Integral transform method: a critical review of kernels for different kinds of observables

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Summary:

- General remarks on integral transform approaches
- Different kernels for different purposes
- Wavelet kernels: results of a model study

Integral transform (IT)

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

One **IS NOT** able to calculate $S(\omega)$

(the quantity of direct physical meaning)

but **IS** able to calculate $\Phi(\sigma)$

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but **IS** able to calculate $\Phi(\sigma)$

In order to obtain $S(\omega)$ one needs to invert the transform

Problem:

Sometimes the “inversion” of $\Phi(\sigma)$ may be problematic

Suppose we want an S(ω) defined as
(for example for perturbation induced inclusive reactions)

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

Scattering states

Energies in the continum

$$S(\omega) = \sum_n \left|\langle n|\Theta|0\rangle\right|^2 \delta(\omega - E_n + E_0)$$

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

1) integrate in **dω** using delta function

2) Use $\sum_n | n \rangle \langle n | = I$

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

$$\langle 0 |\, \Theta^{+}\, K(H-E_0,\sigma)\, \Theta \,| 0 \rangle$$

The calculation of **ANY** transform seems to require, **in principle**, only the knowledge of the ground state!

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

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The calculation of **ANY** transform seems to require, **in principle**, only the knowledge of the ground state!

However,

$K(H-E_0,\sigma)$ can be quite a complicate operator.

So, how to calculate this mean value?

$$\Phi(\sigma) = \boxed{\langle 0|\, \Theta^+ K(H-E_0,\sigma)\, \Theta |0\rangle}$$

If we had to deal with a **"confined"** system one could represent H on **bound states eigenfunctions** $|\nu>$

$$\langle 0|\Theta^+ K(H-E_0,\sigma)\,\Theta|0\rangle =$$

$$\Sigma_{\mu\nu}\,\langle 0|\,\Theta^+\,|\mu\rangle\,\langle\mu|\,K(H_{\mu\nu}-E_0,\sigma)|\nu\rangle\langle\nu|\,\Theta|0\rangle$$

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After diagonalizing $H_{\mu\nu}$ the transform would be simply

$$\Sigma_{\lambda}\;\; K(\varepsilon_{\lambda}- E_0,\sigma)\; |\langle\lambda|\,\Theta|0\rangle|^2$$

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(Up to convergence!)

However, a nucleus is NOT **“confined”!**

The nuclear **H** has positive energy eigenstates and therefore, in general, CANNOT be represented on **b.s. eigenfunctions** $|\nu\rangle$

(Continuum discretization approximation)

THE GOOD NEWS:

The representation of H on **b.s. eigenfunctions $|\nu>$**
and therefore the calculation of the transform via

$$\Phi(\sigma) = \boxed{\sum_\lambda K(\varepsilon_\lambda - E_0, \sigma) \, |\langle\lambda|\,\Theta|0\rangle|^2}$$

is **allowed** for **specific kernels K(ω,σ)!**

No approximation!

Conditions required:

1) $\int S(\omega)\, d\omega < \infty$ $\left(\Rightarrow \int S(\omega)\, d\omega = \langle 0|\Theta^{+}\Theta|0\rangle \right)$

2) $K(\omega,\sigma)$ is a real positive definite function (or linear combination)

3) $\Phi(\sigma) = \int S(\omega)\, K(\omega,\sigma)\, d\omega < \infty$

In fact: if K(ω,σ) is a real positive definite function

$$K(\omega,\sigma) = \kappa^*(\omega,\sigma)\kappa(\omega,\sigma)$$

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$$\langle\ \tilde{\Psi}\ |\ \tilde{\Psi}\ \rangle$$

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$$K(\omega,\sigma) = \kappa^*(\omega,\sigma)\,\kappa(\omega,\sigma)$$

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$$\langle \tilde{\Psi} | \tilde{\Psi} \rangle < \infty \,!$$ (see req.N.3)

$|\tilde{\Psi}\rangle$ has **finite norm** and therefore

can be expanded on **b.s.** functions !!

Moreover, since $\Theta|0\rangle$ has finite norm:

(see condition N.1)

$\Sigma_\nu \; |\nu\rangle\langle\nu|$ $\quad \Sigma_\mu \; |\mu\rangle\langle\mu|$ $\quad \Sigma_\mu \; |\pi\rangle\langle\pi|$

$$\Phi(\sigma) = \langle 0|\Theta^+ \kappa^+(H_{\nu\mu} - E_0, \sigma) \;\; \kappa(H_{\mu\pi} - E_0, \sigma)\, \Theta|0\rangle$$

$$\langle \;\; \tilde{\Psi} \;\; | \;\; \tilde{\Psi} \;\; \rangle$$

… and after diagonalization:

$$\Phi(\sigma) = \boxed{\Sigma_\lambda \; K(\varepsilon_\lambda - E_0, \sigma) \; |\langle\lambda|\,\Theta|0\rangle|^2}$$

Summarizing:

Any integral transform

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

of a structure function $S(\omega)$ such that

1) $$\int S(\omega)\, d\omega < \infty$$

And with a kernel $K(\omega,\sigma)$ such that

2) $K(\omega,\sigma)$ is a real positive definite function (or linear combination)

3) $$\Phi(\sigma) = \int S(\omega)\, K(\omega,\sigma)\, d\omega < \infty$$

… can be calculated by diagonalizing
the H matrix represented on b.s. functions

(Up to convergence!)

$$\Phi(\sigma) = \boxed{\Sigma_\lambda \; K(\varepsilon_\lambda - E_0, \sigma) \; |\langle\lambda| \, \Theta |0\rangle|^2}$$

A side remark on the notation: in

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

σ can also indicate a set of parameters $\sigma_1, \sigma_2, \ldots$

Some examples:

- **Fourier** Transform? NO! the kernel ***Exp (i ω σ)*** is not a real function
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- **Sumudu** transform? YES! the kernel: $(e^{-\mu\,\omega/\sigma1}/\sigma_1 - e^{-\nu\,\omega/\sigma1}/\sigma_1)^{\sigma 2}$
  it has been evaluated with MC methods
  [A.Roggero, F. Pederiva, G.O. , Phys. Rev. B 88, 115138 (2013)]

Some examples:

…..

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- *Moment* transform? YES or NO! The Kernel ω^σ (σ integer) is a real positive definite function, however, $\Phi(\sigma)$ may be ∞ for some σ
- *Other kernels ???*

Which is the best kernel?

Let's remember:

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

In order to obtain $S(\omega)$ one needs to invert the transform

Problem:

Sometimes the "inversion" of $\Phi(\sigma)$ may be problematic

The Laplace Kernel:

$$\Phi(\sigma) = \int e^{-\omega\sigma} S(\omega)\, d\omega$$

In Condensed Matter Physics:

In QCD

In Nuclear Physics:

