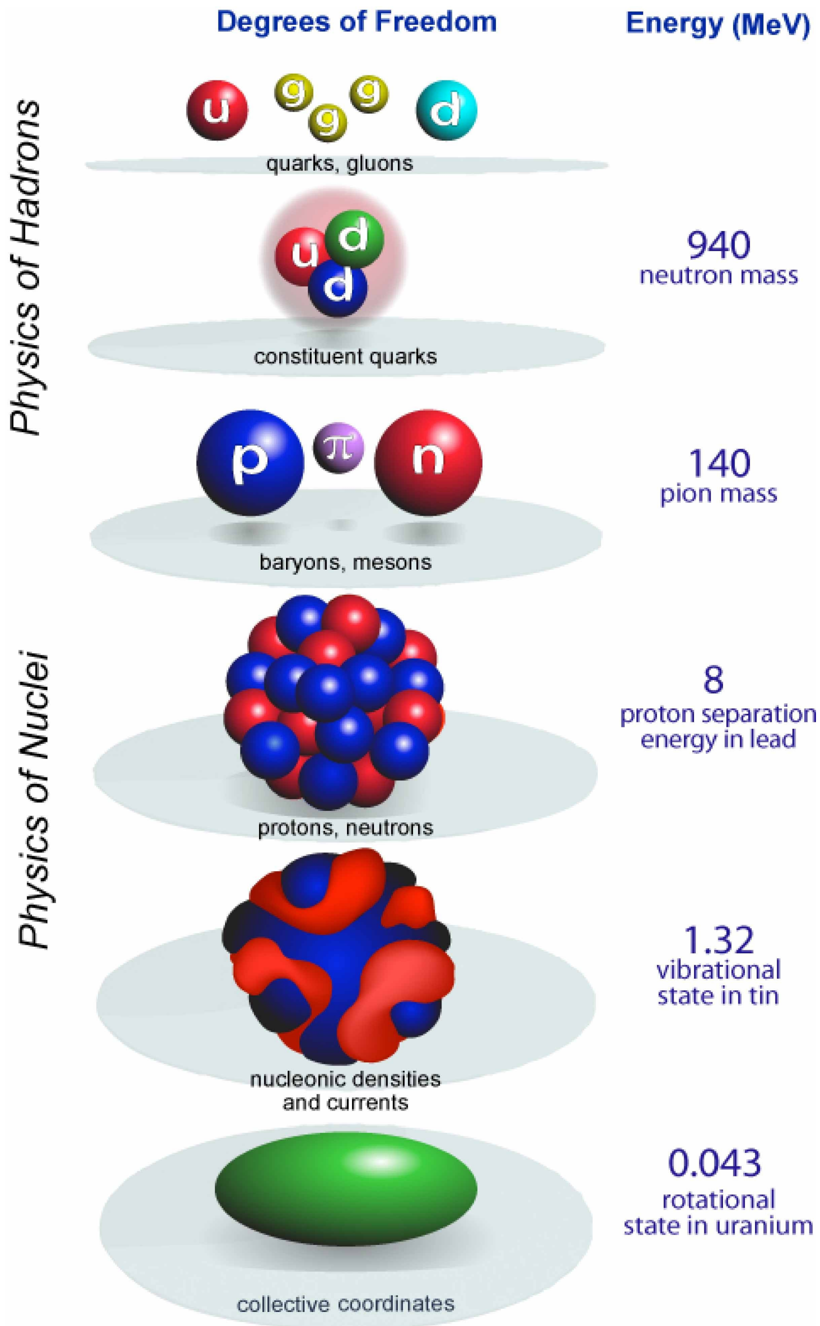
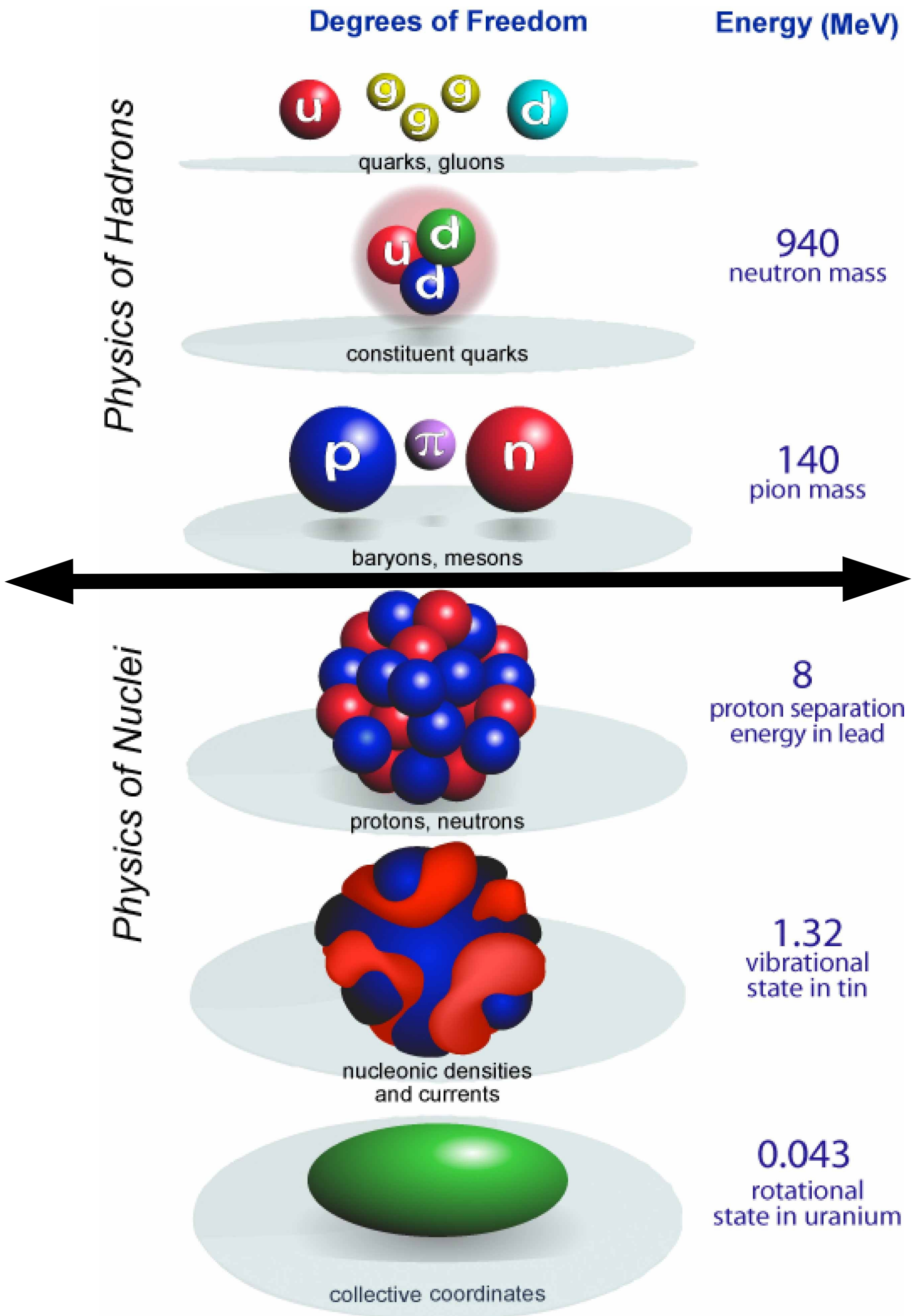
Tutorial: Nuclear Physics with *ab initio* few/many-body methods

Giuseppina Orlandini

UNIVERSITÀ DEGLI STUDI DI TRENTO

INFN

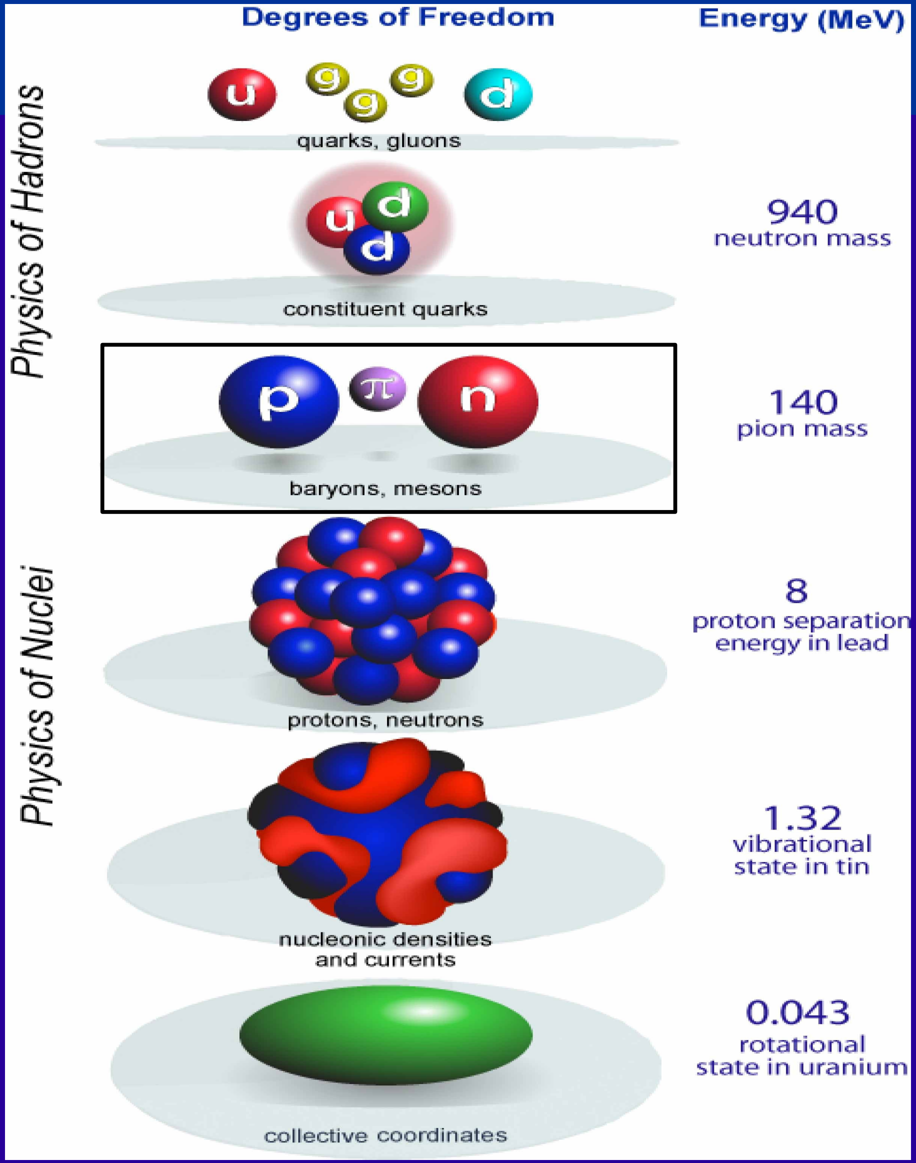

Degrees of Freedom
Energy (MeV)
Physics of Hadrons
Physics of Nuclei
u
g
g
g
d
quarks, gluons
u
d
d
constituent quarks
940
neutron mass
p
π
n
baryons, mesons
140
pion mass
protons, neutrons
8
proton separation
energy in lead
nucleonic densities
and currents
1.32
vibrational
state in tin
collective coordinates
0.043
rotational
state in uranium



FEW / MANY-body

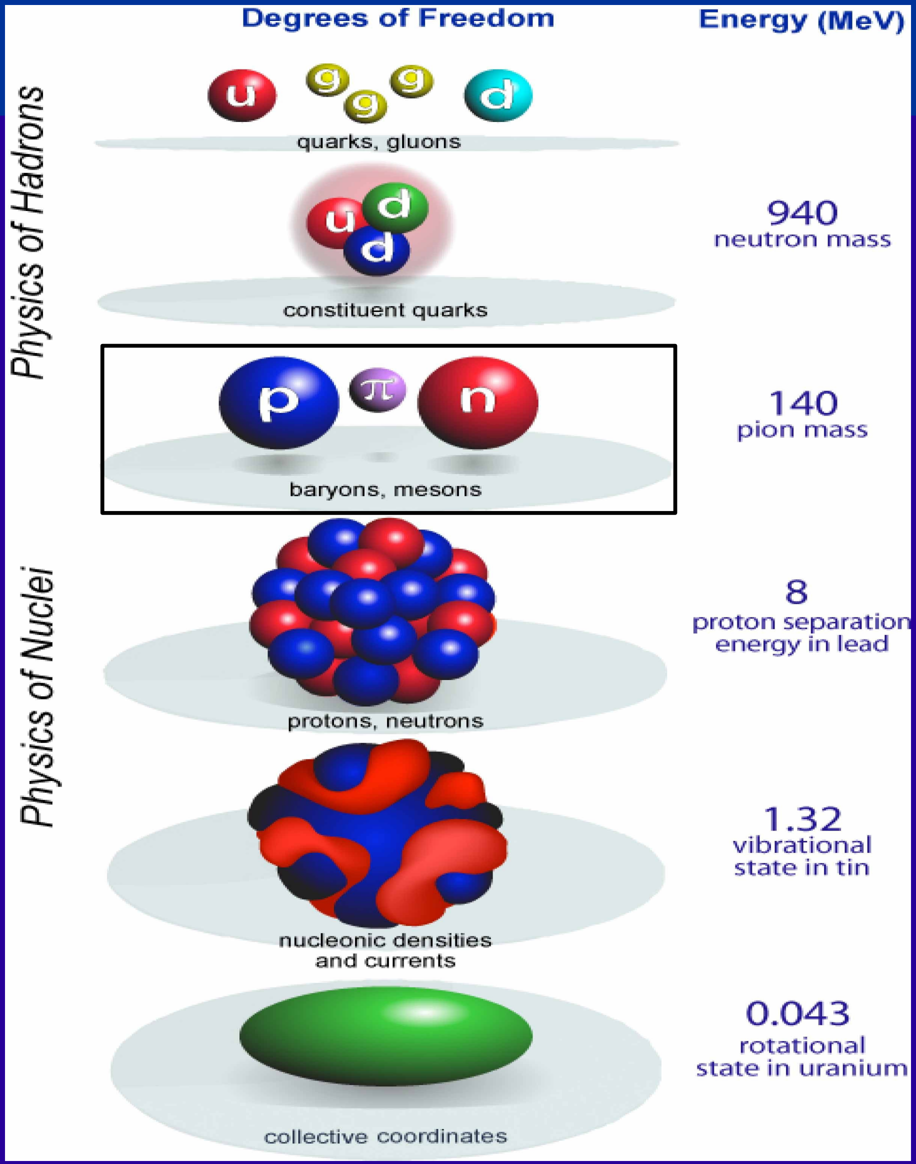
***ab initio* methods**

fundamental issues in nuclear physics:



