Recent applications of integral transform methods

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Summary:

- General remarks on integral transform approaches
- A few useful kernels: **Lorentz**, **Sumudu**
- The **Lorentz** kernel (LIT method) and **Coupled Cluster**
- The **Sumudu** kernel and **Monte Carlo**

Integral transform

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

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One has to use the information $\Phi(\sigma)$ to achieve information on $S(\omega)$ (inversion of the transform) a “good” Kernel has to satisfy two requirements

1) one must be able to calculate the integral transform

2) one must be able to reconstruct the function of interest (invert the transform)

A few examples:

The **moments** of $S(\omega)$ can be considered an IT:

$K(\omega,\sigma) = \omega^{\sigma}$ with σ integer

$$\mathbf{m}_{\sigma} = \boldsymbol{\Phi}(\sigma) = \int d\omega\, \omega^{\sigma}\, S(\omega)$$

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They can be calculated without the knowledge of |n> in the continuum

$$\mathbf{m}_{\sigma} = \langle 0 | \Theta^{+} H^{\sigma} \Theta | 0 \rangle$$

The moments themselves can be considered an IT:

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Unfortunately often only few moments exist.

$$\mathbf{m}_{\sigma} = \int d\omega\, \omega^{\sigma}\, S(\omega) < \infty \;??$$

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

Imaginary $\sigma = \iota\tau$: Laplace Transform

("IMAGINARY TIME" or "EUCLIDEAN" RESPONSES)

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

In Condensed Matter Physics:

Θ = Density Operator

$S(\omega)$ = "Dynamical Structure Function"

$\Phi(\tau)$ is obtained with **Monte Carlo Methods**

In Nuclear Physics:

Θ= Charge or current density operator

$S(\omega)$ = $R(\omega)$ "Response" Function

$\Phi(\tau)$ is obtained with **Monte Carlo Methods**

In QCD

Θ = quark or gluon creation operator

$S(\omega)$ = Hadronic Spectral Function

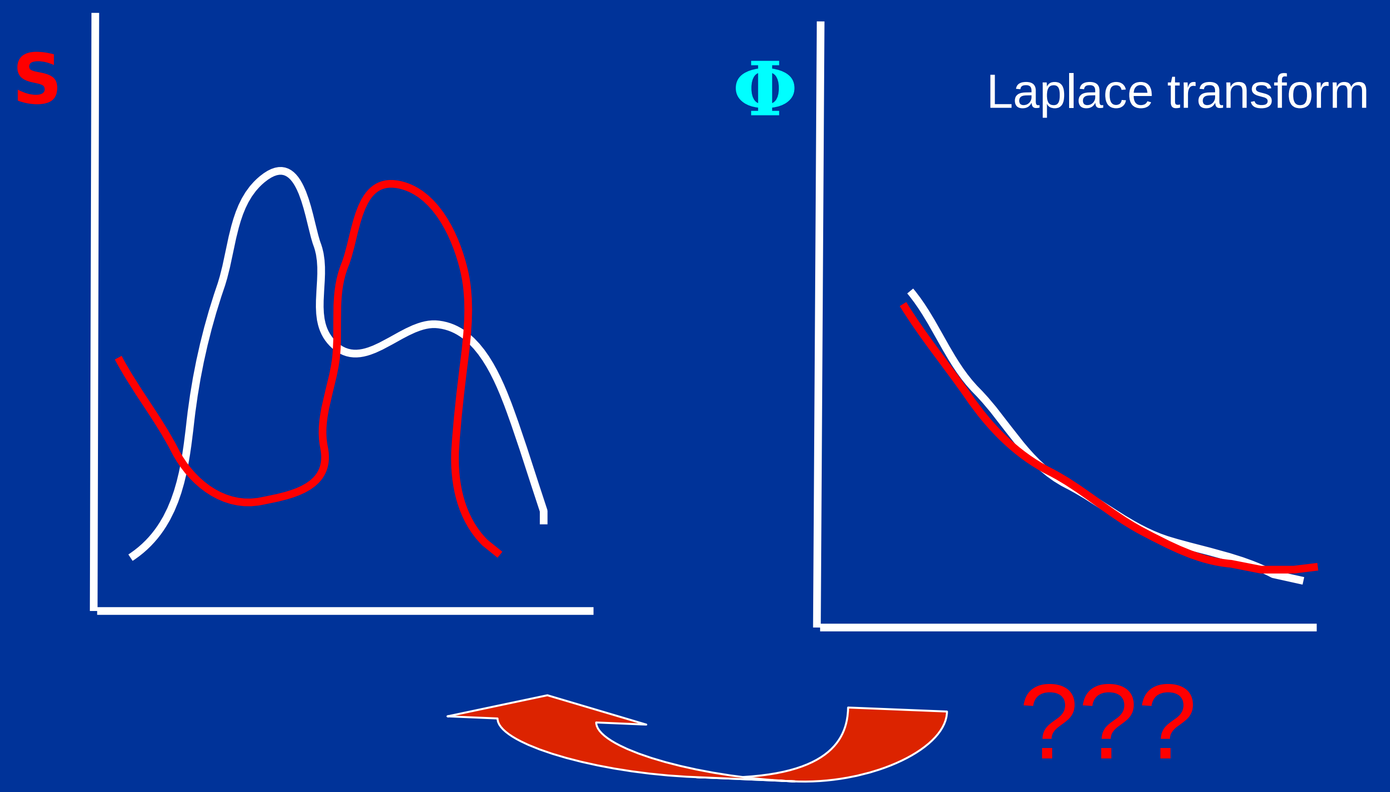
$\Phi(\tau)$ is obtained by moments (OPE - QCD sum rules) or Lattice QCD

Problem:

The "inversion" of $\mathbf{\Phi}$ (τ) may be problematic

("**ill posed problem**")

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



What is the perfect Kernel?

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the delta-function!

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in fact:

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

The **LIT method** is based on the idea to use as kernel one of the "**representations of the delta-function**"

The LIT Kernel is: $K(\omega,\sigma) \sim |(\omega - \sigma)|^{-2}$

with σ **complex:** $\sigma = \sigma_R + i\,\sigma_I$

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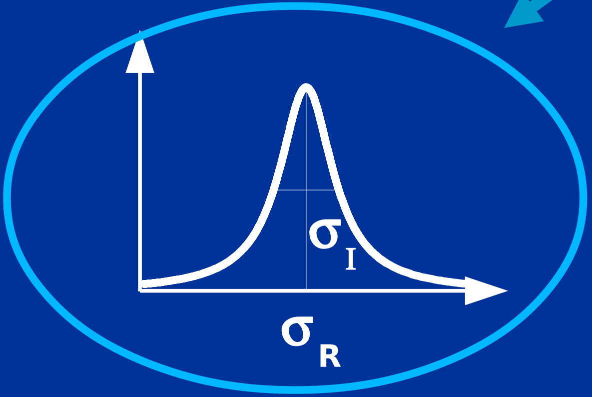
with **σ complex:** $\sigma = \sigma_R + i\,\sigma_I$

Therefore the kernel is a Lorentzian: $K(\omega, \sigma) = \sigma_I/\pi\,[\,(\omega - \sigma_R)^2 + \sigma_I^{\,2}\,]^{-1}$



$$\Phi\,(\sigma_R, \sigma_I) = \sigma_I/\pi \int [(\omega - \sigma_R)^2 + \sigma_I^{\,2}]^{-1}\, S(\omega)\, d\omega$$

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
(controlled resolution with regularization method)

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(Linear response theory)

Reaction cross sections are proportional to

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Green F. $[\Pi(\omega)]$ with poles on the real axis !!

$$\Phi(\sigma_R,\sigma_I) = \sigma_I/\pi \int [(\omega - \sigma_R)^2 + \sigma_I^2]^{-1} S(\omega)\, d\omega < \infty$$

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Green F. **[Π(ω)]** with poles on the complex plane !!

Summarizing:

$$S(\omega) = -1/\pi \, \mathrm{Im} \left[<0| \Theta^{+} (H - E_0 - \omega + \iota\varepsilon)^{-1} \Theta |0> \right]$$

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i.e. represent H on b.s. basis

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NO DISCRETIZATION OF THE CONTINUUM

$$S(\omega) = -1/\pi \, \mathrm{Im}\left[<0|\, \Theta^+ (H - E_0 - \omega + \iota\varepsilon)^{-1}\, \Theta\, |0> \right]$$

ε infinitesimal !

$$\Phi(\sigma_R, \sigma_I) = -\sigma_I/\pi \, \mathrm{Im}\left[<0|\, \Theta^+ (H - E_0 - \sigma_R + \iota\sigma_I)^{-1}\, \Theta\, |0> \right]$$

σ_I finite!