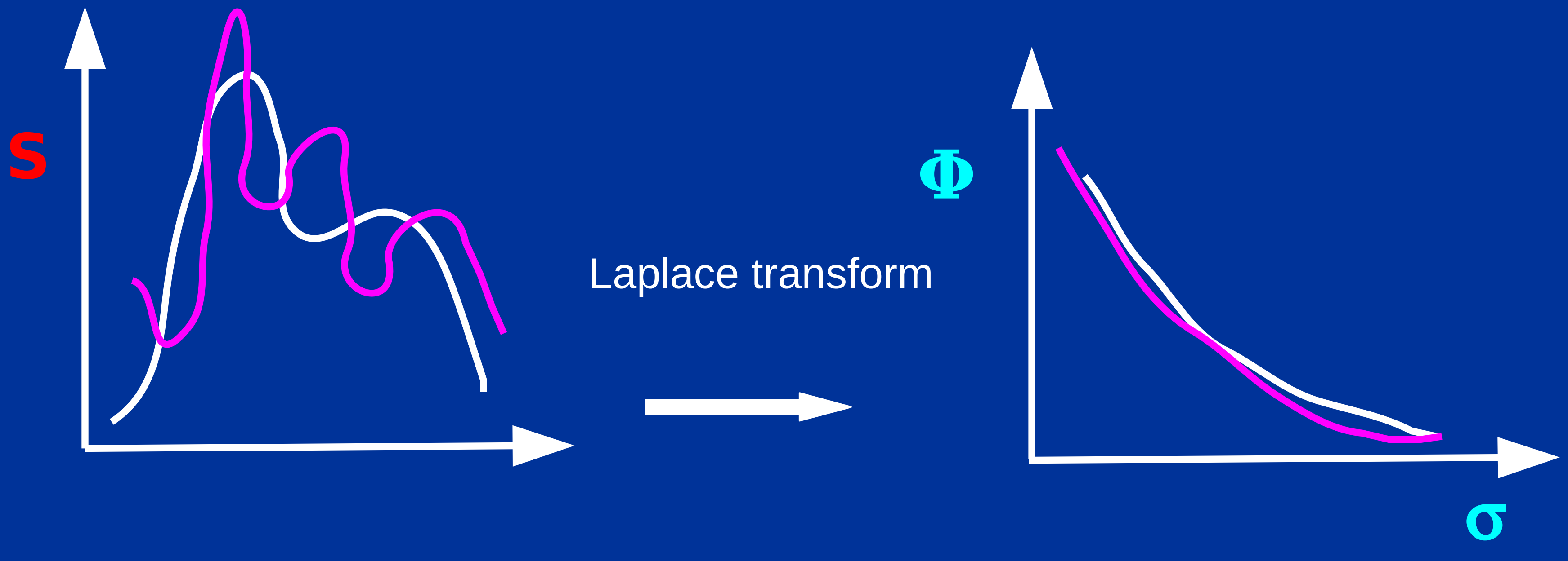
$\sigma = \tau =$ it imaginary time!

$\Phi(\tau)$ is calculated with **Monte Carlo Methods**
and then inverted with methods
based on Bayesian theorem (MEM)

$$\Phi(\sigma) = \int d\omega \; e^{-\omega\sigma} \; S(\omega)$$

It is well known that the numerical inversion of the **Laplace** Transform can be problematic

Illustration of the problem:



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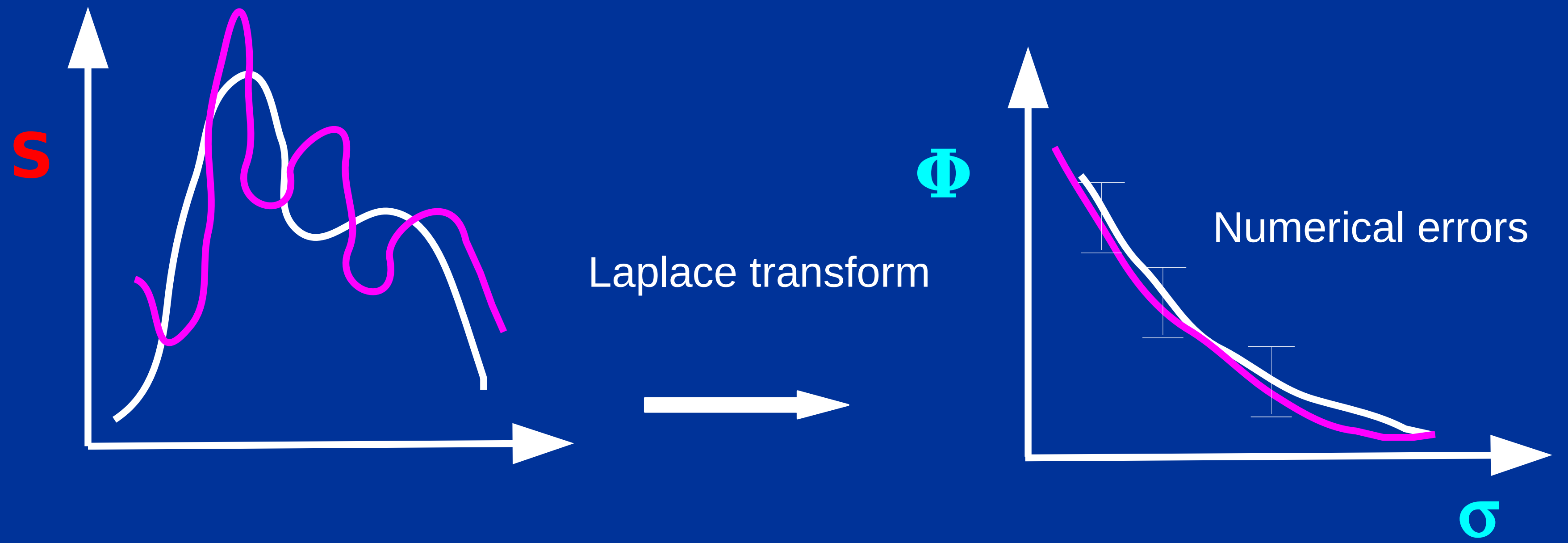

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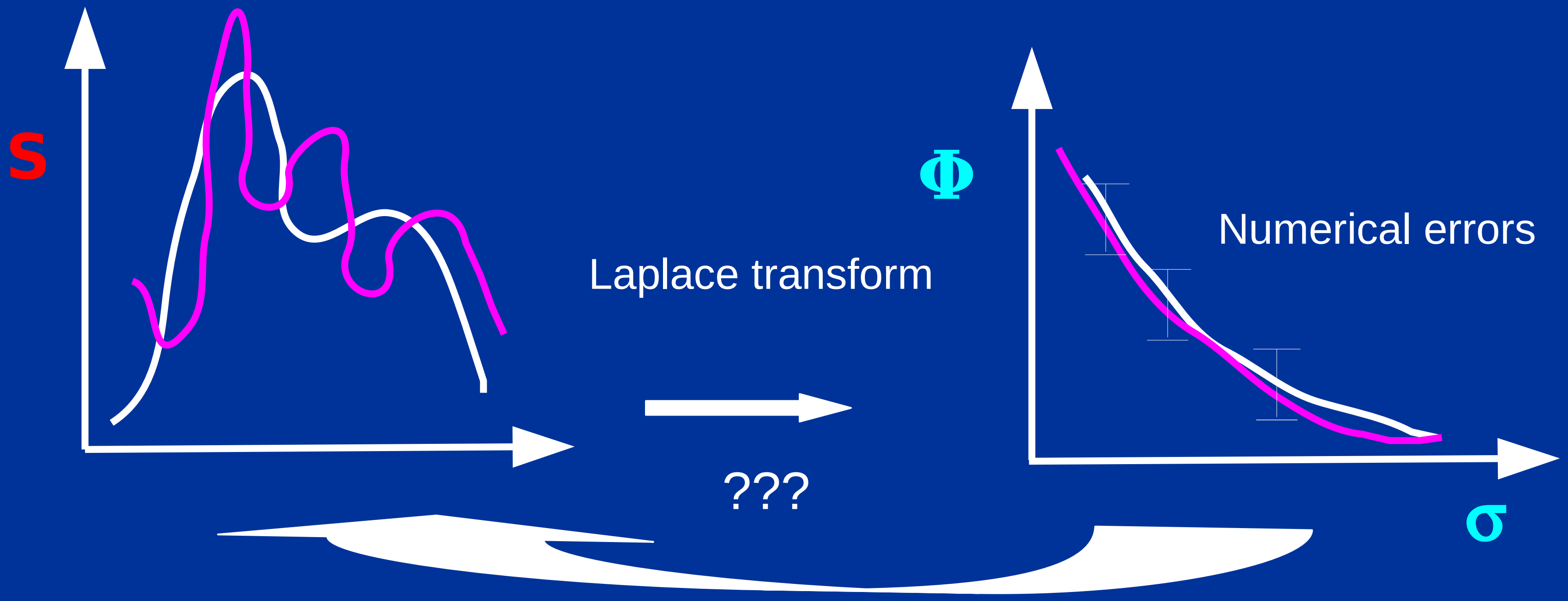


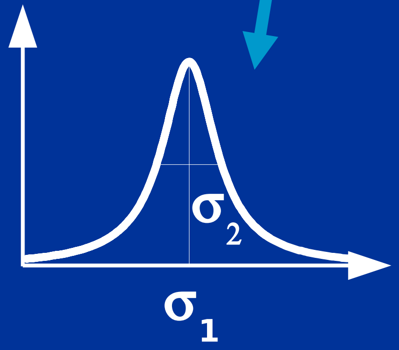
a **“good” Kernel** has to satisfy two requirements

