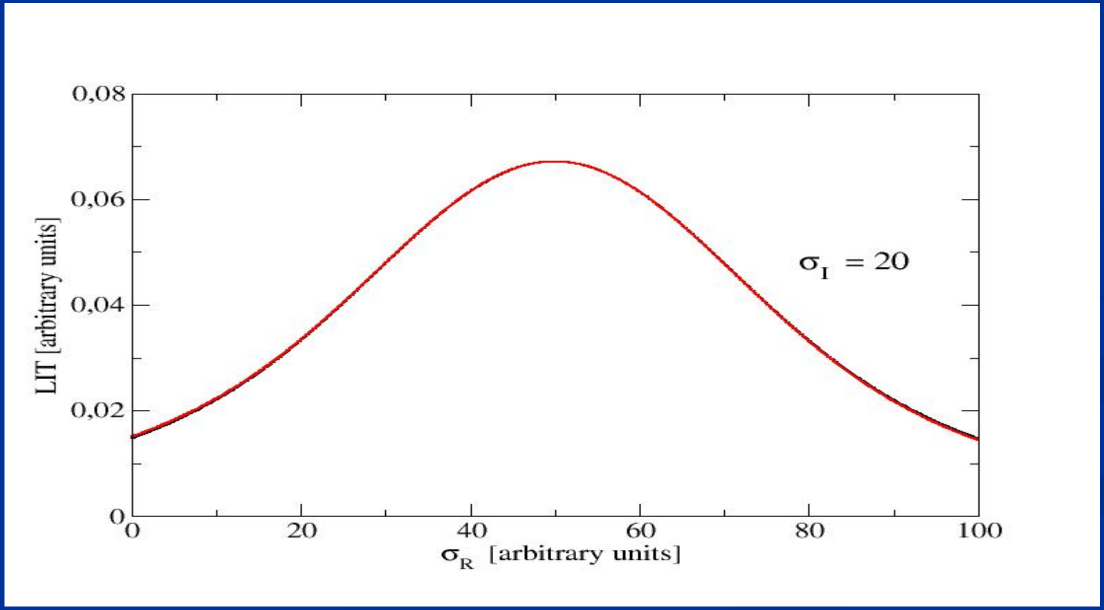


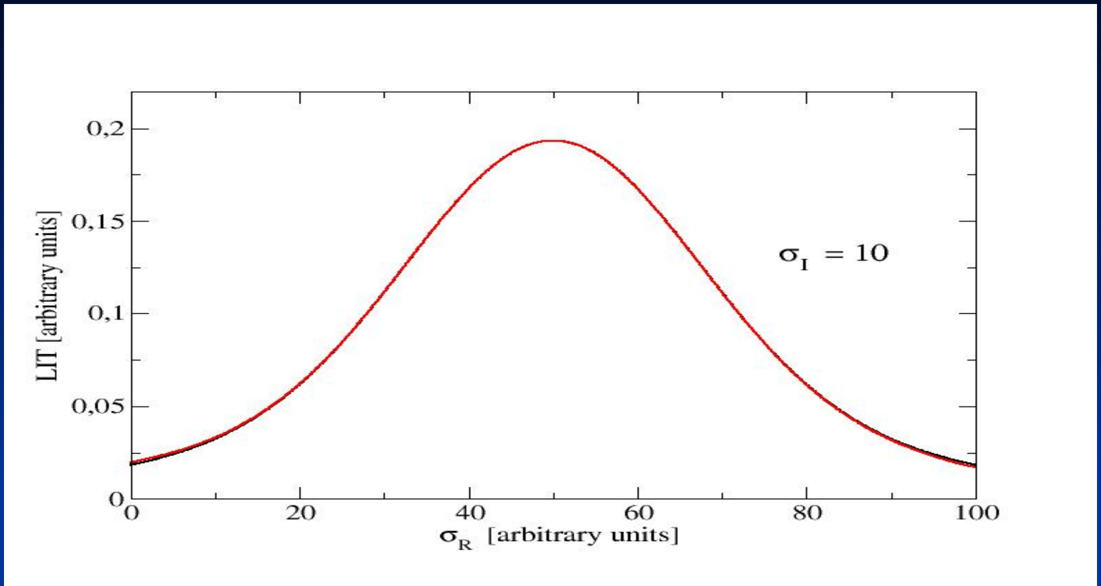
LIT [arbitrary units]
0,012
0,009
σ_I = 50
0
20
40
60
80
100
σ_R [arbitrary units]

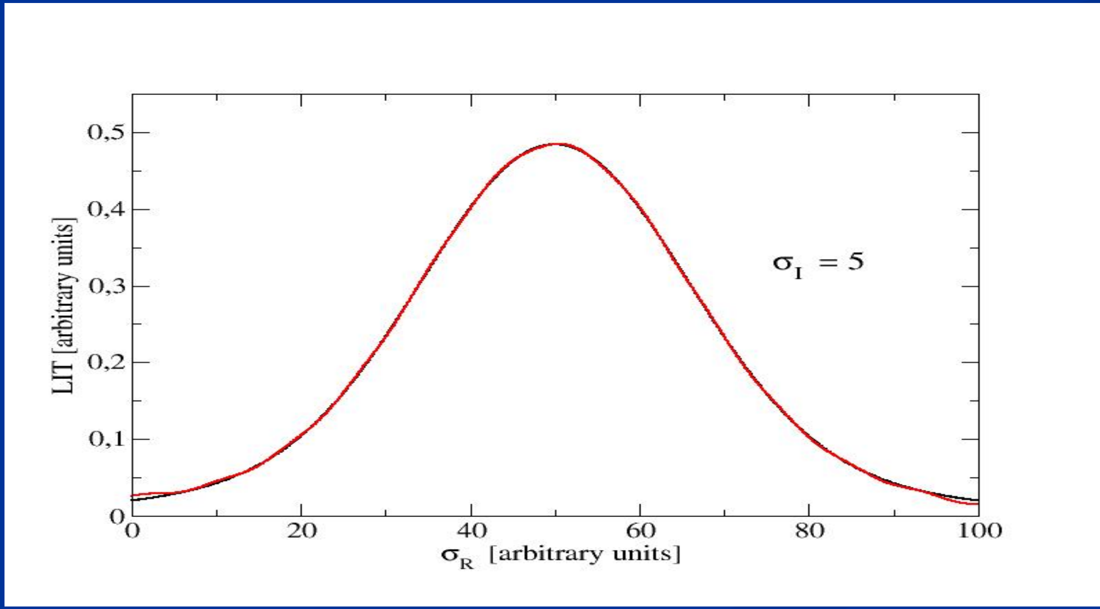

LIT [arbitrary units]
0,012
0,009
σI = 50
0
20
40
60
80
100
σR [arbitrary units]

