Reactions to continuum with bound state methods: the integral transform approach

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Introd. { Reactions to continuum
with bound state methods:

the integral transform approach

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Reactions to continuum

non-perturbative (hadronic)

a + b ----> c + d +...

perturbative (electro-weak)

$\gamma^{(*)}$ + b ----> c + d +...

Where a,b,c,d... are single nucleons or bound nuclear systems
In total: A nucleons involved
A-BODY PROBLEM!

Reactions to continuum

Framework:

- Energies in the non-relativistic regime

  → Non-Relativistic Quantum Mechanics

  *(including **Translation** , **Galileian** , **Rotational** invariances)*

  $[H, \mathbf{P}_{cm}]=0$ $[H, \mathbf{R}_{cm}]=0$ $[H, \mathbf{J}]=0$

- Degrees of freedom: total A nucleons ("microscopic" model)

- $H = T + V$ $V = \Sigma_{ij}\, v_{ij} + (\Sigma_{ijk}\, v_{ijk} + \ldots)$

Digression about potentials for microscopic approaches

(few/not-so-few-nucleon systems)

Before S. Weinberg 1990

V_{ij} :

- generalization of Yukawa idea:

  exchange of pion ----> exchange of mesons (OBEP)

- phenomenological but including symmetries:

phenomenological potentials

to the isospin-invariant case. The available vectors are given by the position, momentum and spin operators for individual nucleons: $\vec{r}_1, \vec{r}_2, \vec{p}_1, \vec{p}_2, \vec{\sigma}_1, \vec{\sigma}_2$. The translational and Galilean invariance of the potential implies that it may only depend on the relative distance between the nucleons, $\vec{r} \equiv \vec{r}_1 - \vec{r}_2$, and the relative momentum, $\vec{p} \equiv (\vec{p}_1 - \vec{p}_2)/2$. Further constraints due to (i) rotational invariance, (ii) invariance under a parity operation, (iii) time reversal invariance, (iv) hermiticity as well as (v) invariance with respect to interchanging the nucleon labels, $1 \leftrightarrow 2$, lead to the following operator form of the potential [7]:

$$\left\{\mathbf{1}_{\text{spin}},\ \vec{\sigma}_1 \cdot \vec{\sigma}_2,\ S_{12}(\vec{r}),\ S_{12}(\vec{p}),\ \vec{L}\cdot\vec{S},\ (\vec{L}\cdot\vec{S})^2\right\} \times \left\{\mathbf{1}_{\text{isospin}},\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right\}, \tag{2.2}$$

where $\vec{L} \equiv \vec{r} \times \vec{p}$, $\vec{S} \equiv (\vec{\sigma}_1 + \vec{\sigma}_2)/2$ and $S_{12}(\vec{x}) \equiv 3\vec{\sigma}_1 \cdot \hat{x}\, \vec{\sigma}_2 \cdot \hat{x} - \vec{\sigma}_1 \cdot \vec{\sigma}_2$ with $\hat{x} \equiv \vec{x}/|\vec{x}|$. The operators entering the above equation are multiplied by scalar operator-like functions that depend on r^2, p^2 and L^2.

- Both OBEP and phenomenological potentials end up in combinations of the same operator terms and a total of about 40 parameters

  (SM: 19 parameters !)

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- Both OBEP and phenomenological potentials end up in combinations of the same operator terms and a total of about 40 parameters (SM: 19 parameters !)
- Parameters are obtained by best fit on deuteron and about 4000 nucleon-nucleon scattering data at E_{cm} below pion threshold (140 MeV)
- χ-square per data: 1.05-1.1 !

Question:

- How do these "perfect" potentials at two-body level perform for A=3?

  Do they reproduce triton binding energy of 8.48 MeV??

Answer:

No!

8.00(5) MeV (OBEP)

7.62(4) MeV (Phen.)

8.481798(3) MeV (EXP)

at least half of an MeV is missing!

The discrepancy in the triton binding energy establishes the importance of **three-body forces** $\mathbf{V_{ijk}}$

Notice:

the assumption $H = T + \sum_{ij} V_{ij}$

is similar to the gravitational problem, namely **only two-body** interactions between A **point-masses** are present.

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However, in classical gravitation when ***3 extended objects*** (e.g. moon-earth-sun) are treated *as* ***point masses --->*** **three-body "*tidal*" forces** arise !!!

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However, in classical gravitation when ***3 extended objects*** (e.g. moon-earth-sun) are treated *as* ***point masses ---> three-body "tidal" forces*** arise !!!

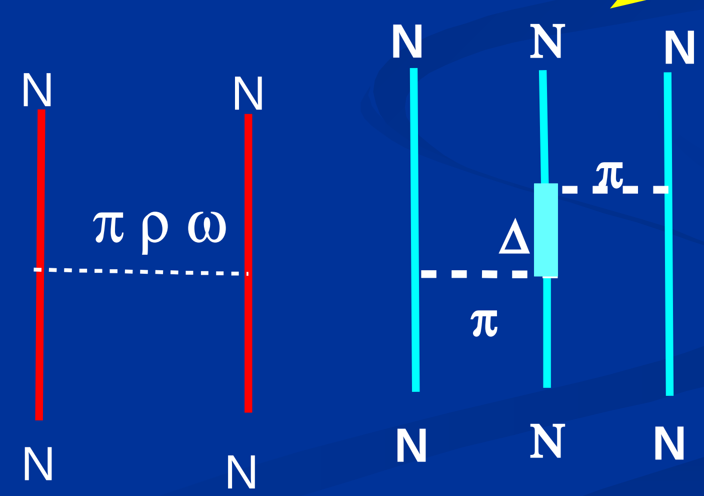
In principle if A non-elementary objects like nucleons are treated as point particles also **3- 4-...N-body forces** should arise.

The nuclear hamiltonian

Kinetic energy

The tidal force

$$H = \sum_{i}^{A-1} \frac{\pi_i^2}{2\mu} + \sum_{ij} V_{ij} + \sum_{ijk} V_{ijk} + \dots$$



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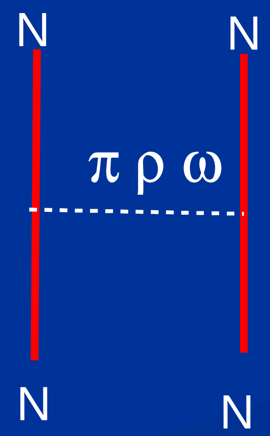
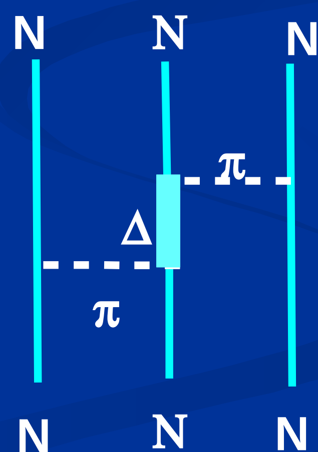




Adds operators of more complicated structure and **one additional parameter fitted on triton binding energy**

How is the ^{4}He binding energy?

28.3(1) MeV (Phen.)
28.2956(6) MeV (EXP)

agree at few tens of MeV level

A less phenomenological approach:

S.Weinberg's idea

1) notice a separation of scale between $Q \sim m_\pi$ and $\Lambda = M_p$

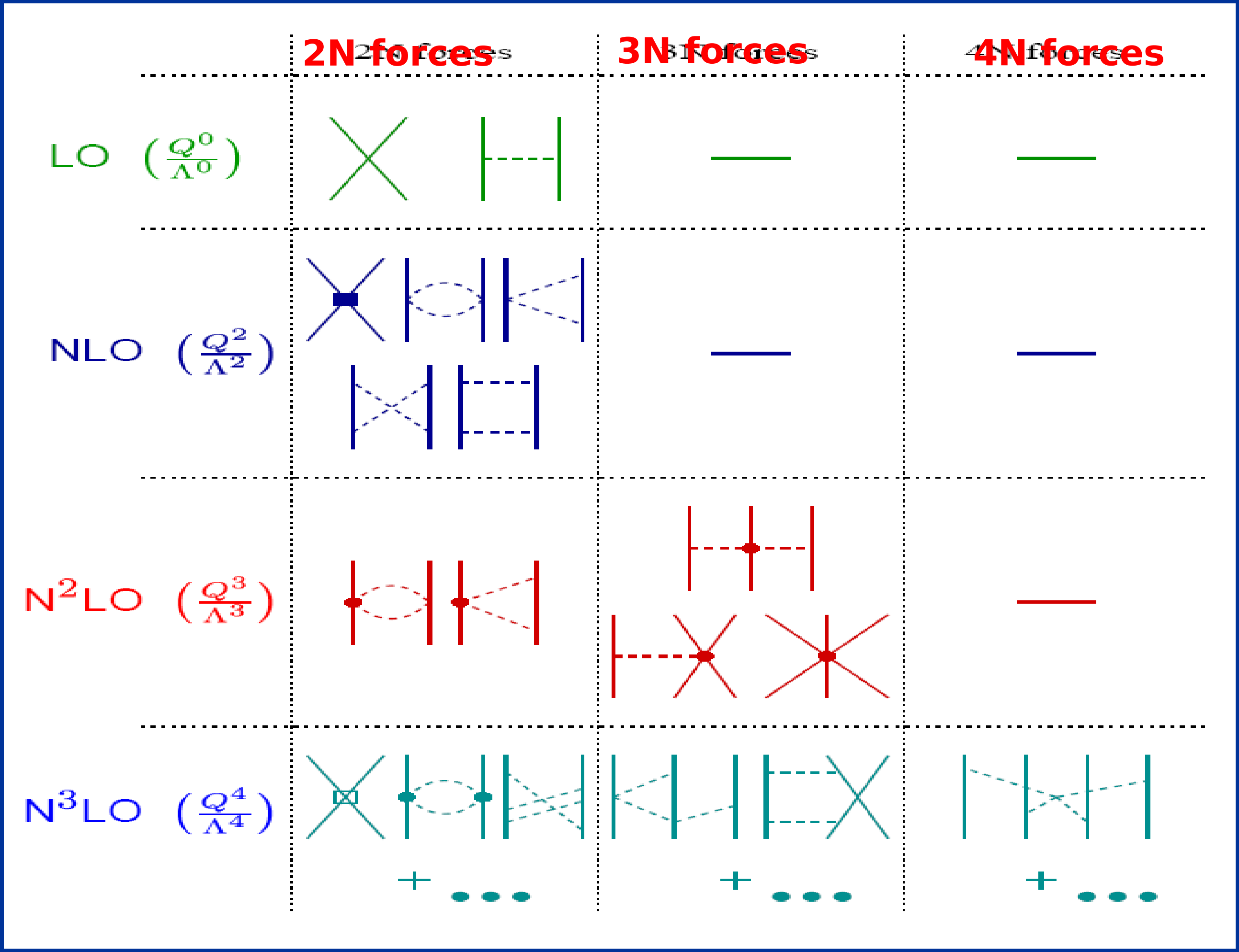
2) write the most general Lagrangian with pions and nucleons as relevant degrees of freedom...

3) ... consistent with QCD symmetries including **chiral symmetry,**

4) expand it in terms of $(Q/\Lambda)^n$

3,4,… nucleon potentials appear! V_{ijk}, V_{ijkl} …

In a hierarchy! 2-body *larger* than 3-body *larger* than 4-body…



END
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- **First order** perturbation theory *(Fermi-Golden Rule)*
- **Linear** Response theory

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- **First order** perturbation theory *(Fermi-Golden Rule)*
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$$\sigma(\omega) \sim \quad |\langle n | \Theta | 0 \rangle|^2 \quad \delta(\omega - E_n + E_0)$$

$$H | n \rangle = E_n | n \rangle$$

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Energy transferred by the perturbative probe

perturbative (electro-weak)

$\gamma^{(*)}$ + b ----> c + d +...

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Ground state of the target
A-body bound state!

perturbative (electro-weak)

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Reactions to continuum

- **First order** perturbation theory *(Fermi-Golden Rule)*
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Fragmented target
A-body continuum state!

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- **First order** perturbation theory *(Fermi-Golden Rule)*
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Property of the target responsible of the interaction with the perturbative probe e.g. charge-current density

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Reactions to continuum

- **First order** perturbation theory *(Fermi-Golden Rule)*
- **Linear** Response theory

$$\sigma(\omega) \sim \sum_n |\langle n | \Theta | 0 \rangle|^2 \delta(\omega - E_n + E_0)$$

perturbative (electro-weak) **INCLUSIVE**

$\gamma^{(*)}$ + b ---> b^* (b^*= c+d+.. *or* e+f+.. *or* ...)

Reactions to continuum

- **First order** perturbation theory *(Fermi-Golden Rule)*
- **Linear** Response theory

$$\sigma(\omega) \sim \sum_n |\langle n | \Theta | 0 \rangle|^2 \delta(\omega - E_n + E_0)$$

$$\sum_n | n \rangle \langle n | = I$$

$$H | n \rangle = E_n | n \rangle$$

Reactions to continuum

PERTURBATIVE INCLUSIVE

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

$S(\omega)$ represents the crucial quantity
Requires the solution of both
the **bound** and **continuum** A-body problem

We see next that in case of non perturbative reactions the crucial quantity for calculating the cross section has a very similar form

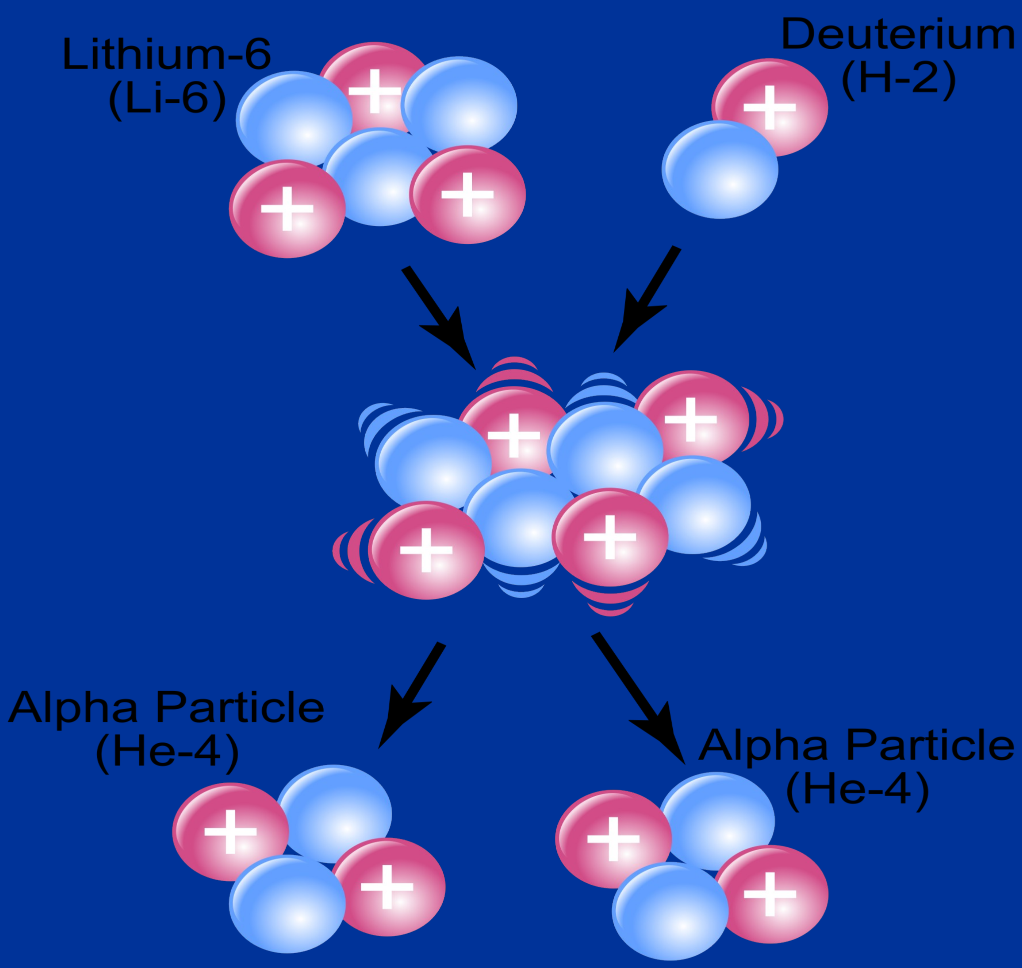
Reactions to continuum

non-perturbative (hadronic)

a + b ----> c + d +...

$$\sigma(\omega) \sim |T_{\beta\alpha}(E)|^2$$

$\mathbf{H}$ is the Hamiltonian of the 8-body system



Lithium-6 – Deuterium Reaction

Reactions to continuum

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General form of T-matrix

(cfr eq. (108) in ch. 5 of Goldberger-Watson Collision Theory)

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$$T_{\beta\alpha}(E) = < \chi_\beta\, \mathcal{V}_\alpha\, \chi_\alpha > \; + \; < \chi_\beta\, \mathcal{V}_\beta\, (E - H + i\,\eta)^{-1} \mathcal{V}_\alpha\, \chi_\alpha >$$

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A-body continuum energy

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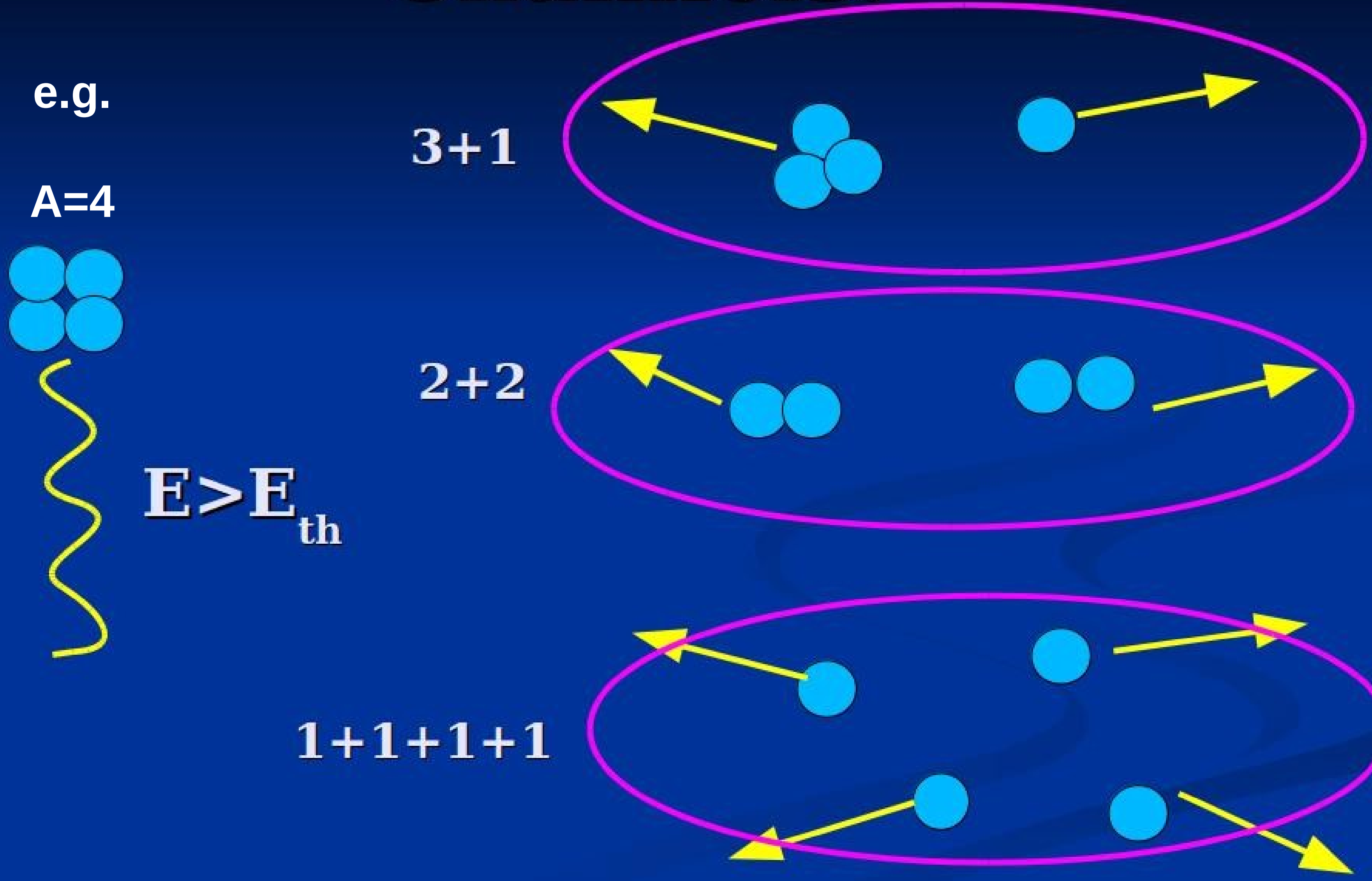
$\chi_{\beta,}$ and χ_α are the "channel functions" (with proper antisymmetrization), namely products of the **bound states** of **a** and b, times a relative Plane Wave

$$|\chi_\alpha> = \mathcal{A} |a>|b> | \mathcal{PW}>$$

Channels:



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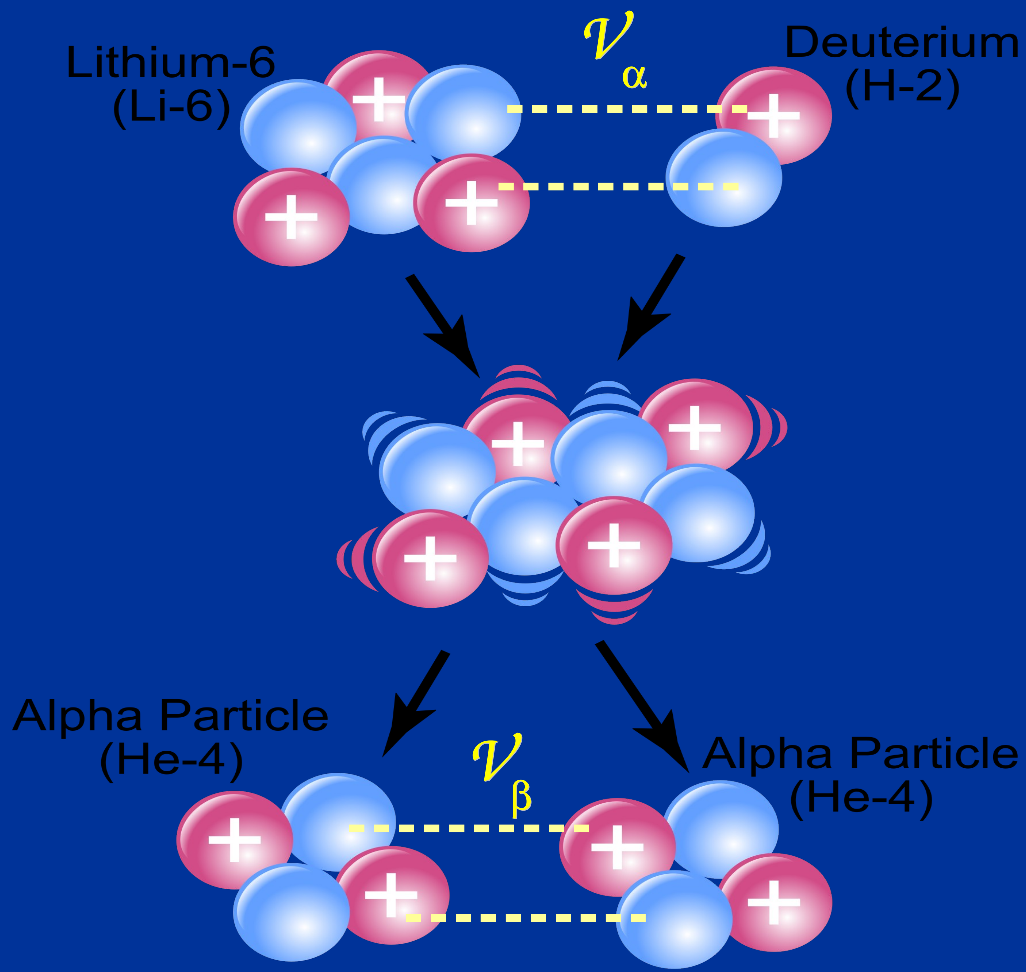

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"easier" part

Very difficult part

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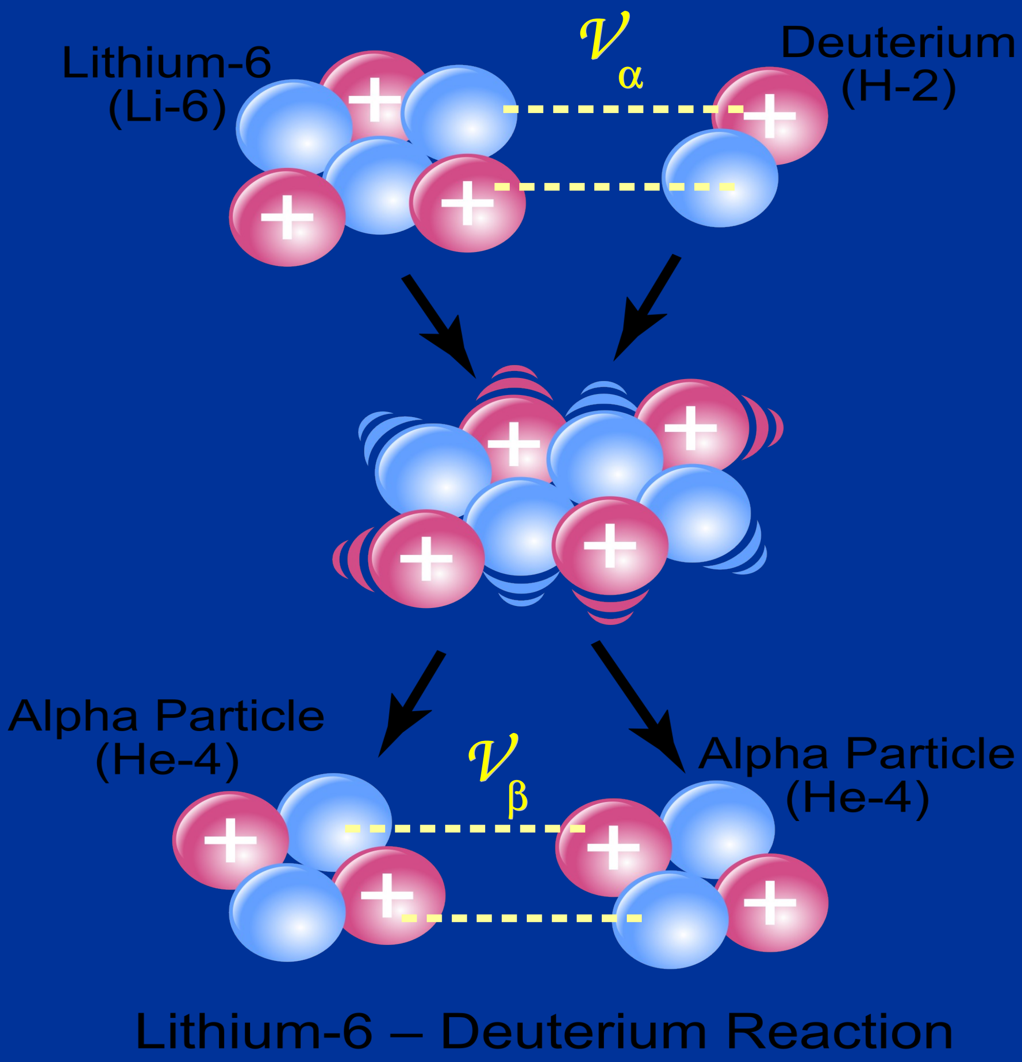
"easier" part

Very difficult part

If we denote $\mathcal{V}_{\alpha,\beta}\, \chi_{\alpha,\beta} = \phi_{\alpha,\beta}$

$\mathcal{V}_{\alpha,\beta}$ is the sum of the potentials between particles belonging to different fragments

H is the Hamiltonian of the 8-body system



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easier part

Very difficult part

$$< \phi_\beta | \;\; (E - H + i\,\eta)^{-1} \; \phi_\alpha >$$

One can manipulate the non trivial part:

$$< \phi_\beta \,|\, (E - H + i\,\eta)^{-1}\, \phi_\alpha > =$$

Step 1) Insert **completeness of eigenstates** |n> of H: $\Sigma_n |n\rangle\langle n| = I$

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$$= \Sigma_n < \phi_\beta | \, n > < n \, | \ (E - H + i\,\eta)^{-1} \ \phi_\alpha > =$$

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Step 1) Insert **completeness of eigenstates** |n> of H: $\Sigma_n |n><n| = 1$

$$= \Sigma_n < \phi_\beta | n > < n | \; (E - H + i\eta)^{-1} \phi_\alpha > =$$

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$$= \int d\omega \, \Sigma_n \delta(\omega - E_n) (E - \omega + i\eta)^{-1} < \phi_\beta | n > < n | \phi_\alpha > =$$

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$$= \int d\omega \ (E - \omega + i\eta)^{-1} \ F_{\alpha\beta}(\omega) =$$

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$$= \int d\omega \, (E - \omega + i\eta)^{-1} F_{\alpha\beta}(\omega) =$$

the problem reduces to calculate the function $F_{\alpha\beta}(\omega)$

$$F_{\alpha\beta}(\omega) = \Sigma_n \delta(\omega - E_n) < \phi_\beta | n > < n | \phi_\alpha >$$

Similar expressions!

Non-Pert.

$$F_{\alpha\beta}(\omega) = \sum_n <\phi_\beta | n><n | \phi_\alpha> \delta(\omega - E_n)$$

Pert.

$$S(\omega) = \sum_n <0 | \Theta^+ | n><n | \Theta | 0> \delta(\omega - E_n + E_0)$$

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$|0\rangle$, $|\phi_\alpha\rangle$, $|\phi_\beta\rangle$ *Needs only to be able to calculate bound states!*

(Remember: $\phi_\alpha = \mathcal{V}_\alpha \chi_\alpha = \mathcal{V}_\alpha \mathcal{A} \, | a \rangle | b \rangle | \mathcal{PW} \rangle$)

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Non-Pert. $$F_{\alpha\beta}(\omega) = \sum_n < \phi_\beta | n > < n | \phi_\alpha > \delta(E_n - \omega)$$

Pert. $$S(\omega) = \sum_n < 0 | \Theta^+ | n > < n | \Theta | 0 > \delta(\omega - E_n + E_0)$$

$| n >$ *All eigenstates of the Hamiltonian, Bound and continuum*

Ab initio methods

 W. Leidemann, G. Orlandini / Progress in Particle and Nuclear Physics 68 (2013) 158–214

"Modern ab initio approaches and applications in few-nucleon physics with A ≥ 4"

that is described by a well-defined microscopic Hamiltonian *H* with *A* nucleon degrees of freedom and where the internal relative motion is treated correctly. If a method enables one to obtain the observable under consideration by solving the relevant quantum mechanical many-body equations, without any uncontrolled approximation, we consider it to be an *ab initio method*. Controlled approximations, however, are allowed. In fact a controlled approximation, e.g. a limited number of channels in a Faddeev calculation, can be increasingly improved up to the point that convergence is reached for the observable. Such a converged result we denote as a *precise ab initio* result. The comparison of *precise ab initio* results with nuclear data then allows an indisputable answer as to whether or not the chosen Hamiltonian appropriately describes the nuclear dynamics. Any uncontrolled approximation in the calculation would not lead to such a clear-cut conclusion. Quite naturally, precise ab initio results obtained with different ab initio methods but with the same Hamiltonian as input, have to agree and are often referred to as *benchmark results.*

- Solution of relevant many-body QM equation for a ***"chosen Hamiltonian"*** **(the only input!)**
- with approximations **improvable** in a **controlled** way
  (→ convergence, error estimate → **benchmark**)

The basic *ab initio* methods

	Few-body: A≤4	Few-body: 4 <A< 12,20,40??
Structure Bound states	• *Faddeev Yakubowski (FY)* • **Diagonalization methods:** ***(on different basis, e.g HH, gaussians...)***	
Reactions scattering states		

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AB INITIO BOUND STATE CALCULATIONS

BE of ^{4}He (exp. 28.296 MeV)

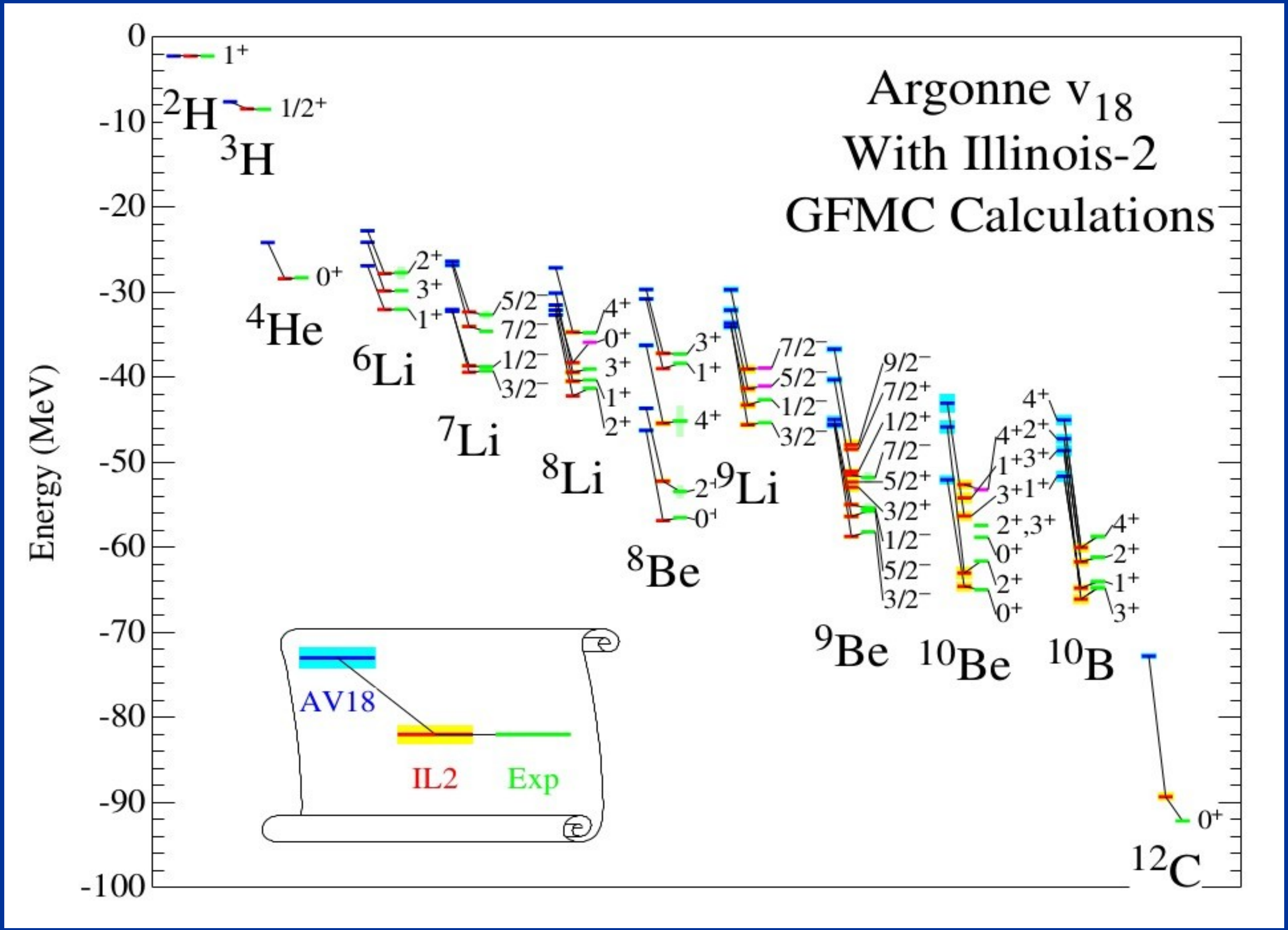
TABLES

TABLE I. The expectation values $\langle T \rangle$ and $\langle V \rangle$ of kinetic and potential energies, the binding energies E_b in MeV and the radius in fm.

Method	$\langle T \rangle$	$\langle V \rangle$	E_b	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	-128.33(10)	-25.94(5)	1.485(3)
CRCGV	102.30	-128.20	-25.90	1.482
SVM	102.35	-128.27	-25.92	1.486
HH	102.44	-128.34	-25.90(1)	1.483
GFMC	102.3(1.0)	-128.25(1.0)	-25.93(2)	1.490(5)
NCSM	103.35	-129.45	-25.80(20)	1.485
EIHH	100.8(9)	-126.7(9)	-25.944(10)	1.486

from H.Kamada et al. (18 auhors 7 groups) PRC 64 (2001) 044001

Green Function Monte Carlo



(no w.f. available!)

Courtesy R.B.Wiringa

No core shell model

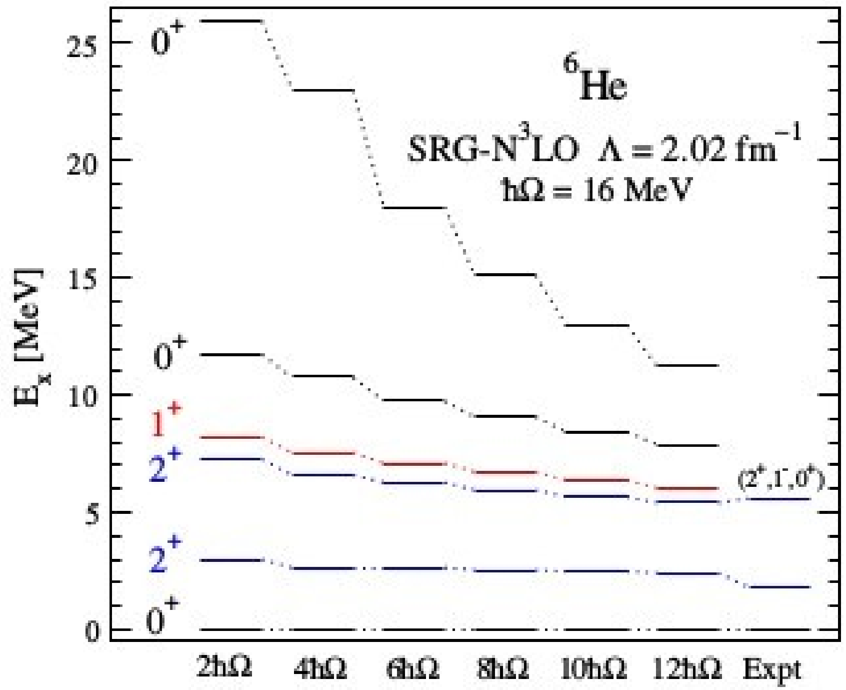


FIG. 1 (color online). Dependence of ^{6}He excitation energies on the size of the HO basis $N_{max}\hbar\Omega$.

S. Baroni, P.Navratil and S. Quaglioni PRL 110, 022505 (2013)

The basic *ab initio* methods

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Reactions scattering states	• *Faddeev Yakubowski (FY)* • *HH Kohn-Variational P. (2 fragments)*	

Why are there so few methods for reactions? Why are they limited to A=3,4?

scattering many-body problem

In configuration space (Schroedinger)

Very difficult to match the asymptotic conditions in the solution of the coupled differential equations

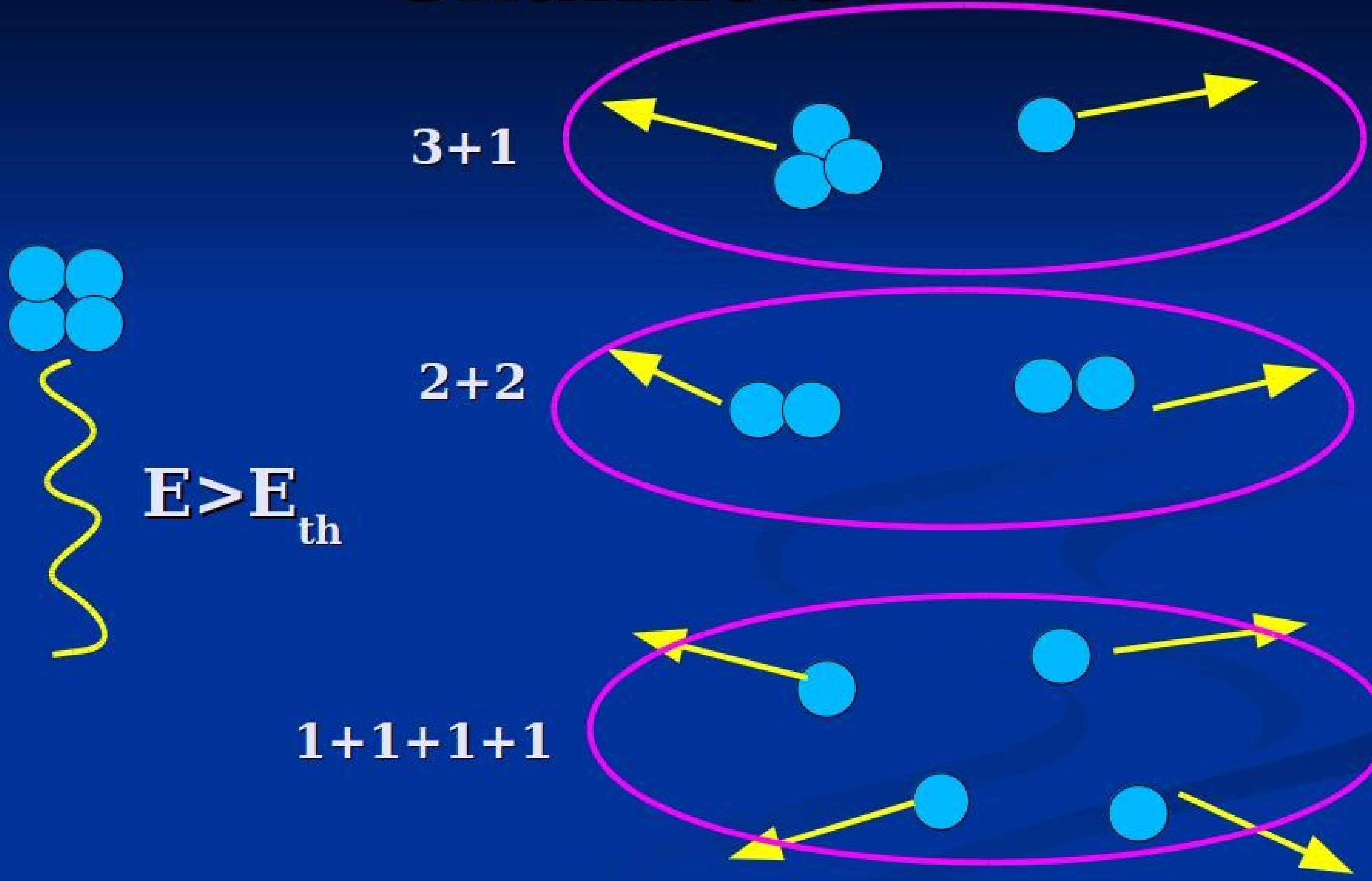
scattering many-body problem

In momentum space (Lippmann-Schwinger)

Very difficult to cope with complicated poles in solving the coupled integral equations

Before reaching the asymptotic condition all channels are coupled!!!