1) one must be able to calculate the integral transform

2) one must be able to invert the transform minimizing uncertainties

The Lorentz kernel:

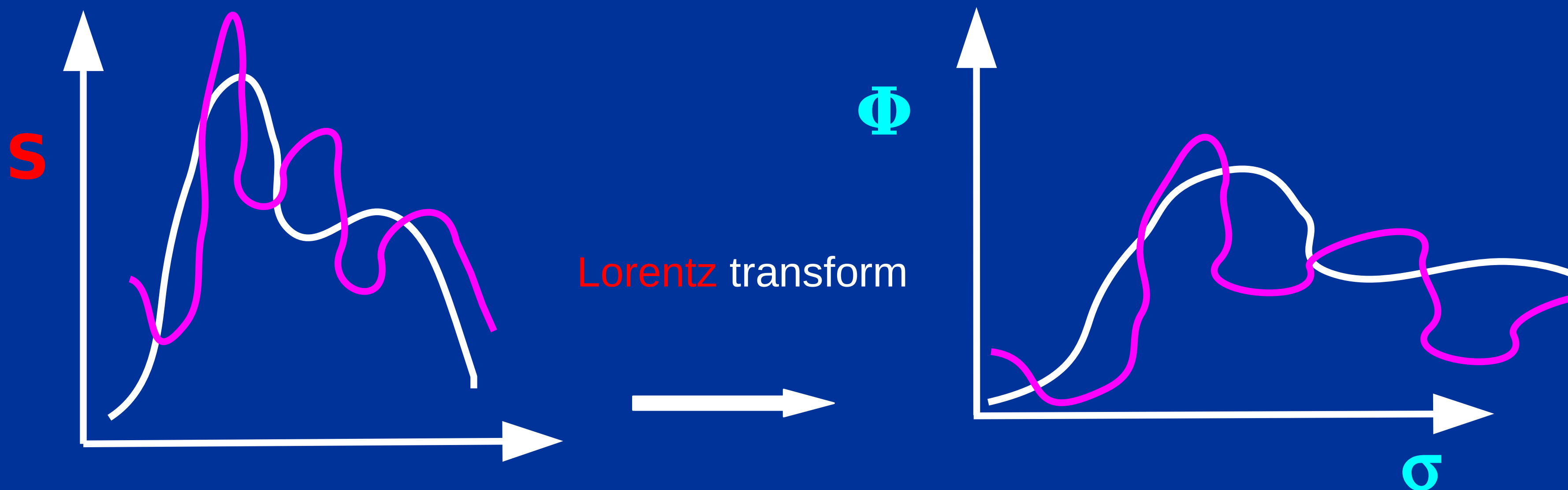
$$K(\omega, \sigma_1, \sigma_2) = [\, (\omega - \sigma_1)^2 + \sigma_2^{\,2} \,]^{-1}$$



It is a representation of the δ-Function !

$$\Phi\,(\sigma_1,\sigma_2) = \int [(\omega - \sigma_1)^2 + \sigma_2^{\,2}]^{-1}\, S(\omega)\, d\omega$$

How can one easily understand why the inversion is **much less** problematic?



blurred, but still distinguishable

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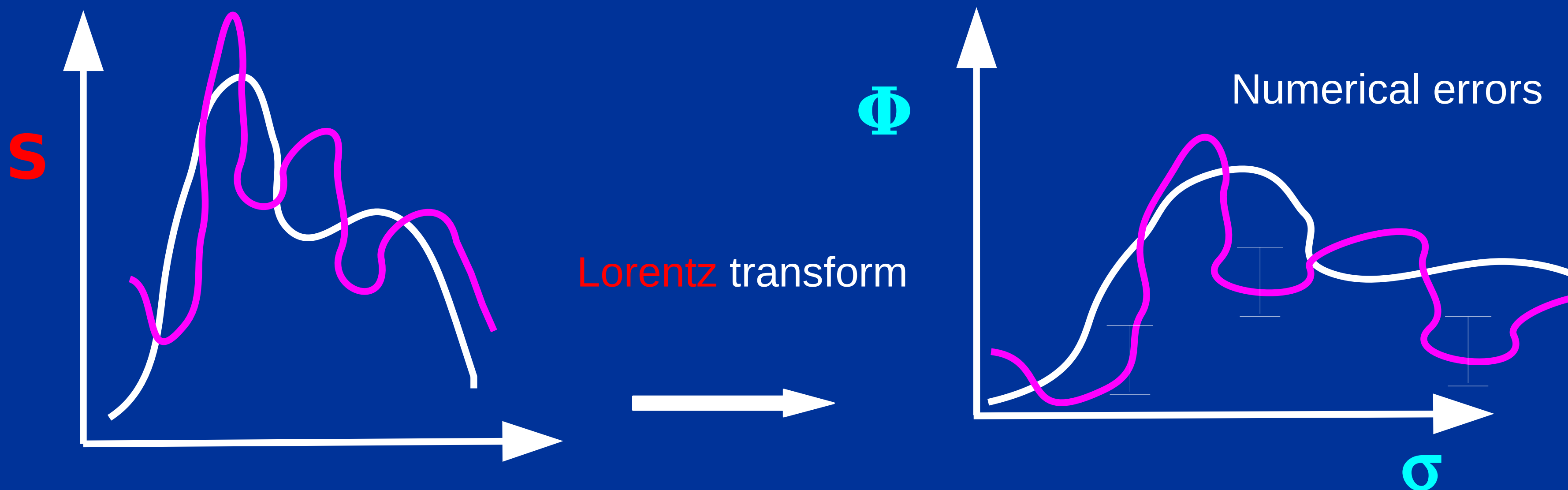
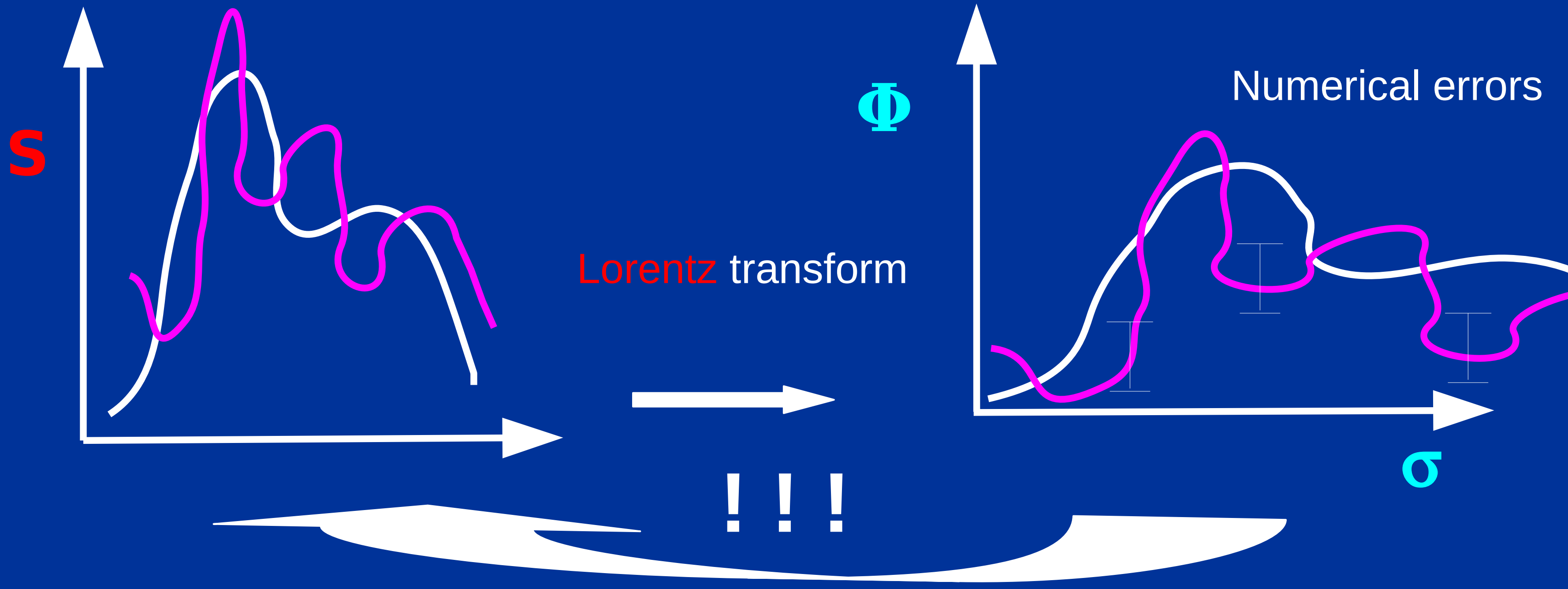


blurred, but still distinguishable also with errors!