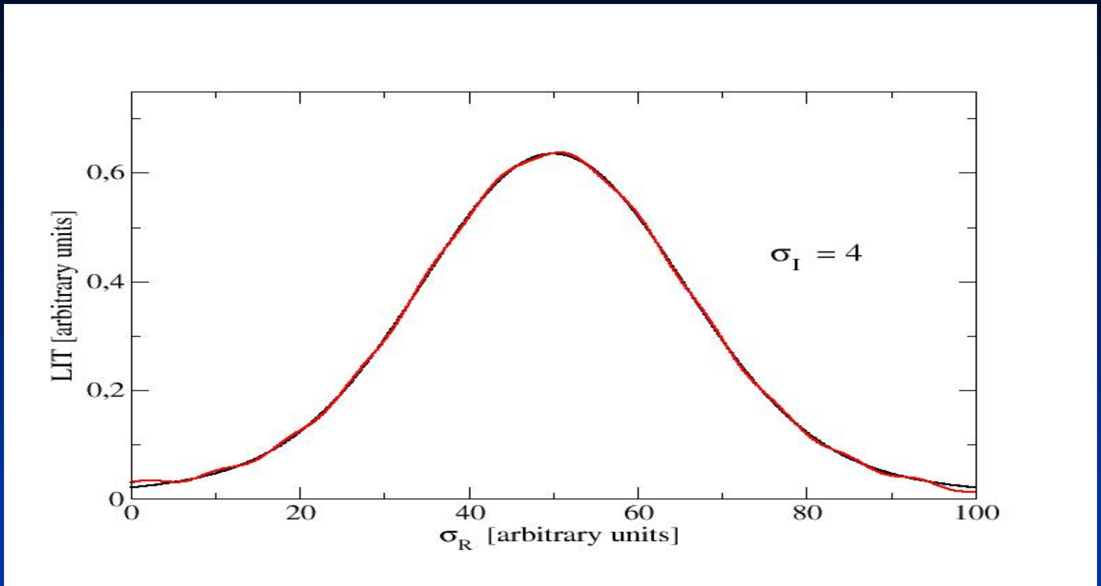

0,08
0,06
0,04
0,02
0
LIT [arbitrary units]
σI = 20
0
20
40
60
80
100
σR [arbitrary units]

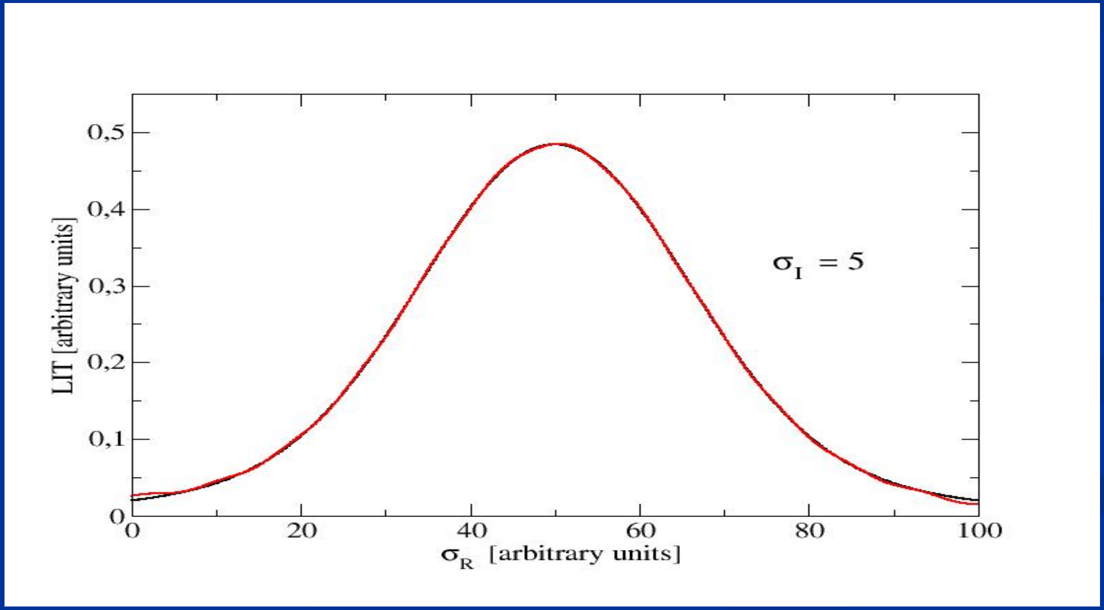

0,2
0,15
0,1
0,05
0
LIT [arbitrary units]
0
20
40
60
80
100
σR [arbitrary units]
σI = 10