Channels:



Today:

- FY solved for scattering states for **A=3** (**1+2, 1+1+1**)
- FY solved for scattering states for **A=4**, however, only up to 3-body break up (**1+3, 2+2, 1+1+2,**

  not yet 1+1+1+1!)

Bochum-Cracow school: (Gloeckle, Witala, Golak, Elster, Nogga...)
Bonn-Lisabon-school (Sandhas, Fonseca, Sauer, Deltuva....)
Config. Space: (Carbonell, Lazauskas...)

Alternative approach to 2+1 or 3+1 scattering:

- **Based on Kohn variational principle**
- **Correct asymptotic conditions**

Pisa School: Kievsky, Viviani, Marcucci...

The basic *ab initio* methods

	Few-body: A≤4	**Few-body: 4 <A< 12,20,40??**
Structure Bound states	• *Faddeev Yakubowski (FY)* • **Diagonalization methods:** *(on different basis, e.g HH, gaussians...)*	• *Green Function Monte Carlo (MC)* • *Coupled Cluster (CC)* *No Core Shell Model (NCSM)* *Effective Interaction Hyperspherical Harmonics (EIHH)*
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The basic *ab initio* methods

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Structure
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- *Faddeev Yakubowski (FY)*
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Reactions
scattering states

- *Faddeev Yakubowski (FY)*
- *HH Kohn-Variational P.*
  (2 fragments)

Integral Transforms Methods (IT)

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 $\Phi(\sigma)$

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 $\Phi(\sigma)$

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 a spectral function S(ω)

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

Scattering states

Energies in the continum

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

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

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

$$\Phi(\sigma) = \Sigma_n K(E_n - E_0, \sigma) < 0 \,|\, \Theta^+ \,|\, n > < n \,|\, \Theta \,|\, 0 >$$

$$= \Sigma_n < 0 \,|\, \Theta^+ K(H - E_0, \sigma) \,|\, n > < n \,|\, \Theta \,|\, 0 >$$

2) Use $\Sigma_n | n > < n | = I$

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

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

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

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

However,

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

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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, which kernel is suitable for calculation of this?

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

One familiar example: sum rules!

Sum rules are a kind of "*Moment* transform"

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

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To obtain $S(\omega)$ the inversion of the transform is equivalent to the reconstruction of $S(\omega)$ by its moments (theory of moments)

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Sum rules are a kind of ***"Moment*** transform"

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

To obtain $S(\omega)$ the inversion of the transform
is equivalent to the reconstruction of $S(\omega)$
by its moments (theory of moments)

however, $\Phi(\sigma)$ may be ∞ for some $\sigma > \bar{\sigma}$!

Another common example:

The Laplace Kernel:

$$\Phi(\sigma) = \int e^{-\omega\sigma} S(\omega)\, d\omega = \langle 0 | \Theta^{+} e^{i(H-E_0)\sigma} \Theta | 0 \rangle$$

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In Condensed Matter Physics:

In QCD

In Nuclear Physics:

The Laplace Kernel:

$$\Phi(\sigma) = \int e^{-\omega\sigma} S(\omega)\, d\omega = \langle 0 | \Theta^{+} e^{-(H-E_0)\tau} \Theta | 0 \rangle$$

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

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

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In Condensed Matter Physics:

In QCD

In Nuclear Physics:

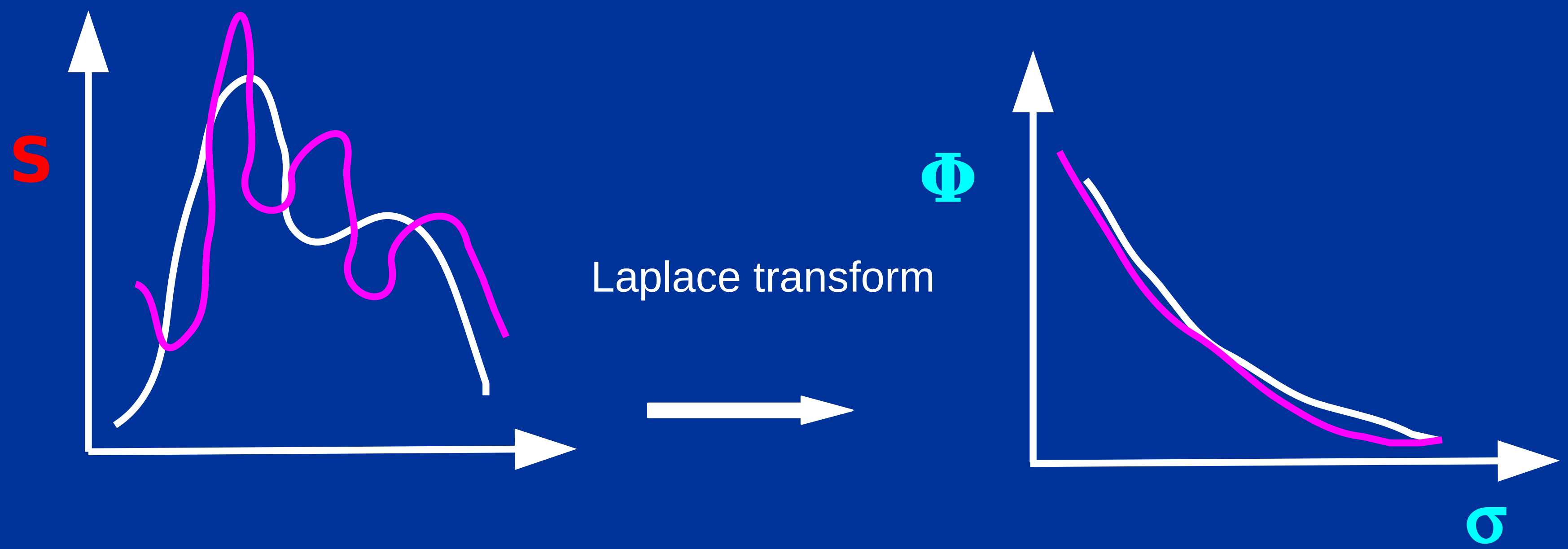
$\sigma = \tau =$ it imaginary time!

$\Phi(\tau)$ 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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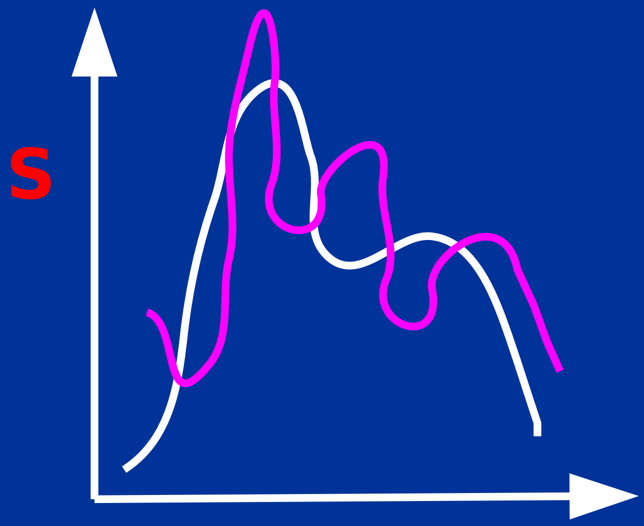
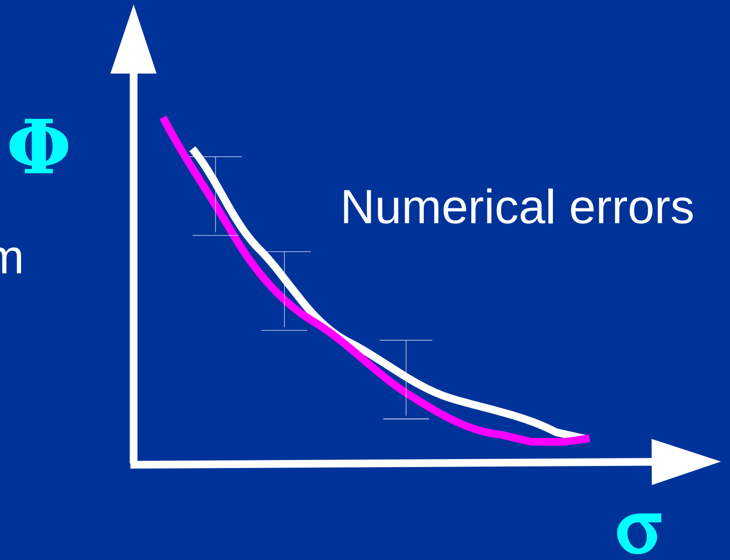


Laplace transform



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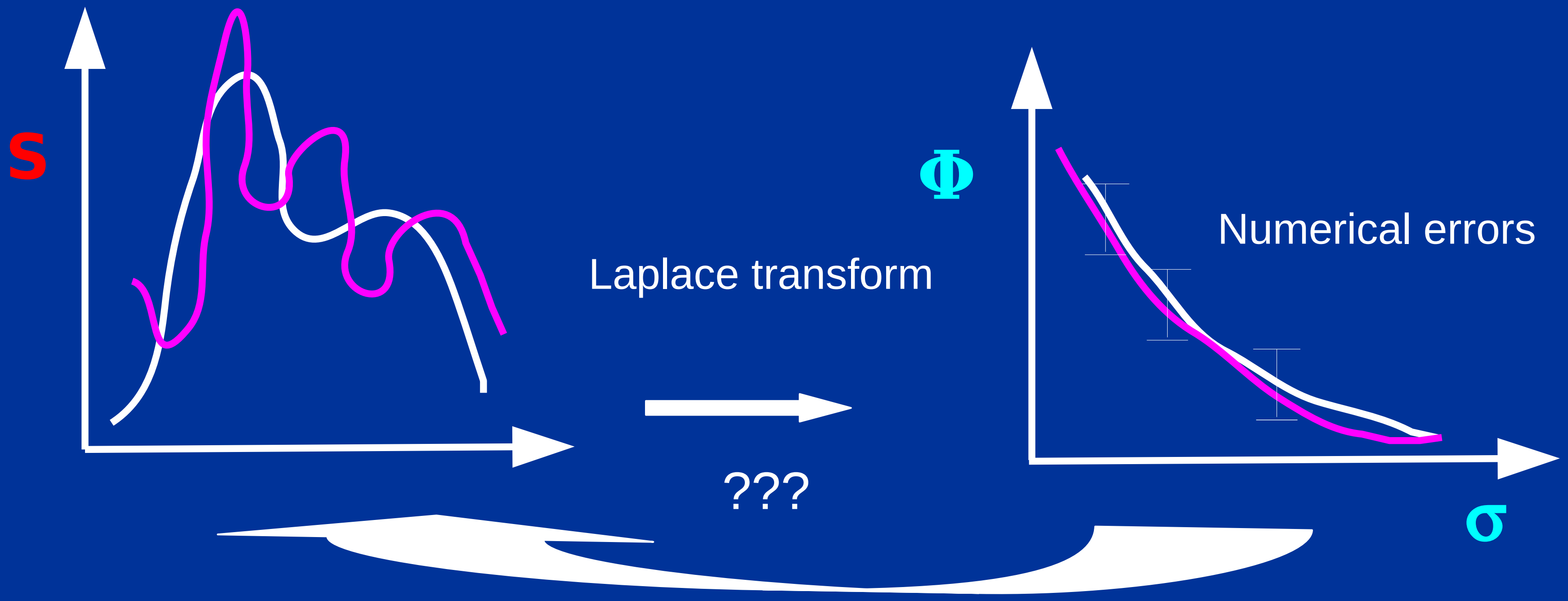

In fact:

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

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Suppose an error

$$[S(\omega) + A \sin(\nu\omega)]$$

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$$\Phi(\sigma) + \Delta\,\Phi(\nu) = \int d\omega \; K(\omega,\sigma)\,[S(\omega) + A \sin(\nu\omega)]$$

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$$\Phi(\sigma) + \Delta\Phi(\nu) = \int d\omega \; K(\omega,\sigma) \left[S(\omega) + A \sin(\nu\omega) \right]$$

$\Delta\Phi(\nu)$ → 0 for very large ν

independently on the amplitude A of the error!

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

Which is the best kernel?

The δ-function!

What would be the “perfect” Kernel?

the delta-function!

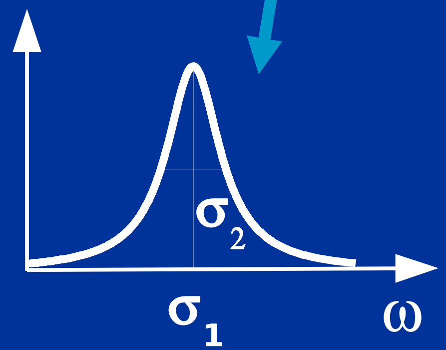
in fact

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

… but what about a representation of the δ-function?

The Lorentzian kernel:

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



It is a representation of the δ-Function

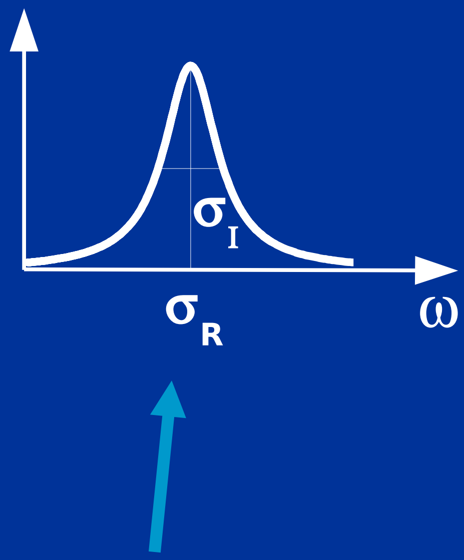
$$\Phi\,(\sigma_1,\sigma_2) = \sigma_2/\pi \int [(\omega - \sigma_1)^2 + \sigma_2{}^2]^{-1}\, S(\omega)\, d\omega$$

Illustration of requirement N.1: one can calculate the integral transform

The LIT Kernel $K(\omega, \sigma) = \sigma_2/\pi \, [\, (\omega - \sigma_1)^2 + \sigma_2^{\,2} \,]^{-1}$

Is equivalent to $K(\omega, \sigma) = \sigma_I/\pi \, (\omega - \sigma)^{-1} \, (\omega + \sigma^*)^{-1}$

with σ complex: $\sigma = \sigma_1 + i\,\sigma_2 = \sigma_R + i\,\sigma_I$



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

Remember!

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

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

$$K(\omega,\sigma)$$

$$\boxed{\Phi(\sigma)} = \int S(\omega)\,(\omega - \sigma)^{-1}\,(\omega + \sigma^*)^{-1}\,d\omega =$$

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$$K(\omega,\sigma)$$

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$$\langle 0|\,\Theta^+\,(H-E_0-\sigma)^{-1}\,(H-E_0-\sigma^*)^{-1}\,\Theta|0\rangle = \langle \tilde{\Psi}|\tilde{\Psi}\rangle$$

main point of the LIT :

Schrödinger-like equation with a source

$$(H - E_0 - \sigma_R - i\,\sigma_I) | \tilde{\Psi} > = \Theta | 0 >$$

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Schrödinger-like equation with a source

$$(H - E_0 - \sigma_R - i\,\sigma_I)\,|\,\tilde{\Psi} > = \Theta|0>$$

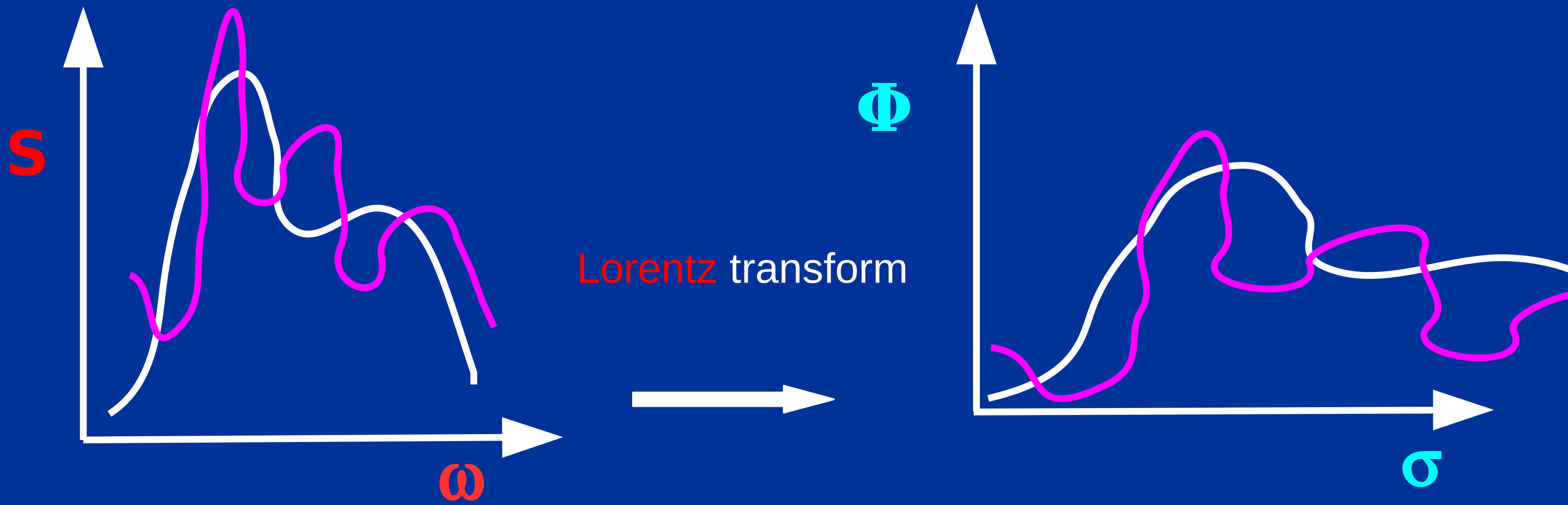
Theorem:

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

conditions → one can apply ***bound state methods***

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

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



blurred, but still distinguishable

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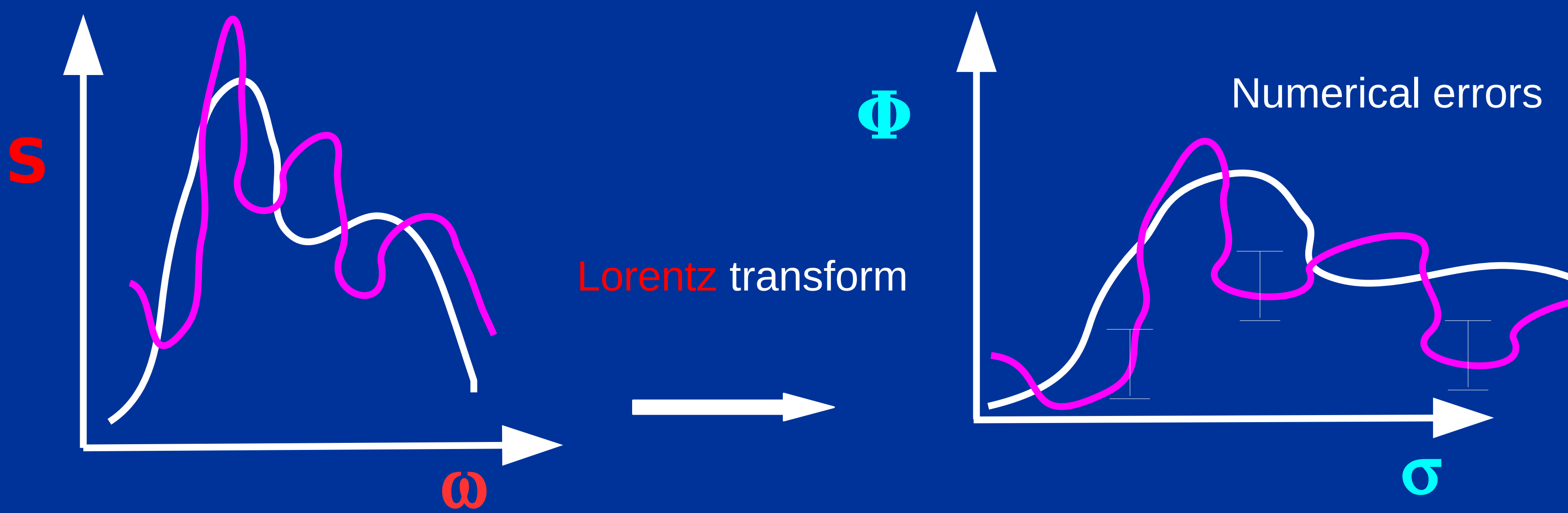
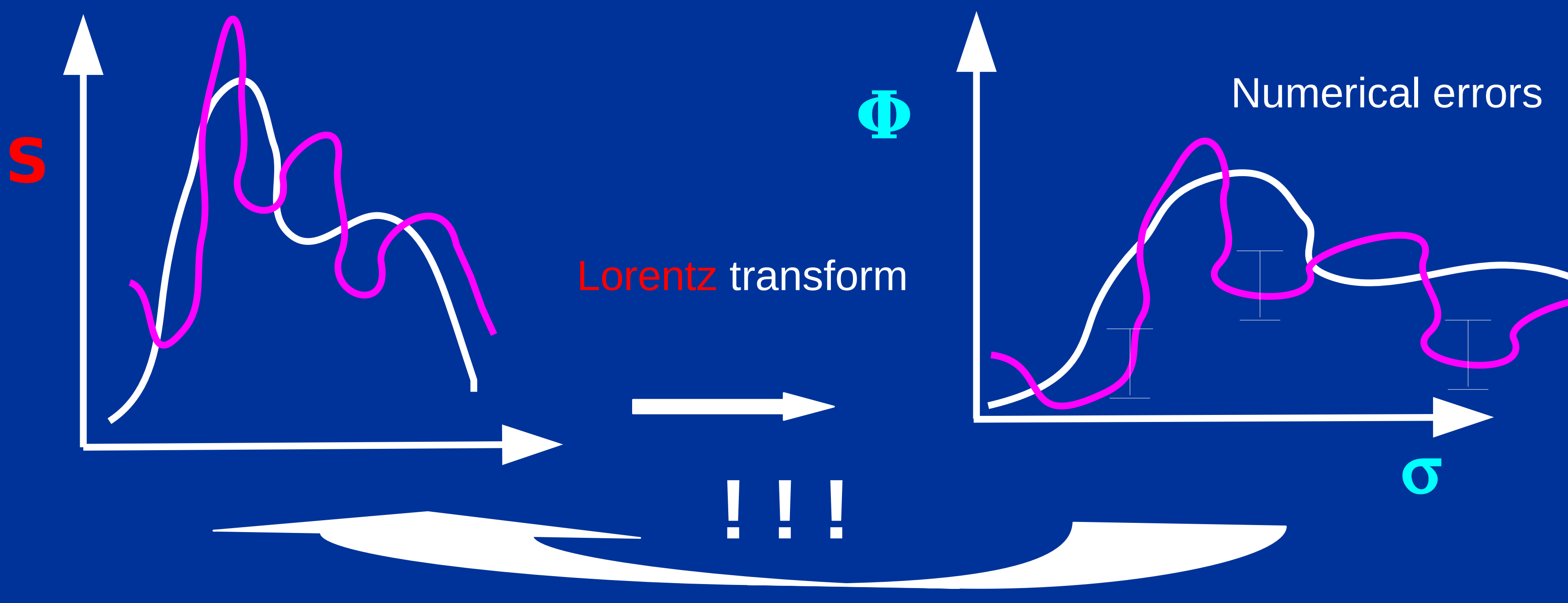


blurred, but still distinguishable also with errors!