How can one easily understand why the inversion is **much less** problematic?

Inversion: “regularization method” at fixed width

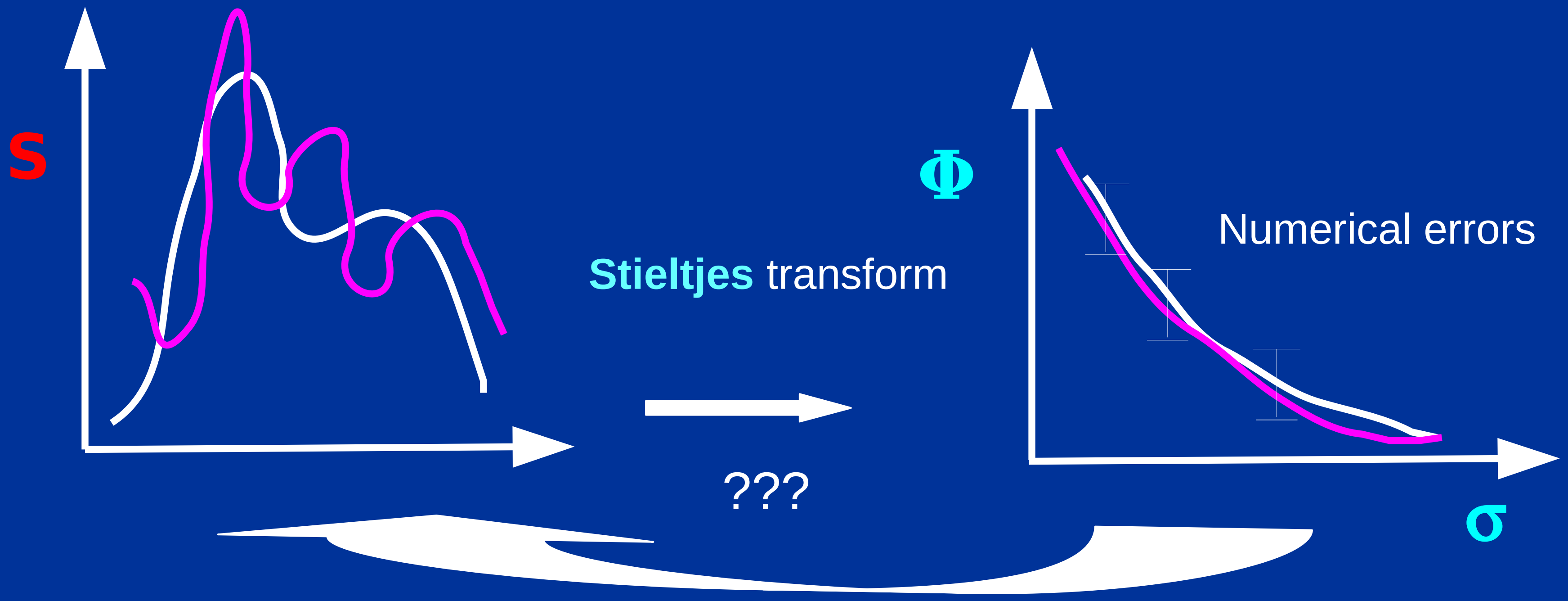


Many successful applications!

The Stieltjes Kernel:

$$K(\omega, \sigma) = (\omega + \sigma)^{-1}$$

Illustration of the problem:
Same as Laplace!



However, it may be useful for another purpose:

In fact:

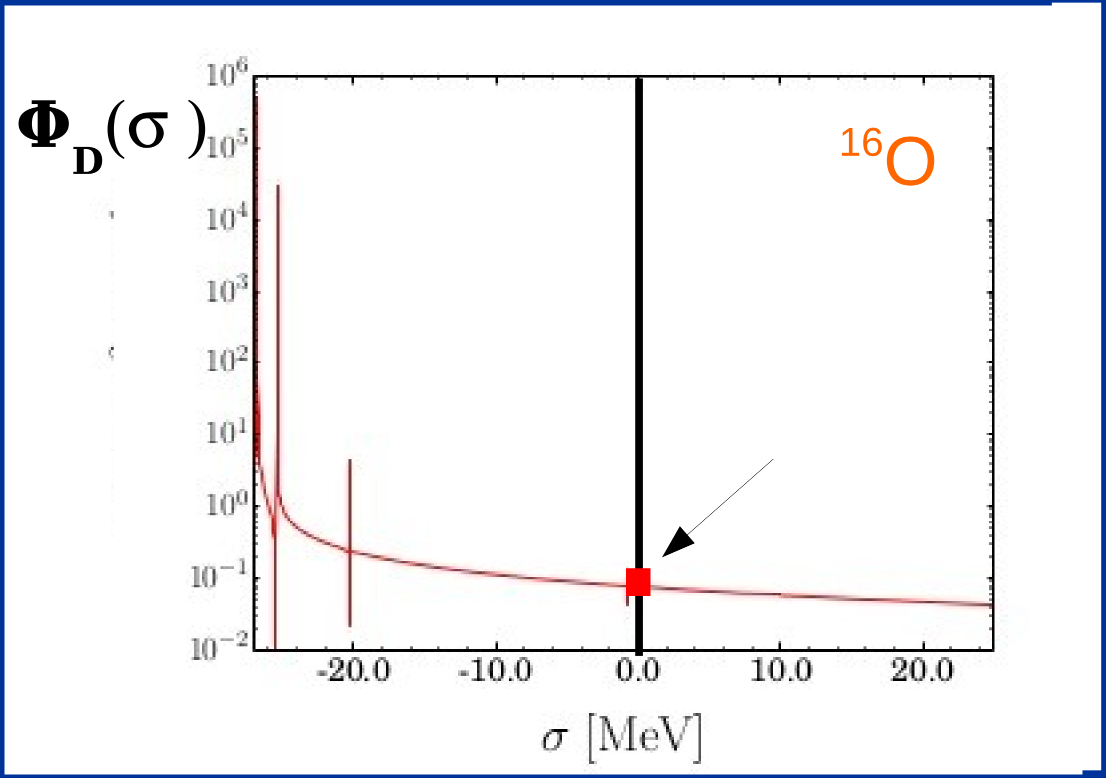
$$\lim_{\sigma \to 0} \Phi(\sigma) = \int S(\omega)\, \omega^{-1}\, d\omega = \alpha_\Theta$$

"generalized polarizability"

e.g. electric polarizability, magnetic susceptibility, compressibility etc… depending on Θ

Recent results on α_Θ with $\Theta = D$ (El. Dipole Polarizability)