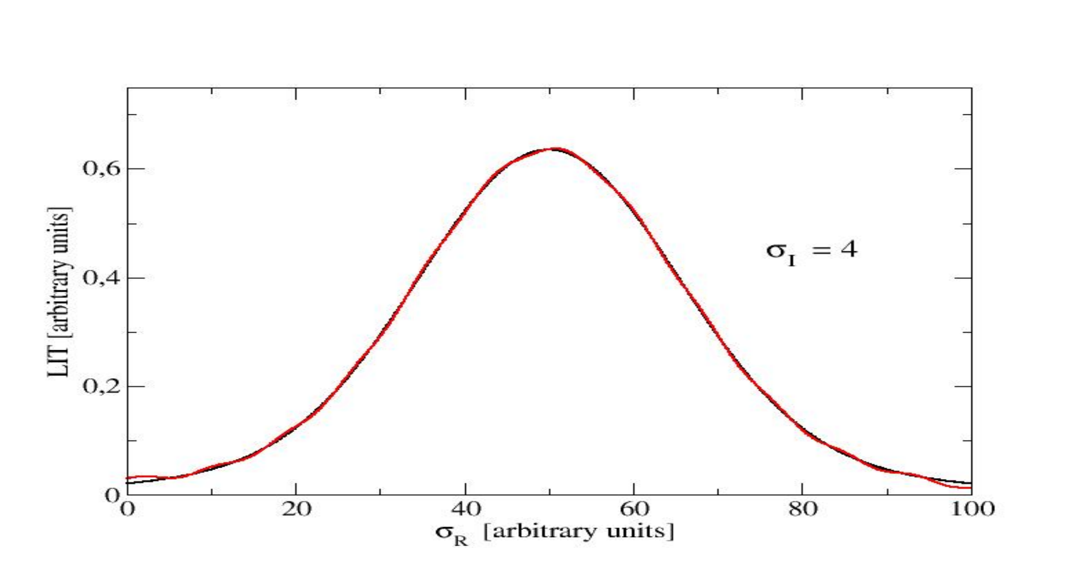

0,08
0,06
0,04
0,02
0
LIT [arbitrary units]
0
20
40
60
80
100
σR [arbitrary units]
σI = 20


LIT [arbitrary units]
0,2
0,15
0,1
0,05
0
20
40
60
80
100
σI = 10
σR [arbitrary units]

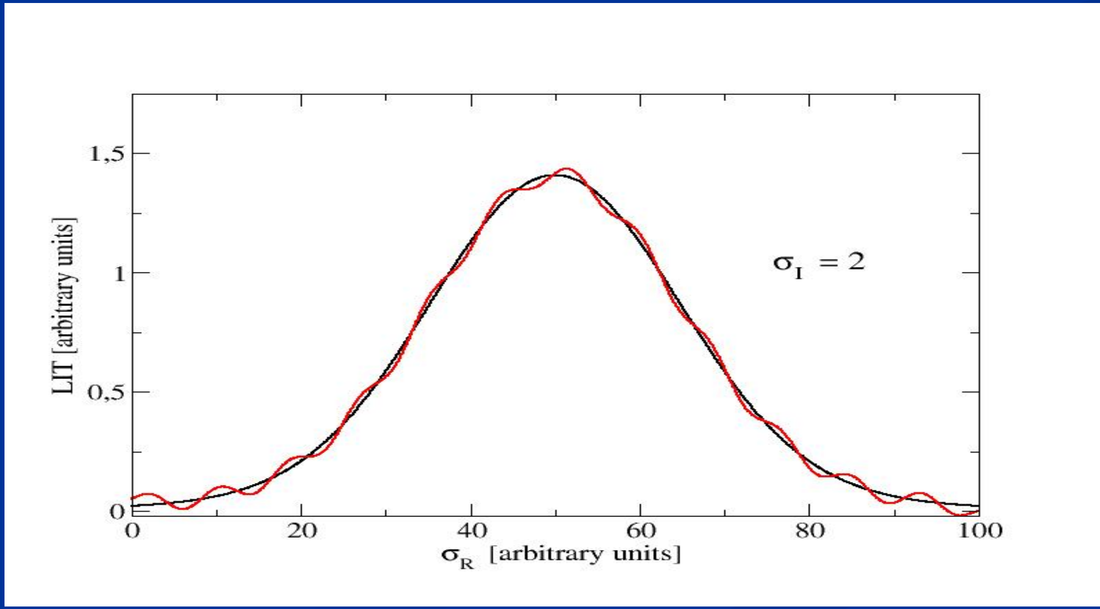

LIT [arbitrary units]
0,5
0,4
0,3
0,2
0,1
0
20
40
60
80
100
σI = 5
σR [arbitrary units]


0,6
0,4
0,2
0
LIT [arbitrary units]
$\sigma_I = 4$
0 20 40 60 80 100
σ_R [arbitrary units]

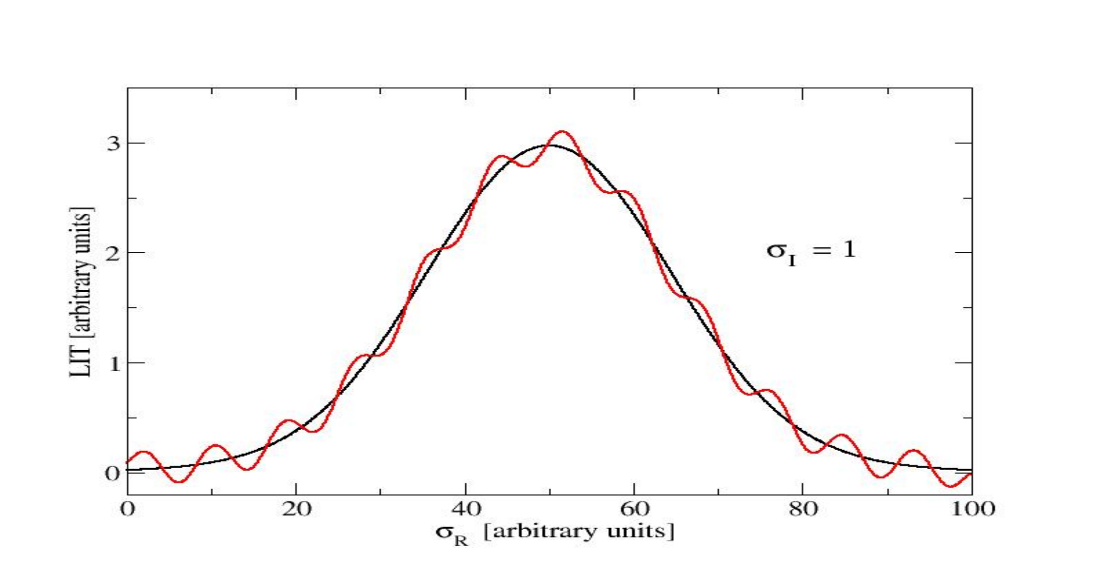

0,5
0,4
0,3
0,2
0,1
0
LIT [arbitrary units]
$\sigma_I = 5$
0 20 40 60 80 100
σ_R [arbitrary units]