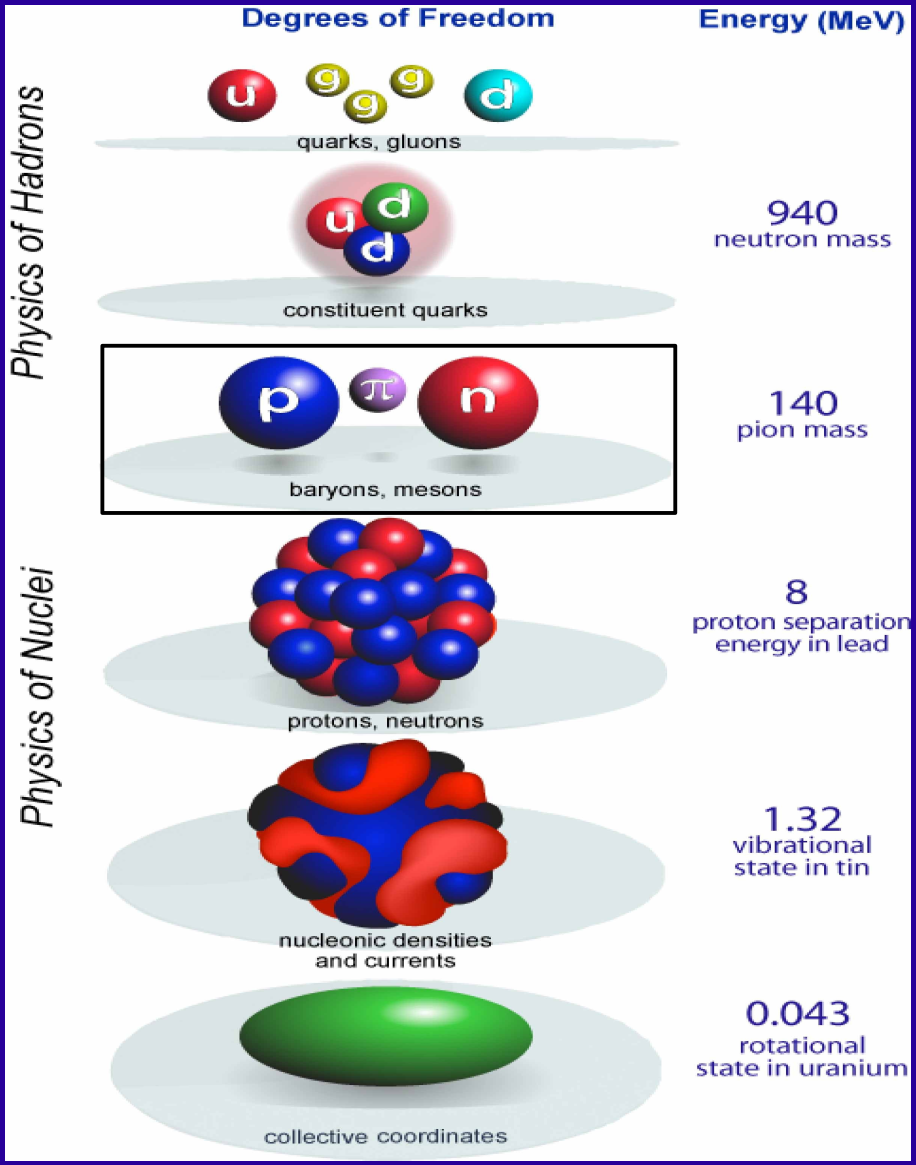
→ **relevant degrees of freedom**

fundamental issues in nuclear physics:



What is the Nuclear Interaction?

fundamental issues in nuclear physics:



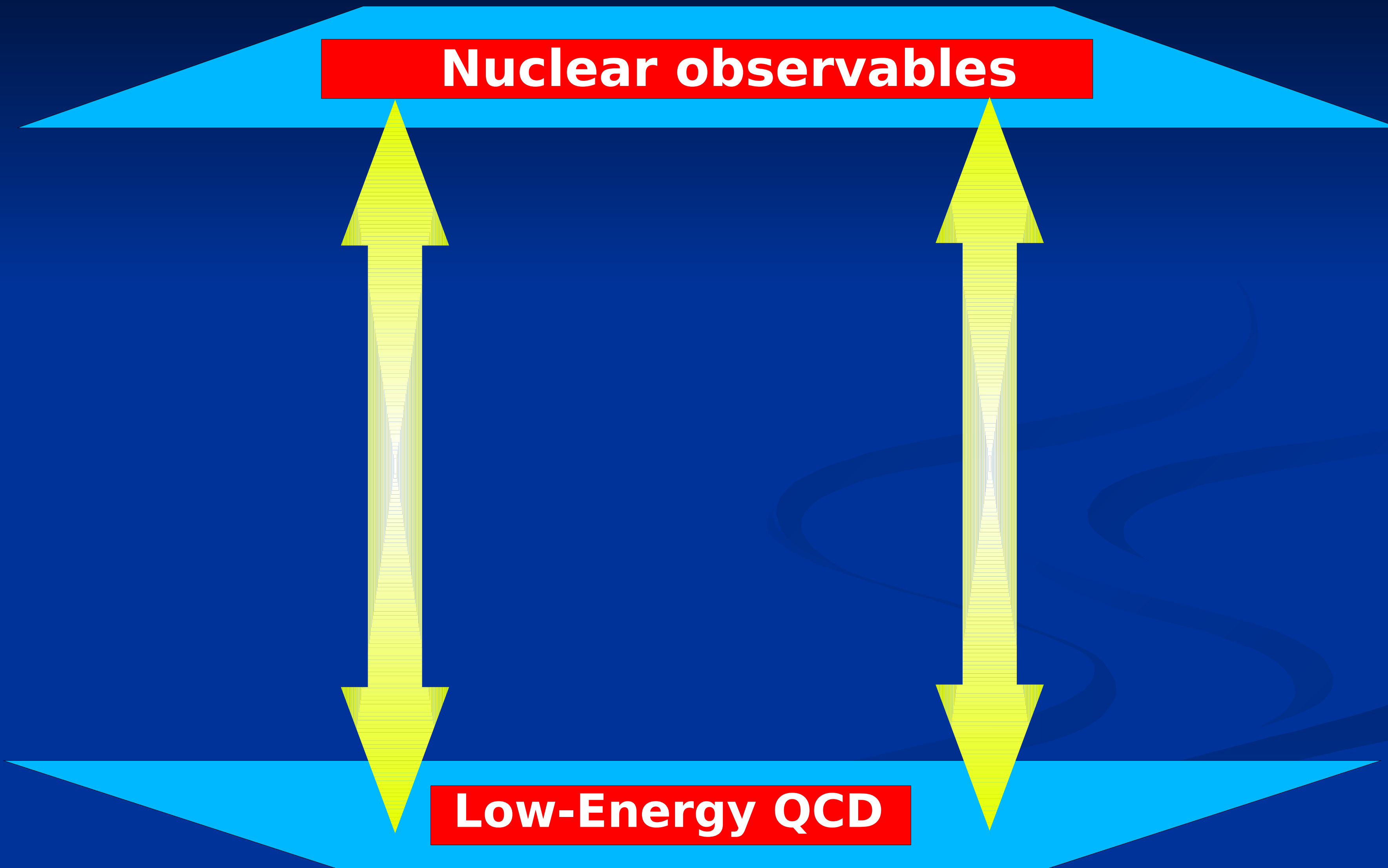
QCD

What is the Nuclear Interaction?

typical MB properties (clusterization, collectivity, mean field properties etc.)

TWO AIMS:

Aim 1: Help building the bridge between **Nuclear Physics** and **QCD**



Aim 1: Help building the bridge between **Nuclear Physics** and **QCD**

Nuclear observables

"effective" degrees of freedom

protons, neutrons, pions

Low-Energy QCD

Aim 1: Help building the bridge between **Nuclear Physics** and **QCD**

Nuclear observables

Nuclear Interactions NN, 3N ...	***Nucleons and pions on the Lattice***

"effective" degrees of freedom

protons, neutrons, pions

Low-Energy QCD

Aim 1: Help building the bridge between **Nuclear Physics** and **QCD**

Nuclear observables

Ab initio **Few/Many-body**

Methods

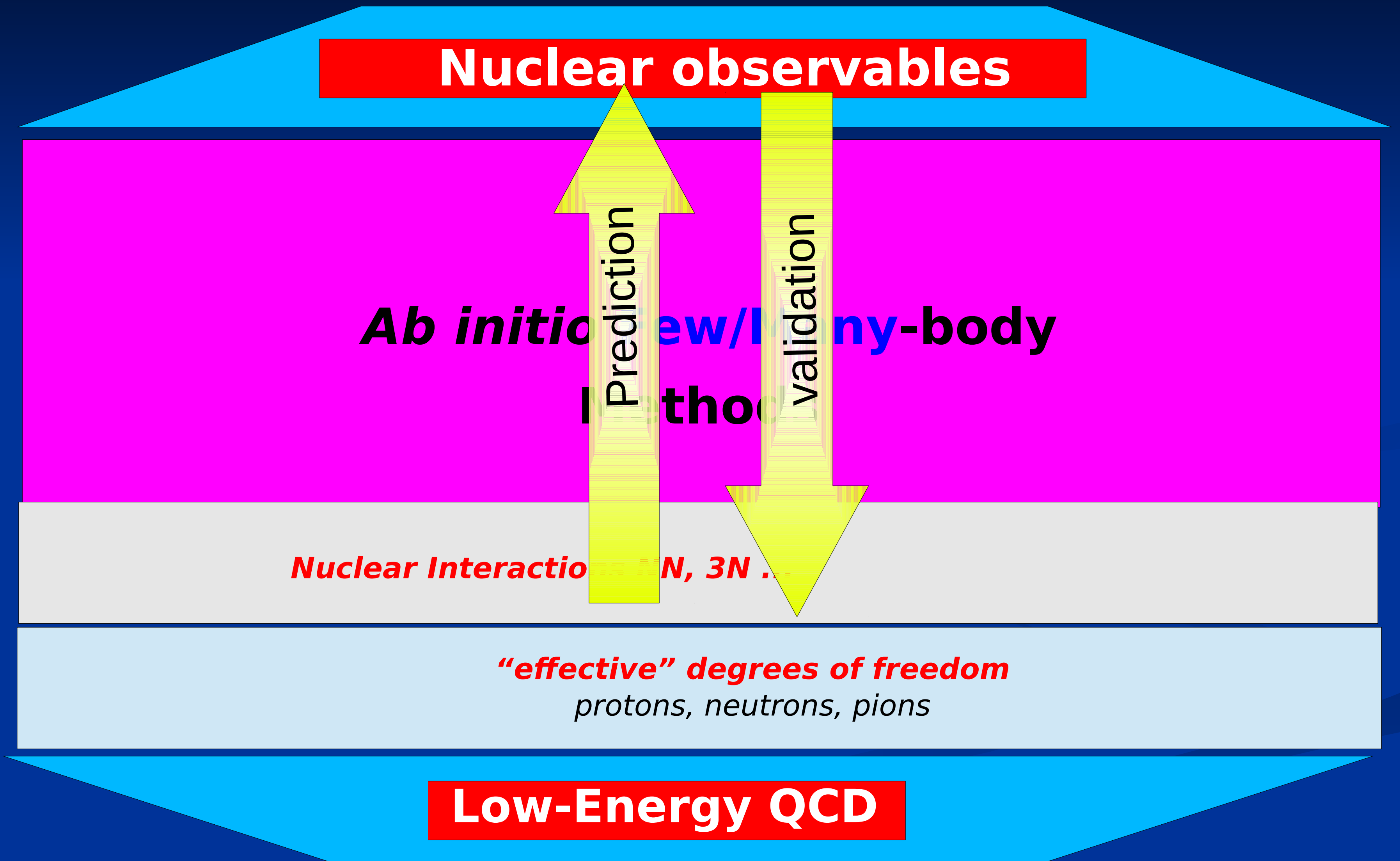
Nuclear Interactions NN, 3N ...

"effective" degrees of freedom

protons, neutrons, pions

Low-Energy QCD

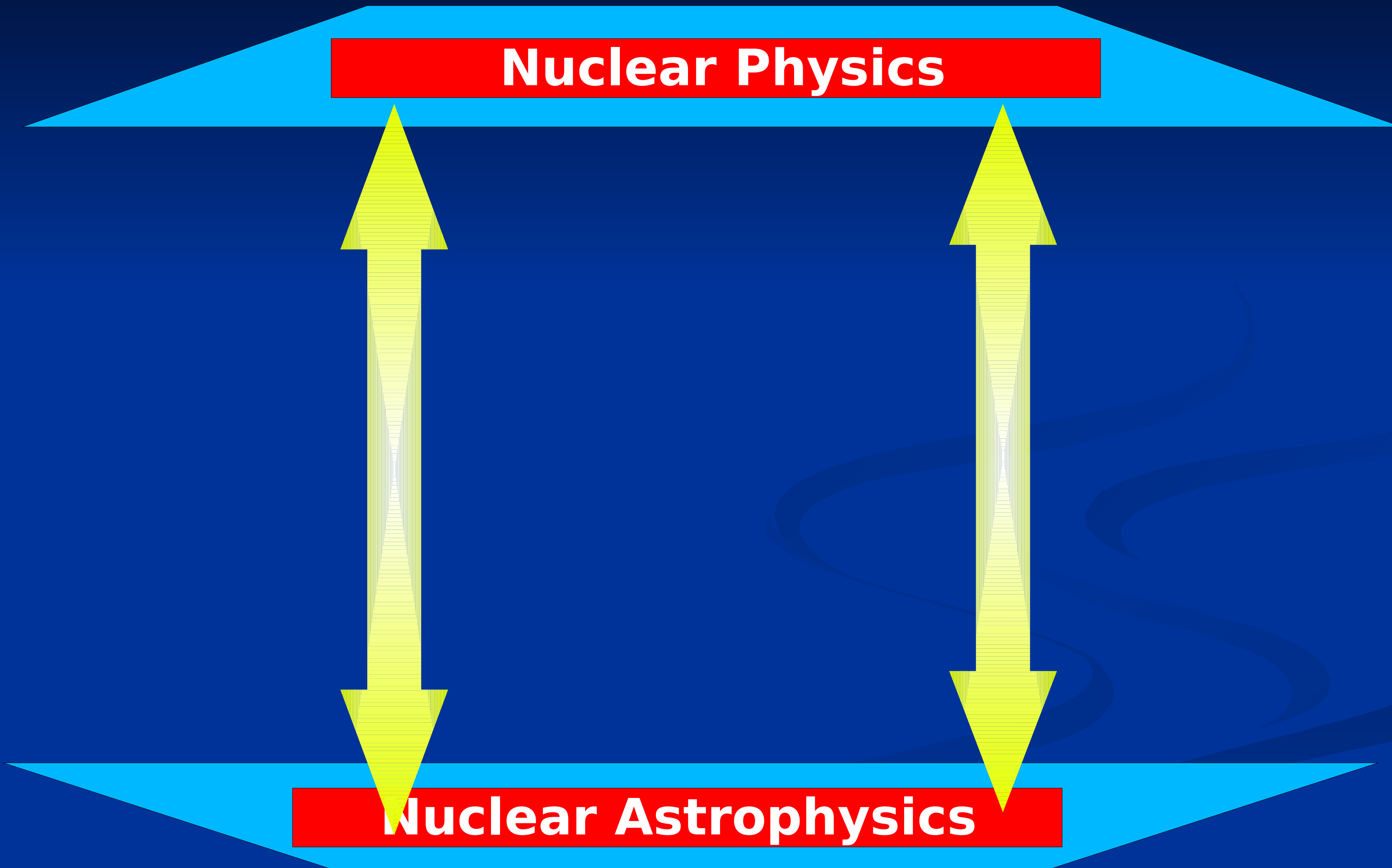
Aim 1: Help building the bridge between **Nuclear Physics** and **QCD**