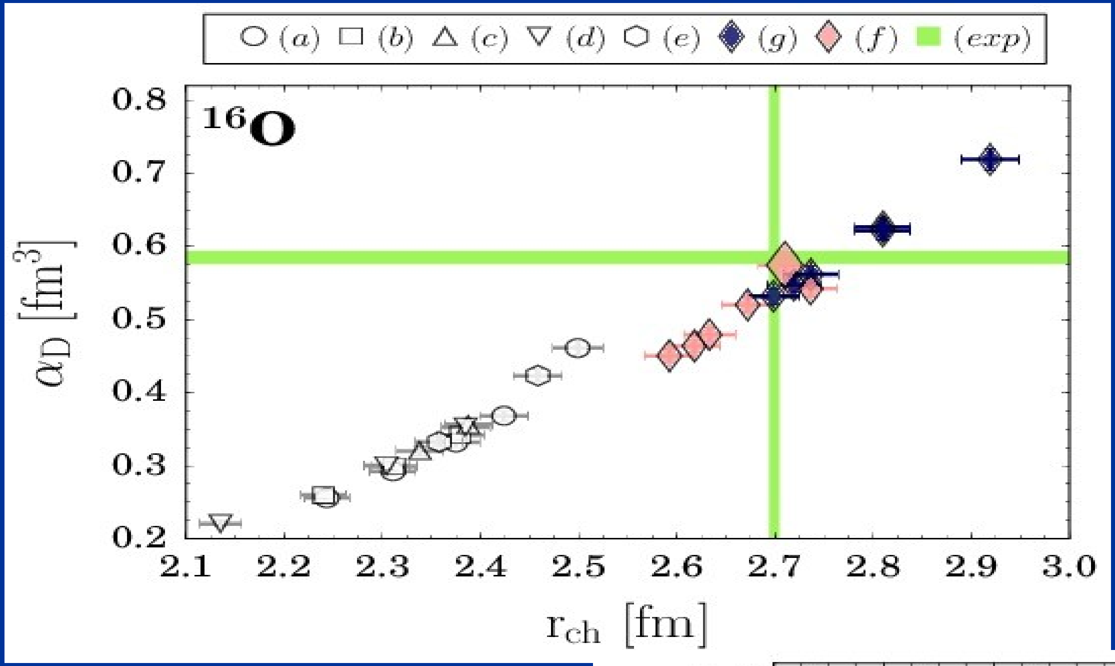
Electric Dipole Polarizability as limit of the Stieltjes transform for σ ---> 0



M.Miorelli et al. nucl.th-arXiv 1604-05381

b.s. expansion: Coupled Cluster

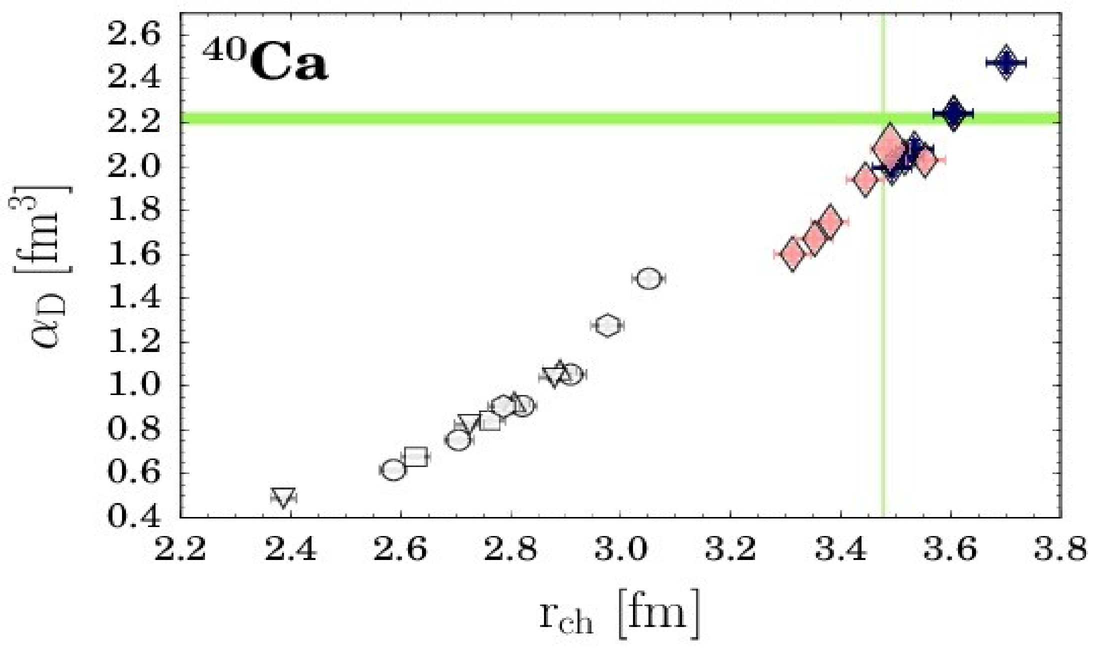
(non hermitian) Lanczos diagonalization



Interesting correlation with the proton charge radius

Role of 3b-force

G. Hagen et al.
Nature Phys. 2016



New Kernels?

What about "**wavelets**"?

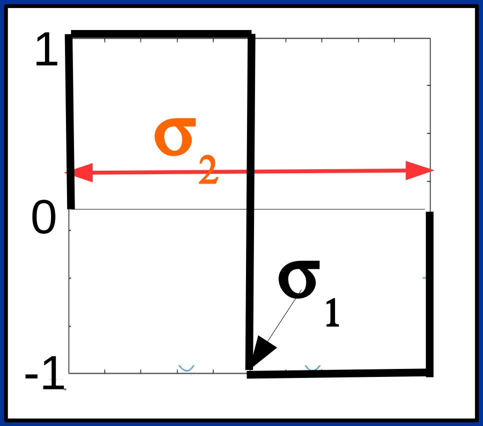
A **wavelet** Kernel is an oscillating function but with a **"window"**.

It has 2 parameters:

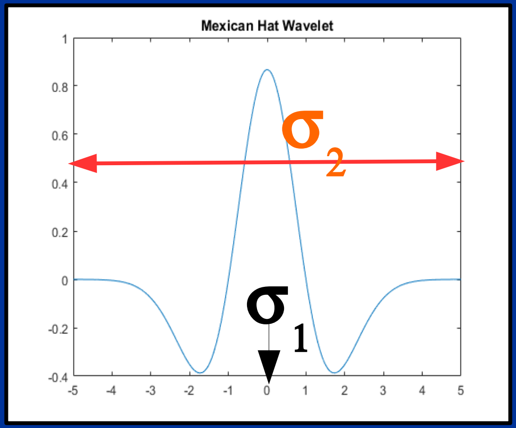
σ_2 drives the frequency of the oscillation

σ_1 drives the position of the window over the ω range

discrete



continuous



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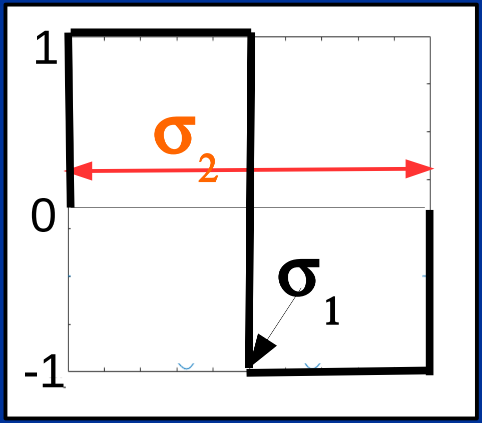
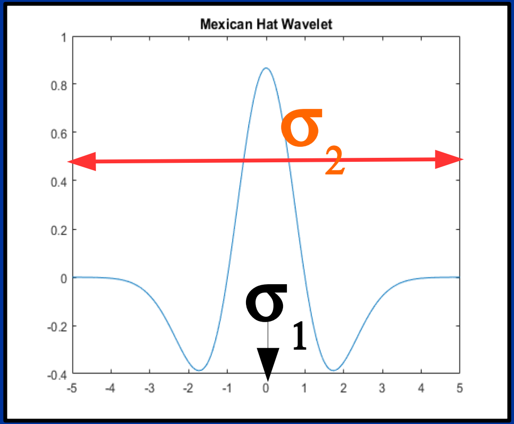


continuous



They combine the power of the Fourier Kernel

(in detecting frequencies of oscillations)

and the Lorentz Kernel

(in picking the information around specific ω ranges)

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σ_2 **drives the position of the window over the ω range**

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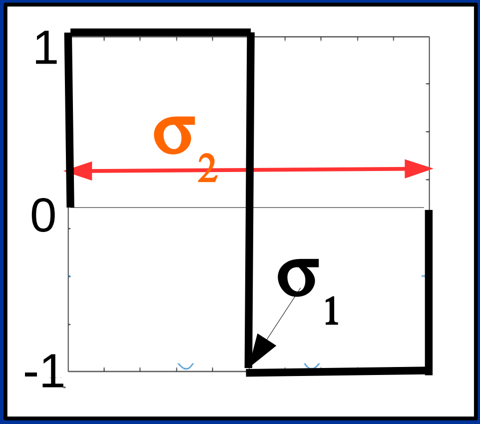