One can use the **Lanczos algorithm** to represent $(H - E_0 - \sigma_R + \iota\sigma_I)^{-1}$ as a continuum fraction **on a bound state basis**

However, in this way one has the Lorentz transform, and one needs to invert it to obtain $S(\omega)$

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

Because the kernel is a representation of the delta-function the inversion is much less “ill posed” and one can get accurate results!

The LIT method

- reduces the continuum problem to a bound state-like problem
- needs only a “good” method for bound state calculations (FY, HH, NCSM, ???)
- has been benchmarked in “directly solvable” systems (A=2,3)

V. D. Efros, W.Leidemann, G.Orlandini, N.Barnea

“The Lorentz Integral Transform (LIT) method
and its applications to
perturbation induced reactions”

J. Phys G: Nucl. Part. Phys.34 (2007) R459-R528

Topical report

Until recently the **LIT** has been calculated with the following b.s. methods

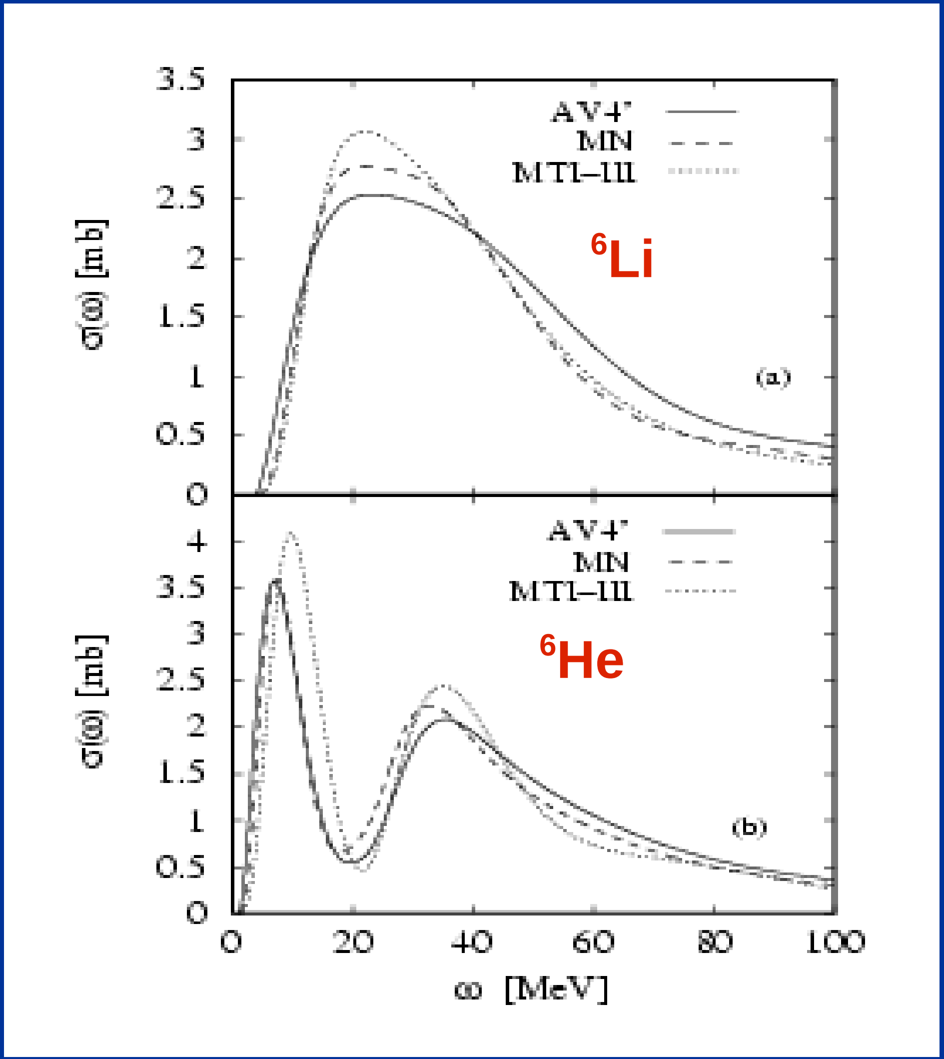
HH, FY, NCSM, EIHH methods

Among the many results there are some interesting ones on the photonuclear cross section

(in the “giant dipole resonance” region)

6-Body E1 excitation

S. Bacca et al.PRL89(2002)052502



LIT + EIHH methods

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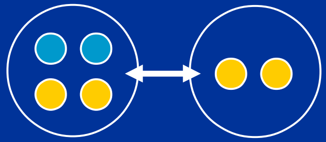
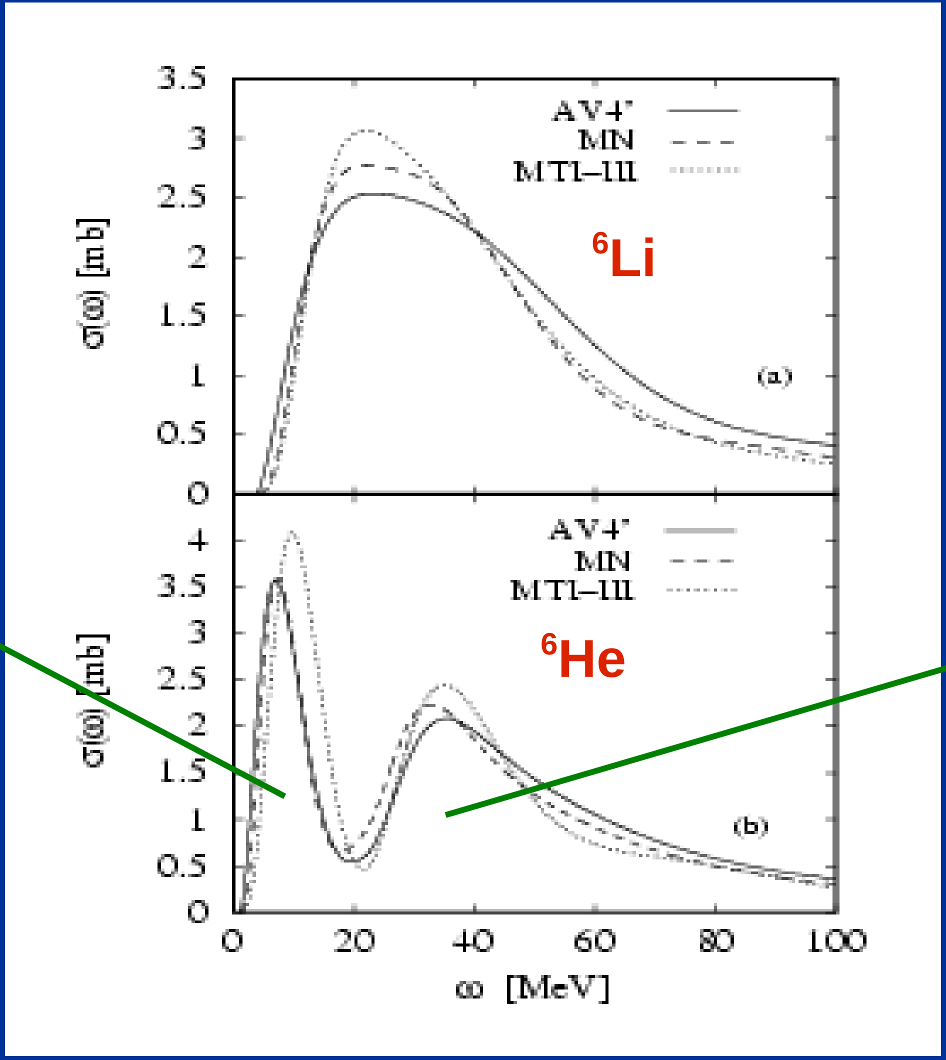
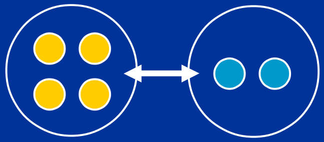


soft mode





classical GT mode

Until recently the **LIT** has been calculated with the following b.s. methods

HH, FY, NCSM, EIHH methods

Typical "**few-body"** methods!

What about “**many-body**” methods ?

Can one access larger A?

Try with Coupled Cluster (CC)

(e^S Theory)

S. Bacca, N. Barnea, G. Hagen, G.O., T. Papenbrock
Phys.Rev.Lett. 111 122502 (1913)

Up to now limited to single-double (CCSD)

LIT+CC:

Remember the expression of the LIT:

$$\Phi(\sigma_R,\sigma_I) = -\sigma_I/\pi \; \mathrm{Im}\, [< 0 \mid \Theta^+ (H - E_0 - \sigma_R + i\sigma_I)^{-1} \Theta \mid 0 >]$$

σ_I finite!