Aim 2: Connections between **Nuclear Physics** and **other fields**

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Nuclear Astrophysics



Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Nuclear Astrophysics

Nuclear Physics

Abundances Nucleosynthesis (Big Bang, Stellar, Explosive)

Nuclear Astrophysics

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.
Nuclear Astrophysics

Nuclear Physics

Astrophysical models

Abundances ***Nucleosynthesis (Big Bang, Stellar, Explosive)***

Nuclear Astrophysics

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Nuclear Astrophysics

Nuclear Physics

Inputs: ***e.g.Electroweak and hadronic processes with nuclei***

Astrophysical models

Abundances ***Nucleosynthesis (Big Bang, Stellar, Explosive)***

Nuclear Astrophysics

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Nuclear Astrophysics

Nuclear Physics

Ab initio **Few/Many-body**

Methods

Inputs: ***e.g.Electroweak and hadronic processes with nuclei***

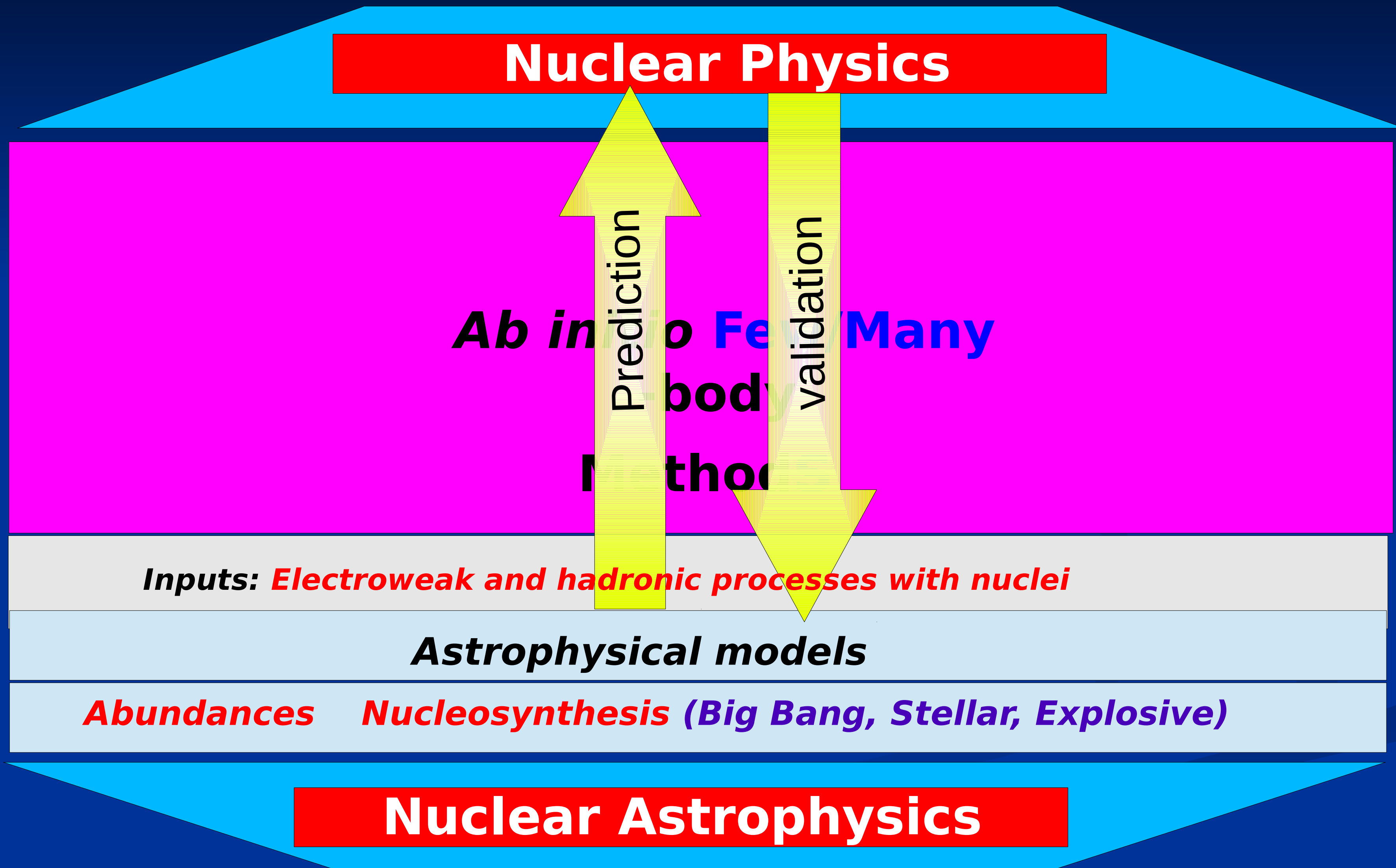
Astrophysical models

Abundances ***Nucleosynthesis*** ***(Big Bang, Stellar, Explosive)***

Nuclear Astrophysics

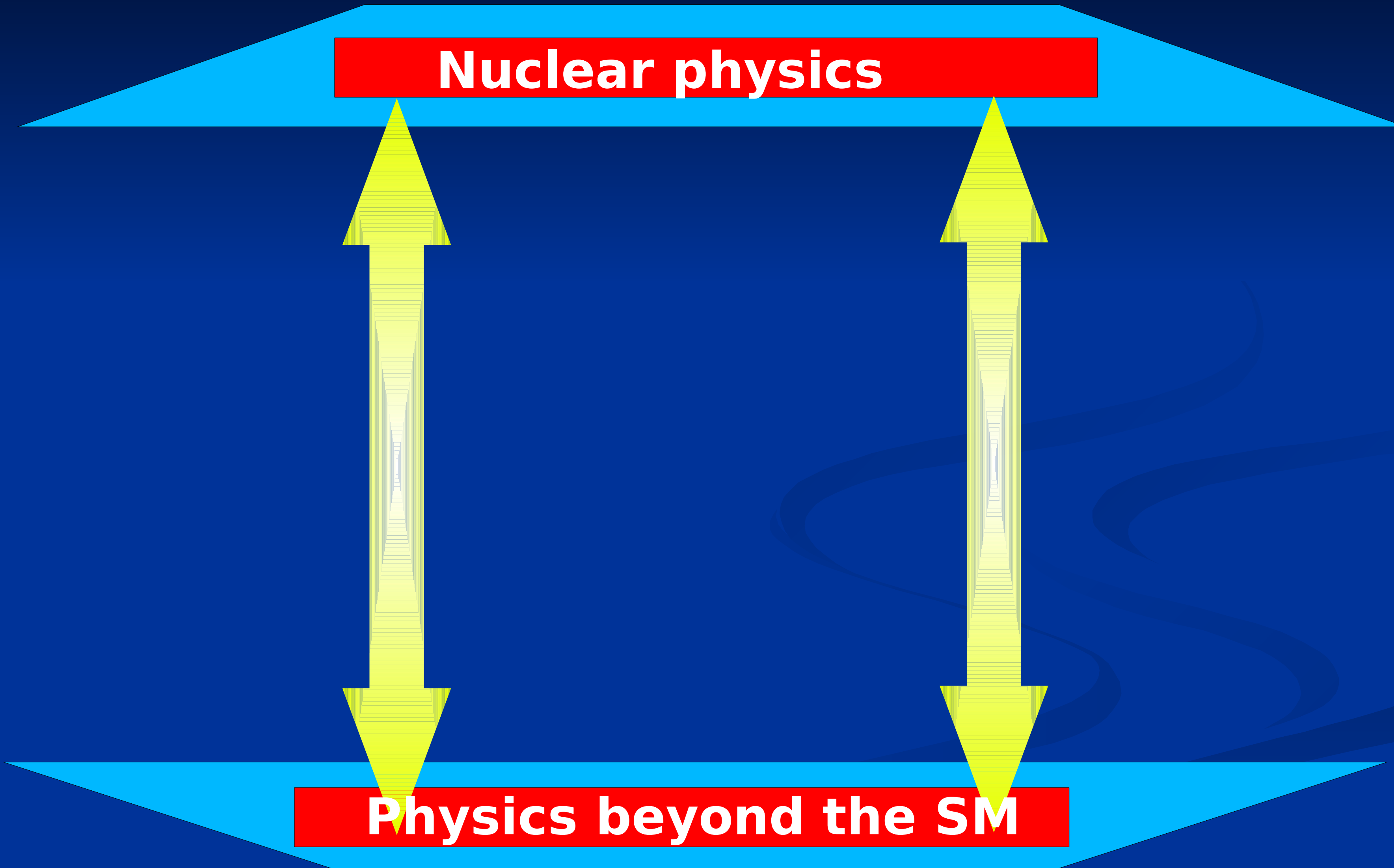
Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Nuclear Astrophysics



Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Physics beyond the standard model



Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Physics beyond the standard model

Nuclear physics

e.g. Time reversal invariance violation in Strong interactions

Physics beyond the SM

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Physics beyond the standard model

Nuclear Physics

Measurement of Electric Dipole Moment in light nuclei

e.g. Time reversal invariance violation in Strong interactions

Physics beyond the SM

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Physics beyond the standard model

Nuclear Physics

Input: ***EDM of light nuclei with $\not{T}$ interaction terms added in the potential***

Measurement of Electric Dipole Moment in light nuclei

e.g. Time reversal invariance violation in Strong interactions

Physics beyond the SM

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Physics beyond the standard model

Nuclear Physics

***Ab initio* Few/Many-body**

Methods

Input: ***EDM of light nuclei with ~~T~~ interaction terms added in the potential***

Measurement of Electric Dipole Moment in light nuclei

Time reversal invariance violation in Strong interactions

Physics beyond the SM

Aim 2: Connections between **Nuclear Physics** and **other fields** e.g.

Physics beyond the standard model

Nuclear Physics

Prediction

validation

***Ab initio* Few-body Methods**

Input: ***EDM of light nuclei with $\not{T}$ interaction terms added in the potential***

Measurement of Electric Dipole Moment in light nuclei

Time reversal invariance violation in Strong interactions

Physics beyond the SM

Ab initio methods

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

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

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 framework:

Non relativistic quantum mechanics

The task:

Solve the Schrödinger equation for a system of **A** nucleons

Respect **Translational/Galileian** invariance

$$[H, \vec{P}_{cm}] = 0 \qquad\qquad [H, \vec{R}_{cm}] = 0$$

Rotational invariance

$$[H, \vec{J}] = 0$$

A classical ~~T~~-invariant hamiltonian:

$$H = \sum_i^A \frac{p_i^2}{2m} + \sum_i W(r_i) + \sum_{ij} \nu_{ij}$$

Mean field

2-body residual interaction

An invariant hamiltonian:

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

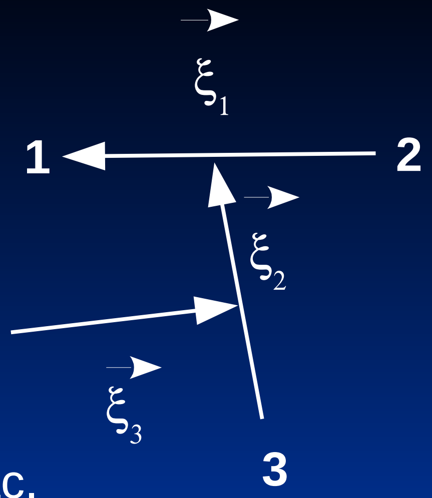
2-body potential

3-body potential

Kinetic energy in terms of A-1

conjugate momenta π_ι of Jacobi coordinates ζ_ι

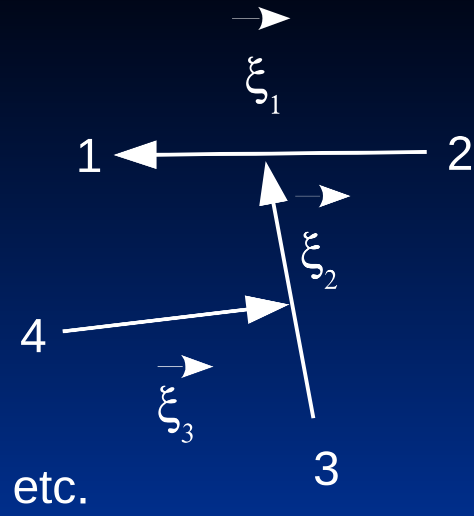
Jacobi coordinates $\vec{\xi}_i$ 1,2 .... A-1



$\vec{\xi}_i$ = distances between each particle "i" and the cm of the previous (A – i) particles

etc.