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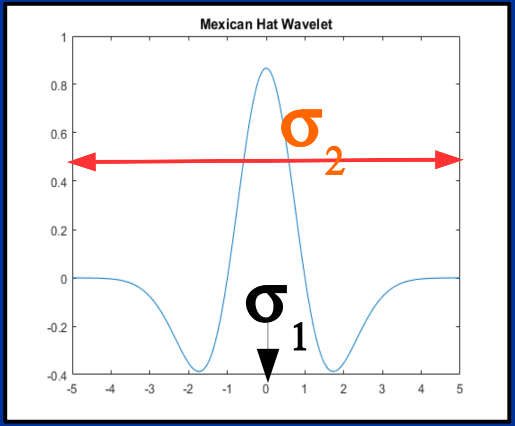
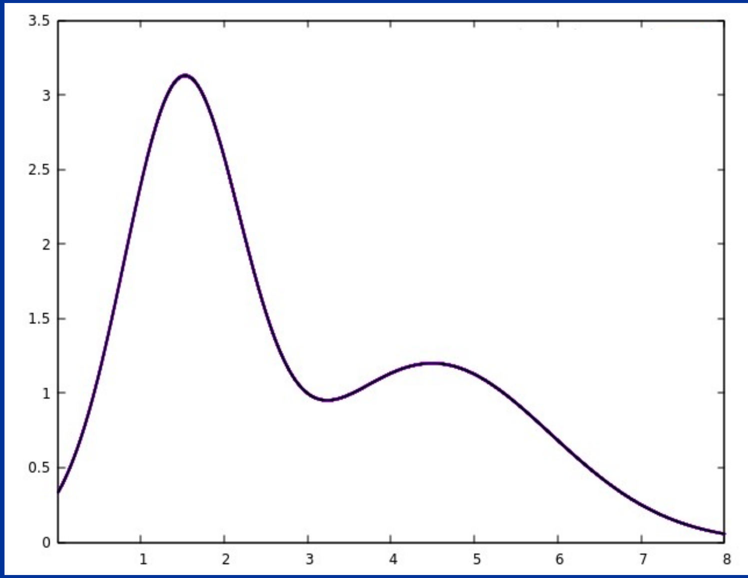


Since wavelets are orthonormal functions in principle their inversion is straightforward !

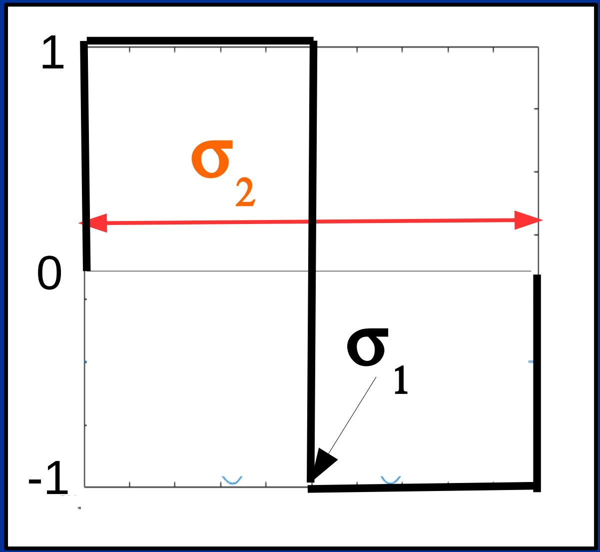
[linear combination of $\Phi(\sigma_1, \sigma_2)$]

A model study
(discrete wavelets)

Our model $S(\omega)$



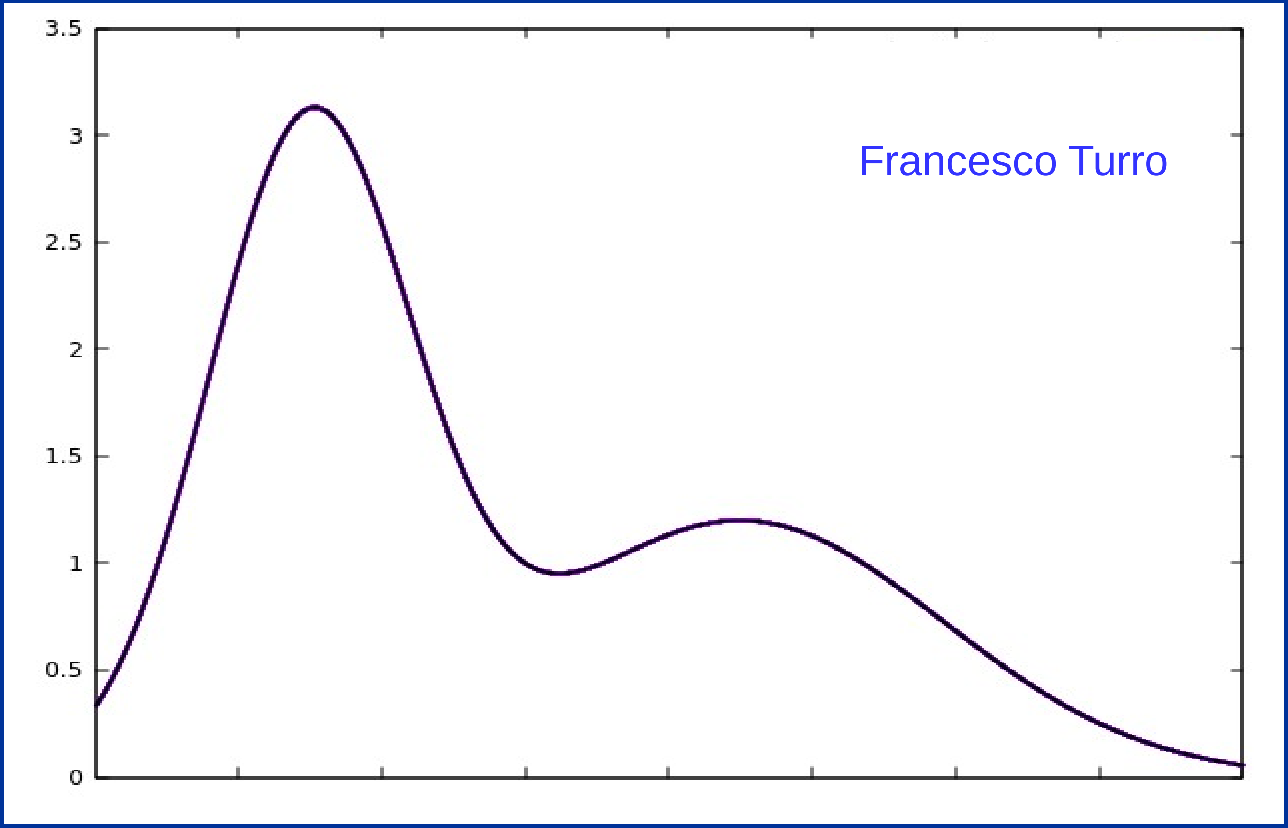
A wavelet kernel



$K(\omega, \sigma_1, \sigma_2)$

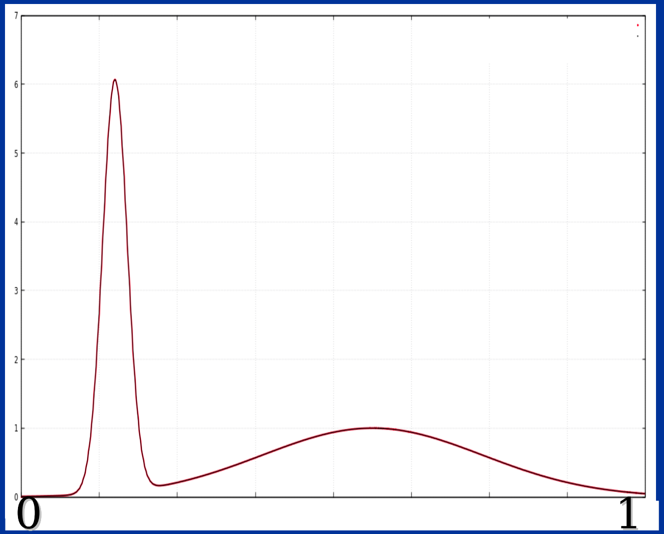
Model S(ω) and reconstructed from wavelet transform:

identical!