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

Inversion: e.g. “regularization method” at fixed width



LIT - Inversion

Inversion method : **regularization** method

(from A.I N.Tikhonov, "Solutions of ill posed problems", Scripta series in mathematics (Winston,1977).

M

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1) Take the following ansatz for the response function $S(\omega)$

$$S(\omega) = \sum_{m=1}^{M} c_m \chi_m(\omega,\alpha_i)$$

with given set of functions χ_m and unknown coefficients c_m

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4) Determine c_m and α_i by best fit on $\Phi(\sigma_R)$

Other remarks on the LIT

Perturbation induced inclusive reactions

Reaction cross sections are proportional to

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

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Green F. **[Π(ω)]** 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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However, in this case since $\Phi(\sigma_R,\sigma_I) < \infty$ and σ_I is finite

one is allowed **to use bound state approaches**,

i.e. represent H on b.s.

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NO DISCRETIZATION OF THE CONTINUUM

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

ε infinitesimal !

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

σ_I finite!

One can use the Lanczos algorithm

to represent $(H - E_0 - \sigma_R + i\sigma_I)^{-1}$ as a continuum fraction

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

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Because the kernel is a representation of the delta-function the inversion is much less ill posed

Many successful applications

See reports:

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

"The Lorentz Integral Transform (LIT) method and its applications toperturbation induced reactions"

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

W.Leidemann, G.Orlandini

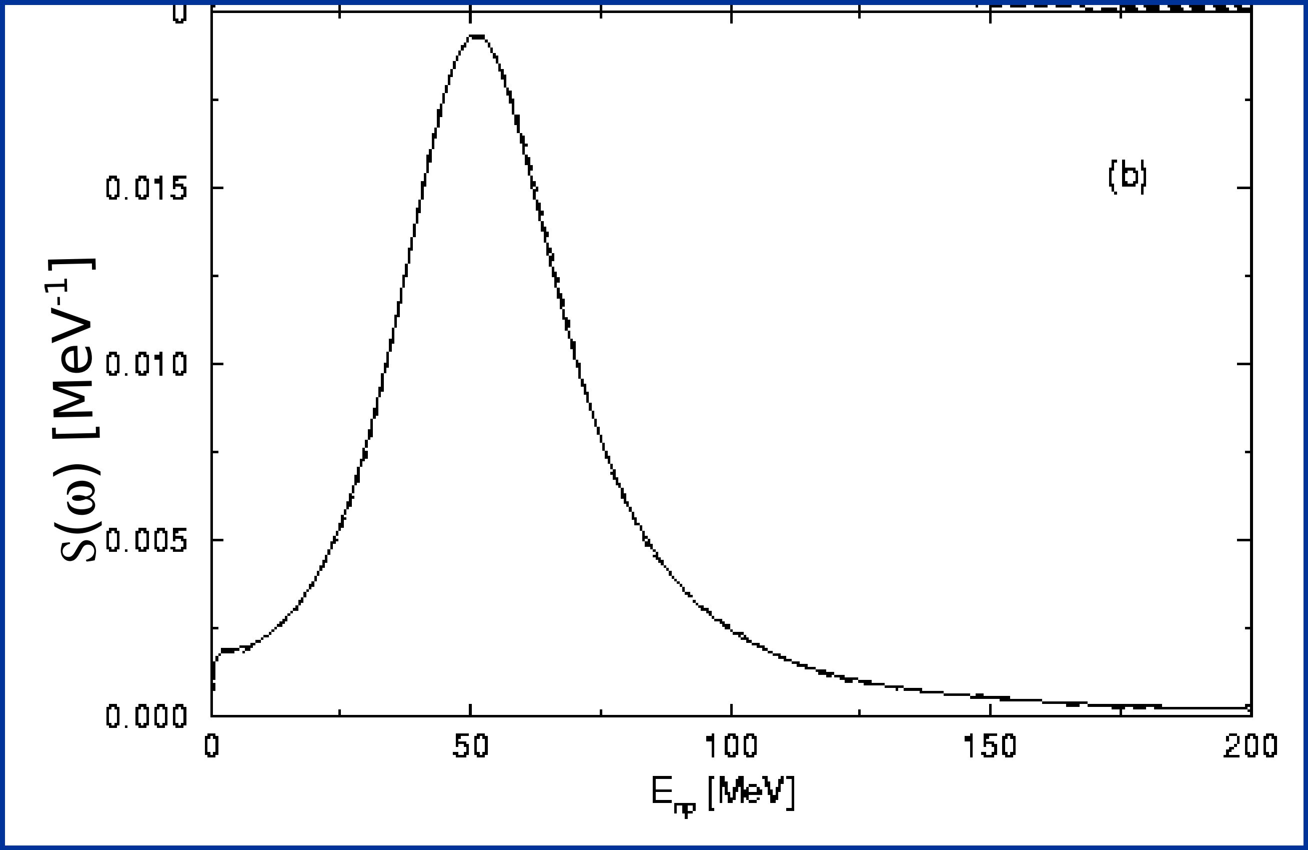
"Modern ab initio approaches and applications in few-nucleon physicswith A ≥ 4"

Progress in Particle and Nuclear Physics 68 (2013) 158–214

Some results with LIT:

test on the Deuteron:

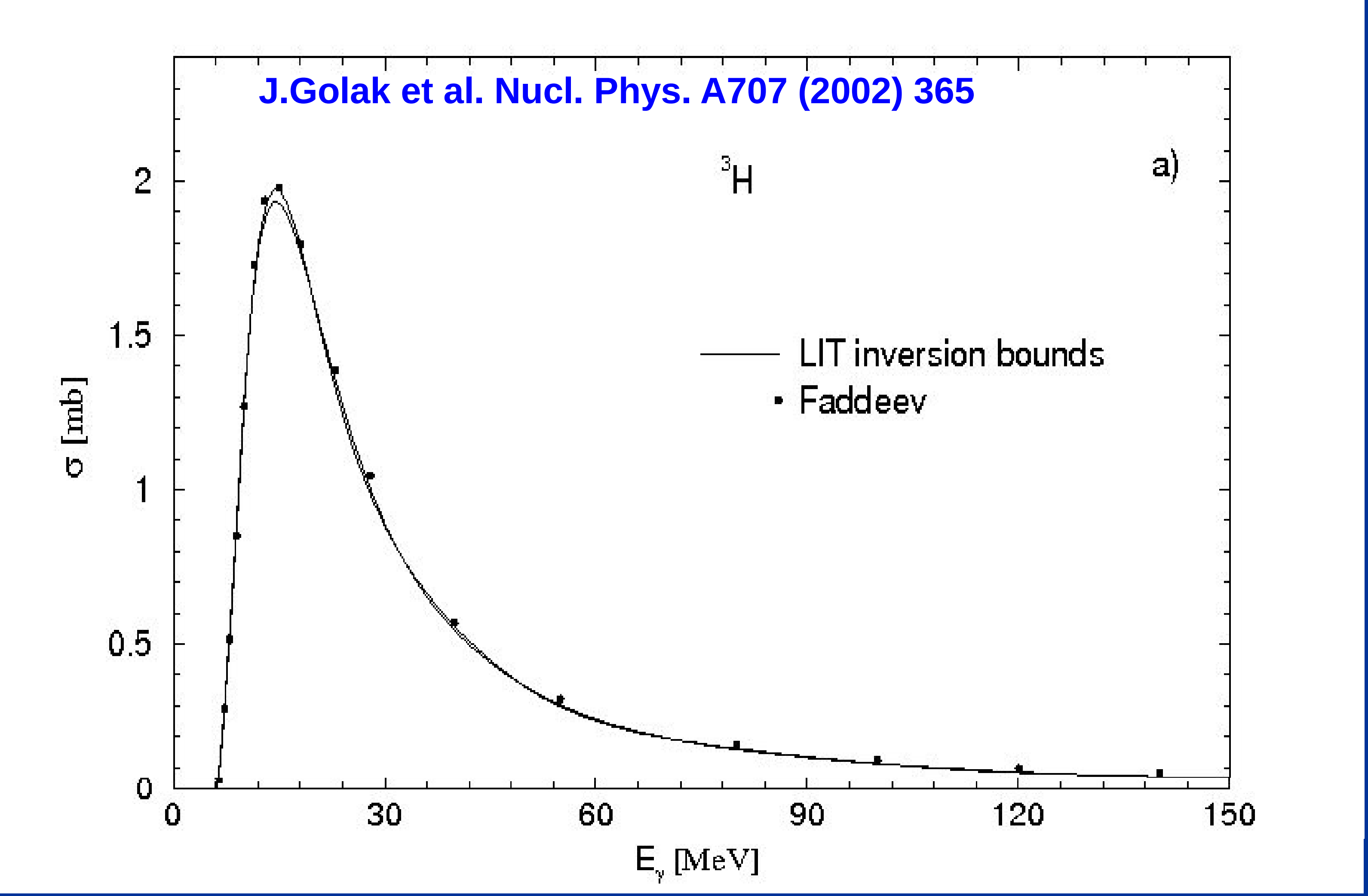
R(ω) is the longitudinal (e,e') response function



Phys Lett. B338 (1994) 130

Benchmark TEST on Triton:

S(ω) is the Dipole Photoabsorption Cross Section



Role of complete 4-body dynamics in the final scattering state

dotted:
Plane Wave Impulse Approximation

Dashed: 2-body force

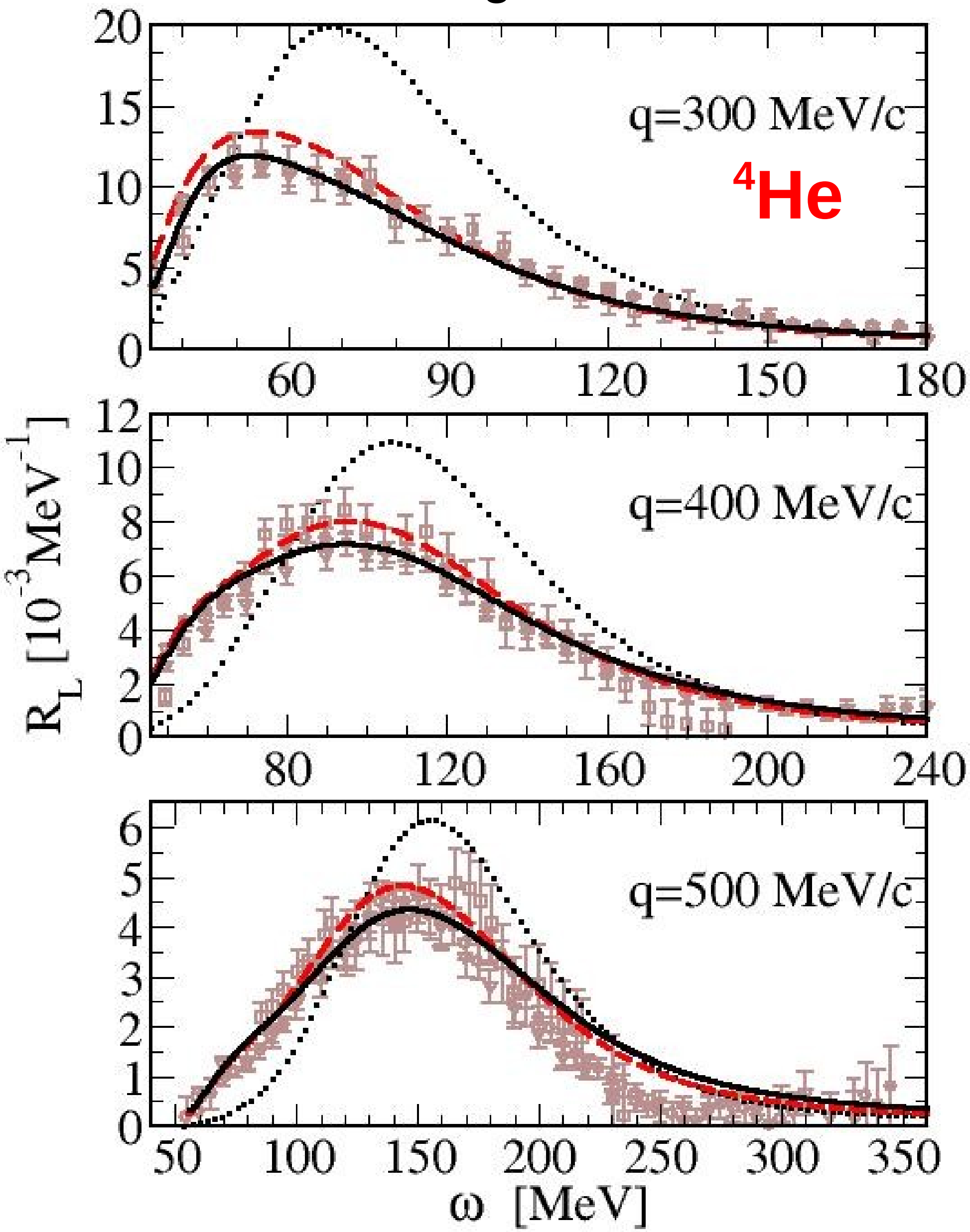
Full: 2+3-body force

S.Bacca et al.,
Phys.Rev.Lett.102:162501 (2009)

Data: Saclay + Bates 1980's

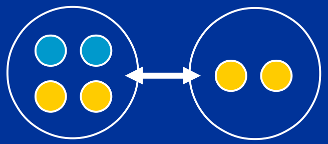
arXiv:0903.0605

Inclusive electron scattering cross section in the longitudinal channel

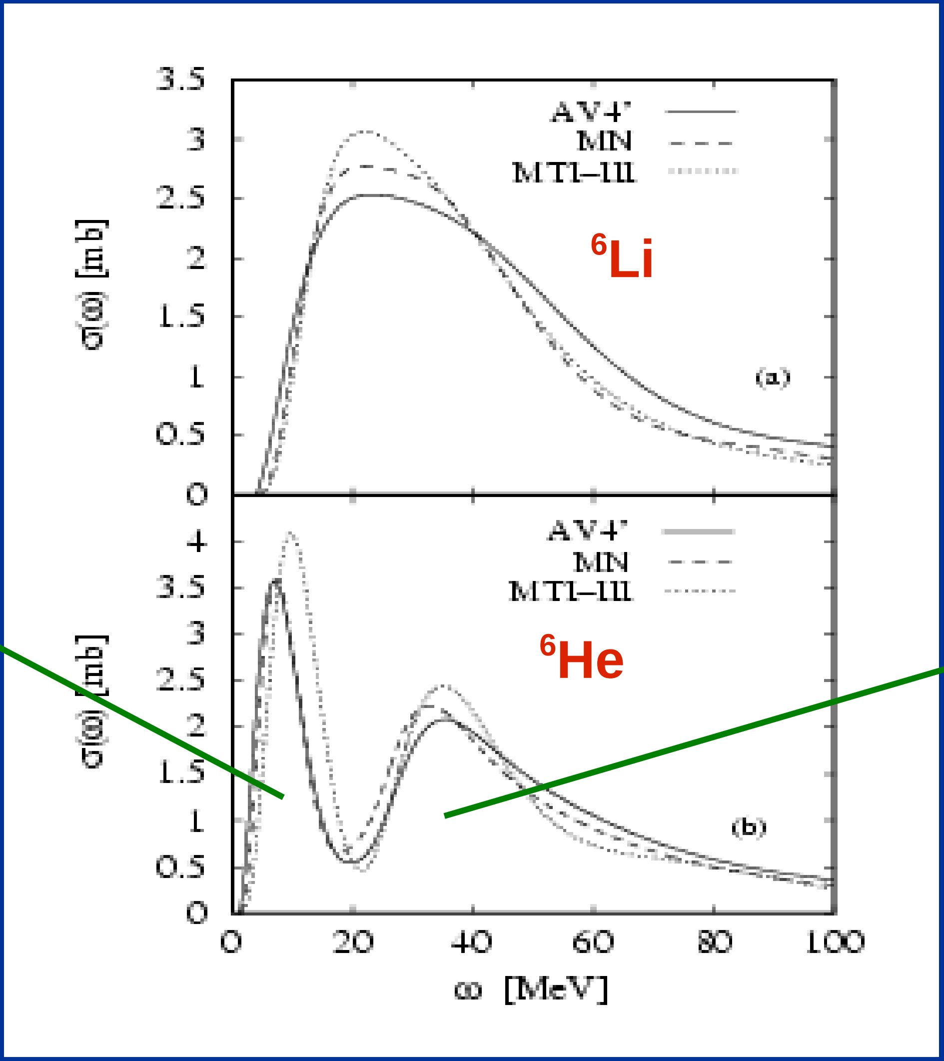


6-Body total photodisintegration

S.Bacca et al. PRL89(2002)052502

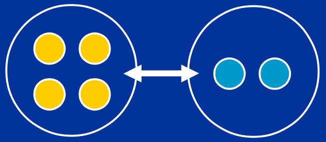


soft mode



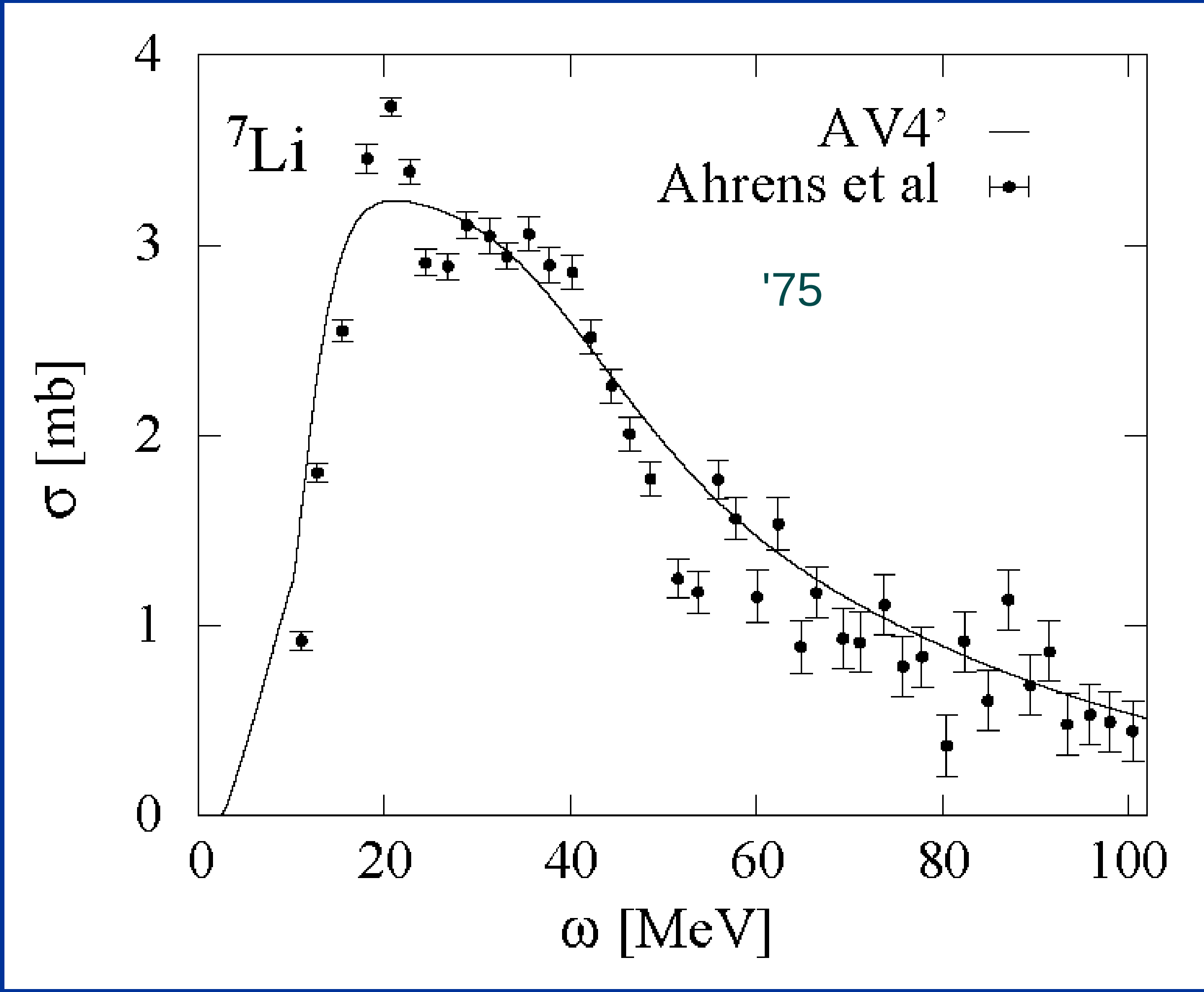
Theory:

LIT+ EIHH



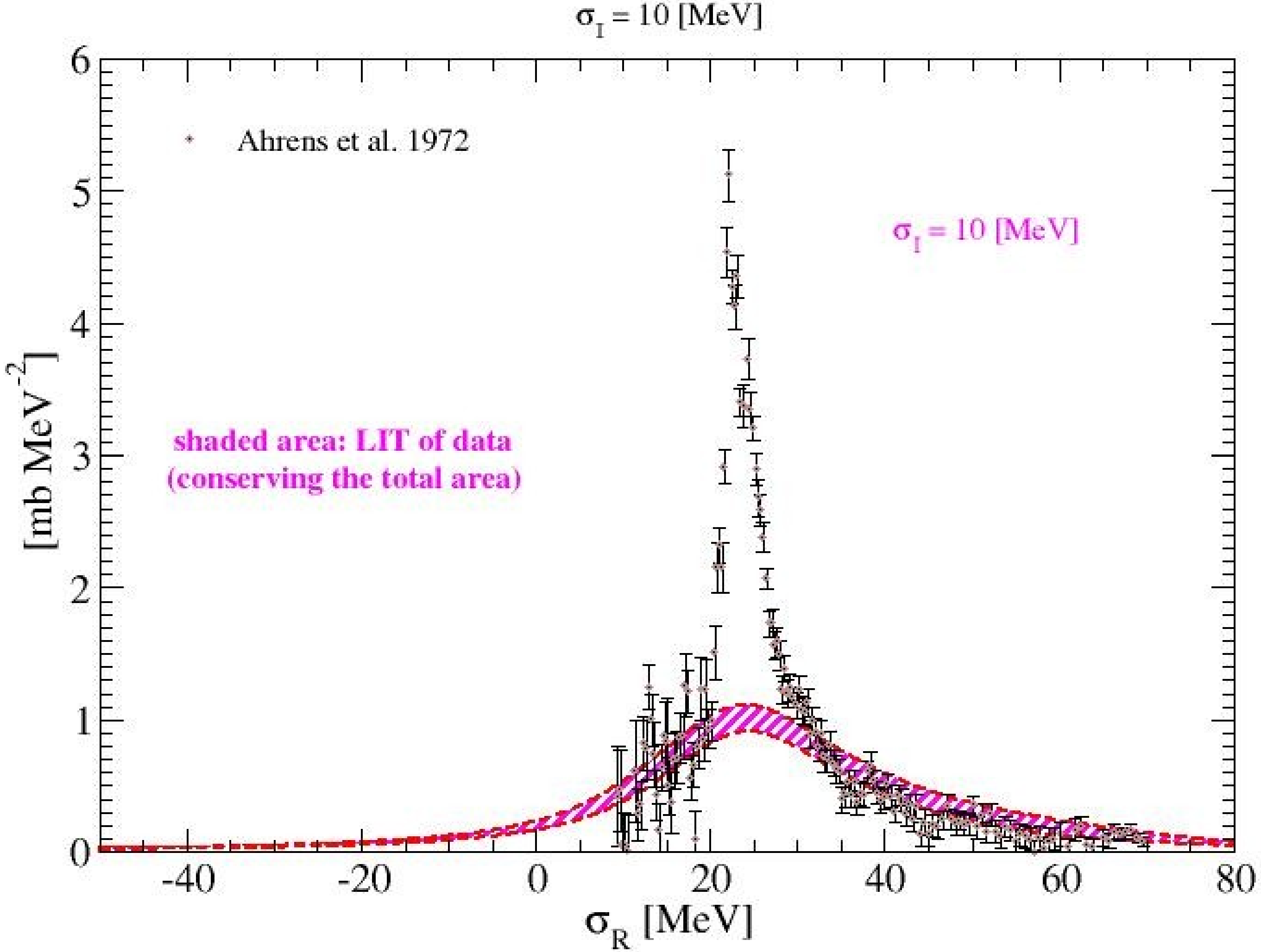
classical GT mode

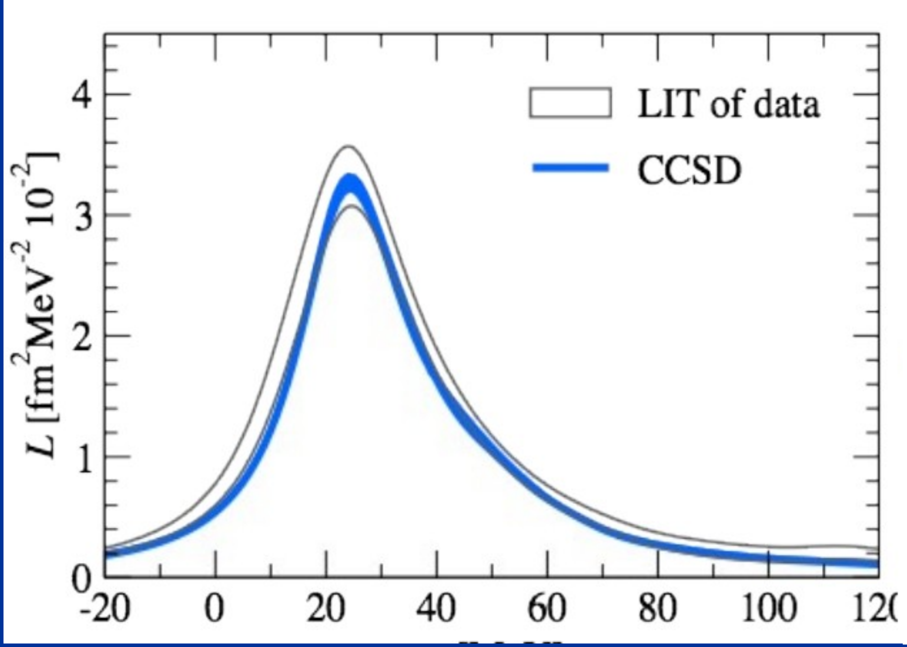
7-Body total photodisintegration with LIT method



S.Bacca et al.
Phys.Lett. B603 (2004) 159-164

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

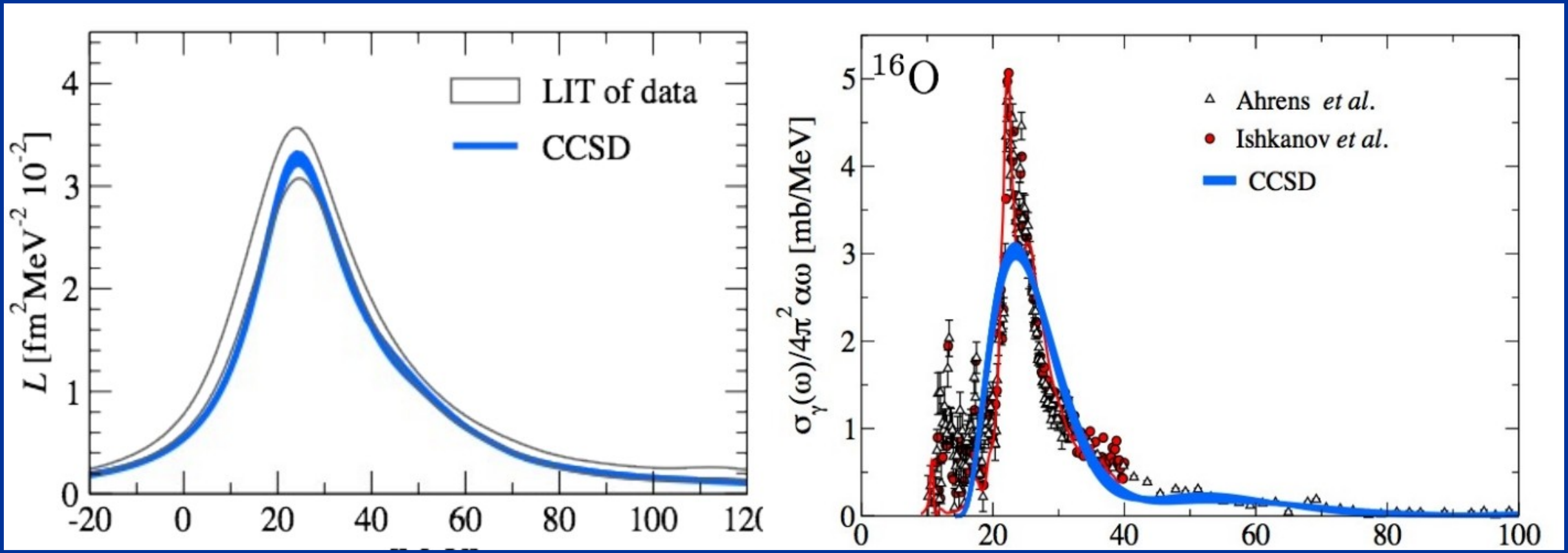




S. Bacca, et al.Phys.Rev.Lett. 111 122502 (1913)

LIT +CC(SD) methods

N3LO EFT 2-body potential only



S. Bacca, et al.Phys.Rev.Lett. 111 122502 (1913)

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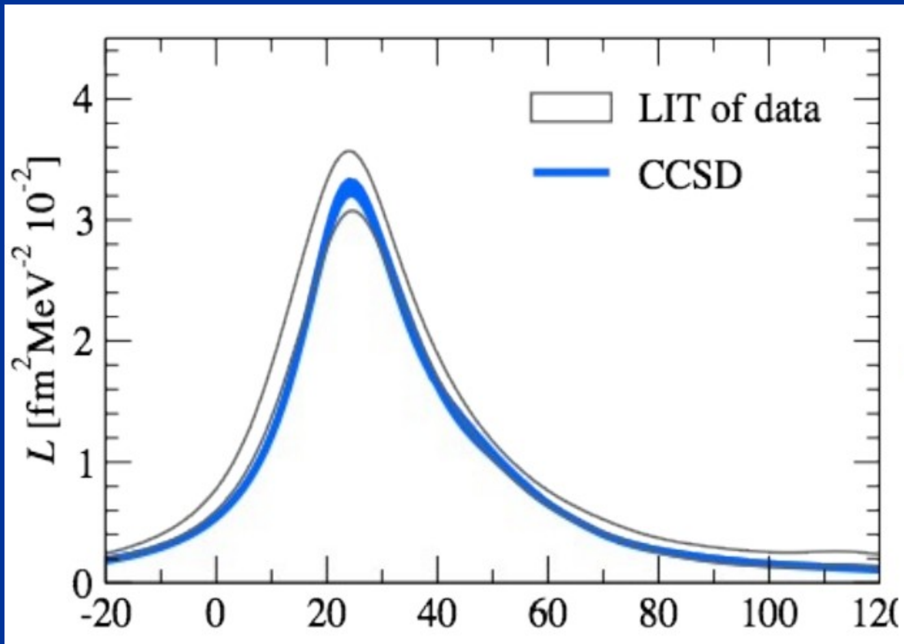
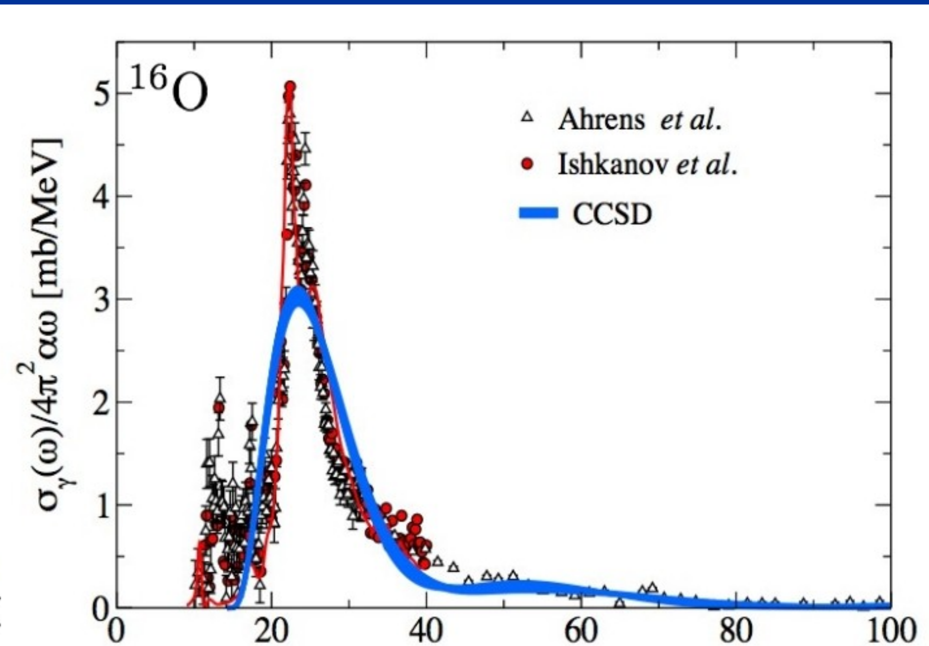
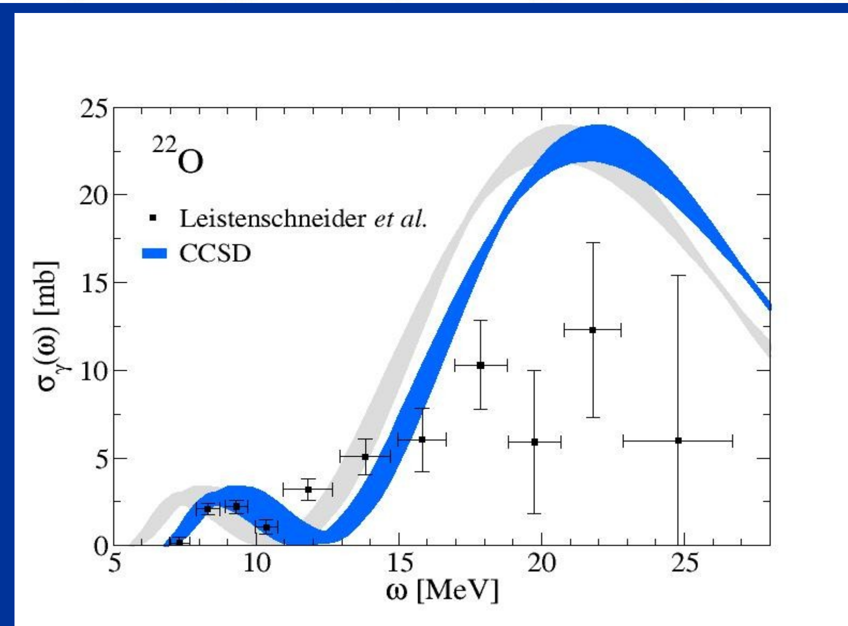




S. Bacca, et al.Phys.Rev.Lett. 111 122502 (1913)

LIT +CC(SD) methods

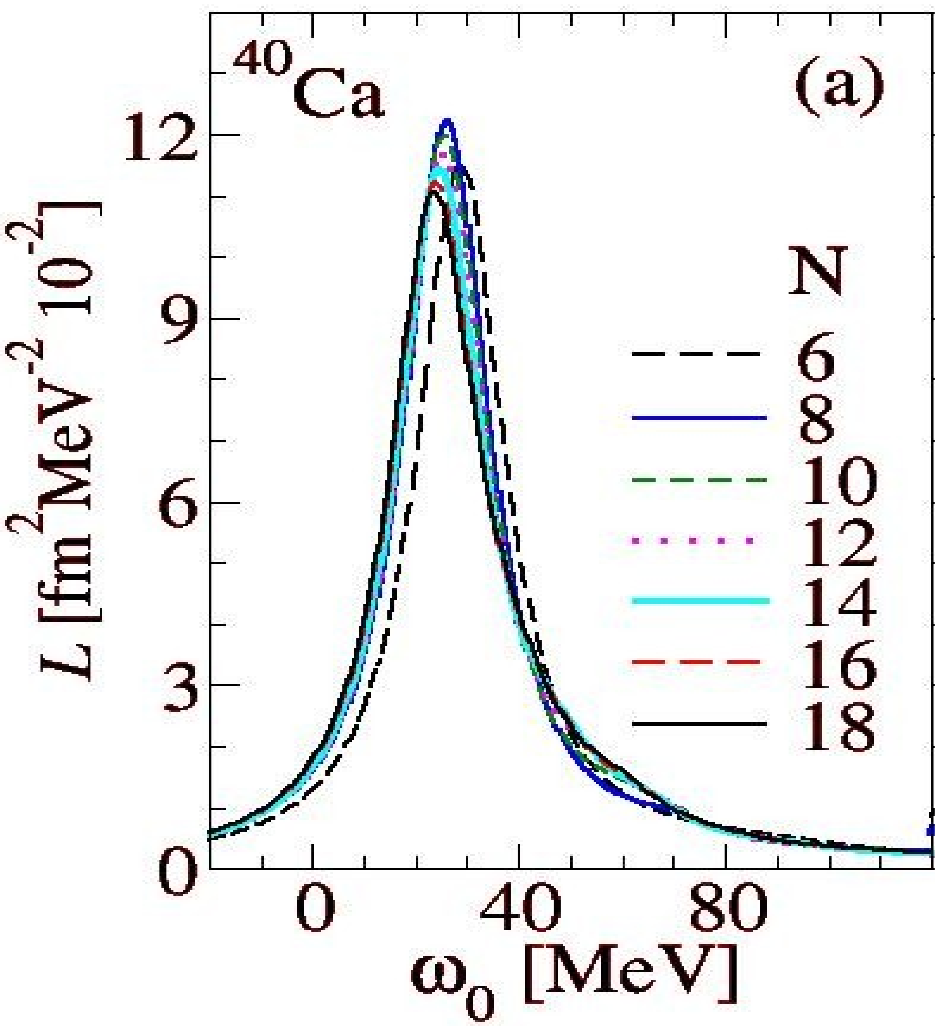
N3LO EFT potential



S. Bacca et al. Phys. Rev. C 90, 064619 (2014)

Mirko Miorelli et al. (Preliminary)

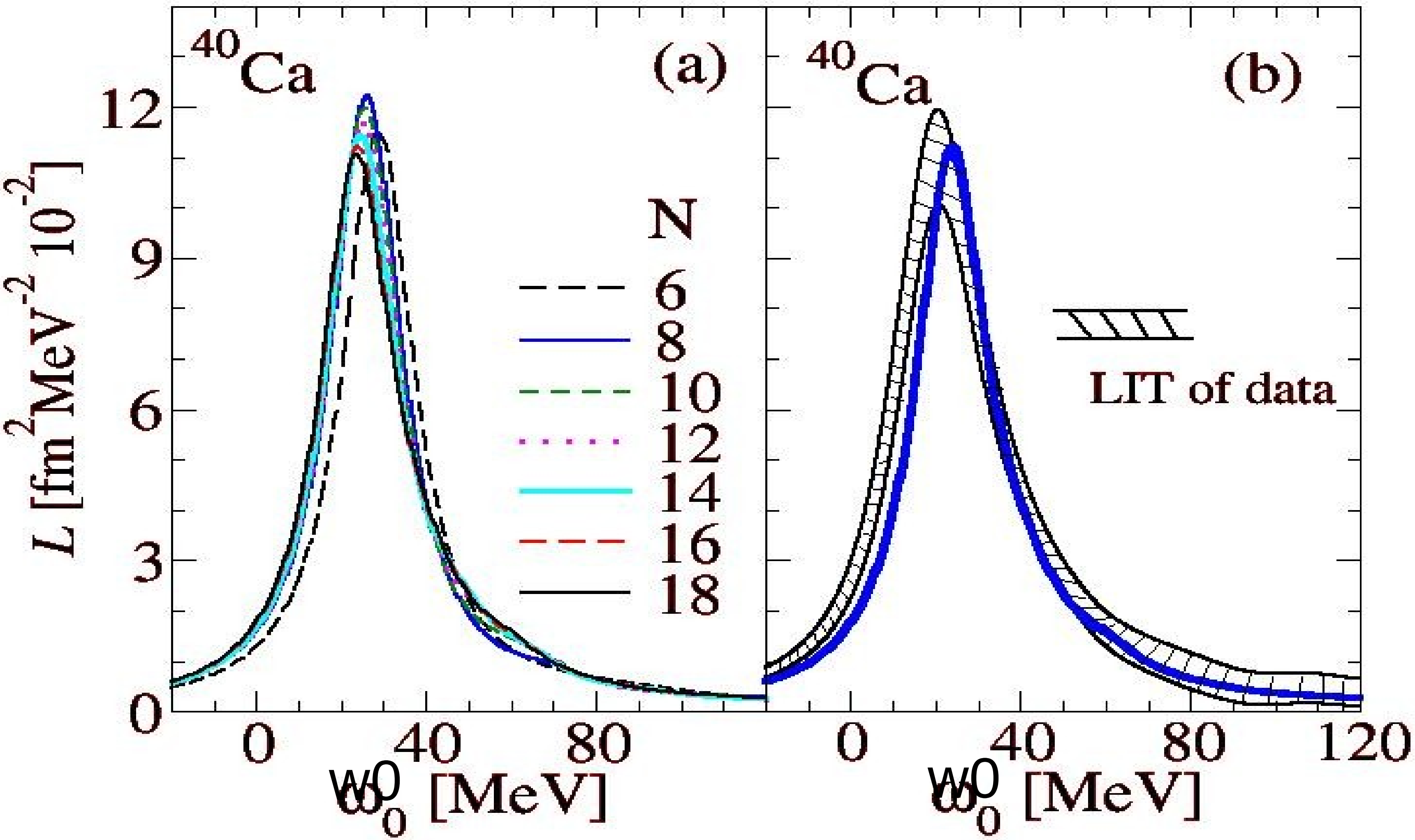
The convergence of the LIT



Mirko Miorelli et al. (Preliminary)

The convergence of the LIT

The comparison with the L I Transformed data



Other kernels?