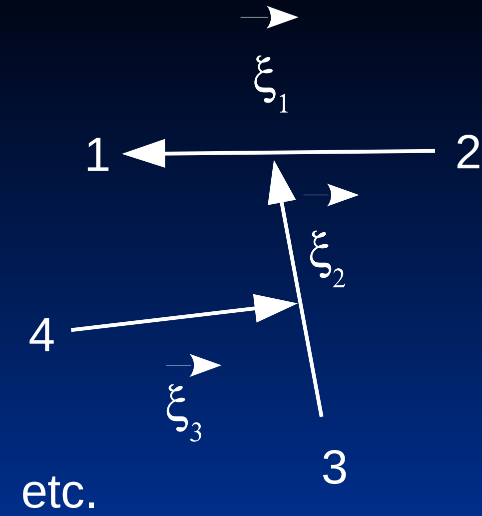
Jacobi coordinates $\vec{\xi}_i$ **1,2 .... A-1**



$\vec{\xi}_i$ = distances between each particle "i" and the cm of the previous (A – i) particles

$$\begin{matrix} \vec{p}_1 & \vec{r}_1 \\ \vec{p}_2 & \vec{r}_2 \\ . & . \\ . & . \\ . & . \\ \vec{p}_A & \vec{r}_A \end{matrix} \quad \xleftrightarrow{\text{transformation}} \quad \begin{matrix} \vec{\xi}_0 = \vec{R}_{CM} & \vec{\pi}_0 = \vec{P}_{CM} \\ \xi_1 & \pi_1 \\ . & . \\ . & . \\ . & . \\ \xi_{A-1} & \pi_{A-1} \end{matrix}$$

Jacobi coordinates $\vec{\xi}_i$ 1,2 .... A-1



$\vec{\xi}_i$ = distances between each particle "i" and the cm of the previous (A – i) particles

$\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_A$ $\quad$ $\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A$ $\quad$ ⟷ transformation ⟷ $\quad$ $\vec{\xi}_0 = \vec{R}_{CM}, \vec{\xi}_1, \ldots, \vec{\xi}_{A-1}$ $\quad$ $\vec{\pi}_0 = \vec{P}_{CM}, \vec{\pi}_1, \ldots, \vec{\pi}_{A-1}$

$$H = \frac{P_{CM}^2}{2M_{CM}} + \frac{\pi_1^2}{2\mu_1} + \frac{\pi_2^2}{2\mu_2} + \ldots\ldots \frac{\pi_{A-1}^2}{2\mu_{A-1}} + V(\vec{\xi}_1, \vec{\xi}_2, \ldots\ldots \vec{\xi}_{A-1})$$

→ **Invariant H**

→ in general **NON** separable

Remarks:

- When expressed in terms of Jacobi coordinates, even a 2-body potential becomes of “A-body nature”
- The translation invariant wave function is highly *correlated* (i.e. particles are not independent) beyond the correlation due to the dynamics

Remarks:

- Coping with T&G invariances, as well as Pauli principle at the same time, is one of the problems that makes difficult to extend some ab initio approaches to large A
- (*No Slater Determinants!*) 

Possible questions:

- Can a comparison between measured and calculated observables help discriminating among OBEP, Phenomenological, EFT potentials?
- Can it help discriminating between different versions of EFT potentials?
- *(Are such questions "well posed"?)*

To answer such questions one needs to solve the Schrödinger equation with an ab initio method and calculate several observables

The basic *ab initio* methods

	Few-body: A≤4	F/M-body:4<A< 12,20,40..??
Structure: Bound state observables		
Reactions: Cross sections (Scatt. states)		

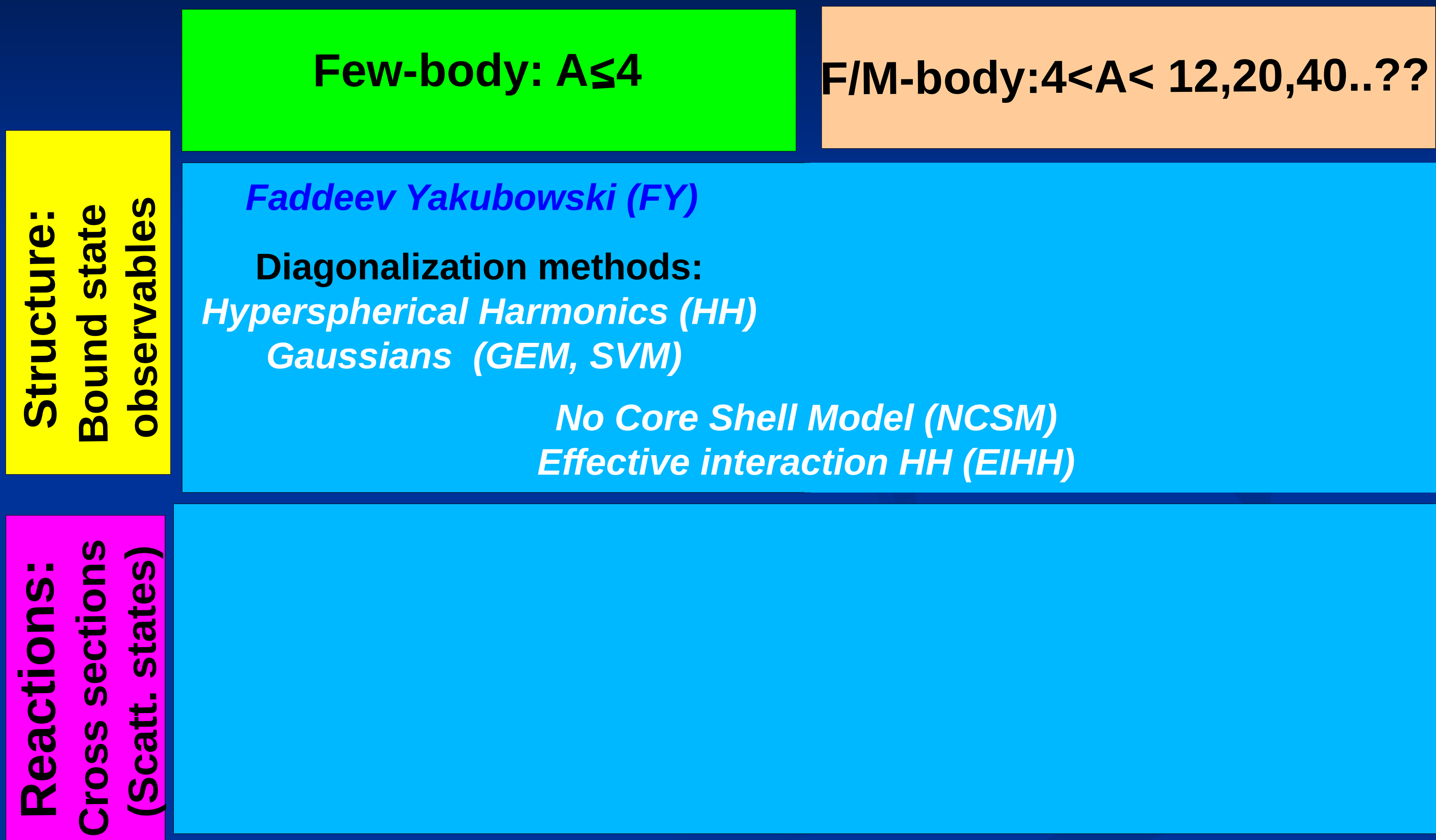
The basic *ab initio* methods

	Few-body: A≤4	F/M-body:4<A< 12,20,40..??
Structure: Bound state observables	*Faddeev Yakubowski (FY)*	
Reactions: Cross sections (Scatt. states)		

The basic *ab initio* methods

	Few-body: A≤4	**F/M-body:4<A< 12,20,40..??**
Structure: Bound state observables	*Faddeev Yakubowski (FY)* **Diagonalization methods:** ***Hyperspherical Harmonics (HH)*** ***Gaussians (GEM, SVM)***	
Reactions: Cross sections (Scatt. states)		

The basic *ab initio* methods



The basic *ab initio* methods

Tomorrow !
Francesco Pederiva

Few-body: A≤4

F/M-body:4<

Faddeev Yakubowski (FY)

Monte Carlo methods
(GFMC,AFDMC)

Diagonalization methods:
Hyperspherical Harmonics (HH)
Gaussians (GEM, SVM)

No Core Shell Model (NCSM)
Effective interaction HH (EIHH)

Structure:
Bound state observables

Reactions:
Cross sections (Scatt. states)

The basic *ab initio* methods

Tomorrow !
Francesco Pederiva

Few-body: A≤4

F/M-body:4<

Structure:
Bound state observables

Faddeev Yakubowski (FY)

Monte Carlo methods
(GFMC,AFDMC)

Diagonalization methods:
Hyperspherical Harmonics (HH)
Gaussians (GEM, SVM)

??Coupled Cluster (CC)??

No Core Shell Model (NCSM)
Effective interaction HH (EIHH)

Reactions:
Cross sections (Scatt. states)

HH: A nice alternative to the HO basis, inspired by the 2-body problem:

$\vec{\pi}_1$ $\quad$ $\vec{\xi}_1$

$$H_{int} = \frac{\vec{p}^{\,2}}{2\mu} + V(\vec{r})$$

$\vec{\xi}_1$

1 $\longrightarrow$ 2

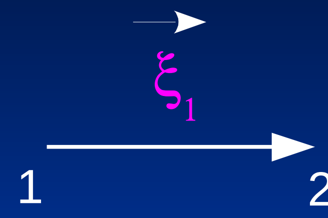
$$\vec{\xi}_1 = r,\ \theta,\ \phi$$

spherical coordinates

HH: A nice alternative to the HO basis, inspired by the 2-body problem:

$\vec{\pi}_1 \uparrow \qquad \vec{\xi}_1 \nearrow$

$$H_{int} = \frac{p^2}{2\mu} + V(\vec{r})$$



$\vec{\xi}_1 = r, \ \theta, \ \phi$

spherical coordinates

$T \sim \Delta_r -$ L^2/r^2

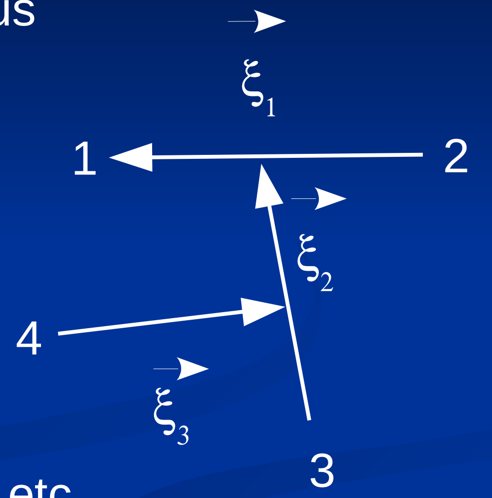
the good basis are **spherical** harmonics **$Y_{lm}(\theta, \phi)$**

eigenfunctions of **angular momentum L^2**

EXTEND THAT IDEA TO A>2

HYPERSPHERICAL COORDINATES

ξ_1		ρ	← hyperradius
θ_1		α_1	
ϕ_1		α_{2}	
.	transform ! →	.	
.		.	
.		.	hyperangles
.		.	
		.	
		.	
ξ_{A-1}			
θ_{A-1}			
ϕ_{A-1}		α_{3A-4}	

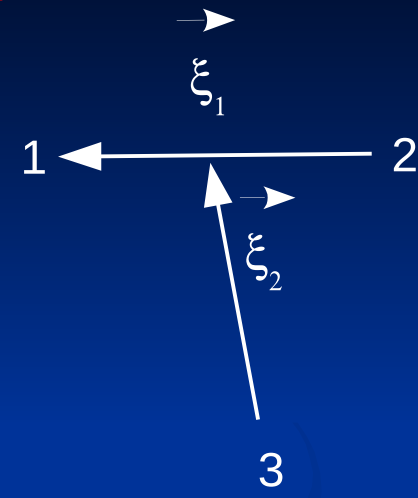


etc.

HOW ARE HYPERRADIUS ρ AND HYPERANGLES α'_ι DEFINED ???

HOW ARE HYPERRADIUS ρ AND HYPERANGLES α'_ι DEFINED ???

e.g. for **3** particles



ξ_1

θ_1

ϕ_1

ξ_2

θ_2

ϕ_2

transform →

$$\rho^2 = \xi_1^{\,2} + \xi_2^{\,2}$$

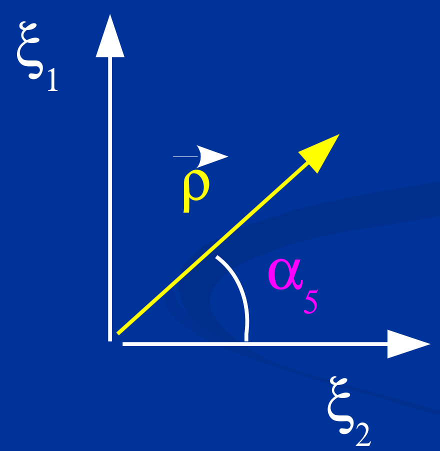
$$\alpha_1 = \theta_1$$

$$\alpha_2 = \phi_1$$

$$\alpha_3 = \theta_2$$

$$\alpha_4 = \phi_2$$

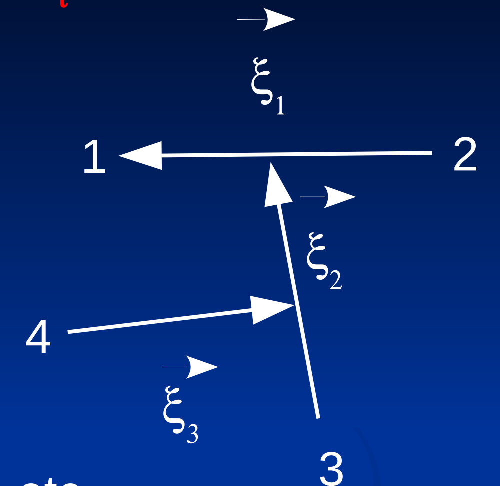
$$\alpha_5 = \text{arcos}(\xi_2/\rho)$$



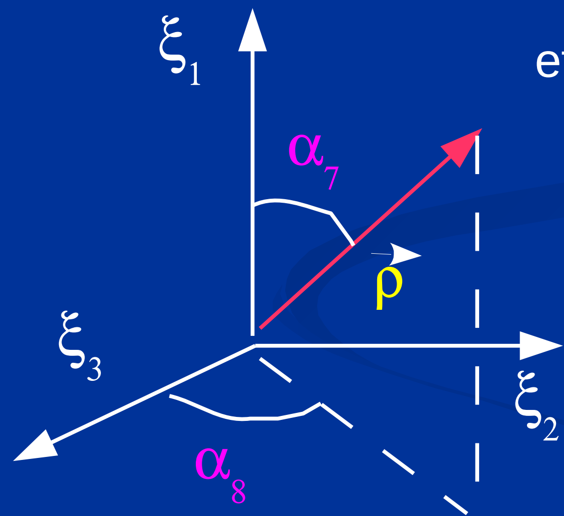
HOW ARE HYPERRADIUS ρ AND HYPERANGLES α'_ι DEFINED ???

e.g. for **4** particles

ξ_1		$\rho^2 = \xi_1^{\ 2} + \xi_2^{\ 2} + \xi_3^{\ 2}$
θ_1		$\alpha_1 = \theta_1$
ϕ_1		$\alpha_2 = \phi_1$
ξ_2		$\alpha_3 = \theta_2$
θ_2	transform →	$\alpha_4 = \phi_2$
ϕ_2		$\alpha_5 = \theta_3$
ξ_3		$\alpha_6 = \phi_3$
θ_3		$\alpha_7 = \ldots$
ϕ_3		$\alpha_8 = \ldots$



etc.



2 body: **SPHERICAL** HARMONICS

$T \sim \Delta_r - L^2 / r^2$

the good basis are $Y_{lm}(\theta, \phi)$ **spherical** harmonics

eigenfunctions of **angular momentum** L^2

A body: **HYPERSPHERICAL** HARMONICS

$T \sim \Delta_\rho - K^2 / \rho^2$

the good basis are $Y_{K \ldots}(\alpha_1, \ldots \alpha_{3A-4})$ **hyperspherical** harmonics

eigenfunctions of **hyperangular momentum** K^2

SUMMARIZING:

$$H_{int} = 1/\mu \, (\Delta_\rho - K^2 / \rho^2) + V(\xi_1, \xi_2, \dots \xi_{A-1})$$

Hyperspherical Harmonics basis

$$\Psi = \sum_{N\,K\,\dots\dots} L_N(\rho)\, Y_{K\,\dots}(\alpha_1, \dots \alpha_{3A-4})$$

$L_N(\rho)$ = Laguerre Polynomials (exp [- a ρ])

PROBLEM N.1 : **ANTISYMMETRIZATION of HH IS NON TRIVIAL ! (no Slater Determinants!)**

“ by hand ” : cumbersome! possible only for A=3,4

SOLUTIONS

1) an algorithm based on relations between O(N) and S_N

Novoselsky & Katriel PRA 49 (1994) 833
Novoselsky & *Barnea* PRA 51 (1995) 2777

2) an algorithm based on property of the Casimir operator of S_N

M. Gattobigio, A. Kievsky, M. Viviani, Phys.Rev.C, 83, 024001 (2011);
S.Deflorian, N.Barnea, W.Leidemann, G.O.i, Few-Body Syst. 54, 1879 (2013);

PROBLEM N.2 : SLOW CONVERGENCE IN QUANTUM NUMBER [K] = {K....}

essentially for two reasons

1) for increasing A the # of quantum numbers {K, ... } increases
i.e. each combination of values corresponds to a state

→ **for increasing A one has lots of states even for K small**

BIG MATRICES (FULL!)