Now use the similarity transformations inserting

$e^{T} e^{-T} = 1$

$$\Phi(\sigma_R, \sigma_I) = -\sigma_I/\pi \, \mathrm{Im} \, [< 0 \,|\, \Theta^{+} (H - E_0 - \sigma_R + i\sigma_I)^{-1} \Theta \,|\, 0 >]$$

Insert $e^{T} e^{-T} = 1$

After inserting $e^T e^{-T} = 1$ one has

$$\Phi(\sigma_R, \sigma_I) =$$

$$-\sigma_I/\pi \, \mathrm{Im} \, [< 0 \,|\, e^T \, \overline{\Theta}^+ \, (\overline{H} - E_0 - \sigma_R + i\sigma_I)^{-1} \, \overline{\Theta} \, e^{-T} | \, 0 >]$$

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Similarity Transf. ANSATZ!: $e^{-T} | 0 \rangle = | SD \rangle$

$$\bar{\Theta} = e^{-T}\, \Theta\, e^{T}$$

$$\bar{H} = e^{-T}\, H\, e^{T}$$

Difficulties:

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Similarity Transf. ANSATZ!: $e^{-T} | 0 > = | SD >$

1) $< 0 | e^{T} \neq < SD |$!!

therefore one has $| SDR >$ and $< SDL |$

2) $\bar{H}$ is a non hermitian !!

Solutions:

$$\Phi(\sigma_R, \sigma_I) =$$

$$-\sigma_I/\pi \, \mathrm{Im} \, [< 0 \,|\, e^{T} \bar{\Theta}^{+} (\bar{H} - E_0 - \sigma_R + i\sigma_I)^{-1} \bar{\Theta} \, e^{-T} | \, 0 >]$$

1) < SDL | = < SDR | $(1+\Lambda)$ where Λ is known in the standard CCSD(T)

2) use the **non** hermiitian **Lanczos** algorithm to rewrite $\bar{H}$ as a continuous fraction

Because of the exponential e^T

all **A**-body correlations of the kind

$(T^{[1]})^m$ $(T^{[2]})^n$ (A=m+2n) are included!

We have applied it to ^{16}**O** total photoabsorption cross section

GDR

$$\Theta = \sum_i z_i \; \tau_i^3$$

With chiral EFT potential at **N3LO**

First we have validated the method on ^{4}He

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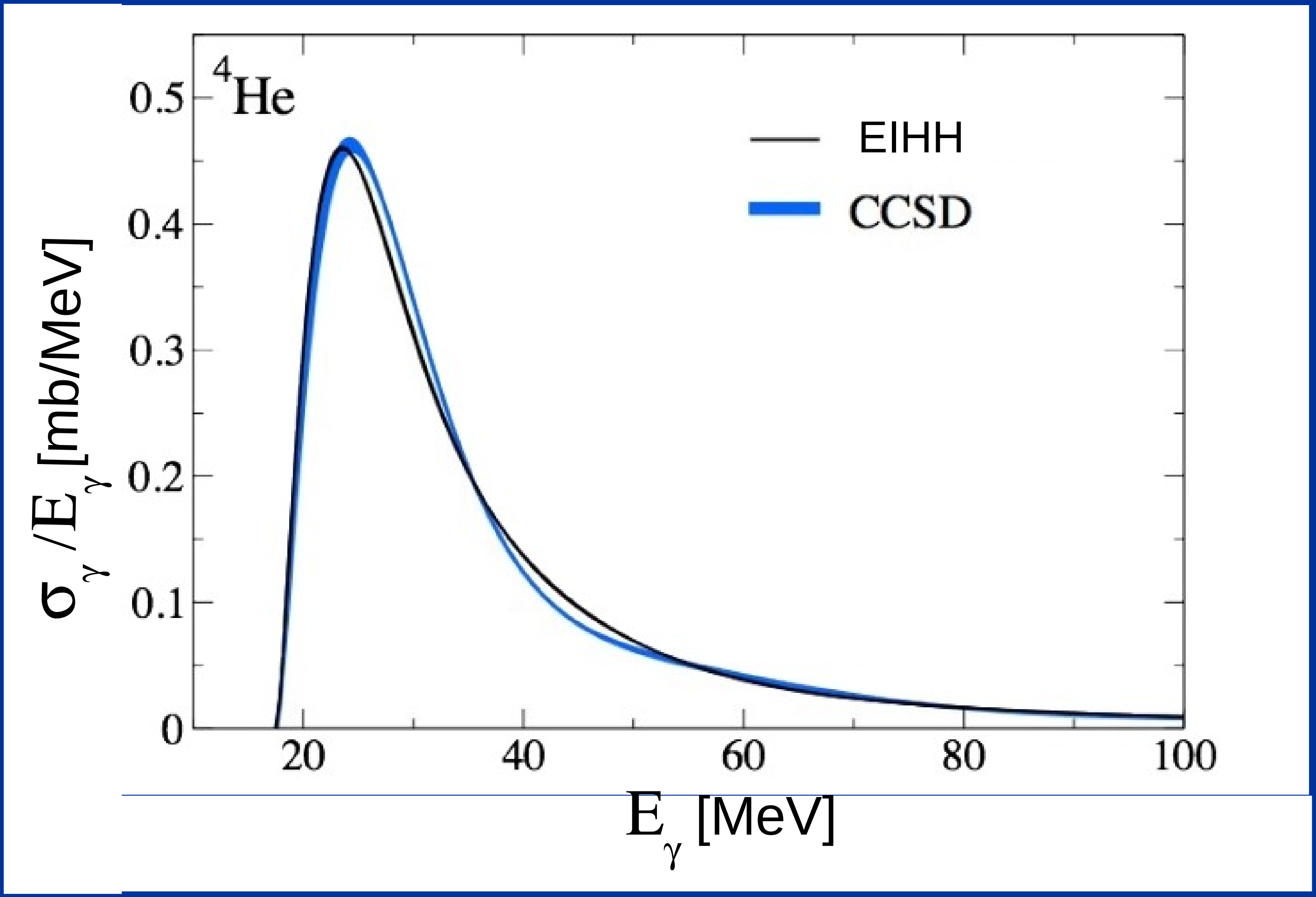
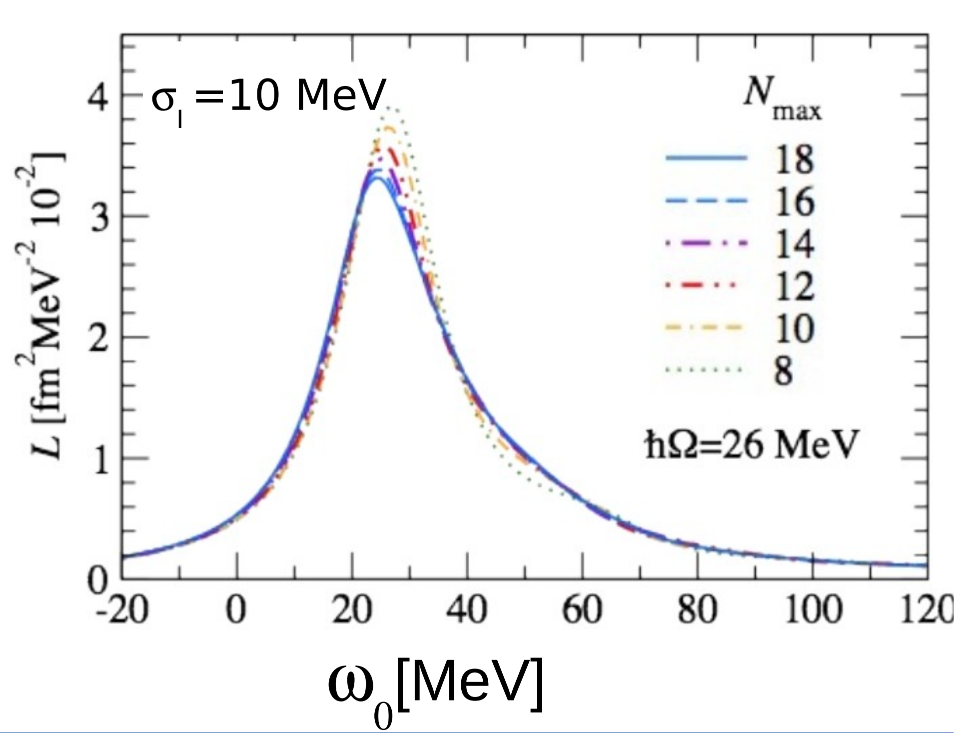


Good agreement !