A Transform with a kernel suitable for Monte Carlo methods:

[A.Roggero, F. Pederiva, G.O. Phys. Rev. B 88, 115138 (2013)]

combination of Sumudu kernels:

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

$$\nu/\mu = b/a \qquad \nu - \mu = \frac{\ln[b] - \ln[a]}{b-a} \qquad b > a > 0 \text{ integer}$$

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

A Transform with a kernel suitable for Monte Carlo methods:

[A.Roggero, F. Pederiva, G.O. Phys. Rev. B 88, 115138 (2013)]

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

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

Finite sum of Laplace Kernels!

A Transform with a kernel suitable for Monte Carlo methods:

[A.Roggero, F. Pederiva, G.O. Phys. Rev. B 88, 115138 (2013)]

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

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

$$\tau(P,k,\sigma) = \log(b/a)\,[P\,a/(b-a) + k\,] / \sigma$$

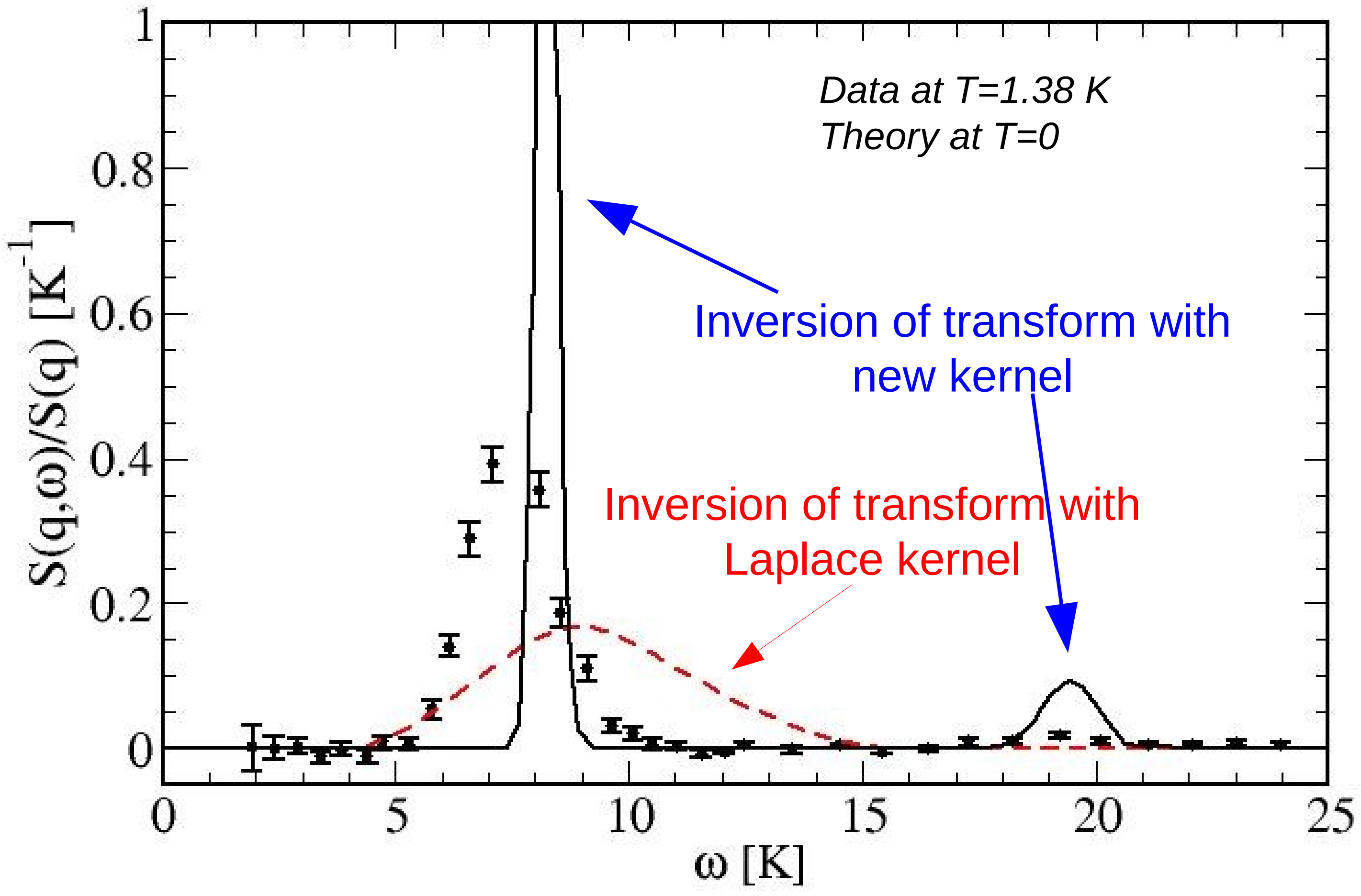
Small width ---> large P ---> **large** imaginary time

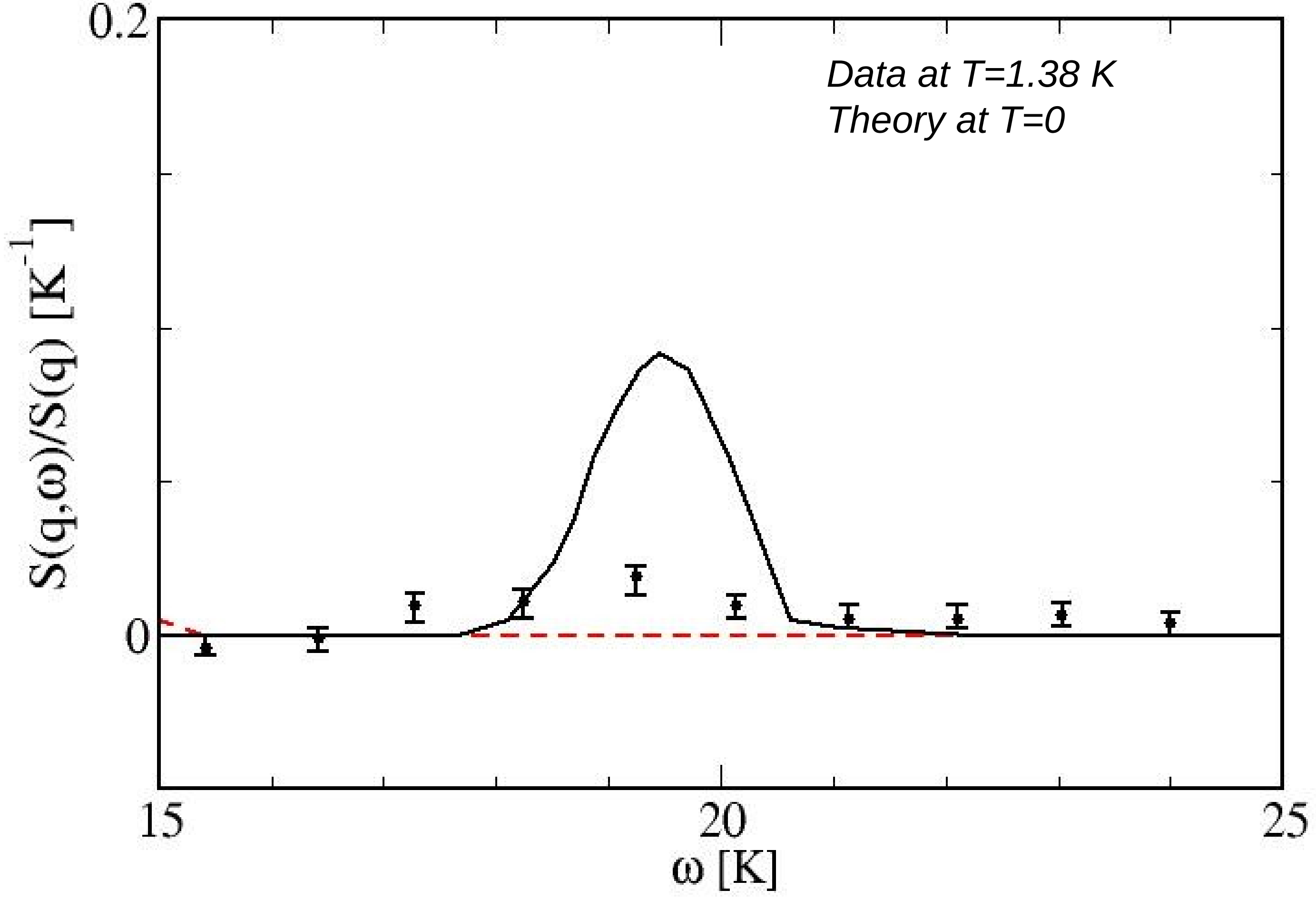
Bosonic system: Liquid Helium

The transform is calculated with AFDMC and then inverted with MEM

[A.Roggero, F. Pederiva, G.O. Phys. Rev. B 88, 115138 (2013)]

Bosonic system: Liquid Helium





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

But what are other kernels suitable for diagonalization methods on finite norm basis functions

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

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

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

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

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

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

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

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

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

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

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

(Up to convergence!)

For Lorentzian kernels

$$K_L(\omega - E_0,\sigma) = \sigma_I/\pi \ [(\omega - \sigma_R)^2 + \sigma_I^{\,2}]^{-1}$$

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

Convolution of transition m.e. at discrete energies with Lorentzian functions ***(see S(ω) in RPA!)***

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

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

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

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

3) $K(\omega,\sigma)$ is a real positive definite function of ω
(or linear combinations)

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

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

In fact: if $K(\omega,\sigma)$ is a real positive definite function

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

$$\Phi(\sigma) = \underbrace{\langle 0|\Theta^+ \kappa^+(H-E_0,\sigma)}_{\langle \tilde{\Psi}|}\ \underbrace{\kappa(H-E_0,\sigma)\,\Theta|0\rangle}_{|\tilde{\Psi}\rangle}$$

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

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

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

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

$< \infty$! (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)

$$\sum_\nu |\nu\rangle\langle\nu| \qquad \sum_\mu |\mu\rangle\langle\mu| \qquad \sum_\mu |\pi\rangle\langle\pi|$$

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

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

… 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!)

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

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 $\sigma_1, \sigma_2, \ldots$

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 Φ (σ) may be problematic

New Kernels?

What about “wavelets”?

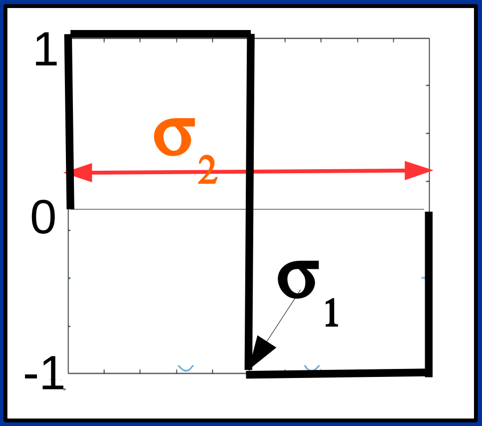
A **wavelet** Kernel is an oscillating function but with a **"window"**.

It has 2 parameters:

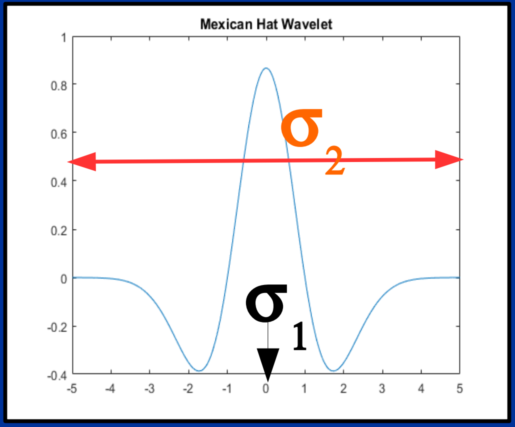
σ_2 **drives the frequency of the oscillation**

σ_1 **drives the position of the window over the ω range**

discrete



continuous



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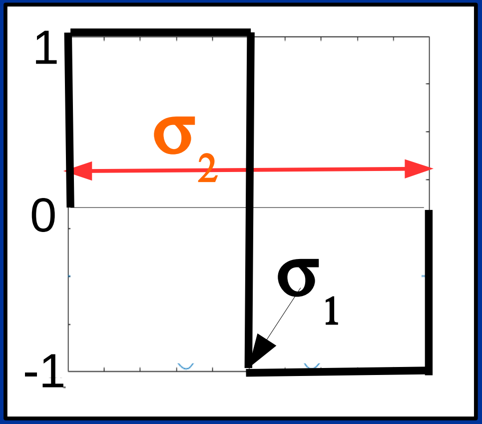
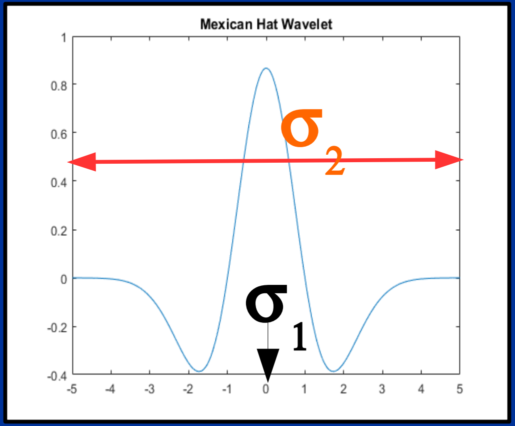


continuous



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)

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

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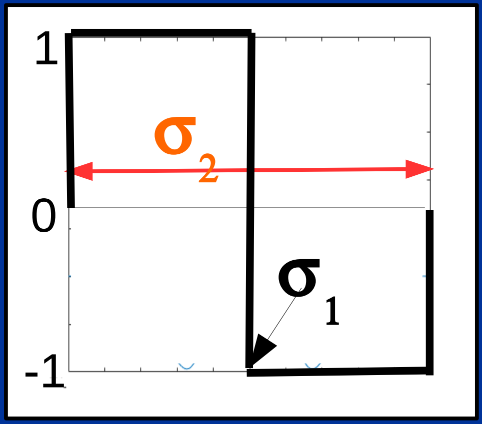
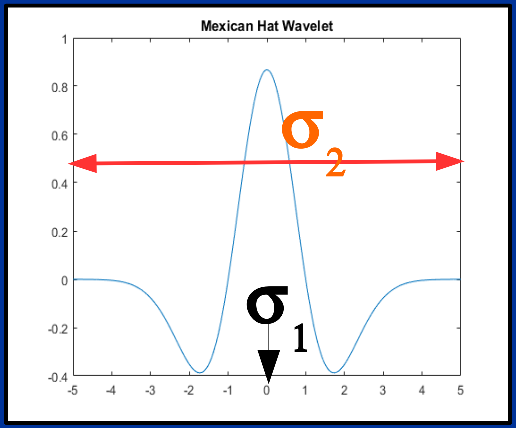
σ_1 drives the frequency of the oscillation

σ_2 drives the position of the window over the ω range

discrete



continuous



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

[linear combination of Φ (σ_1 ,σ_2)]

Integral transform (IT)

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

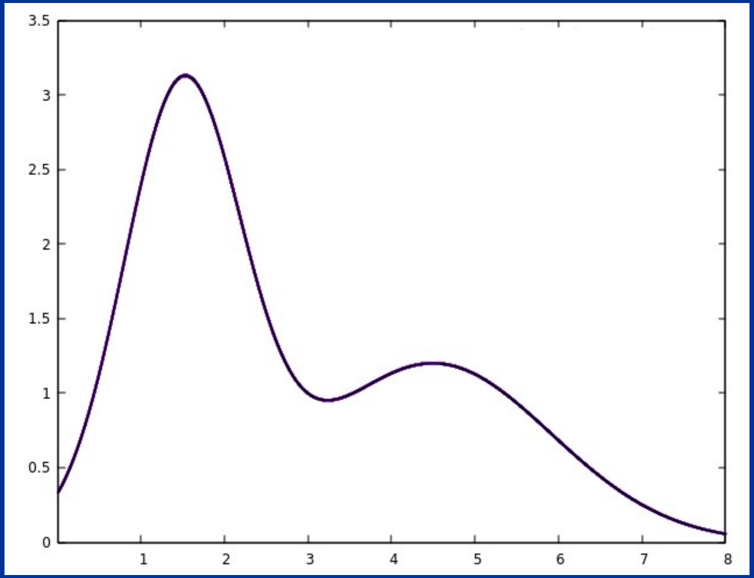
If $K(\omega,\sigma) \equiv K_\sigma(\omega)$ represents an orthogonal basis

$\Phi(\sigma) = \Phi_\sigma$ represent the coefficients of the expansion

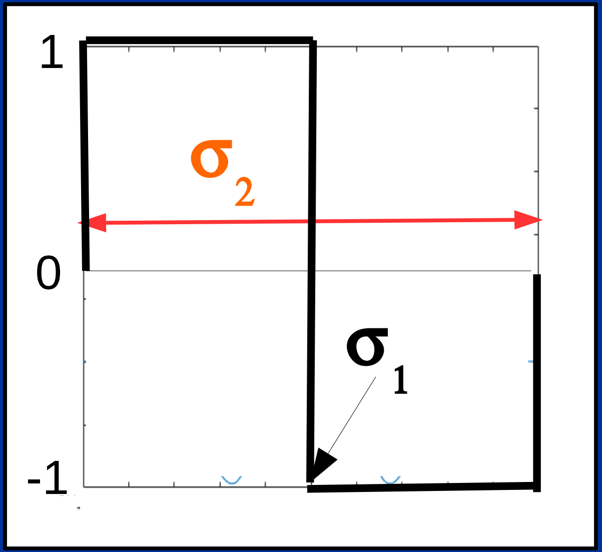
then $$S(\omega) = \sum_\sigma \Phi_\sigma K_\sigma(\omega)$$

A model study
(discrete wavelets)