2) strong short range repulsion of the potential

HOW TO SPEED UP THE CONVERGENCE?

SOLUTION:

Construct **EFFECTIVE INTERACTIONS** **by** ***Similarity Transformations***

Suzuki-Lee (NCSM, EIHH)

Similarity Renormalization Group (NCSM, CC)

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

No core shell model

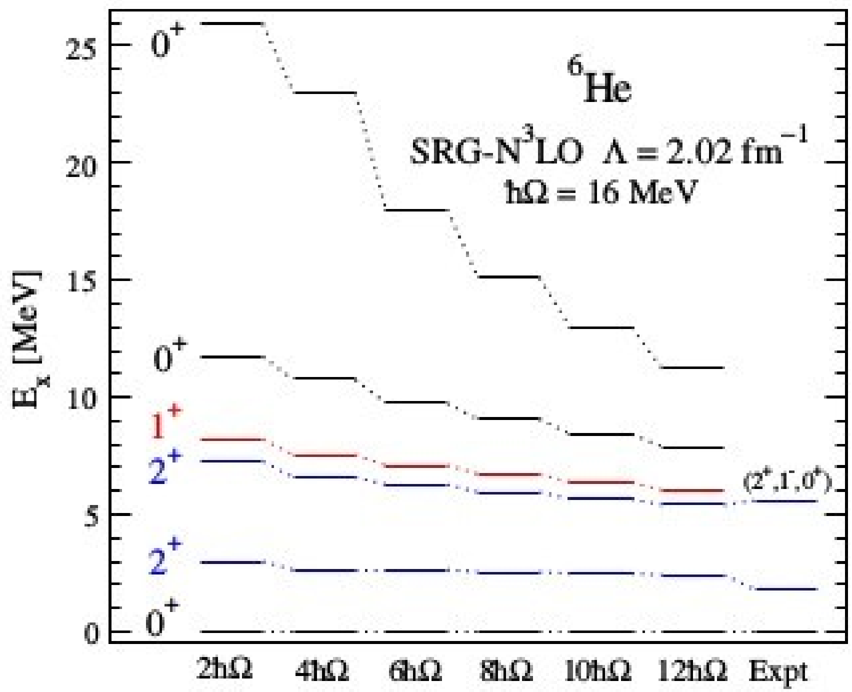


FIG. 1 (color online). Dependence of ^{6}He excitation energies on the size of the HO basis $N_{max}\hbar\Omega$.

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

The basic *ab initio* methods

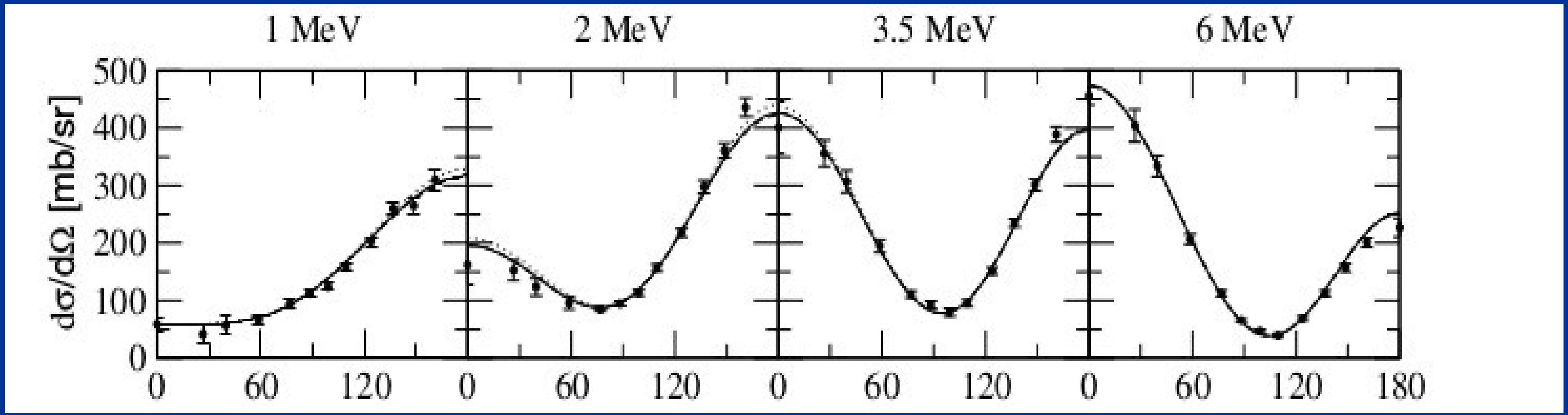
	Few-body (A≤4)	Few-body (4<A< 12,20,40??)
Structure: Bound state observables	*Faddeev Yakubowski (FY)* Diagonalization methods: *Hyperspherical Harmonics (HH)* *Gaussians (GEM, SVM)*	Monte Carlo methods *(GFMC,AFDMC)* *??Coupled Cluster (CC)??*
	No Core Shell Model (NCSM) *Effective interaction HH (EIHH)*	
Reactions: Cross sections (Scatt. states)		

The basic *ab initio* methods

	Few-body (A≤4)	**Few-body (4<A< 12,20,40??)**
Structure: Bound state observables	*Faddeev Yakubowski (FY)* **Diagonalization methods:** *Hyperspherical Harmonics (HH)* *Gaussians (GEM, SVM)*	**Monte Carlo methods** *(GFMC,AFDMC)* *??Coupled Cluster (CC)??*
	No Core Shell Model (NCSM) *Effective interaction HH (EIHH)*	*No Core Shell Model (NCSM)* *Effective interaction HH (EIHH)*
Reactions: Cross sections (Scatt. states)	**Faddeev Yakubowski (FY)** **HH Kohn-variational**	

Benchmark calculation of n-^{3}H and p-^{3}He scattering

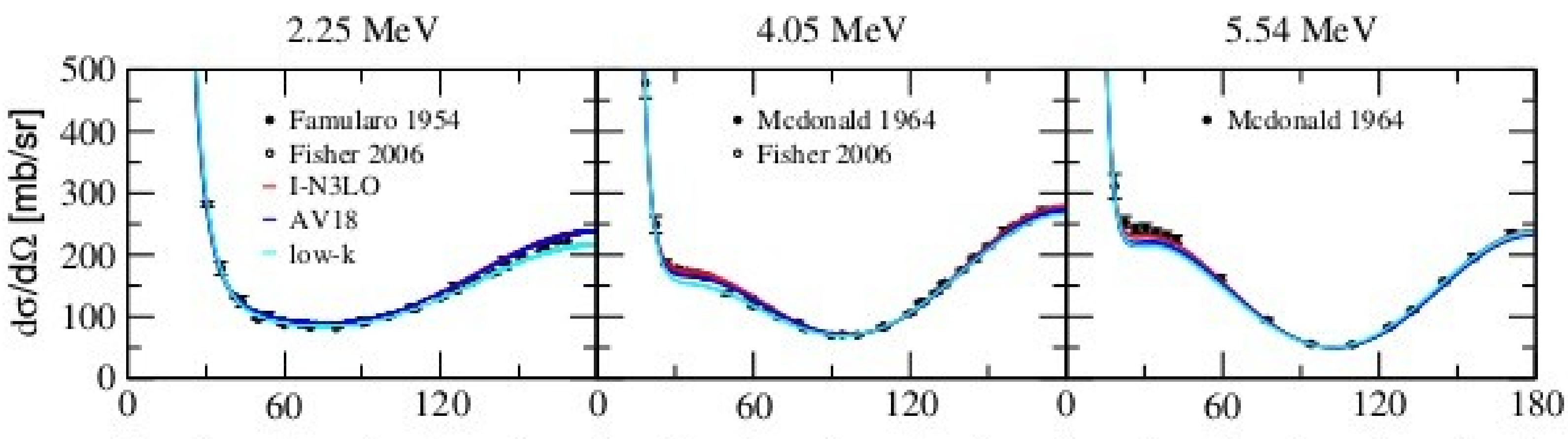
3 methods: **FY momentum space, FY configuration space, HH Kohn variational**



M. Viviani, A. Deltuva, R. Lazauskas, J. Carbonell, A. C. Fonseca, A. Kievsky, L.E. Marcucci, and S. Rosati Phys. Rev. C 84, 054010 (2011)

Benchmark calculation of n-^{3}H and p-^{3}He scattering

3 different potentials

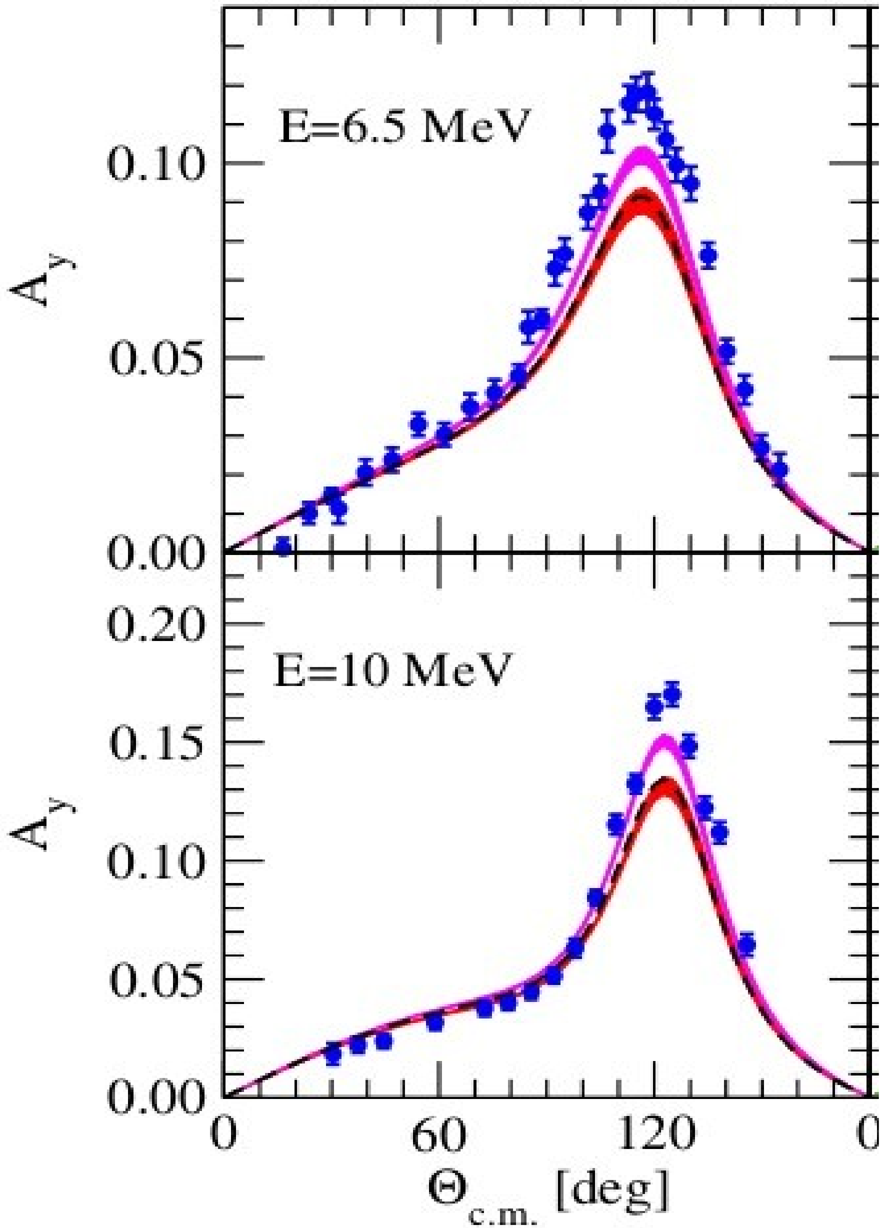


M. Viviani, A. Deltuva, R. Lazauskas, J. Carbonell, A. C. Fonseca, A. Kievsky, L.E. Marcucci, and S. Rosati Phys. Rev. C 84, 054010 (2011)

A_y puzzle:

n - d elastic scattering with polarized neutrons

"A_y puzzle"

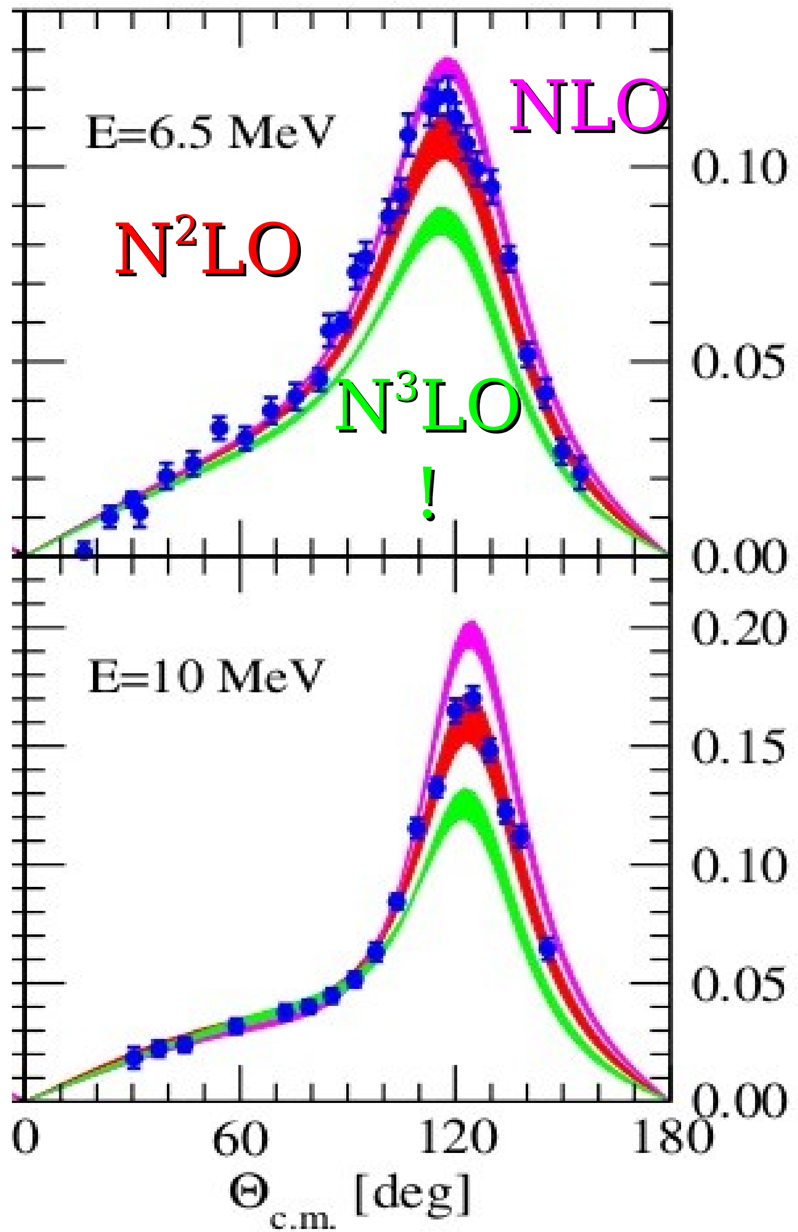


Phen. NN

Phen.NN+NNN

J. Golak, R. Skibinski, K. Topolnicki, H. Witala,a, E. Epelbaum, H. Krebs, H. Kamada, Ulf-G. Meissner, V. Bernard, P. Maris, J. Vary, S. Binder, A. Calci, K. Hebeler8, J. Langhammer, R. Roth, A.Nogga, S. Liebig, and D. Minossi
Eur. Phys. J. A (2014) 50: 177

"A_y puzzle" remains with EFT potentials!