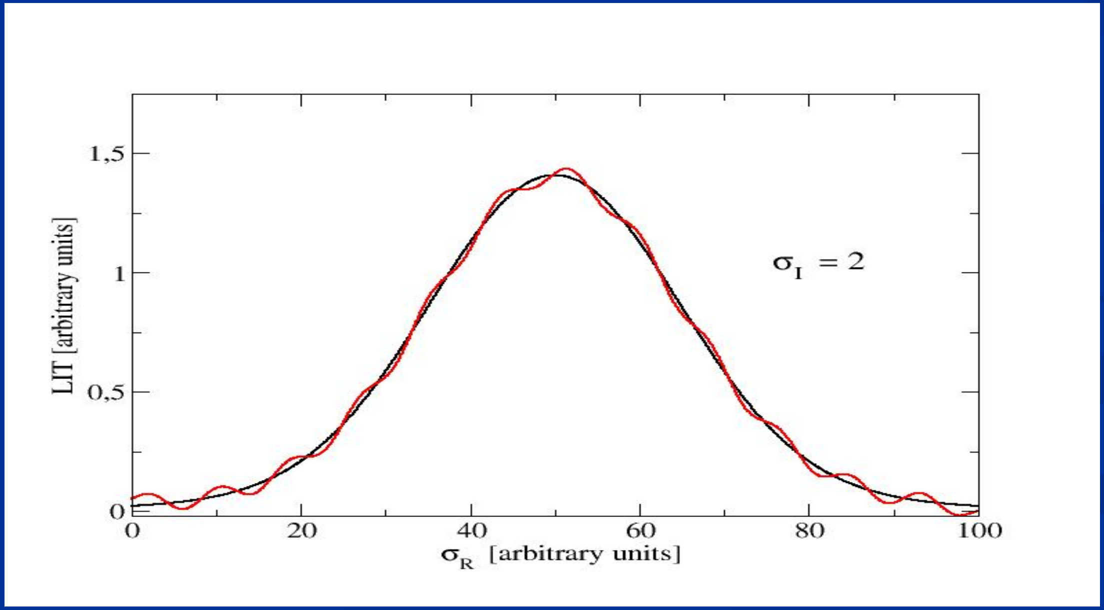
LIT [arbitrary units]
0,6
0,4
0,2
0
0
20
40
60
80
100
σ_R [arbitrary units]
σ_I = 4



LIT [arbitrary units]
1,5
1
0,5
0
0
20
40
60
80
100
σ_R [arbitrary units]
σ_I = 2



LIT [arbitrary units]
$\sigma_I = 1$
σ_R [arbitrary units]



LIT [arbitrary units]
$\sigma_I = 2$
σ_R [arbitrary units]

Conclusion:

LIT method is a method with a controlled resolution

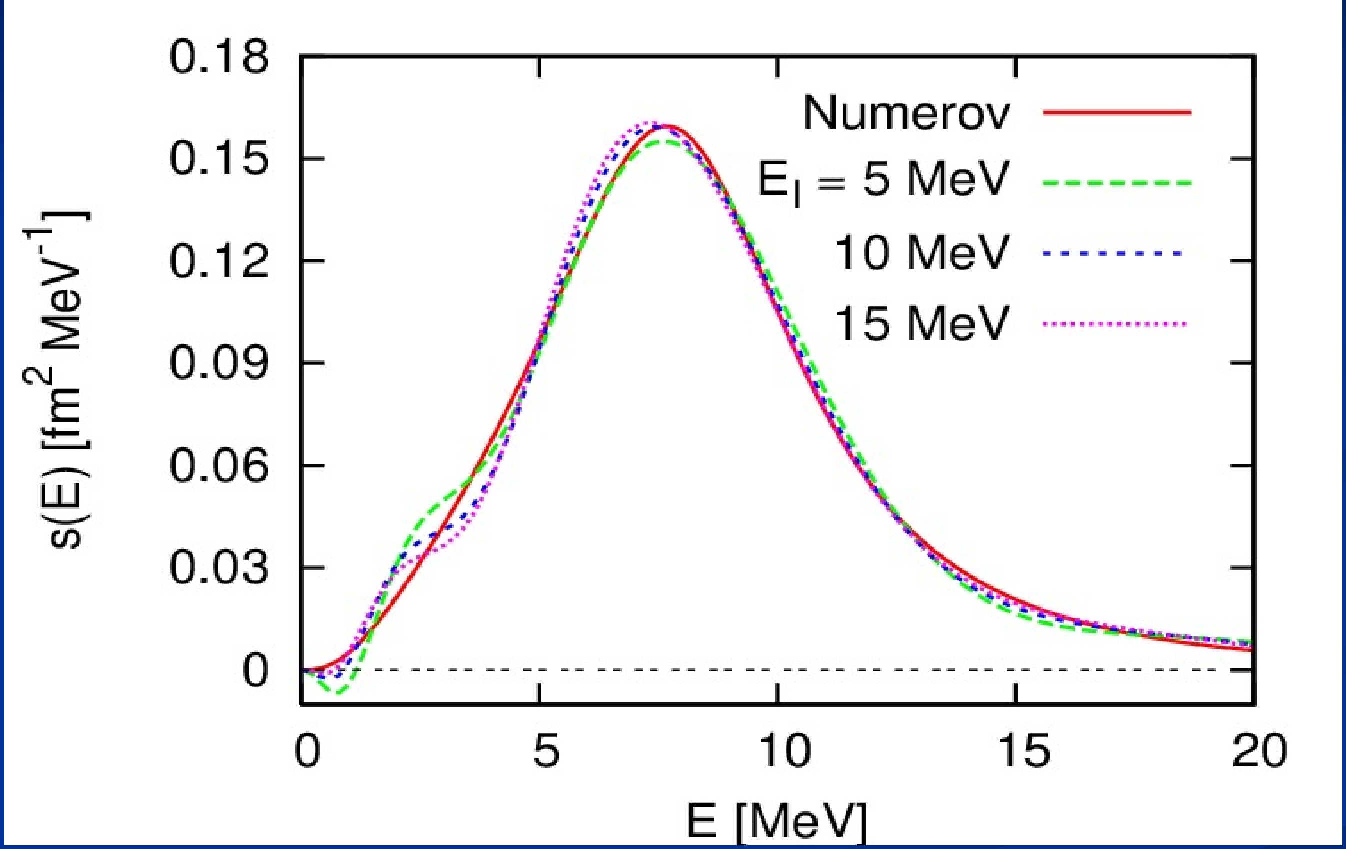
Consequence: discard inversions with structures having a width smaller than σ_I