Our model $S(\omega)$



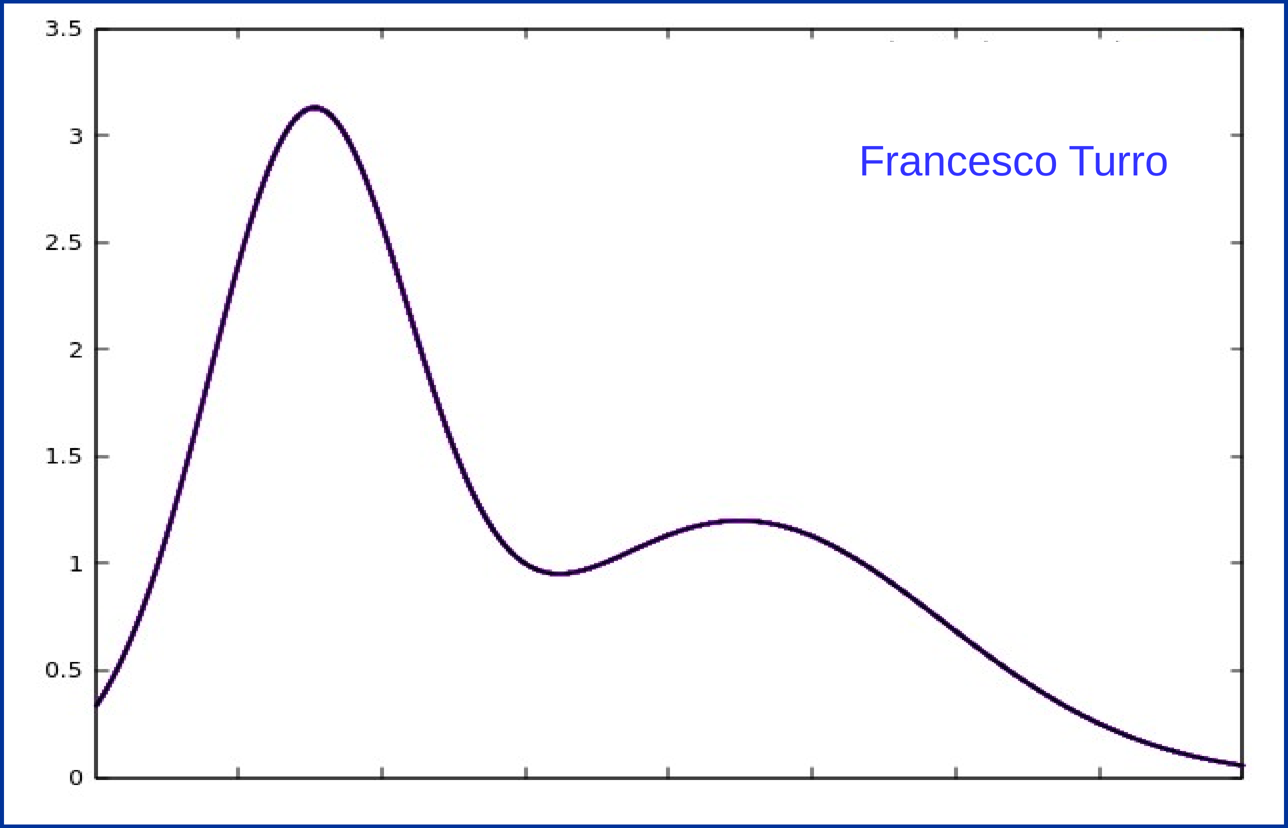
A wavelet kernel



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

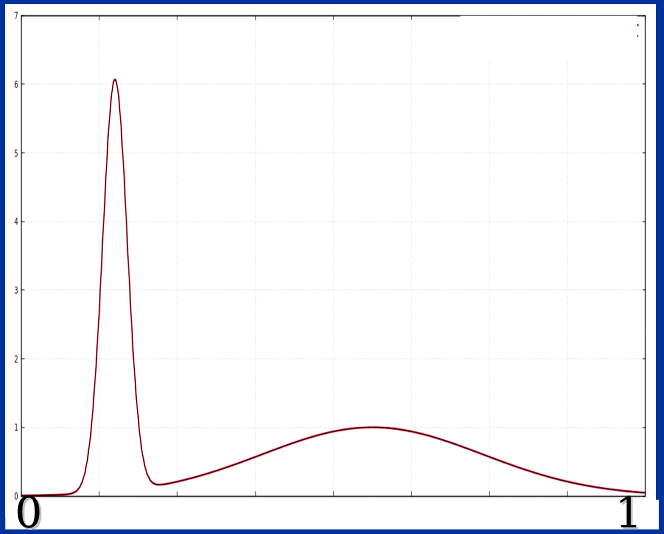
Model S(ω) and reconstructed from wavelet transform:

identical!

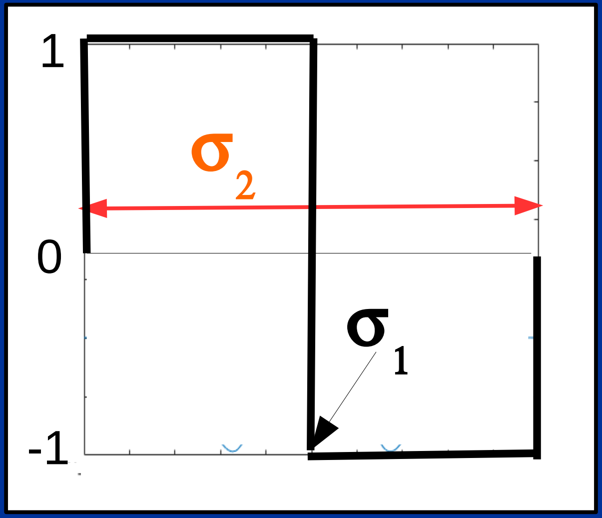


Another model study
(narrow resonance, discrete wavelets)

Our model S(ω)



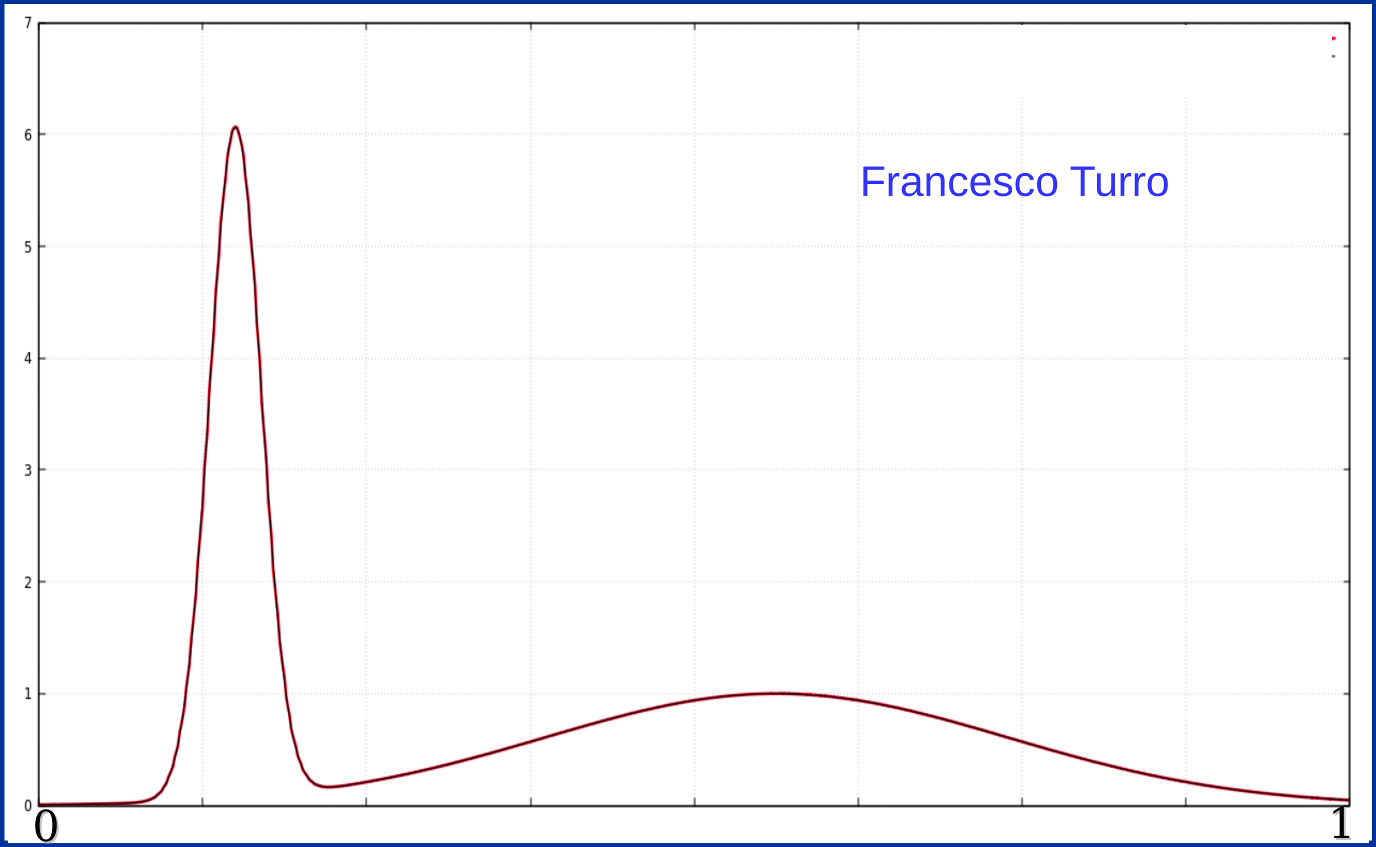
A wavelet kernel



K(ω, σ_1, σ_2)

Model S(ω) and reconstructed from wavelet transform:

again identical!

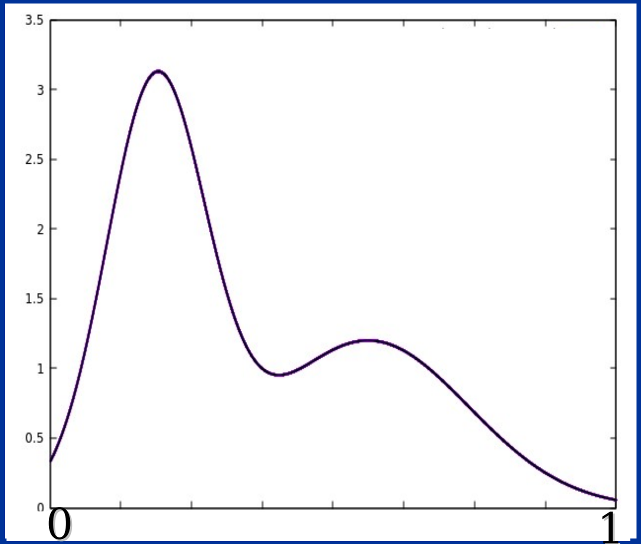


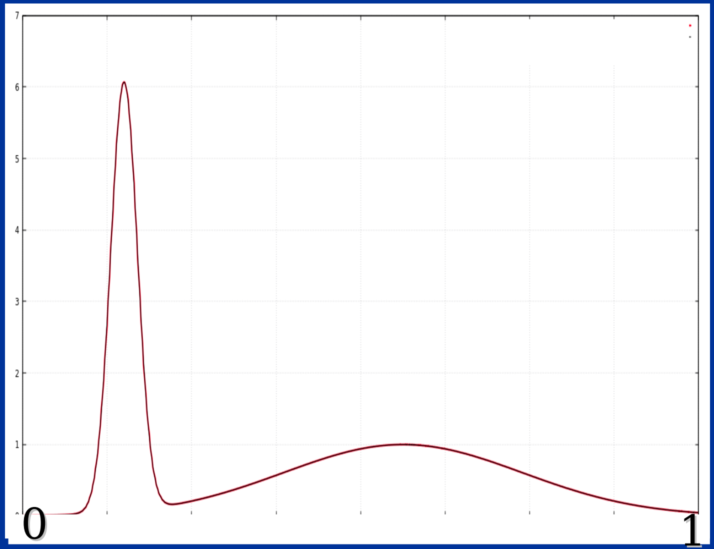
Which information has been used to reconstruct S(ω) ???

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

values of K(ω, σ_1, σ_2) with different widths

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

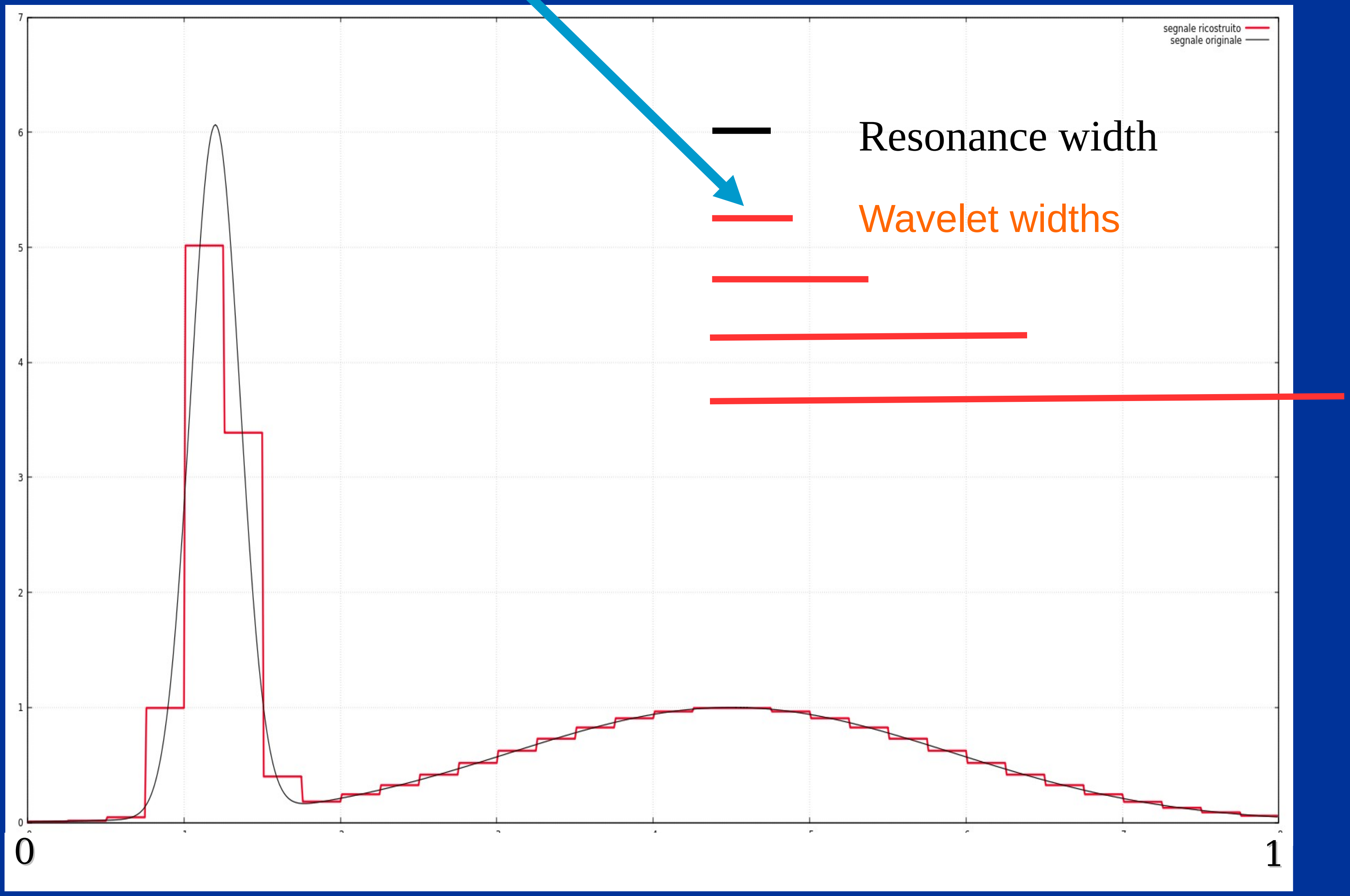




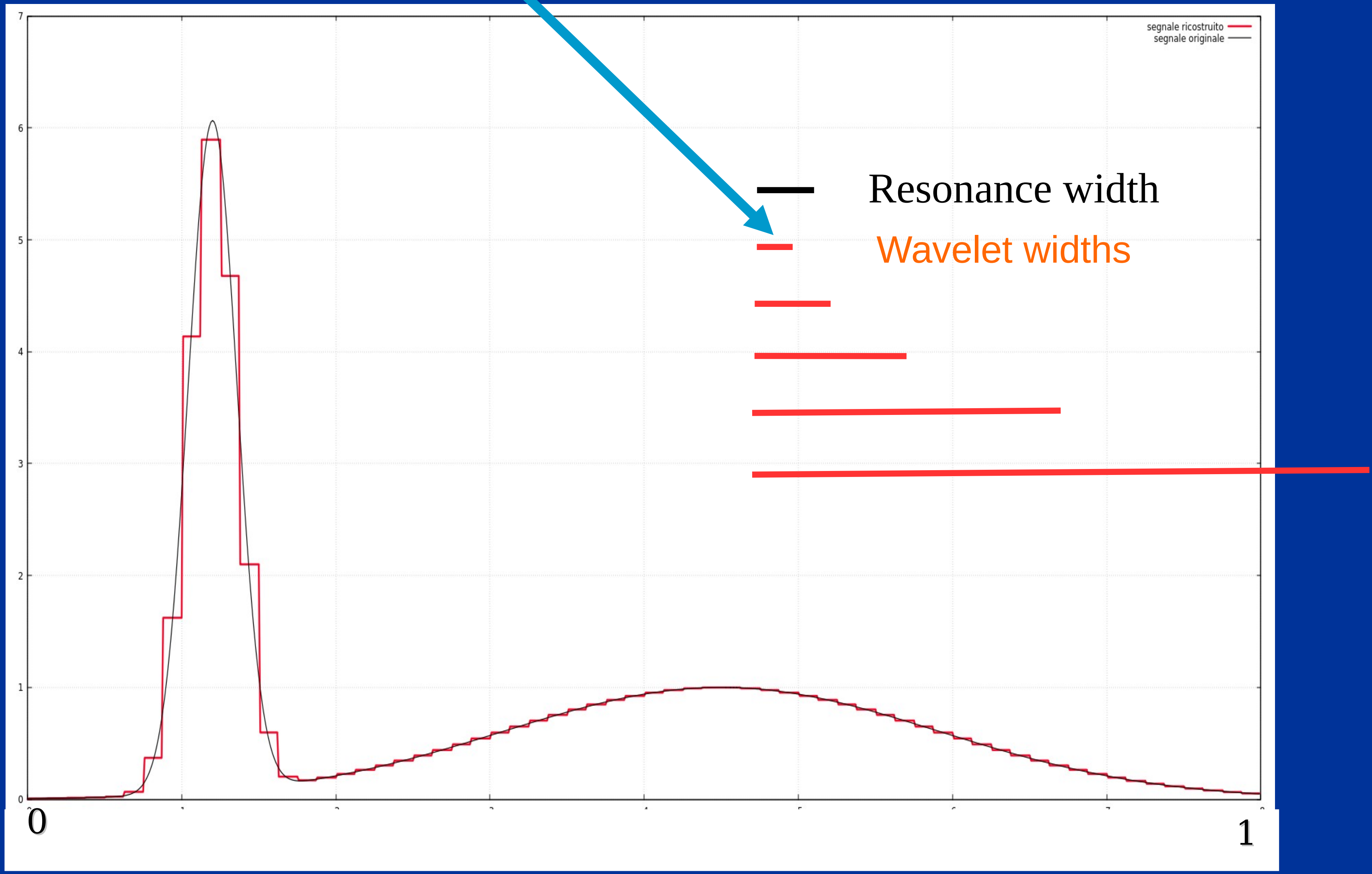
namely a lot of different resolutions up to $\sigma_2 = 0.03$!!!

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):



Acknowledgements

to all people who have taken part in the
IT adventure over 20 years

- Victor Efros
- Winfried Leidemann
- Nir Barnea
- *Sonia Bacca*
- *Sofia Quaglioni*
- Ed Tomusiak
- The CC people (Gaute Hagen, Thomas Papenbrock, *Mirko Miorelli*...)
- The MC people (Francesco Pederiva, *Alessandro Roggero*
- *...*

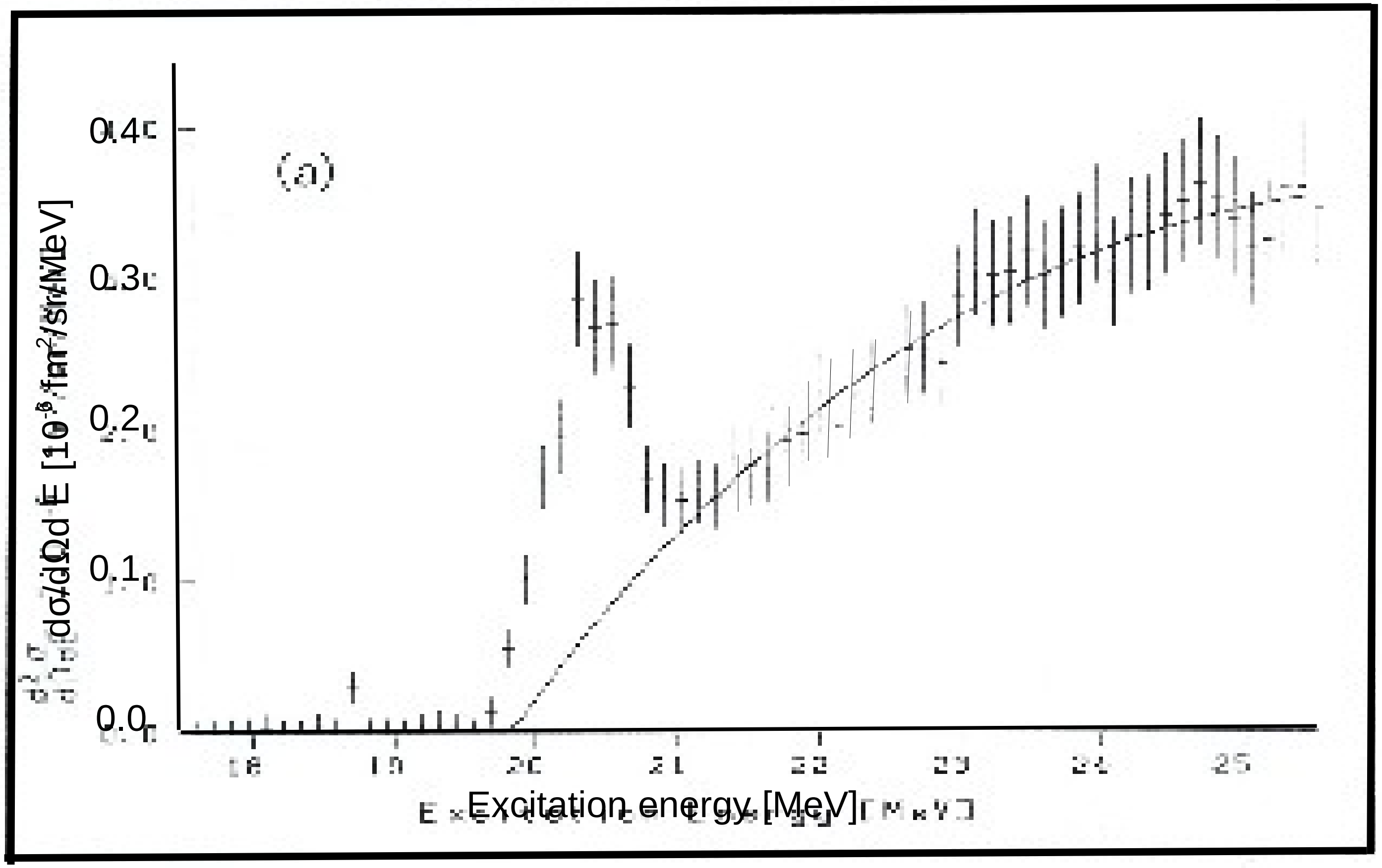
Thanks to the organizers for the invitation!!