J. Golak, R. Skibinski, K. Topolnicki, H. Witala,a, E. Epelbaum, H. Krebs, H. Kamada, Ulf-G. Meissner, V. Bernard, P. Maris, J. Vary, S. Binder, A. Calci, K. Hebeler8, J. Langhammer, R. Roth, A.Nogga, S. Liebig, and D. Minossi

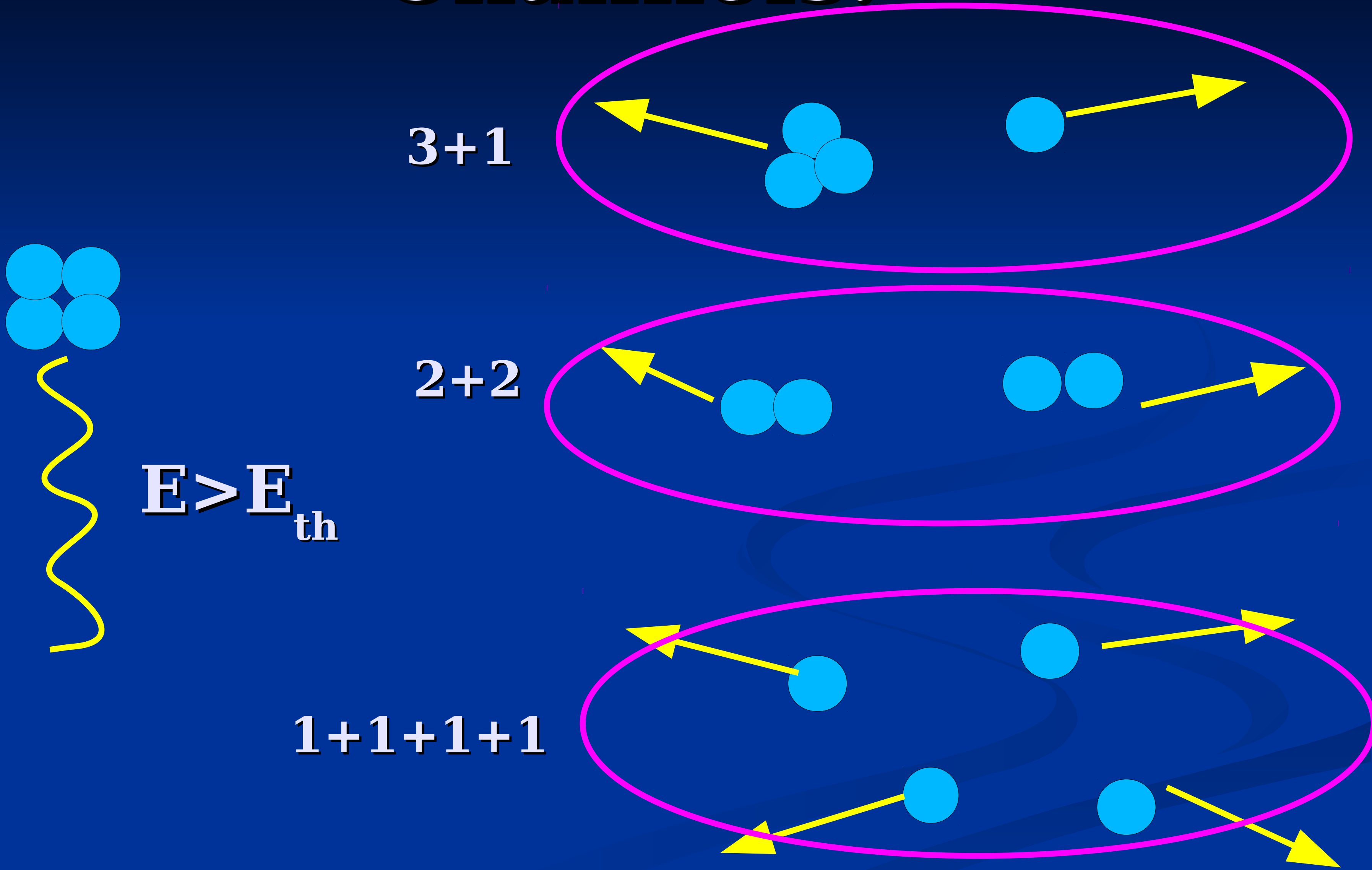
Eur. Phys. J. A (2014) 50: 177

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

Account for the asymptotic conditions in the w.f. for positive energies

(scattering many-body problem!)

Channels:



Before reaching the asymptotics condition all those channels interfere

FY equations:

n compact integral equations

(coupled Lippmann-Schwinger-like equations):

- for A=3 **n**=3
- for A=4 **n**=28
- for A=5 **n** too many !!!
- ...

Today:

- FY: **A=3** cross sections at energies where all channels (**1+2,1+1+1**) contribute
- FY: **A=4** cross sections at energies where all channels (**1+3, 2+2, 1+1+2**) contribute

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

Alternative approach:

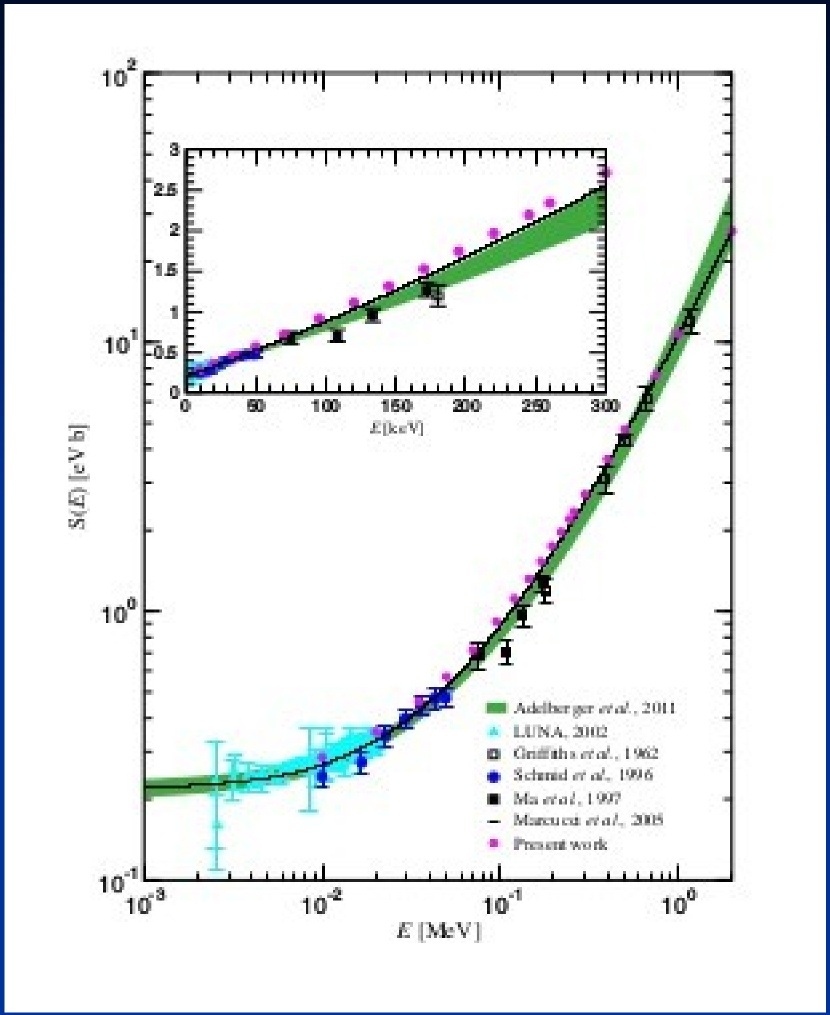
- Configuration space
- Based on Kohn variational principle
- Correct asymptotic conditions

Pisa School: Kievsky, Viviani, Marcucci...

An interesting Astrophysical application:

- **Recent Planck Satellite results:**
  Apparent **disagreement** between Cosmic Microwave Background (CMB) and primordial deuterium abundance
- **Crucial input:**
  d(p,γ)^{3}He rate at Big Bang Nucleosynthesis (BBN) temperature range (E = 30-300 keV)
- **Existing measurements:**
  unclear, new Luna experiment is planned

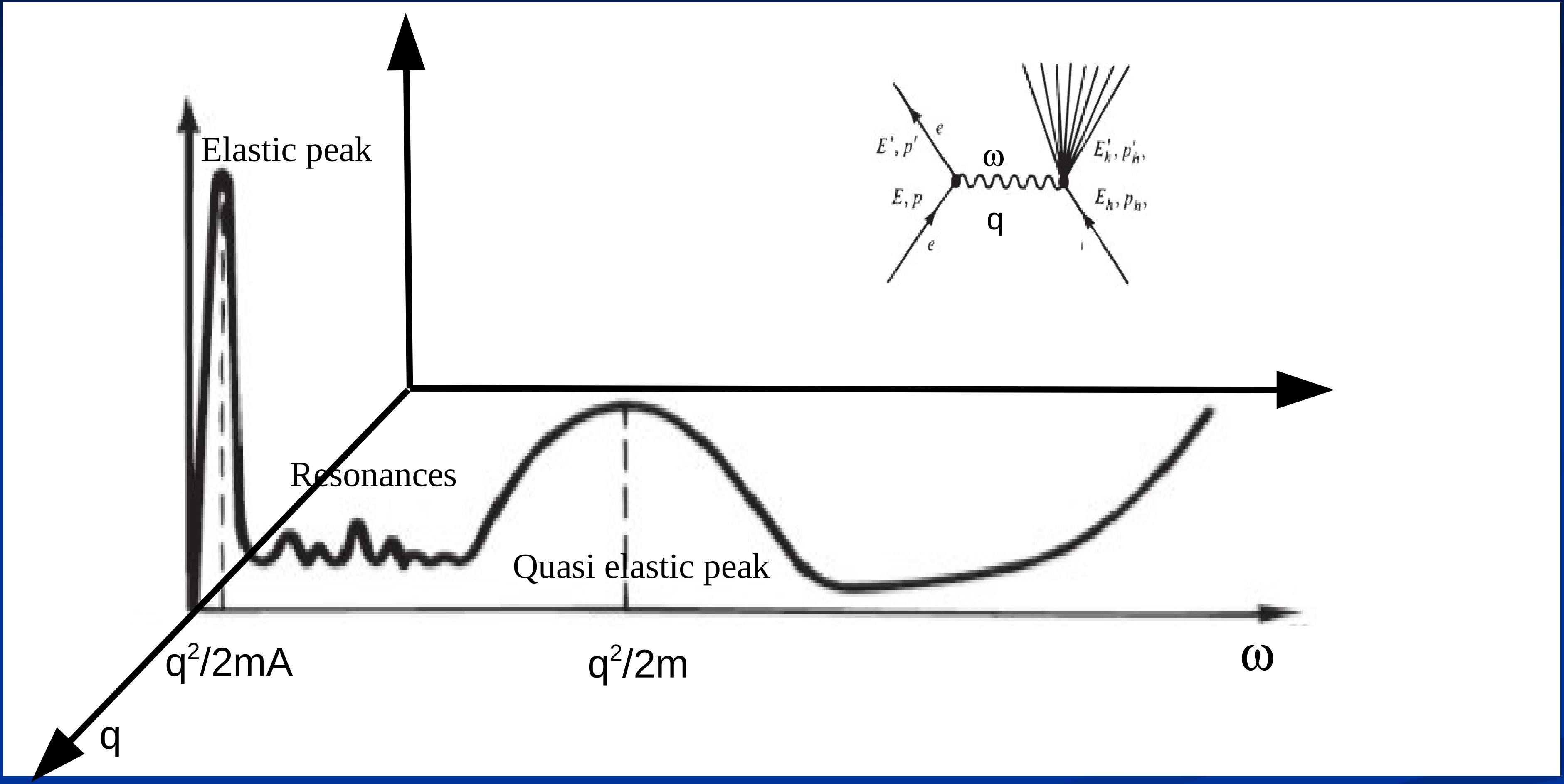
- **Disgreement becomes agreement if:**
  d(p,γ)^{3}He rate 10% higher than measured



Phen.NN+NNN
+ Many-body currents
(however from EFT)

L.E. Marcucci, G. Mangano, A. Kievsky and M. Viviani
Phys. Rev. Lett. 116, 102501 (2016)

Nuclear spectrum



Remarks on the problem of scattering w.f.:

- The information on wave functions is redundant, since they are not observable

Remarks on the problem of scattering w.f.:

- The information on wave functions is redundant, since they are not observable
- Observables are matrix elements on w.f., namely integrals, i.e. less information is needed

Remarks on the problem of scattering w.f.:

- The information on wave functions is redundant, since they are not observable
- Observables are matrix elements on w.f., namely integrals, i.e. less information is needed
- Point directly to matrix elements!

The basic *ab initio* methods

Few-body (A≤4)

Few-body (4<A< 12,20,40???)

Structure
Bound states

Faddeev Yakubowski (FY)

Diagonalization methods:
Hyperspherical Harmonics (HH)
Gaussians (GEM, SVM)

Monte Carlo methods
(GFMC,AFDMC)

??Coupled Cluster (CC)??

No Core Shell Model (NCSM)
Effective interaction HH (EIHH)

Reactions
scattering states

Faddeev Yakubowski (FY)

HH Kohn-variational

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

REMEMBER:

$S(\omega)$ is the observable! **$S(\omega) = 1/\pi \, Im \left[\Pi(\omega)\right]$**, where

$$\Pi(\omega) = \int <|\Theta^{\dagger}(t)\, \Theta(0)|> e^{\,i\omega t}\, dt$$

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

Green F. with poles on the real axis

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

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

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

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

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

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

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.

So, how to calculate this mean value?

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

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

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

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

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

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

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

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

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

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

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

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

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!)