Another model study
(narrow resonance, discrete wavelets)

Our model $S(\omega)$



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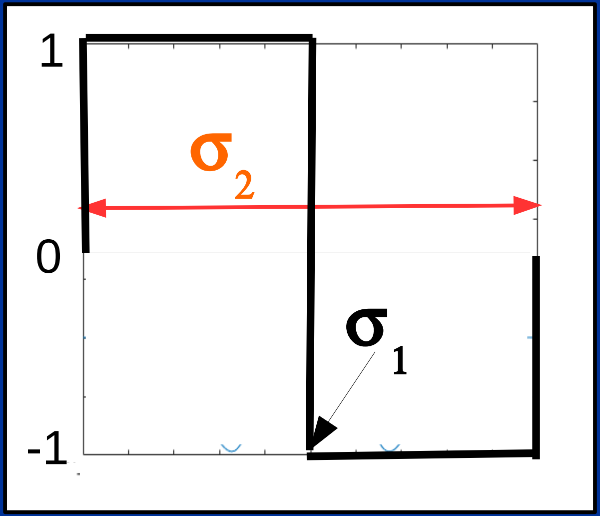

$K(\omega, \sigma_1, \sigma_2)$

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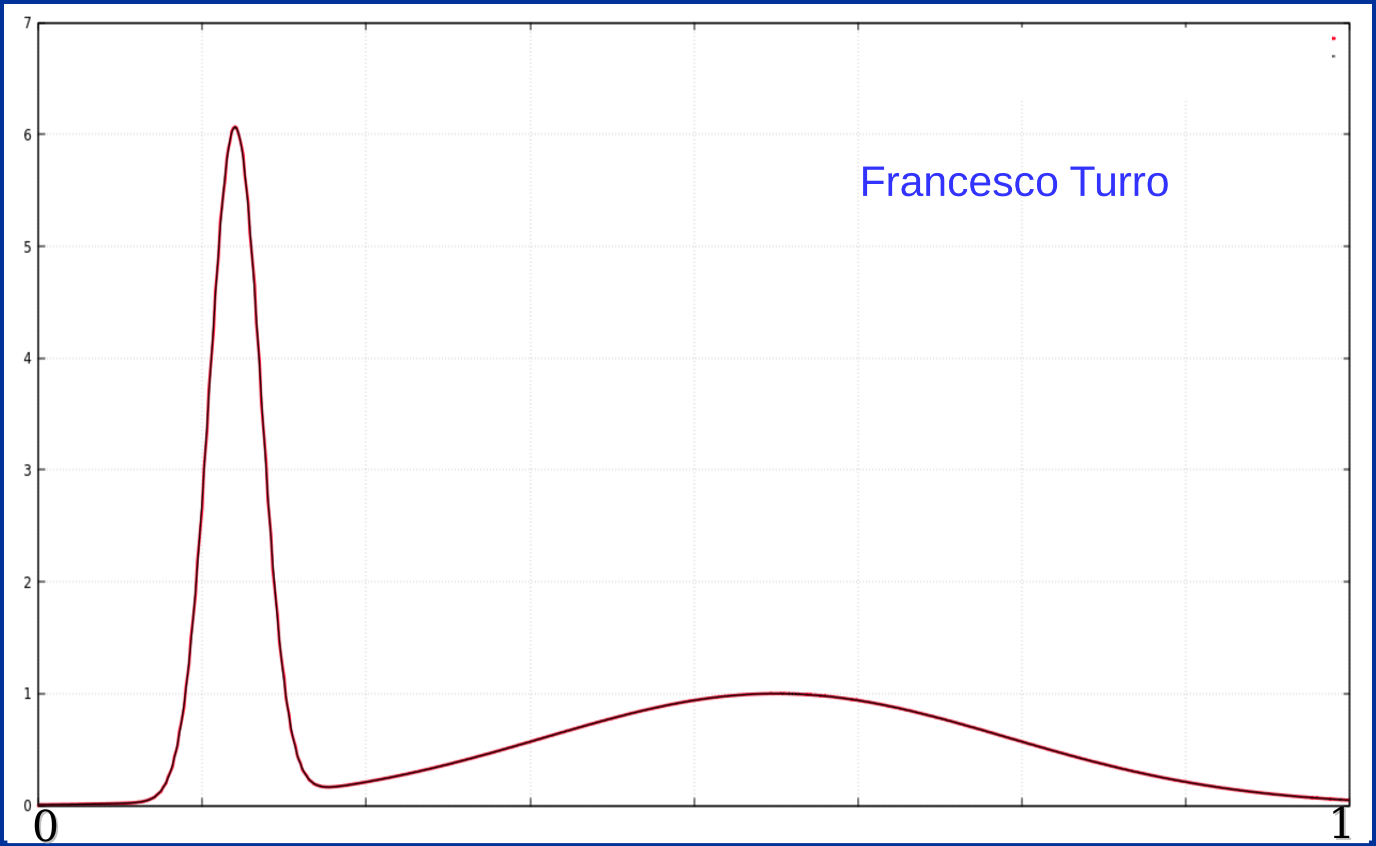
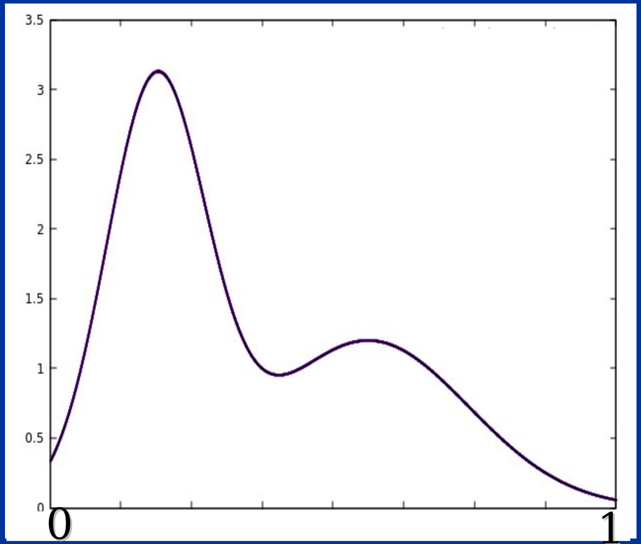


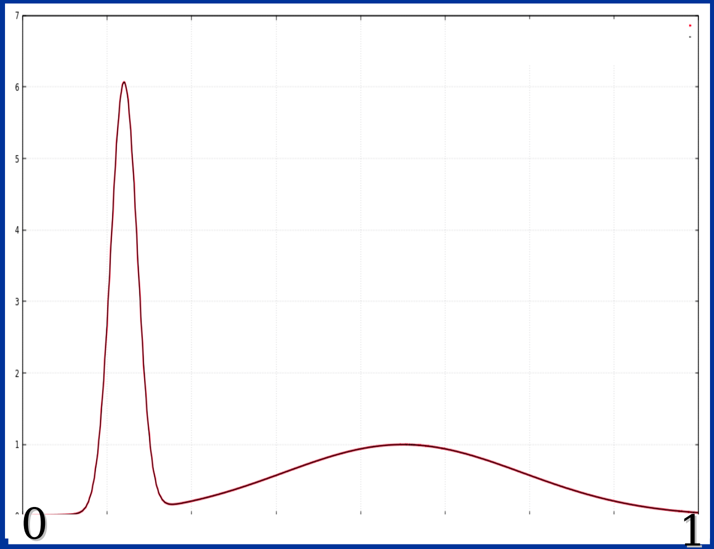
Which information has been used to reconstruct S(ω) ???