Example from the literature that things can go wrong

Y. Suzuki, W. Horiuchi, D. Baye, Prog. Theor. Phys. 123, 547 (2010)

Electric dipole Photodisintegration of a three-particle system interacting via a hypercentral potential

Model is equivalent to a one-body problem in which the hypercentral potential is represented by a central one and a nucleon with orbital angular momentum 3/2 bound in this potential passes to the continuum state with orbital angular momentum 5/2



From: Y. Suzuki, W. Horiuchi, D. Baye, Prog. Theor. Phys. 123, 547 (2010)

Reconsideration of the same Problem

(V.D. Efros, WL, V.Yu. Shalamova)

Calculation of wave functions and LIT: HO expansion

- Inversion with an extreme numerical precision
- Our standard inversion method

In both cases inversion with basis function set

$\chi_{\mathbf{n}}(E) = E^m \exp(-\alpha E/n)$ with m=3

(E^3 behaviour at threshold)

Results

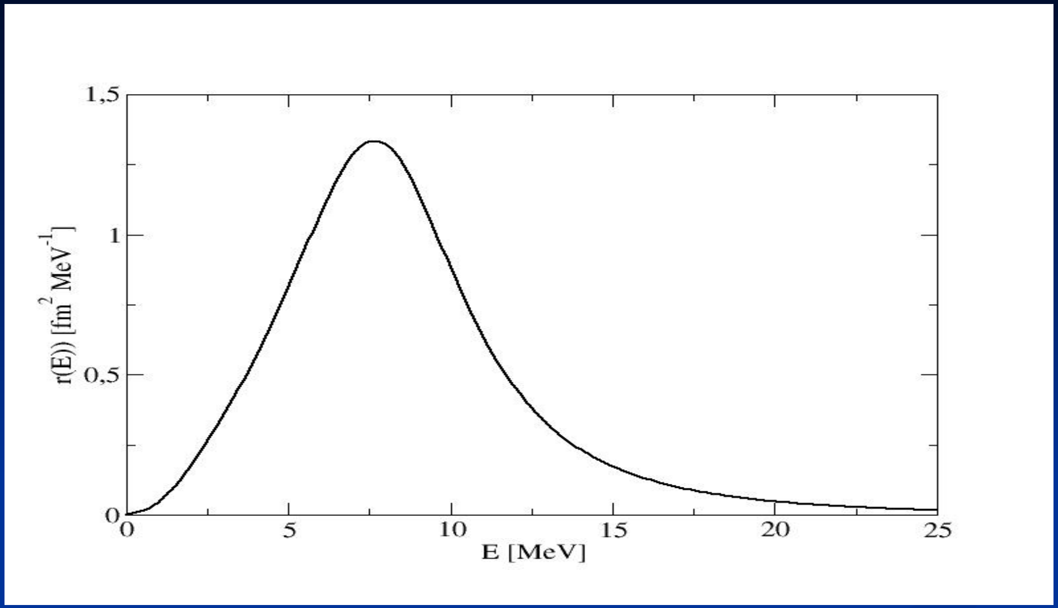
Ground-state energy: -3.49262845170356(1) MeV

Continuum state: Phase shifts with precision of 7 digits

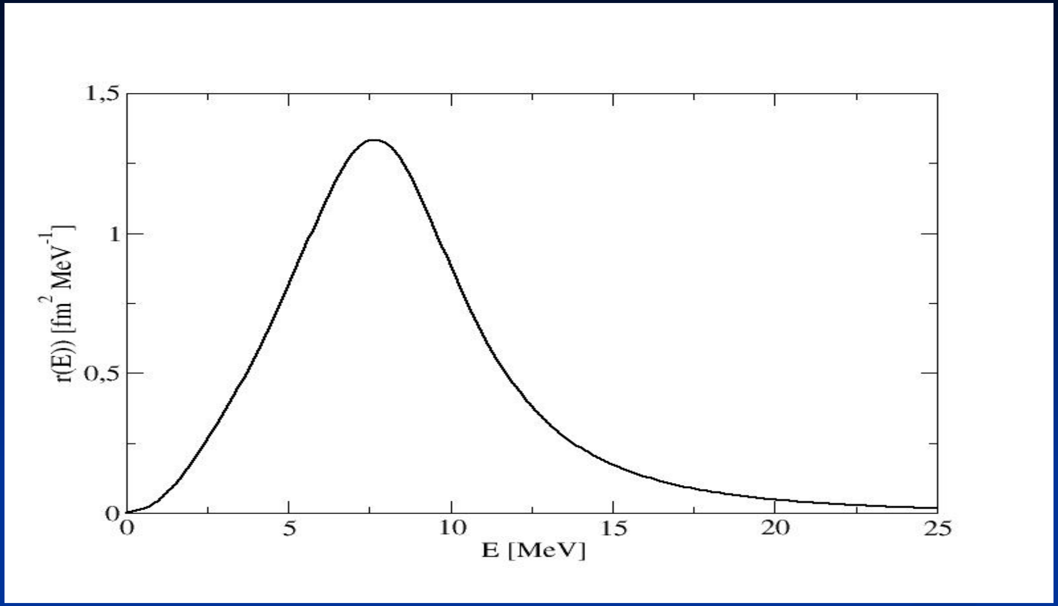
Response function with precision of 5 digits