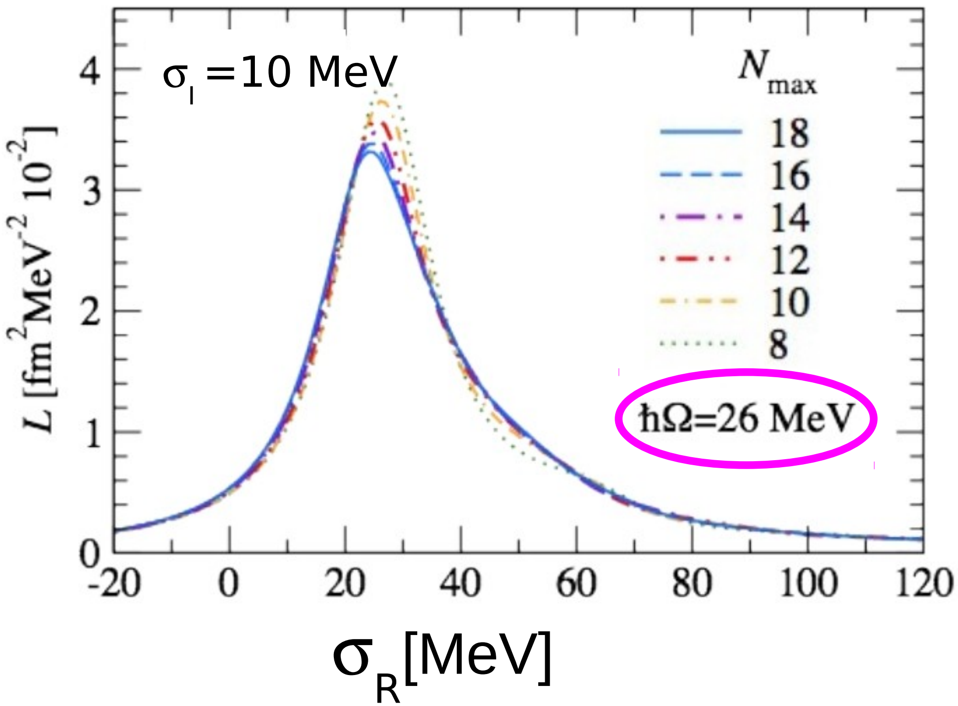
^{16}O

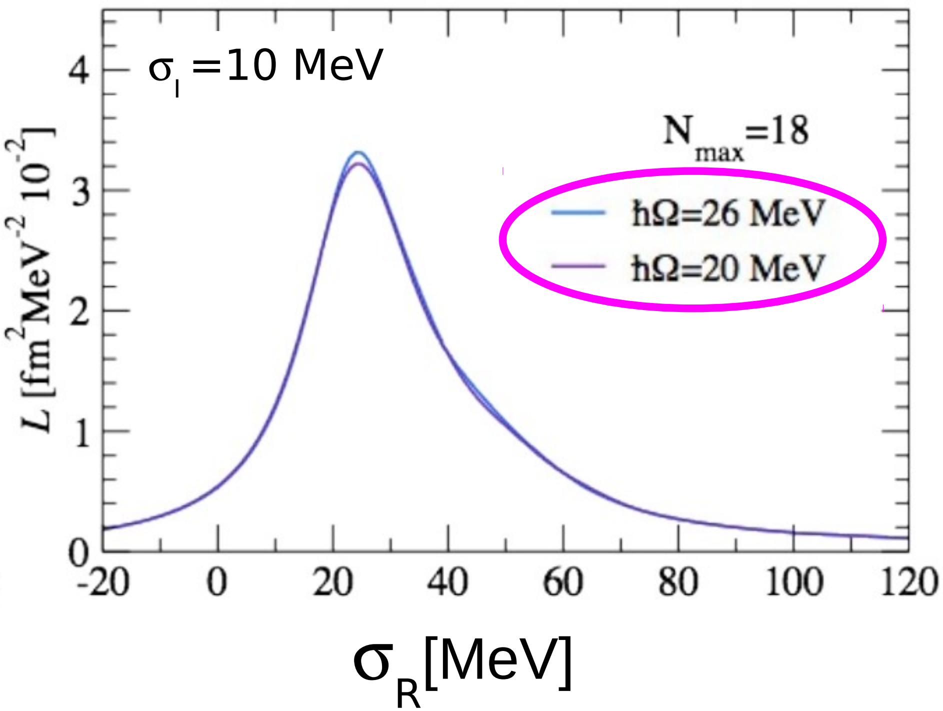
^{16}O : Convergence of the LIT



Good convergence!

^{16}O : H.O. parameter dependence

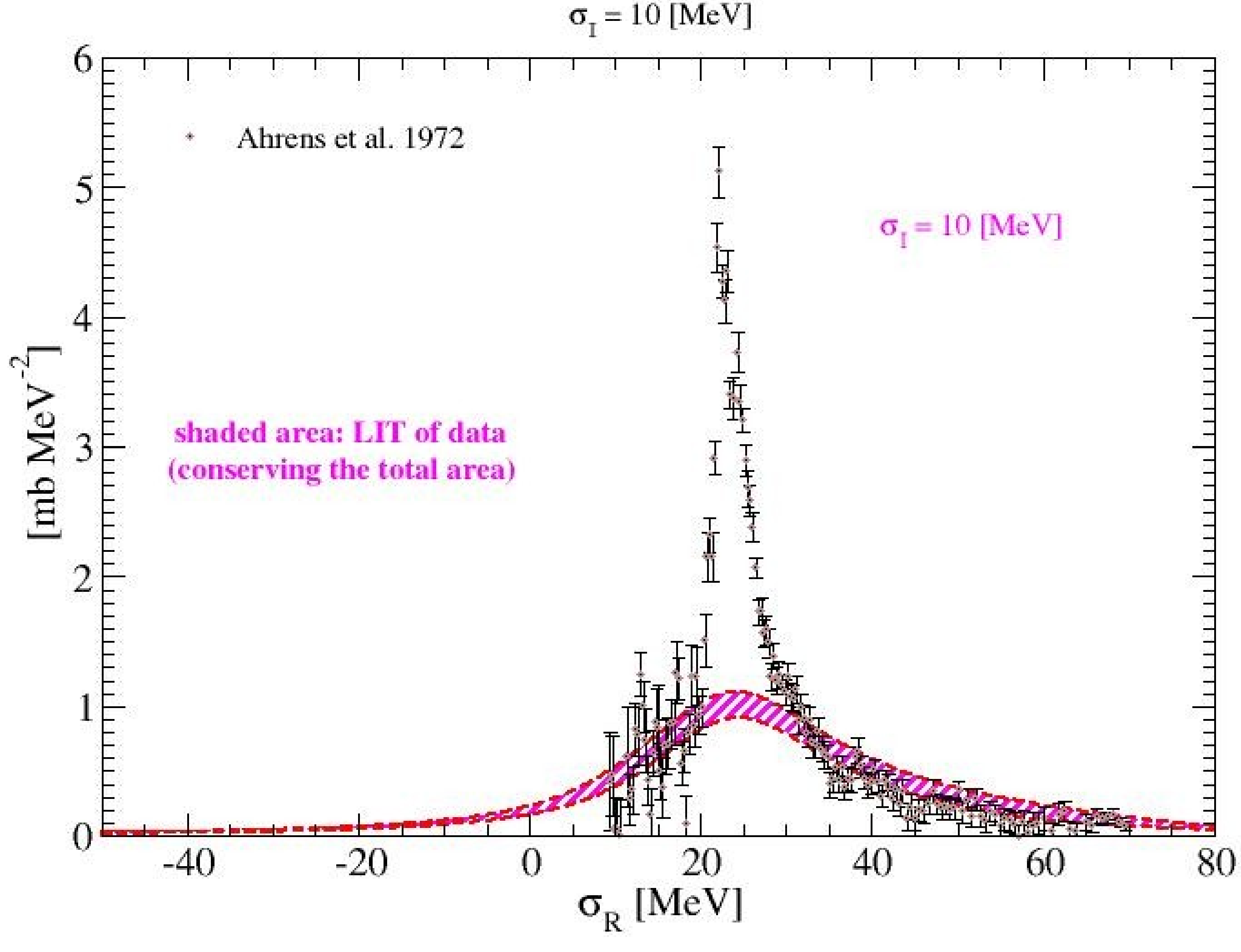




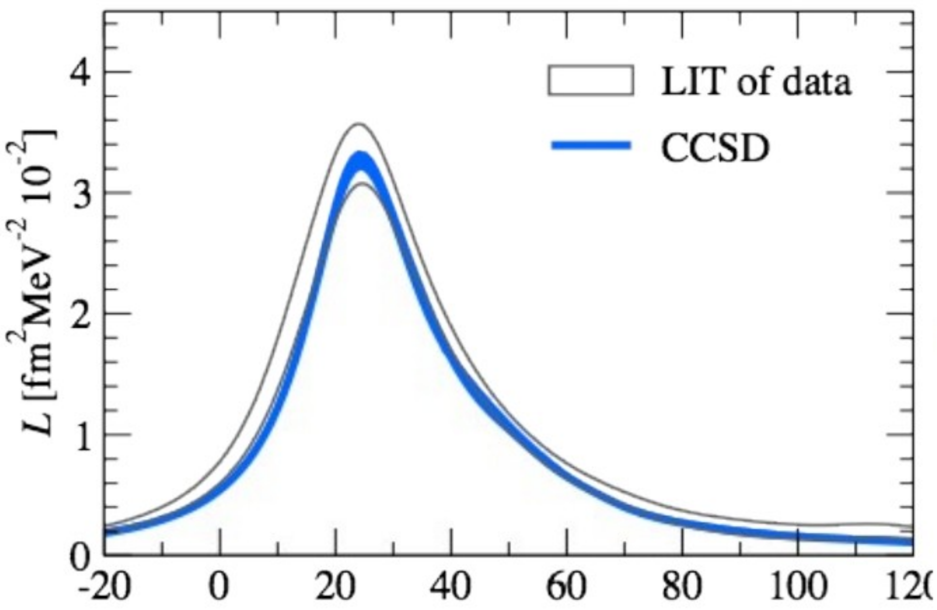
Good convergence!