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

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 $\sigma_1, \sigma_2, \ldots$

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 Φ (σ) 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:

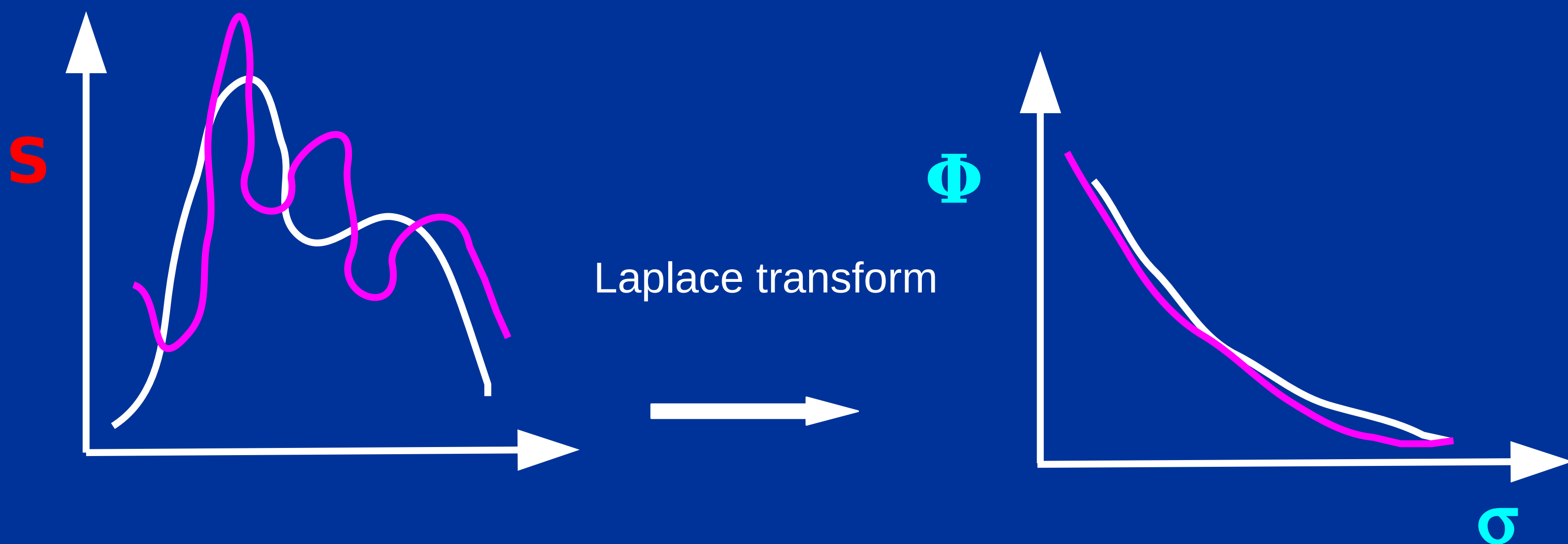


Illustration of the problem:

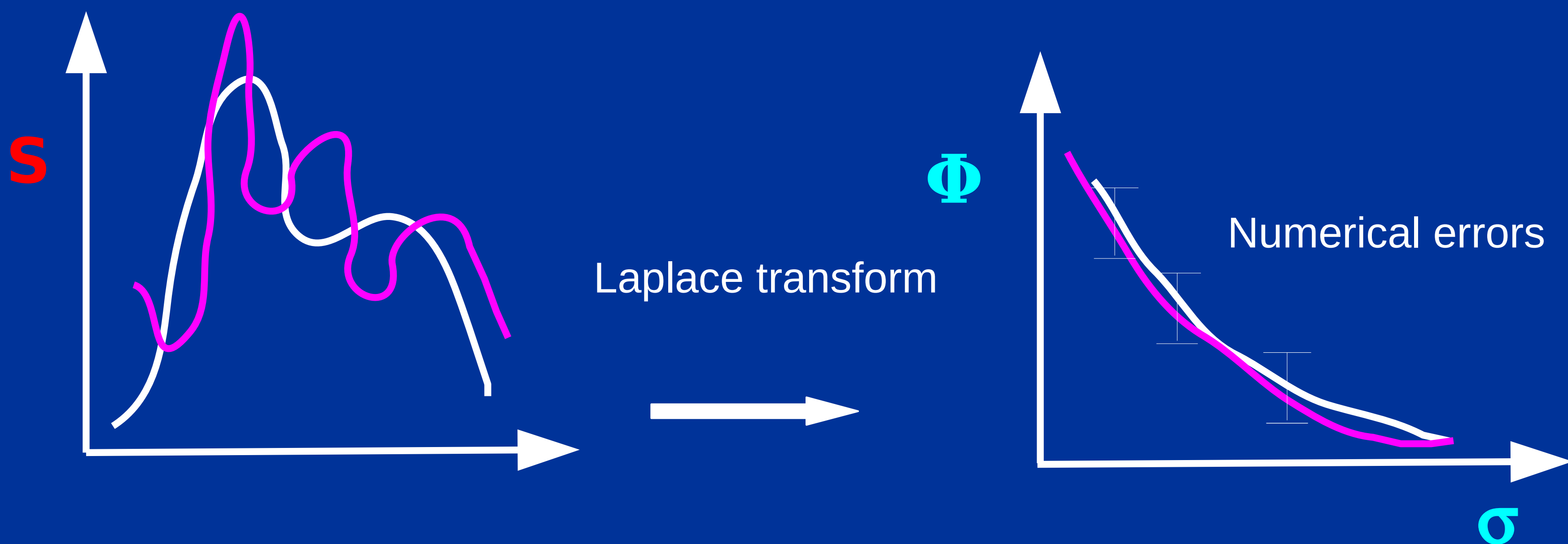
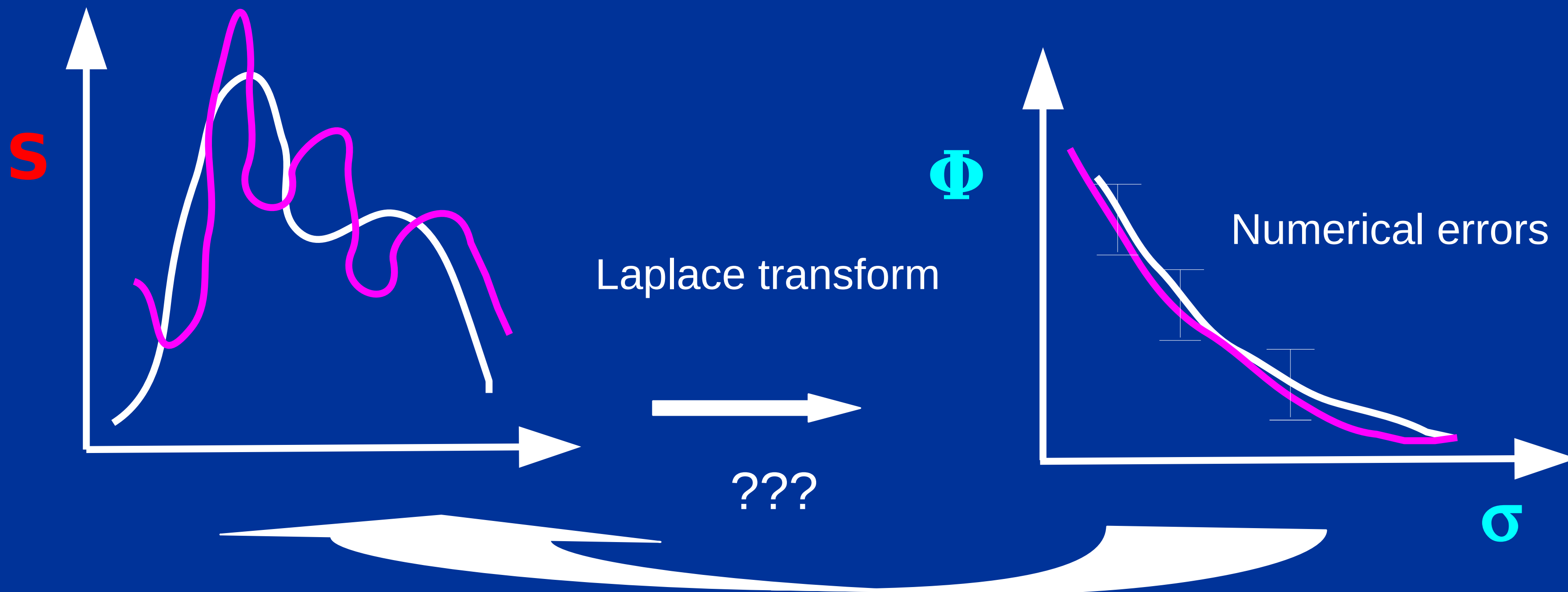


Illustration of the problem:



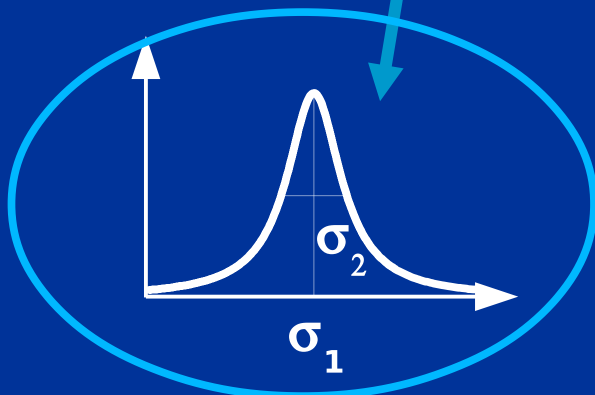
a **“good” Kernel** has to satisfy two requirements

1) one must be able to calculate the integral transform

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

The Lorentz kernel:

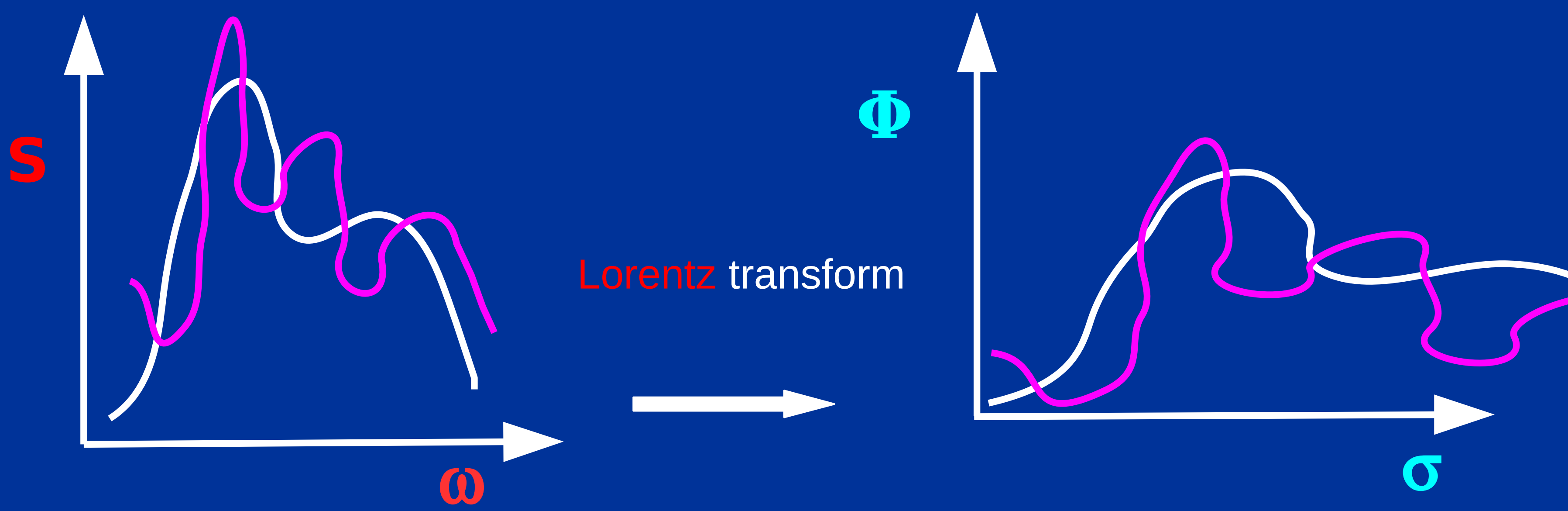
$$K(\omega, \sigma_1, \sigma_2) = [\,(\omega - \sigma_1)^2 + \sigma_2^{\,2}\,]^{-1}$$



It is a representation of the δ-Function !

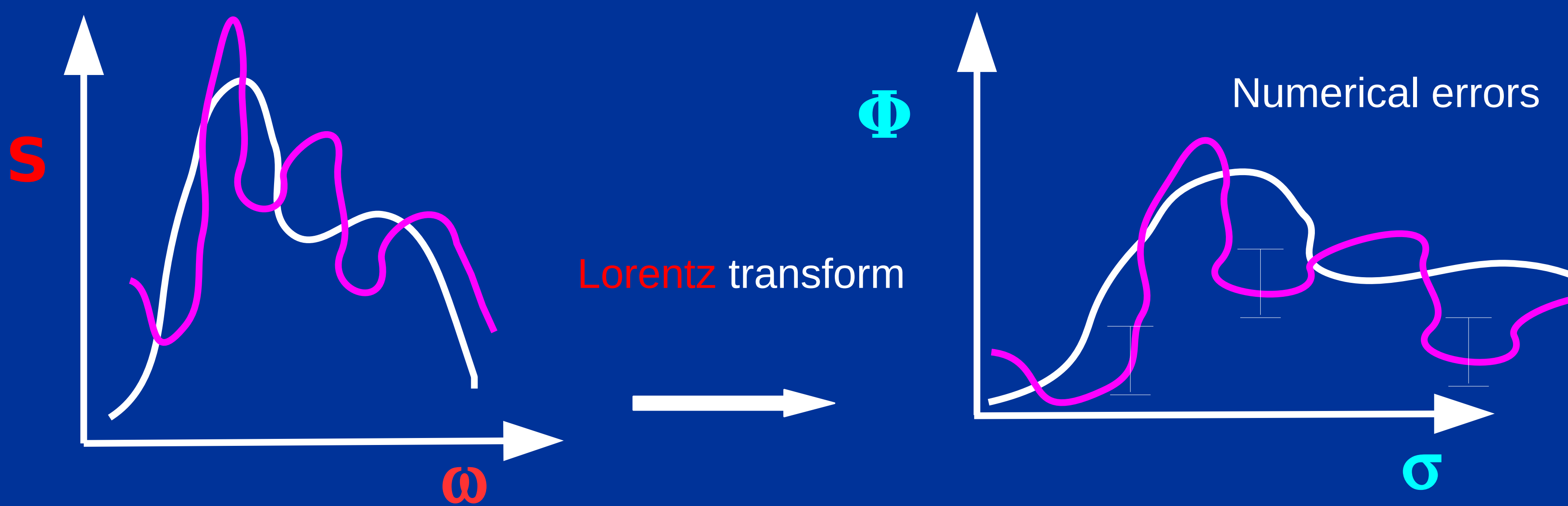
$$\Phi\,(\sigma_1,\sigma_2\,) = \int [(\omega - \sigma_1)^2 + \sigma_2^{\,2}\,]^{-1}\, S(\omega)\, d\omega$$