LIT with precision of 7 digits

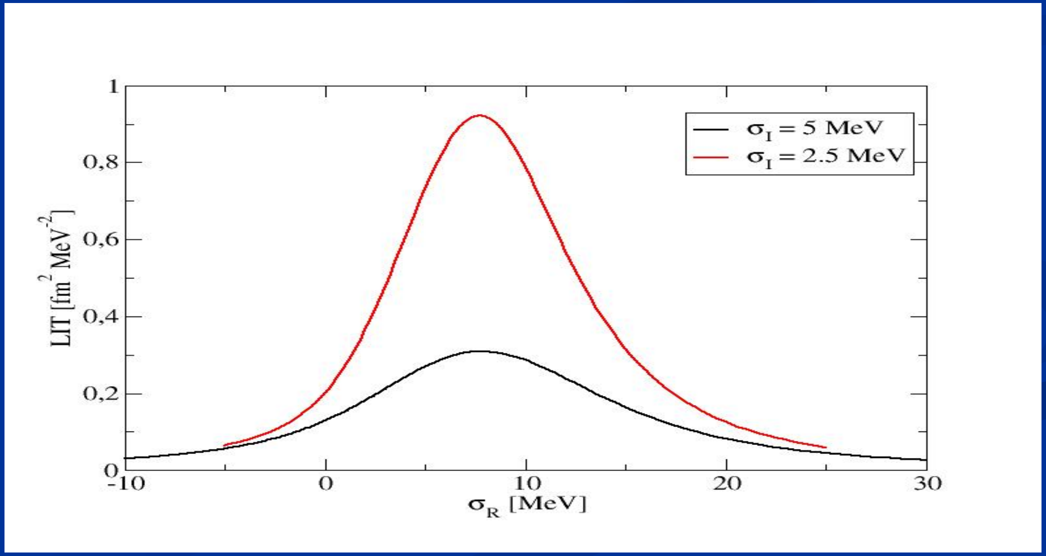
Our calculated response function



Our calculated response function



Our calculated LIT



Inversion calculated with quadrupole precision

For a given number of basis functions N a very precise search for the value of α that leads to the overall best fit to the calculated LIT is made. Recall definition of basis functions:

$$\chi_{\mathbf{n}}(E) = E^{m} \exp(-\alpha E/n) \quad \text{with } m=3$$

Inversion calculated with quadrupole precision

Given the number of basis functions N very precise search for the value of α leading to the overall best fit to the calculated LIT. Recall definition of basis functions:

σ_I = 5 MeV

		N				
E	exact	30	35	40	45	50
1	0.044	-0.042	0.012	0.015	0.009	0.005
2	0.177	0.215	0.178	0.196	0.198	0.237
3	0.354	0.361	0.363	0.357	0.356	0.349
4	0.564	0.559	0.559	0.561	0.562	0.564
8	1.321	1.322	1.321	1.321	1.321	1.322
12	0.452	0.452	0.452	0.452	0.452	0.452
16	0.130	0.130	0.130	0.130	0.130	0.130
20	0.048	0.048	0.048	0.048	0.048	0.048

σ_I = 2.5 MeV

		N						
E,	exact	10	15	20	23	25	27	28
1	0.044	0.107	0.113	0.029	0.044	0.044	0.041	0.043
2	0.177	0.118	0.158	0.167	0.186	0.183	0.176	0.184
3	0.354	0.390	0.358	0.362	0.355	0.355	0.356	0.355
4	0.564	0.571	0.561	0.560	0.563	0.563	0.563	0.563
8	1.321	1.311	1.321	1.321	1.321	1.321	1.321	1.321
12	0.452	0.454	0.452	0.452	0.452	0.452	0.452	0.452
16	0.130	0.131	0.130	0.131	0.131	0.131	0.130	0.131
20	0.048	0.048	0.049	0.049	0.049	0.049	0.048	0.049

Now to our standard inversion method (double precision)