Small HO dependence:
use it as error bar!

Exper. LIT of the photoabsorption cross section of ^{16}O



Comparison between the Exp. and Theor. LIT's



σ_R[MeV]

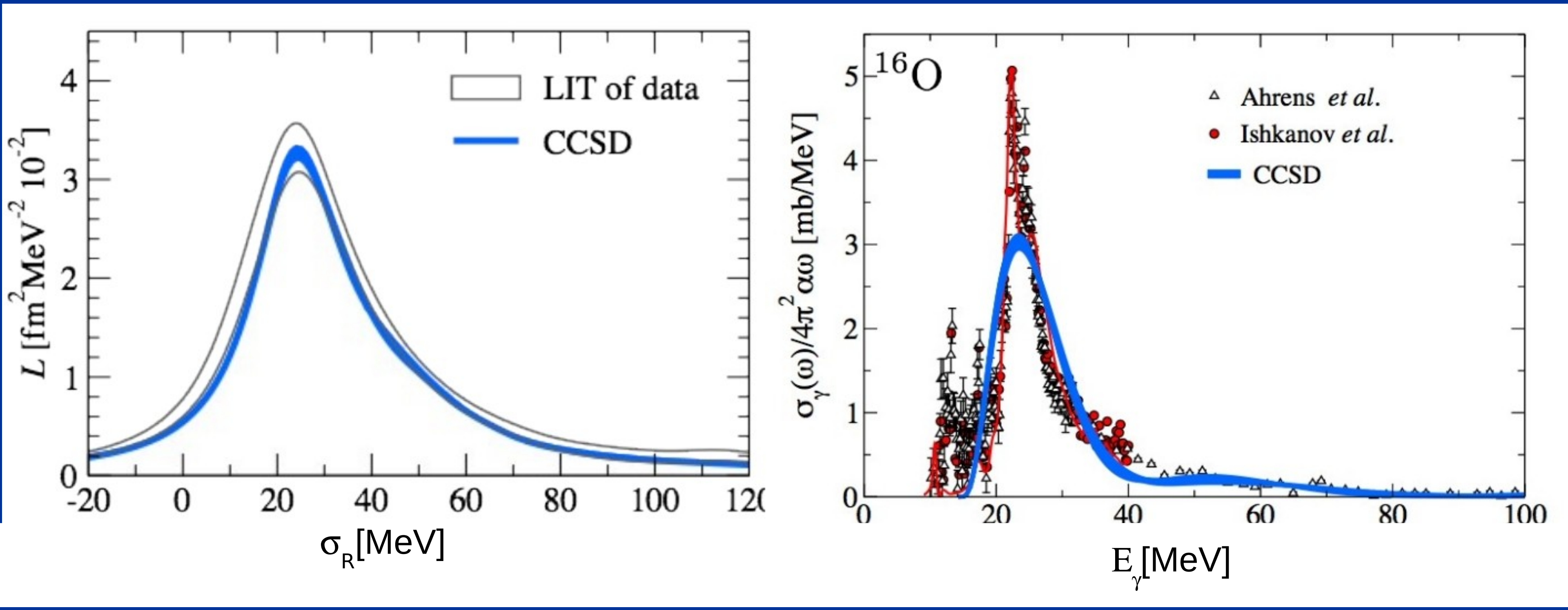
σ_I =10 MeV

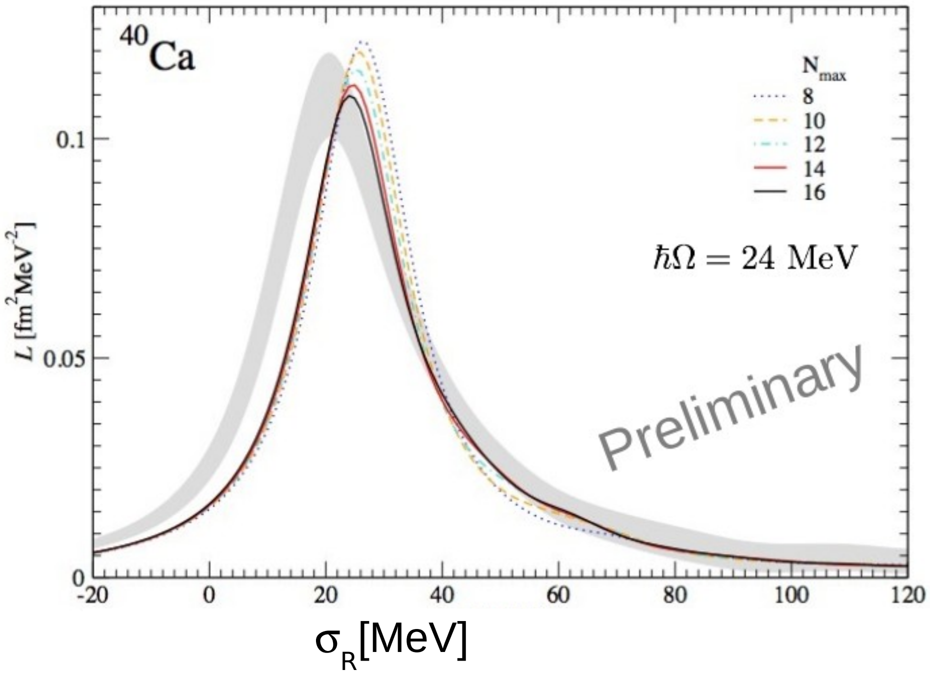
The width of the GDR is around 6 MeV

Our width is 10 MeV

We can try to invert the LIT

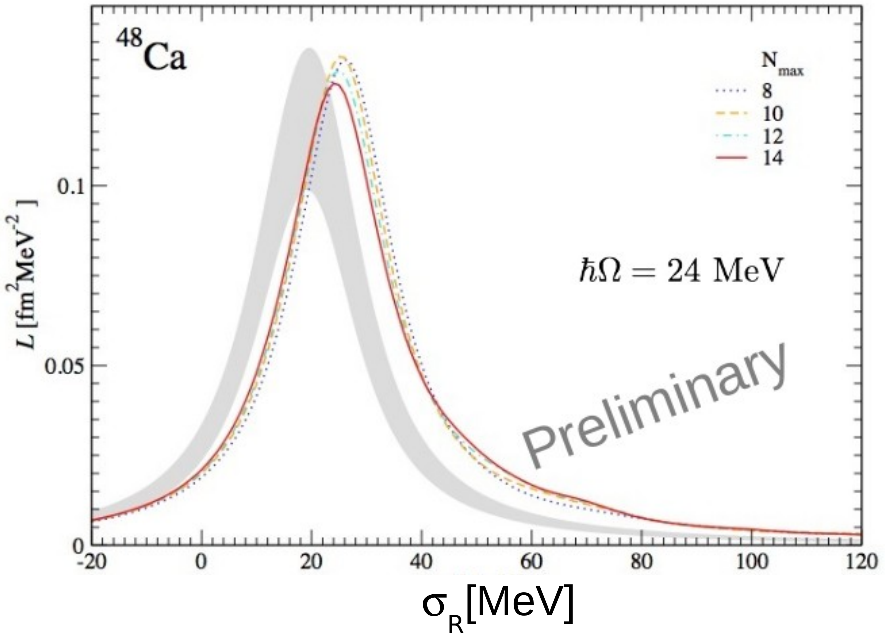
Comparison between the Exp. and Theor. LIT's





Mirko Miorelli

σ_I =10 MeV



A good kernel for Monte Carlo methods:

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(A.Roggero, F. Pederiva, G.Orlandini Phys. Rev. B 88, 115138 (2013))

combination of Sumudu kernels:

$$K_P(\omega, \sigma) = N\,\sigma \left(\frac{e^{-\mu\,\omega/\sigma}}{\sigma} - \frac{e^{-\nu\,\omega/\sigma}}{\sigma} \right)^P$$

$$\nu/\mu = b/a \qquad \nu - \mu = \frac{\ln[b] - \ln[a]}{b - a}$$

$b > a > 0$ integer

A good kernel for Monte Carlo methods:

(A.Roggero, F. Pederiva, G.Orlandini arXiv-1209.5638)

3. arXiv:1209.5638

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$$K_P(\omega , \sigma) \xrightarrow[P \to \infty]{} \delta(\omega - \sigma)$$

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s. arXiv:1209.5638

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$$= N \sum_k^P (-1)^k \binom{k}{P} e^{-\tau(P,k,\sigma)\, \omega}$$

Finite sum of Laplace Kernels!