0^+ Resonance in ^{4}He

Position at E_R = 20.1 MeV, (i.e. **above** the ^{3}H-p threshold)

Γ = 270±70 keV - **Strong** evidence in electron scattering

G. Koebschall et al./ Quasi bound state in ^{4}He Nucl. Phys. A405, 648 (1983)



The 0^+ resonance of ^4He is a typical isoscalar monopole excitation

Isoscalar monopole excitation operator

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

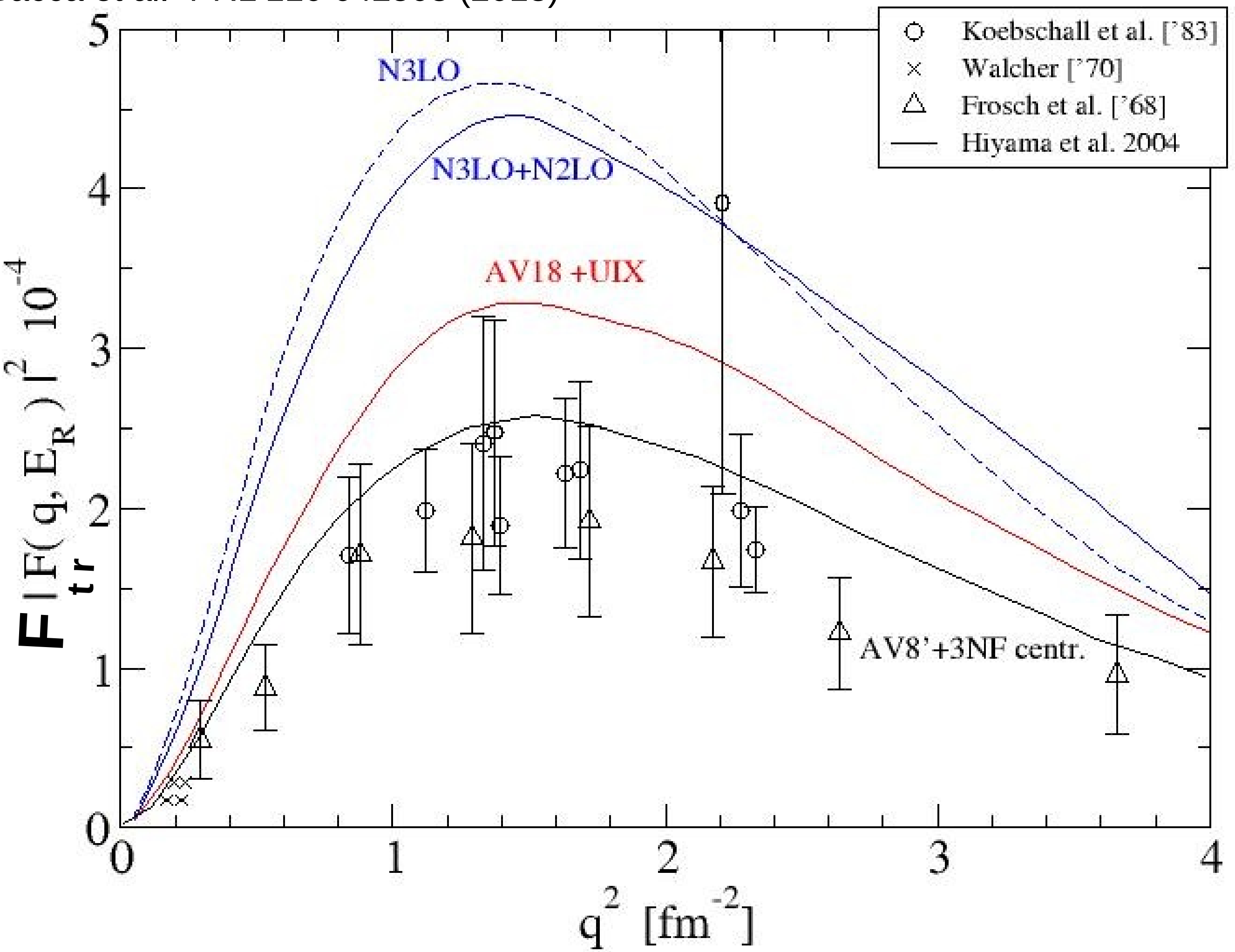
$$\sum_i j_0(q \cdot r_i)$$

An interesting aspect of this resonance: its **transition form factor** as a "prism" of nuclear potentials

In S.Bacca et al. PRL 110 042503 (2013), we have calculated $S_M(q,\omega)$ via the Lorentz Integral Transform **(LIT)** **m**ethod and looked in particular at the **transition form factor** for two different realistic potentials (**N3LO+N2LO, AV18 +UIX**)

Very large potential dependence !!!

S.Bacca et al. PRL 110 042503 (2013)



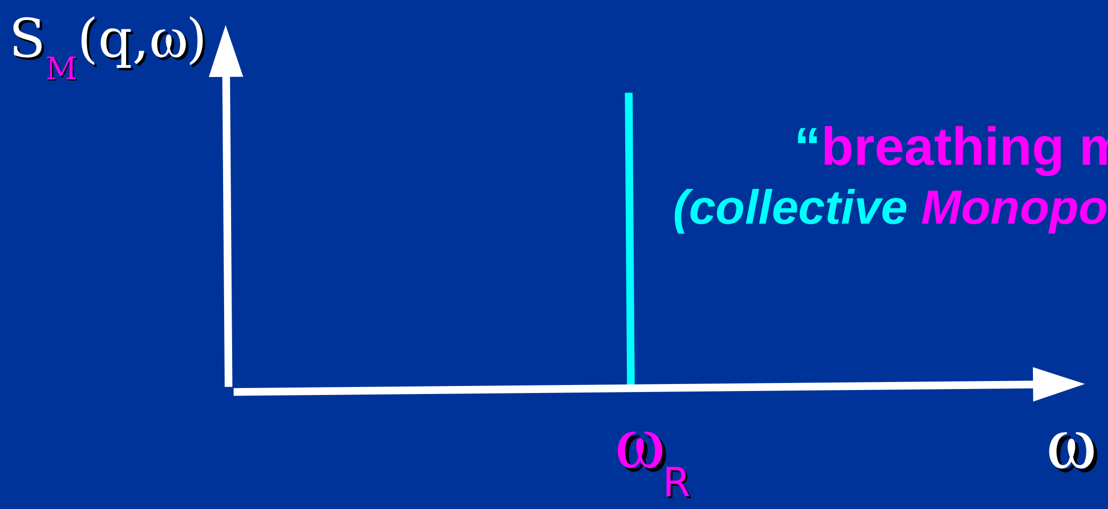
When the first measurements of the 0^+ resonance of ^{4}He appeared in 1965 (*Frosch et al.*) Werntz and Ueberall asked the interesting question:

Is the 0^+ resonance of ^{4}He a *collective breathing mode?*

Their simple breathing mode model (***density scaling***) implies

a) the breathing mode exhausts the energy weighted sum rule

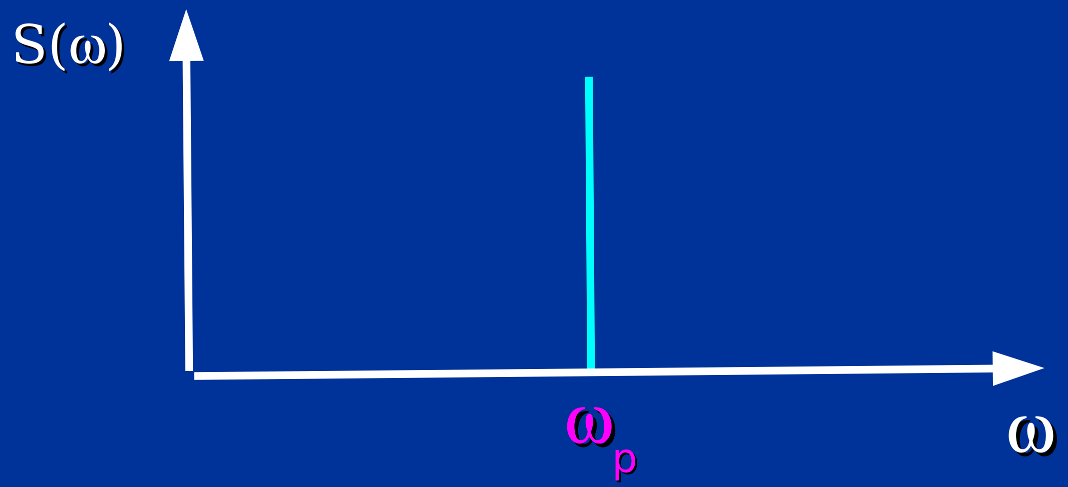
b) the transition density $|< 0^+_R | \Sigma_\iota \, \delta(\mathbf{r}-\mathbf{r}_\iota) \, | 0>|^2$ changes sign at $r = <r^2>^{1/2}$



"*Sum Rules* provide useful yardsticks for measuring qua

D.Rowe in "Nuclear Collective motion" 1970

if the situation is of extreme collectivity all *Sum Rules* are 100% "exhausted"



Sum Rules

$$m_0 = \int S(\omega)\, d\omega = \frac{1}{2} \langle 0|\, \{\Theta,\ \Theta\}\, |0\rangle$$

(T+V)

=

$$m_1 = \int S(\omega)\, \omega\, d\omega = \frac{1}{2} \langle 0|\, [\, \Theta, [H,\ \Theta]]\, |0\rangle$$

$$m_2 = \int S(\omega)\, \omega^2\, d\omega = \frac{1}{2} \langle 0|\{\Theta, H\}\{H, \Theta\}|0\rangle$$

etc.

Sum Rules

$$m_0 = \int S_M(q,\omega)\, d\omega = \frac{1}{2} \langle 0|\, \{M, M\}\, |0\rangle$$

$$m_1 = \int S_M(q,\omega)\, \omega\, d\omega = \frac{1}{2} \langle 0|\, [M, [\mathbf{H}, M]]\, |0\rangle$$

$$m_2 = \int S_M(q,\omega)\, \omega^2\, d\omega = \frac{1}{2} \langle 0|\{M,H\}\{H,M\}|0\rangle$$

At low-q MODEL INDEPENDENT SUM RULE for local potentials

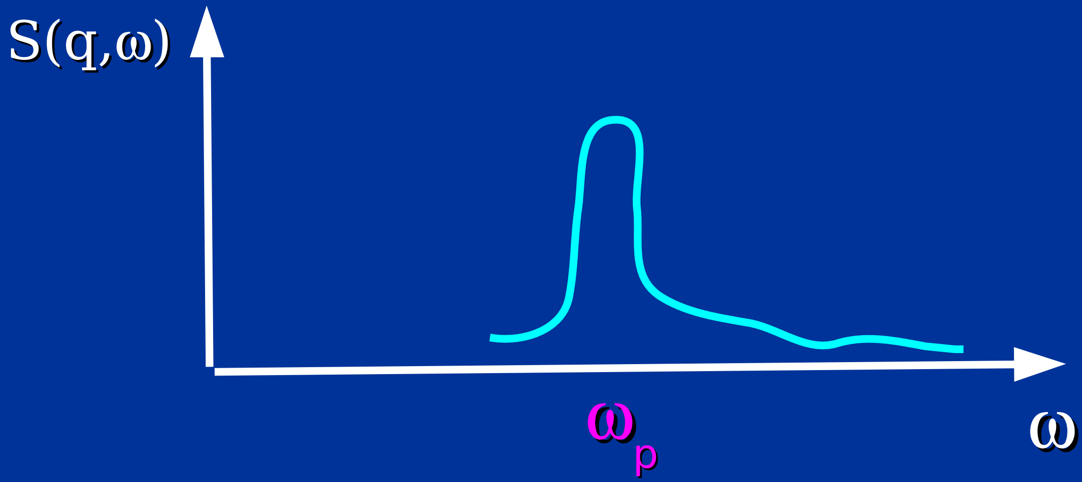
etc.

$$\mathbf{m_1 = m_1(T) = \frac{2A}{m} \langle r^2 \rangle}$$

“Sum Rules provide useful yardsticks for measuring quantitatively the degree of collectivity of a given excited state”

D.Rowe in “Nuclear Collective motion” 1970

However, if the situation is



m_o has to be considered to avoid emphasizing right o left background

"Sum Rules provide useful yardsticks for measuring quantitatively the degree of collectivity of a given excited state"

D.Rowe in "Nuclear Collective motion" 1970

"A typical isoscalar collective state exhausts something like 50% of $\boldsymbol{m_0}$*"*

D.Rowe in "Nuclear Collective motion" 1970

What about the small nucleus ^4He?

Sum rules:

q	$\lvert F_{\mathcal{M}}(q)\rvert^2$	m_0	m_1	r_0	r_1
$[\frac{\mathrm{MeV}}{\mathrm{c}}]$			[MeV]	%	%
50	0.00034	0.00063	0.021	53	34
	0.00024	0.00064	0.018	38	28
100	0.0042	0.0085	0.262	50	34
	0.0031	0.0086	0.258	37	25
200	0.0248	0.0683	2.42	36	22
	0.0190	0.0710	2.48	27	16
300	0.0297	0.129	5.89	23	11
	0.0242	0.139	6.33	17	8
400	0.0154	0.126	8.43	12	4
	0.0141	0.143	9.39	10	3

N3LO+N2LO

AV18+UIX

Sum rules:

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N3LO+N2LO

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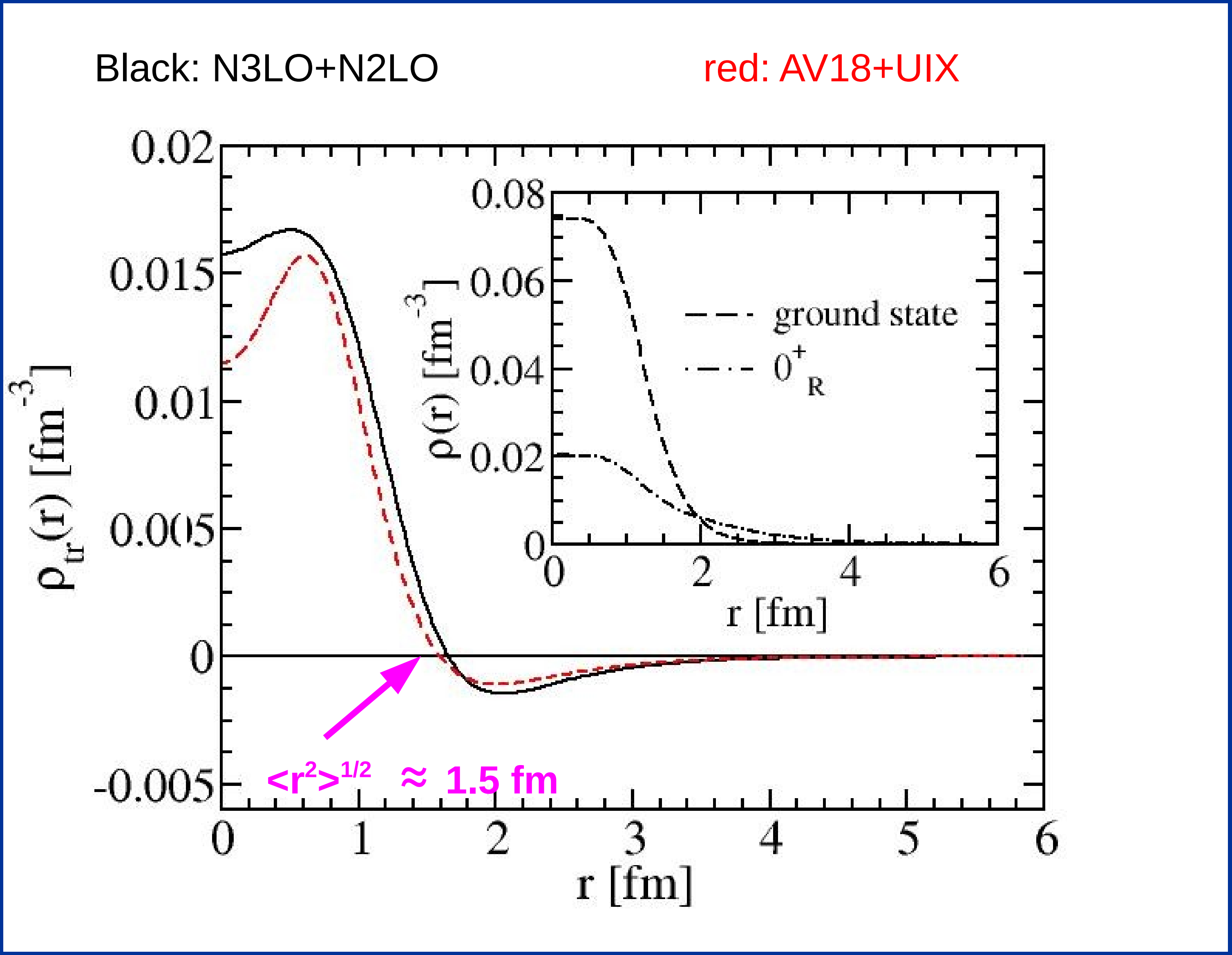
b) the transition density $|\langle 0^+_R| \Sigma_\iota \, \delta(r-r_\iota) \, | 0\rangle|^2$ changes sign at $r = \langle r^2\rangle^{1/2}$



Conclusion

Is the *0^+* *resonance* of the α-particle a "*breathing mode*" ???

Acknowledgements

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- Victor Efros
- Winfried Leidemann
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- *Sofia Quaglioni*
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- The MC people (Francesco Pederiva, *Alessandro Roggero*
- *...*

Thanks to the organizers for the invitation!!

Some examples:

- **"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
- **Laplace** transform? YES! the kernel $Exp(-\omega\sigma)$ is real and $\Phi(\tau) < \infty$

  (in this case σ represents the imaginary time $\tau = it$, is generally evaluated with MC methods)
- **Stieltjes** transform? YES! the kerne:l $1/(\omega + \sigma)$

  [V.D.Efros, Sov. J. Nucl.. Phys. 91, 949 (1985)]
- **Lorentz** transform? YES! the kernel: $[(\omega - \sigma_1)^2 + \sigma_2^{\ 2}]^{-1}$

  V.D.Efros, W.Leidemann, **G.O.** , Phys Lett. B338 (1994) 130]
- **Sumudu** transform? YES! the kernel: $(e^{-\mu\,\omega/\sigma 1}/\sigma_1 - e^{-\nu\,\omega/\sigma 1}/\sigma_1)^{\sigma 2}$

  it has been evaluated with MC methods

  [A.Roggero, F. Pederiva, **G.O.** , Phys. Rev. B 88, 115138 (2013)]

In general we have to do with

$$F_{ab}(\omega) = \sum\!\!\!\!\int_n \langle a | n \rangle \langle n | b \rangle \; \delta(E_n - \omega)$$

Using $\lim_{\eta \to 0} \eta \; (x - \alpha - \iota\eta)^{-1} = \mathcal{P}(x - \alpha - \iota\eta)^{-1} + \iota\,\pi\,\delta(x - \alpha)$

and closure $\sum_n | n \rangle \langle n | = I$

$$F_{ab}(\omega) = 1/\pi \; Im \left\{ \langle a | \frac{1}{(H - \omega - \iota\eta)} | b \rangle \right\}$$