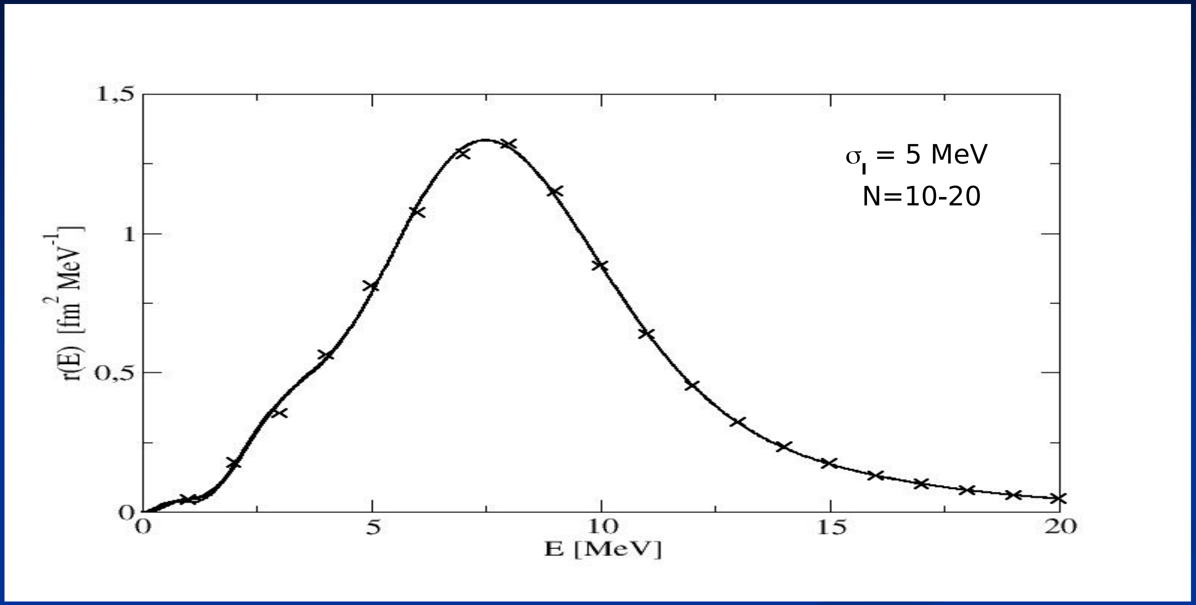
Search for best α value on a grid

Here $\alpha(j) = \frac{1000}{j}$ with j = 1, 2, 3, ..., 1500

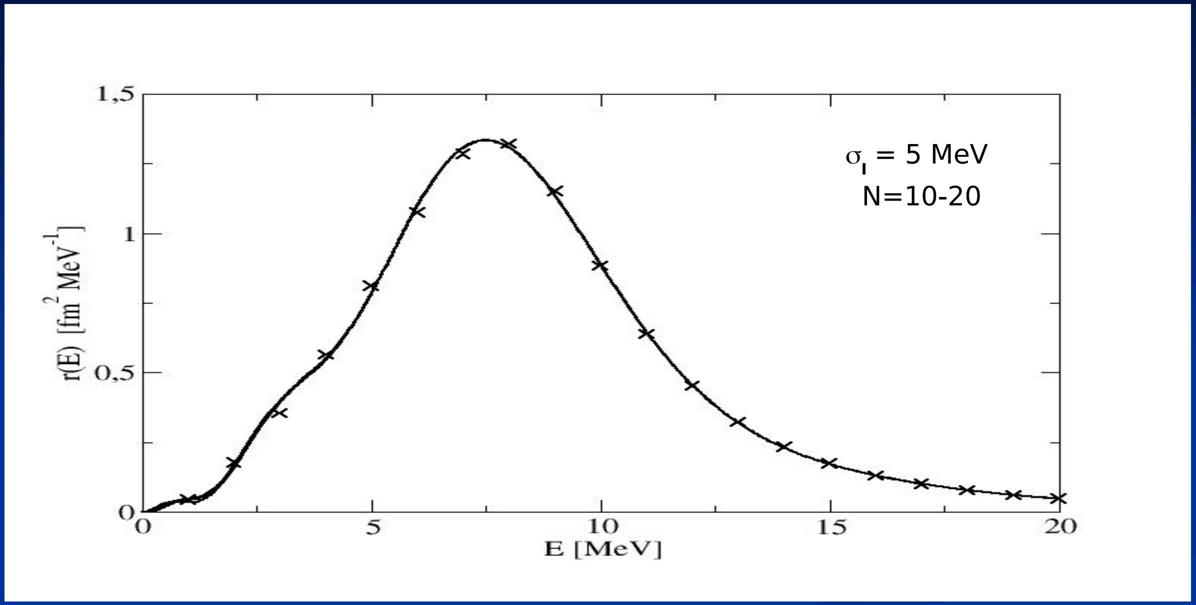
But discard inversions with

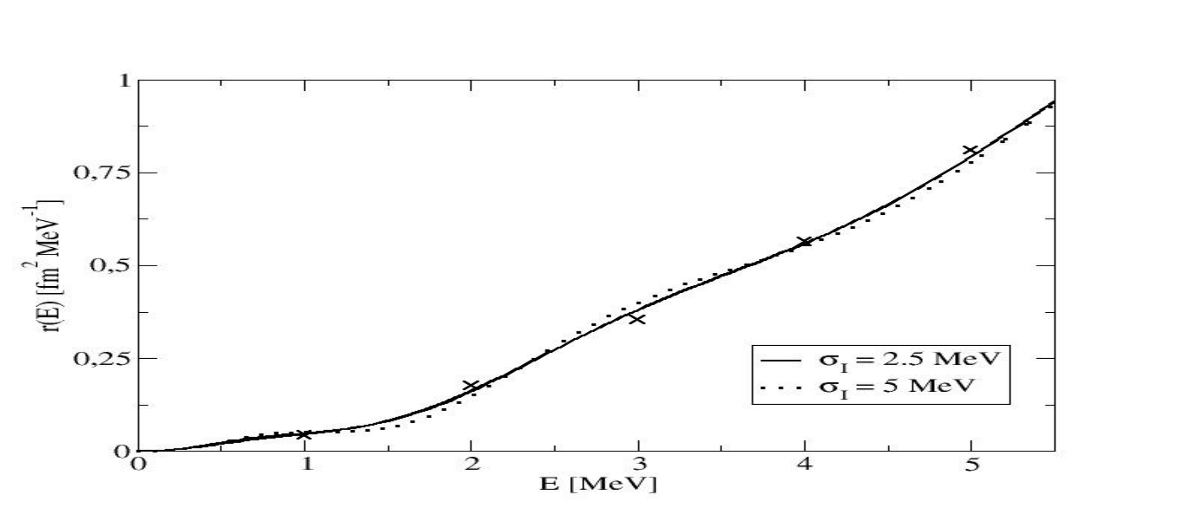
- a not positive definite response
- a response having structures of a width smaller than σ_I

Inversion Results



Inversion Results





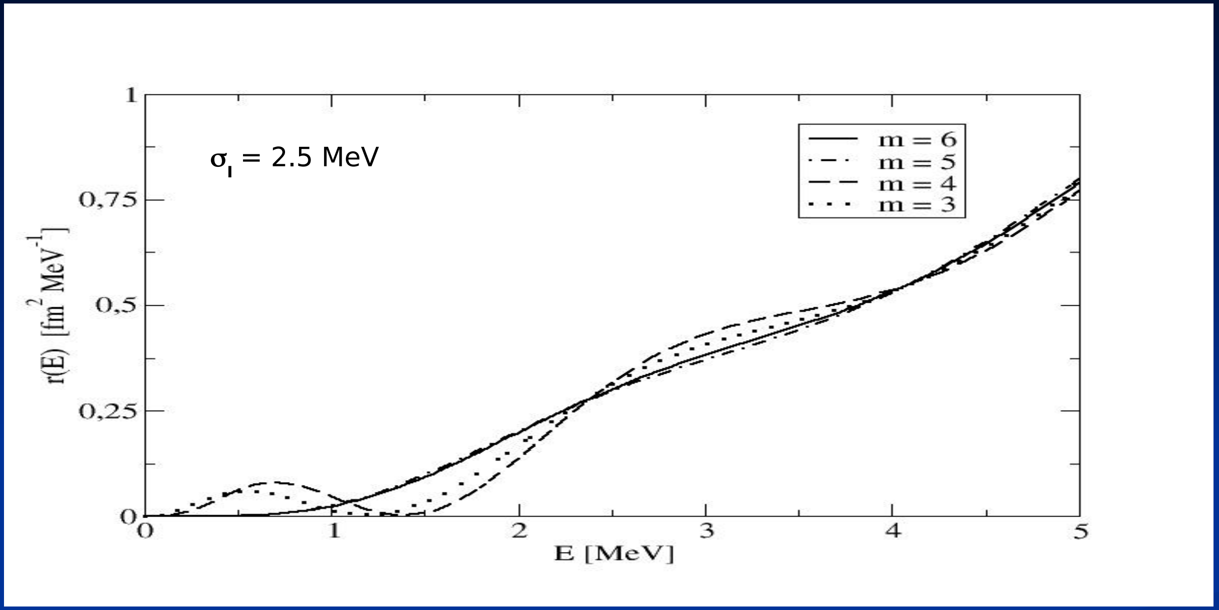
Conclusion:

Difficult to get rid off unwanted structures at threshold

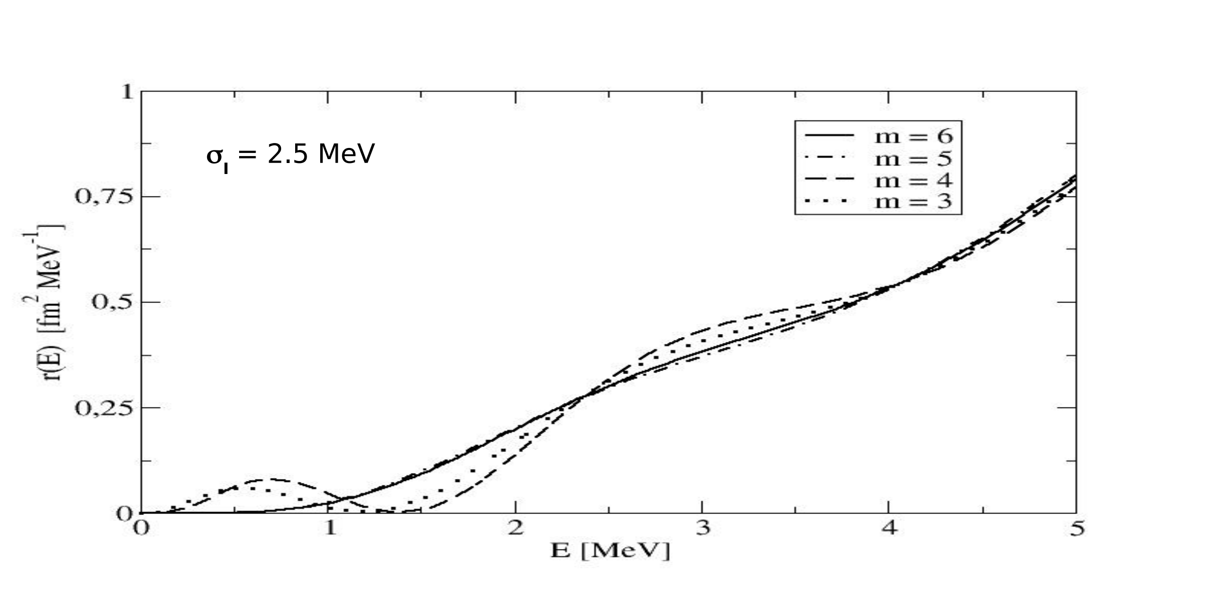
Conclusion:

Difficult to get rid off unwanted structures at threshold

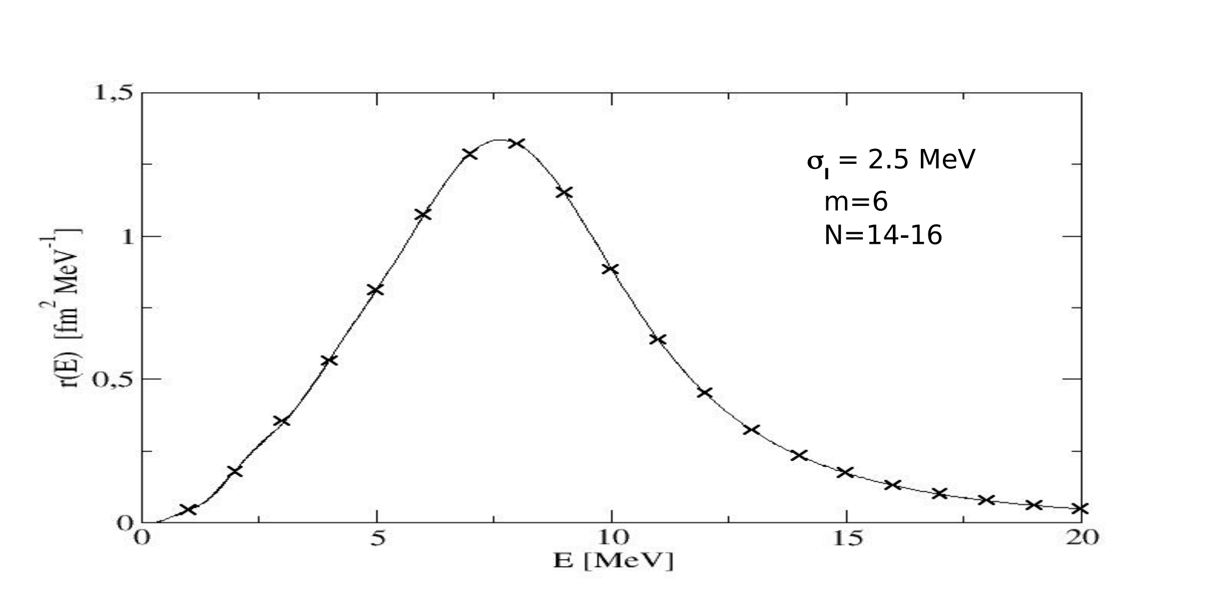
Modify threshold behaviour implemented in basis functions



Different threshold behaviour: E^m with m = 3, 4, 5, 6 and N=8



σ_I = 2.5 MeV
m = 6
m = 5
m = 4
m = 3
r(E) [fm^2 MeV^{-1}]
E [MeV]



σ_I = 2.5 MeV
m=6
N=14-16
r(E) [fm^2 MeV^{-1}]
E [MeV]

Conclusion

Our standard inversion method leads to reliable results when obeying the rules of the inversion game:

discard inversions with a negative response function

minimize structures having a width smaller than σ_I

Summary

LIT method

- reduces a continuum state problem to a bound-state like problem
- is a method with a controlled resolution
- leads to reliable results for a `controlled` inversion