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Small width ---> large P ---> **large** imaginary time

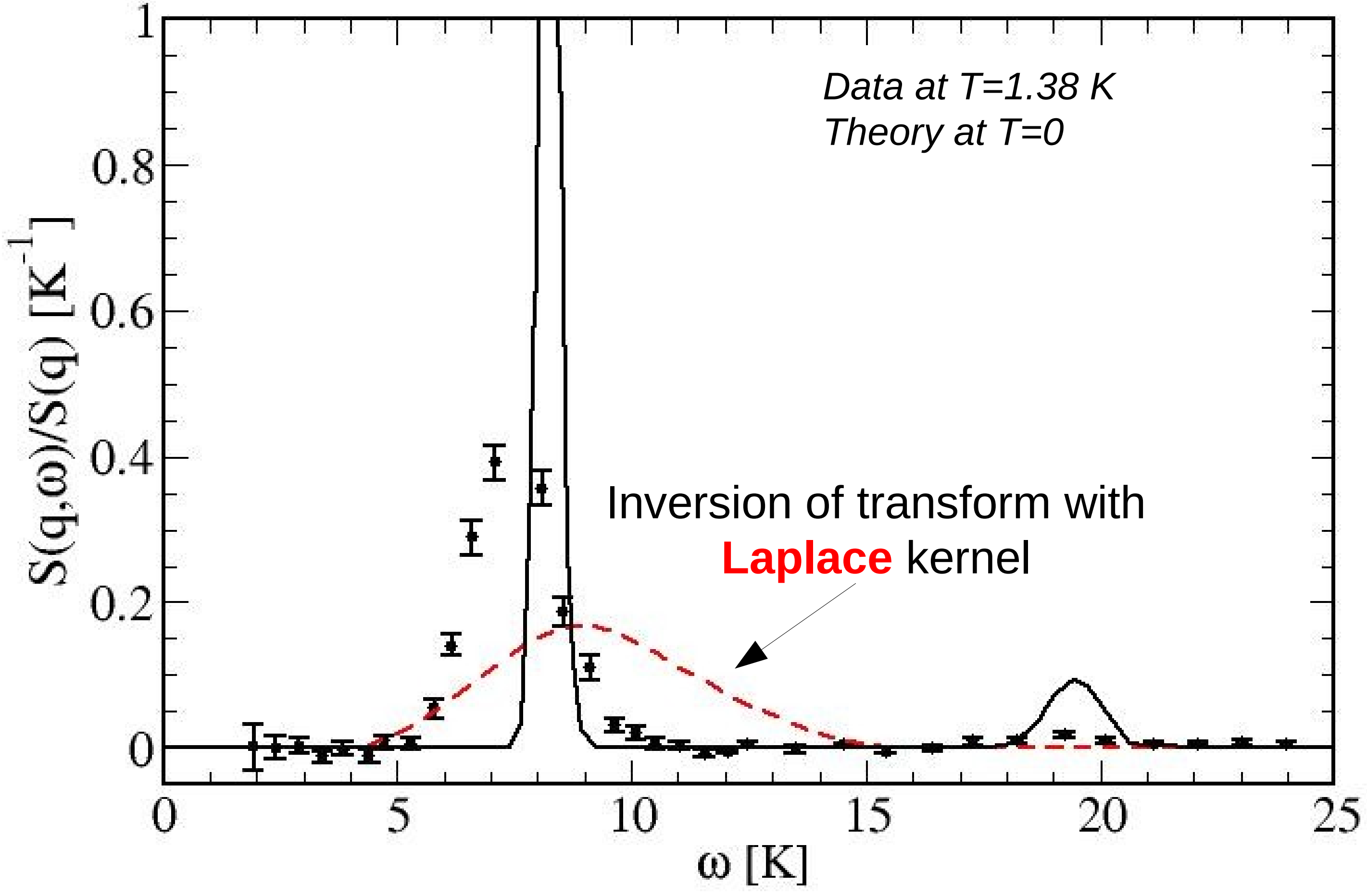
(**Zero** width ---> P = ∞ ---> **infinite** τ !!!)

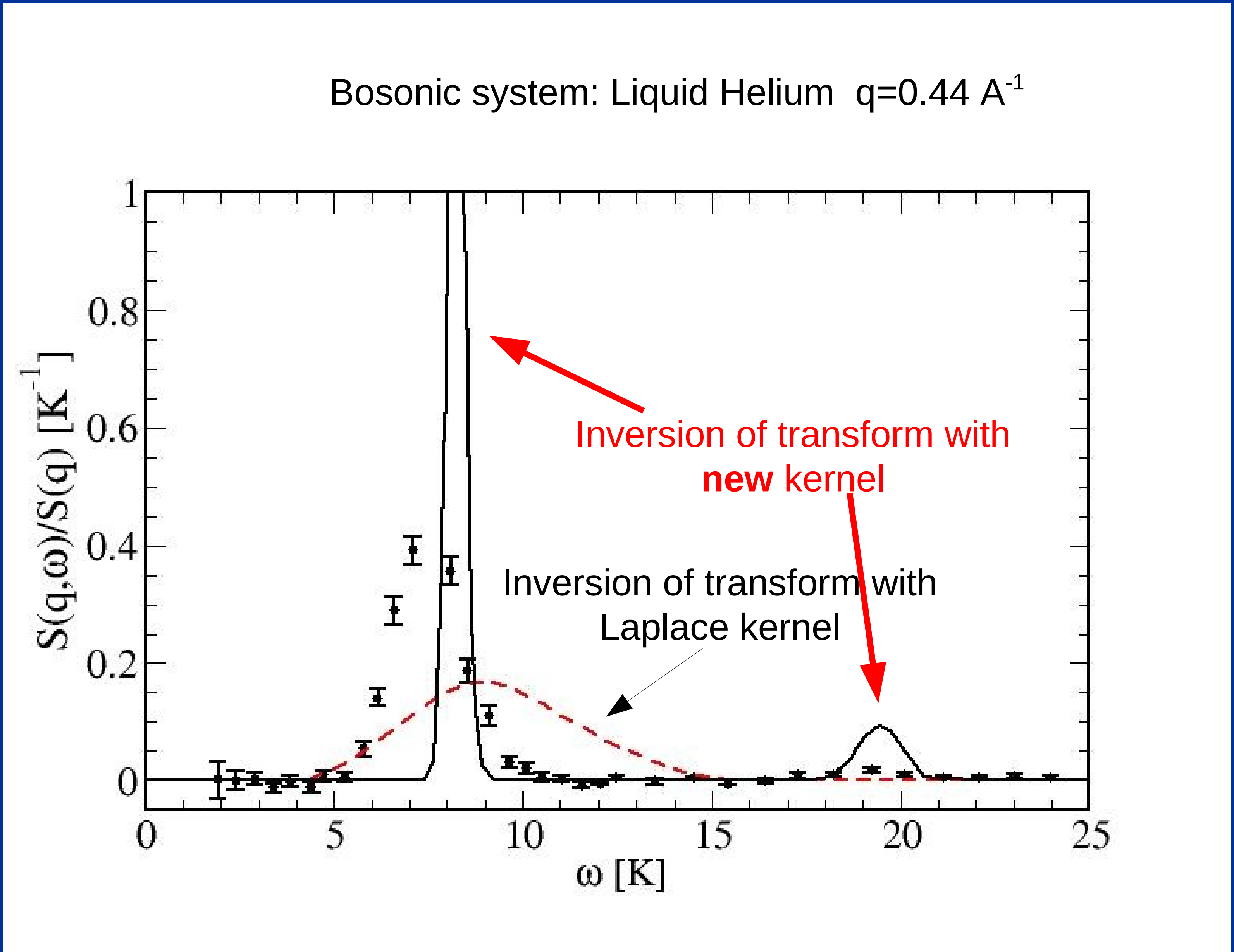
First application for bosons

(no sign problem)