Which information has been used to reconstruct $S(\omega)$???

values of $K(\omega, \sigma_1, \sigma_2)$ with different widths

$\sigma_2 = 1/2^J$, J=1-5

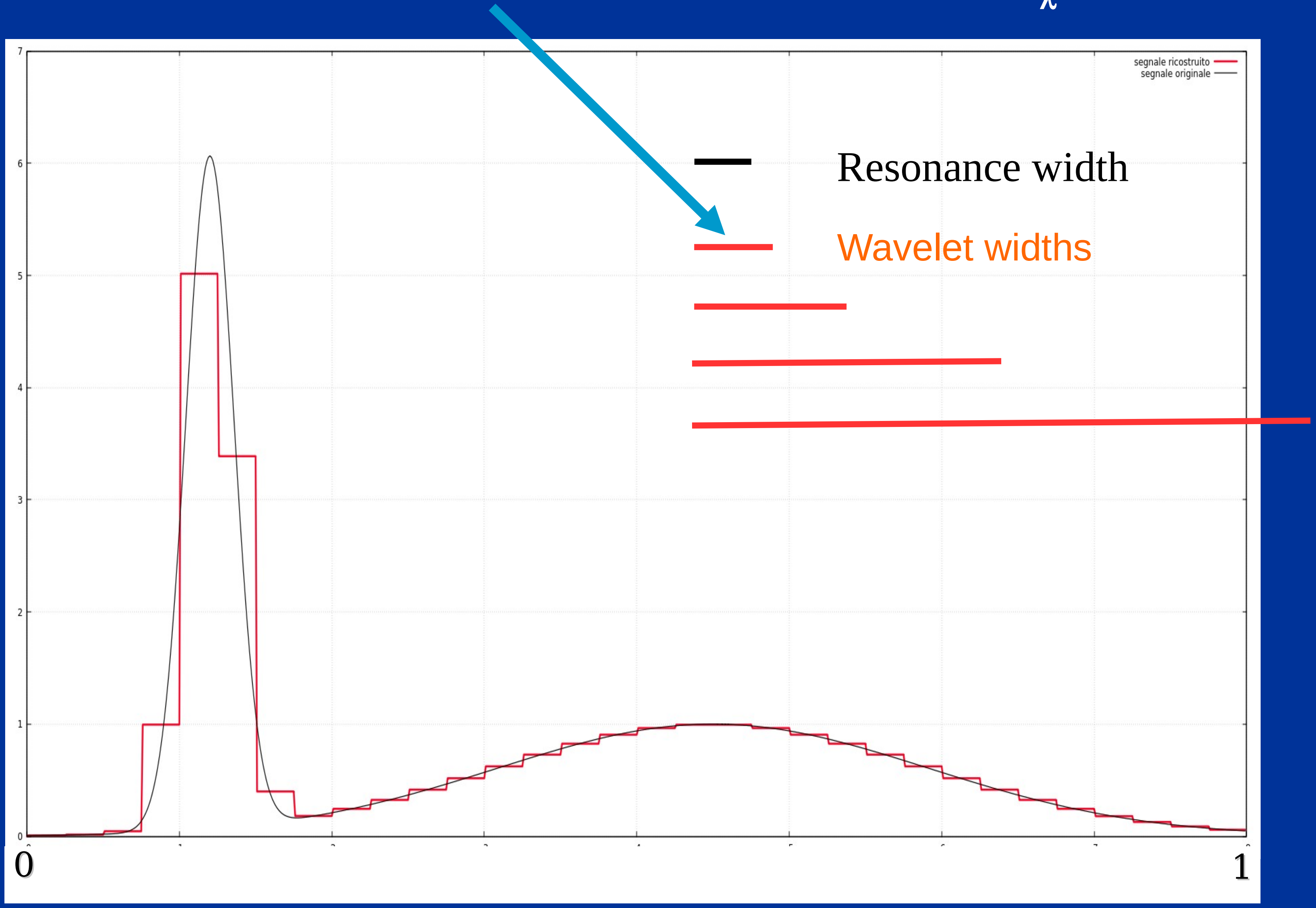




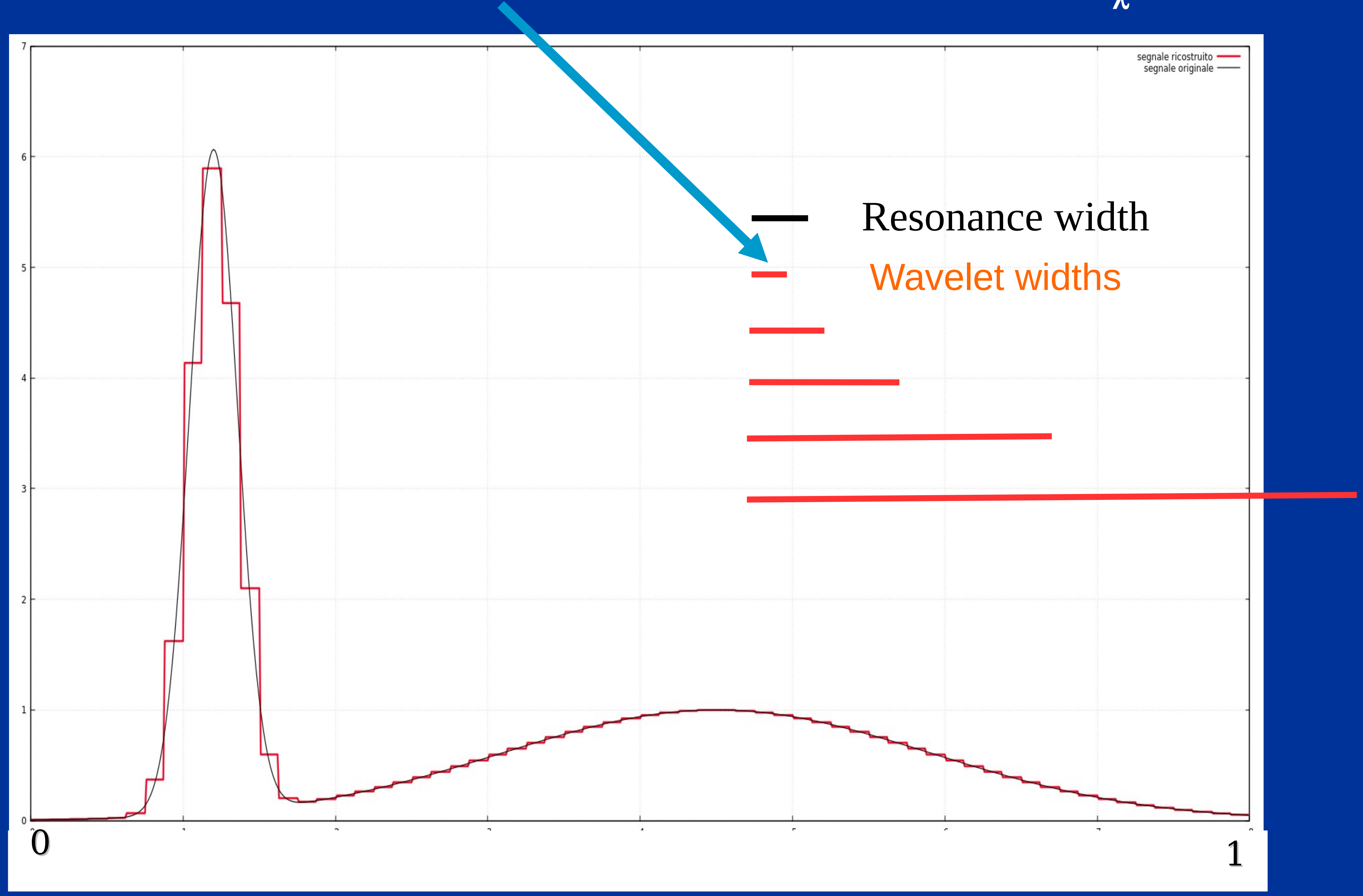
namely a lot of different resolutions up to $\sigma_2 = 0.03$!!!

This may not be possible with diagonalization in realistic cases!

Hp. on smallest "resolution" (low density of ε_λ):



Hp. on smallest “resolution” (higher density of ε_λ):



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- **Wavelets** may be an interesting alternative

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- Integral transform approaches are very powerful ab initio methods for cross sections in the continuum
- In many cases they reduce continuum problem in a b.s. problem
- Good kernels are representations of the delta-functions (the width of the delta-function representation represents the resolution of the problem)
- **Wavelets** may be an interesting alternative
- Still a lot to be explored !!!

Thank you for your attention!

Then:

$\sum_\mu |\mu\rangle\langle\mu|$

$$\Phi(\sigma) = \langle 0|\Theta^+ \kappa^+(H-E_0,\sigma) \quad \kappa(H-E_0,\sigma)\,\Theta|0\rangle$$

$$\langle \tilde{\Psi} | \tilde{\Psi} \rangle$$