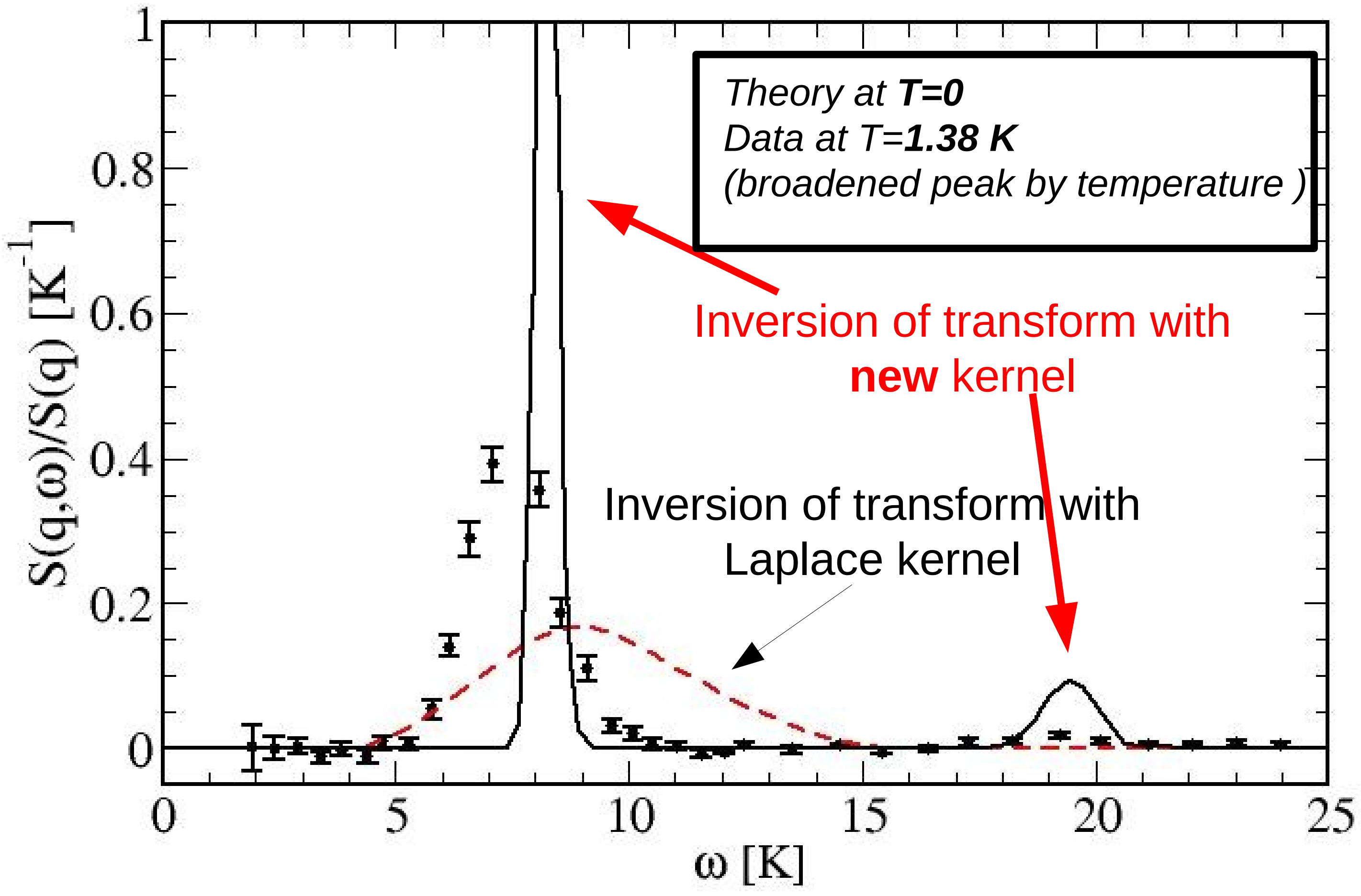
The transform is calculated with Reptation MC and then inverted

Bosonic system: Liquid Helium q=0.44 A^{-1}

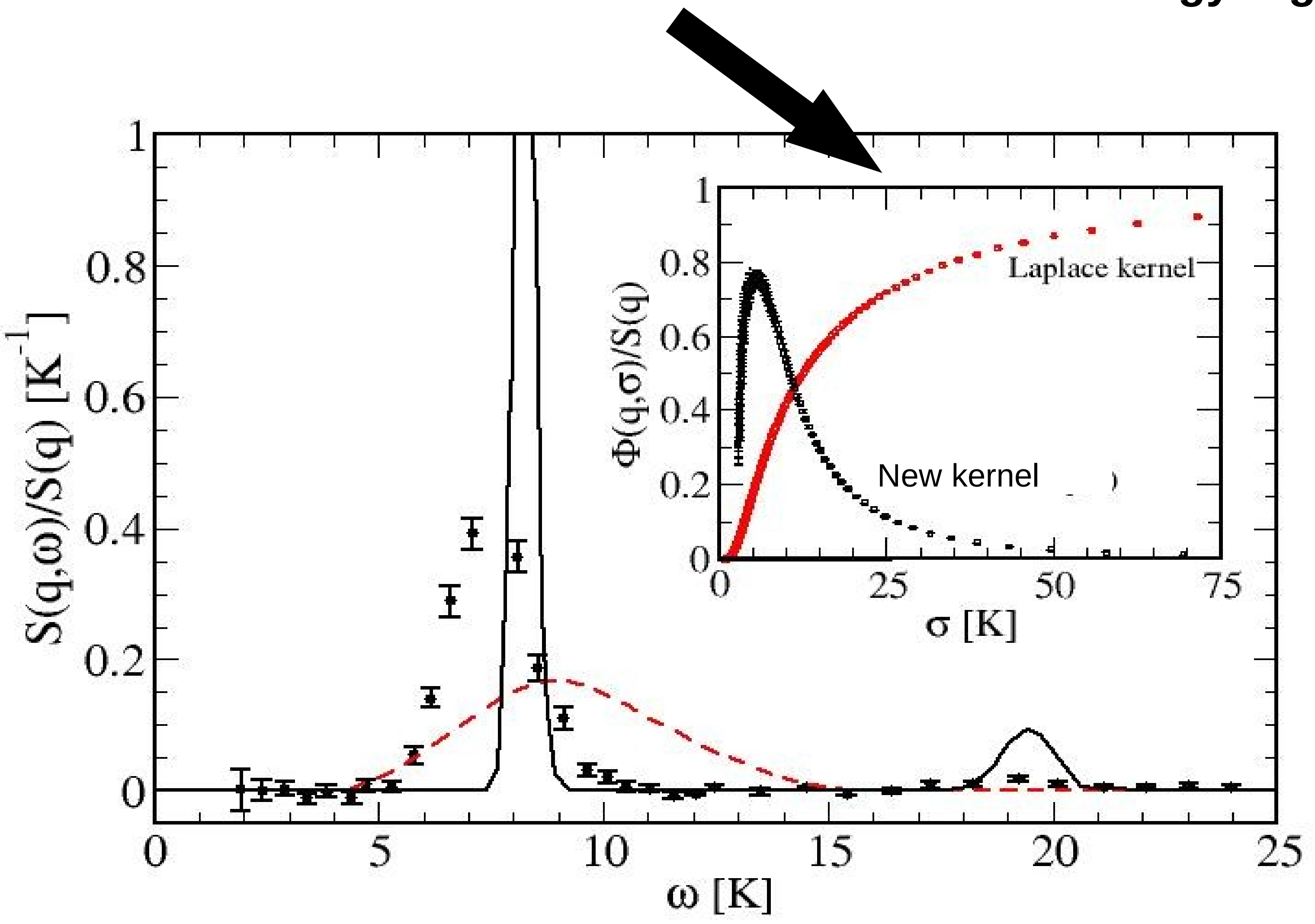



Bosonic system: Liquid Helium q=0.44 A-1
Inversion of transform with new kernel
Inversion of transform with Laplace kernel
S(q,ω)/S(q) [K-1]
ω [K]
0
5
10
15
20
25
0.2
0.4
0.6
0.8
1

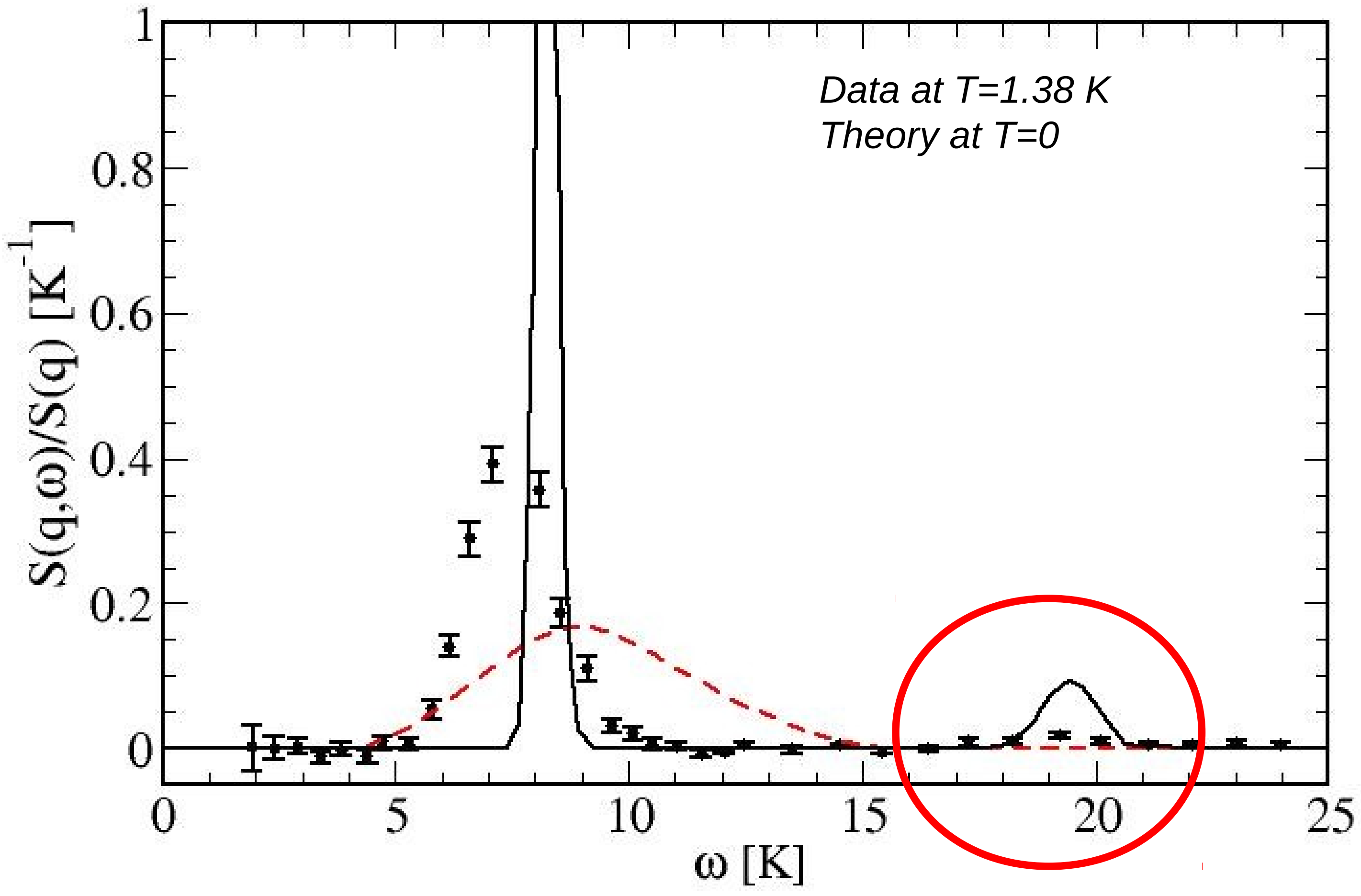
Bosonic system: Liquid Helium q=0.44 A^{-1}

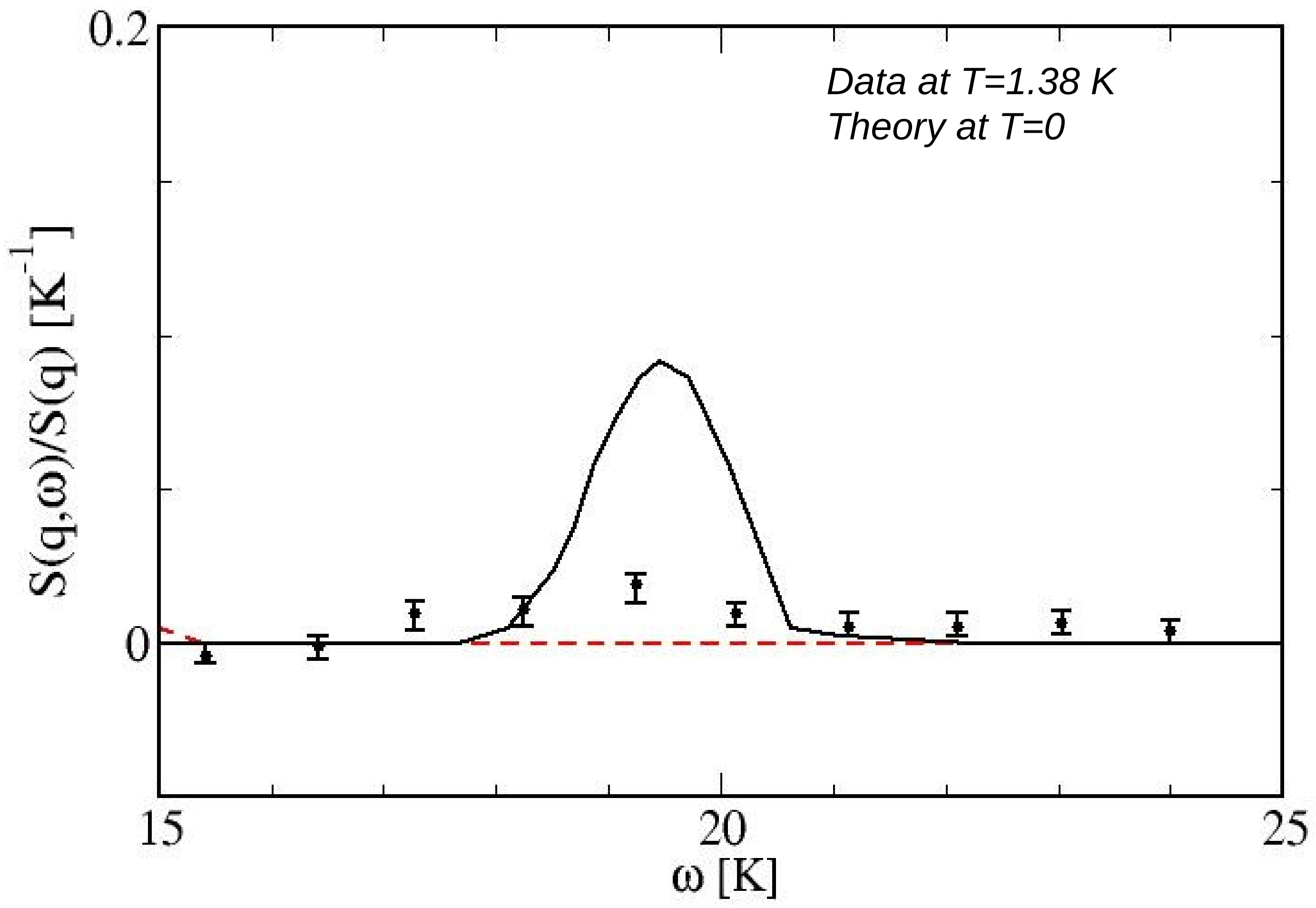


Look at teh different form of the 2 kernels on that energy region !!



Bosonic system: Liquid Helium




0.2
0
15
20
25
ω [K]
S(q,ω)/S(q) [K^-1]
Data at T=1.38 K
Theory at T=0

conclusions

1) Integral transform approaches are very powerful ab initio methods for cross sections in the continuum

2) Good kernels are representations of the delta-functions (provided that one can calculate the integral transform !)

The work presented here has been done in collaboration with

- Victor Efros (Moscow)
- Nir Barnea (Jerusalem)
- Sonia Bacca (TRIUMF)
- Gaute Hagen (ORNL)
- Thomas Papenbrock (ORNL)
- Winfried Leidemann (Trento)
- Francesco Pederiva (Trento)
- *Alessandro Roggero (Trento)*
- *Mirko Miorelli (Trento)*

Now use the similarity transformations inserting

$e^{T}e^{-T} = 1$

$$\Phi(\sigma_R, \sigma_I) = -\sigma_I/\pi \, \mathrm{Im}\, [< 0 \,|\, \Theta^{+} (H - E_0 - \sigma_R + i\sigma_I)^{-1} \Theta \,|\, 0 >]$$

Insert $e^{T}e^{-T} = 1$

$T = T^{[1]} + T^{[2]} + T^{[3]} + T^{[4]} + \ldots$

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CCSD

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Insert $e^{T}e^{-T}=1$

$$T = T^{[1]} + T^{[2]} + T^{[3]} + T^{[4]} + \ldots$$

CCSDT

$$S(\omega) = -1/\pi \; \mathrm{Im} \left[<0|\, \Theta^{+} (H - E_0 + \iota\varepsilon)^{-1} \,\Theta\, |0> \right]$$

ε infinitesimal !

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ε infinitesimal !

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σ_I finite!