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



blurred, but still distinguishable

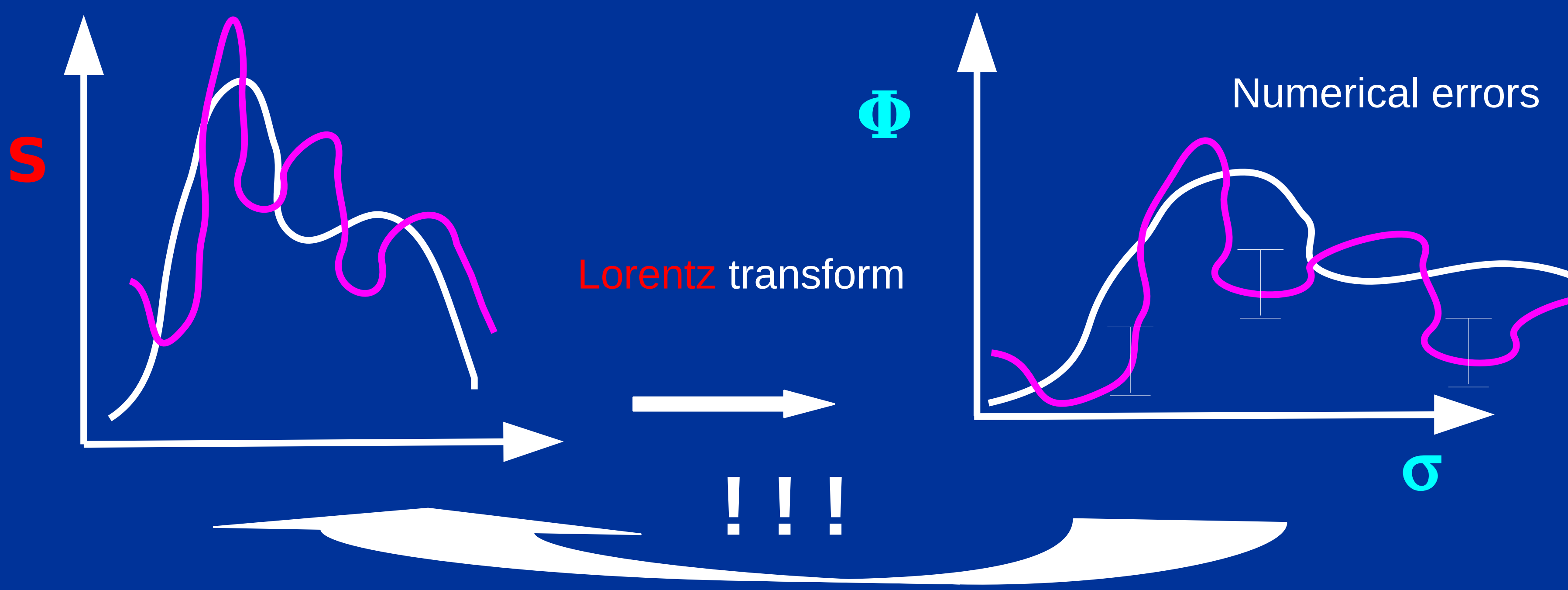
How can one easily understand why the inversion is **much less** problematic?



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



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

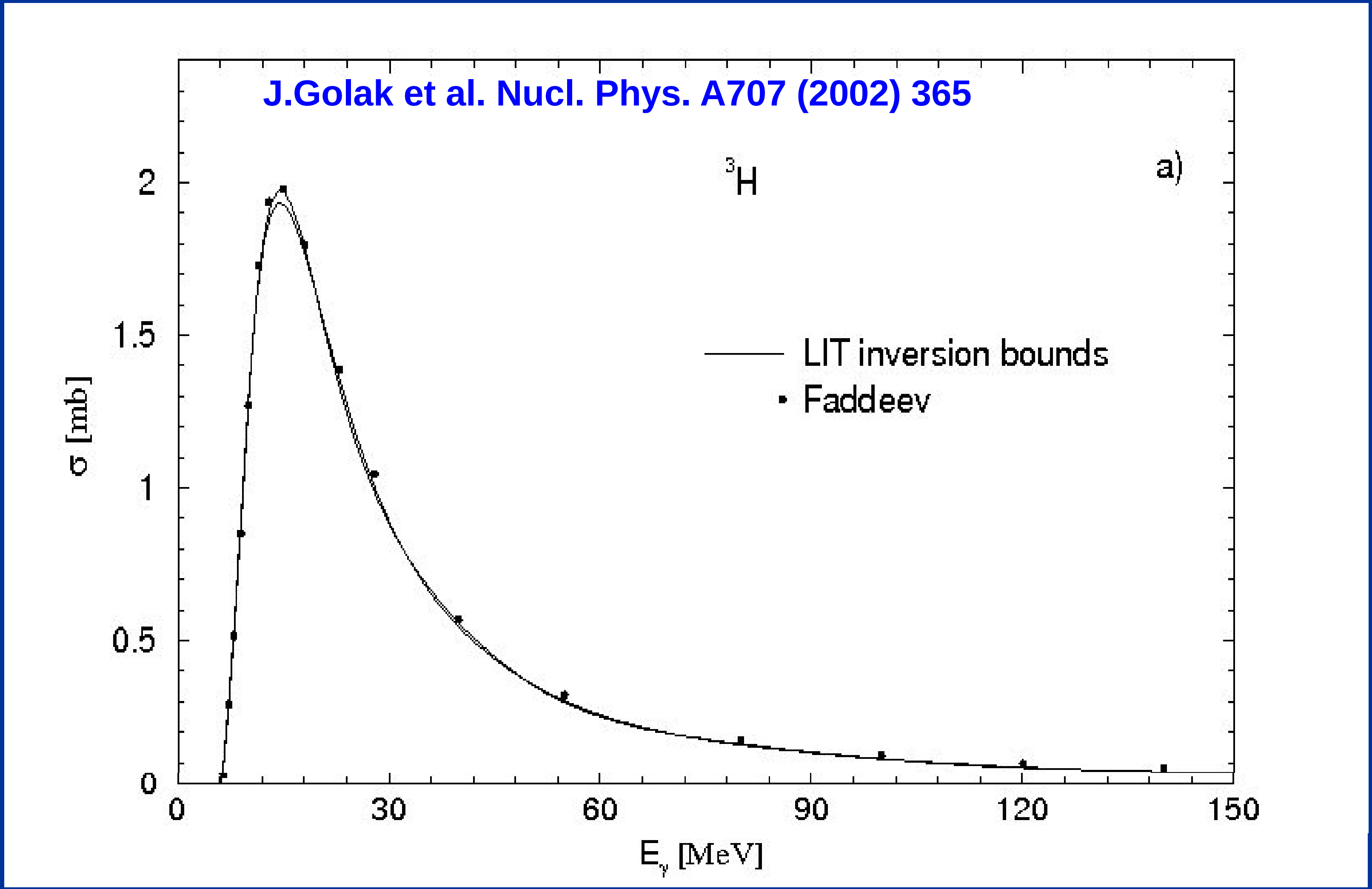
"Modern ab initio approaches and applications in few-nucleon physicswith A ≥ 4"

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

Some results with LIT:

Benchmark TEST on the Triton:

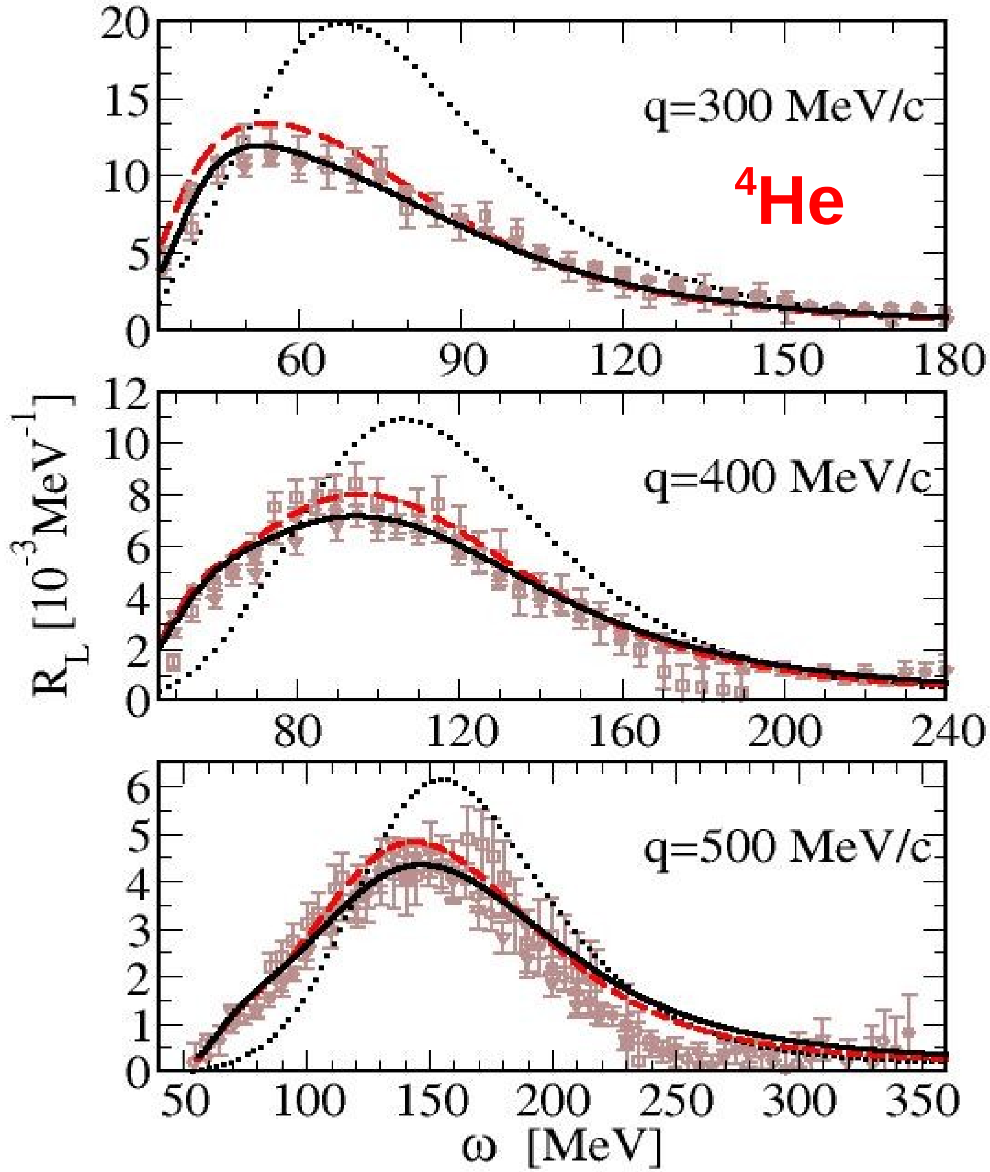
$S(\omega)$ is the Dipole Photoabsorption Cross Section



Ex. N.1:
Inclusive electron scattering cross section on ^{4}He (longitudinal channel)

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

Inclusive electron scattering cross section in the longitudinal channel



dotted: ***Plane Wave Impulse Approximation***

Dashed: 2-body force

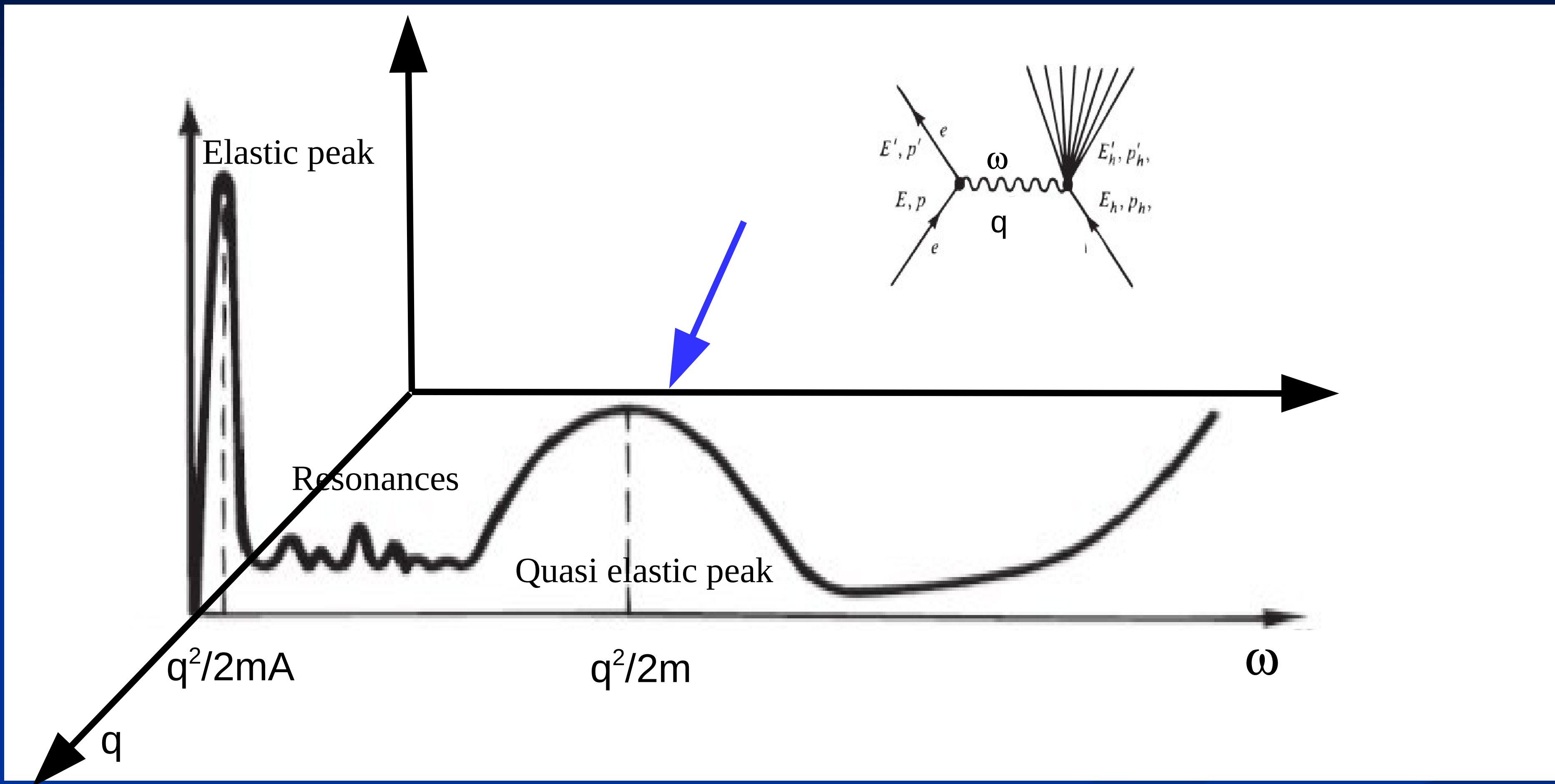
Full: 2+3-body force

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

Data: Saclay + Bates 1980's

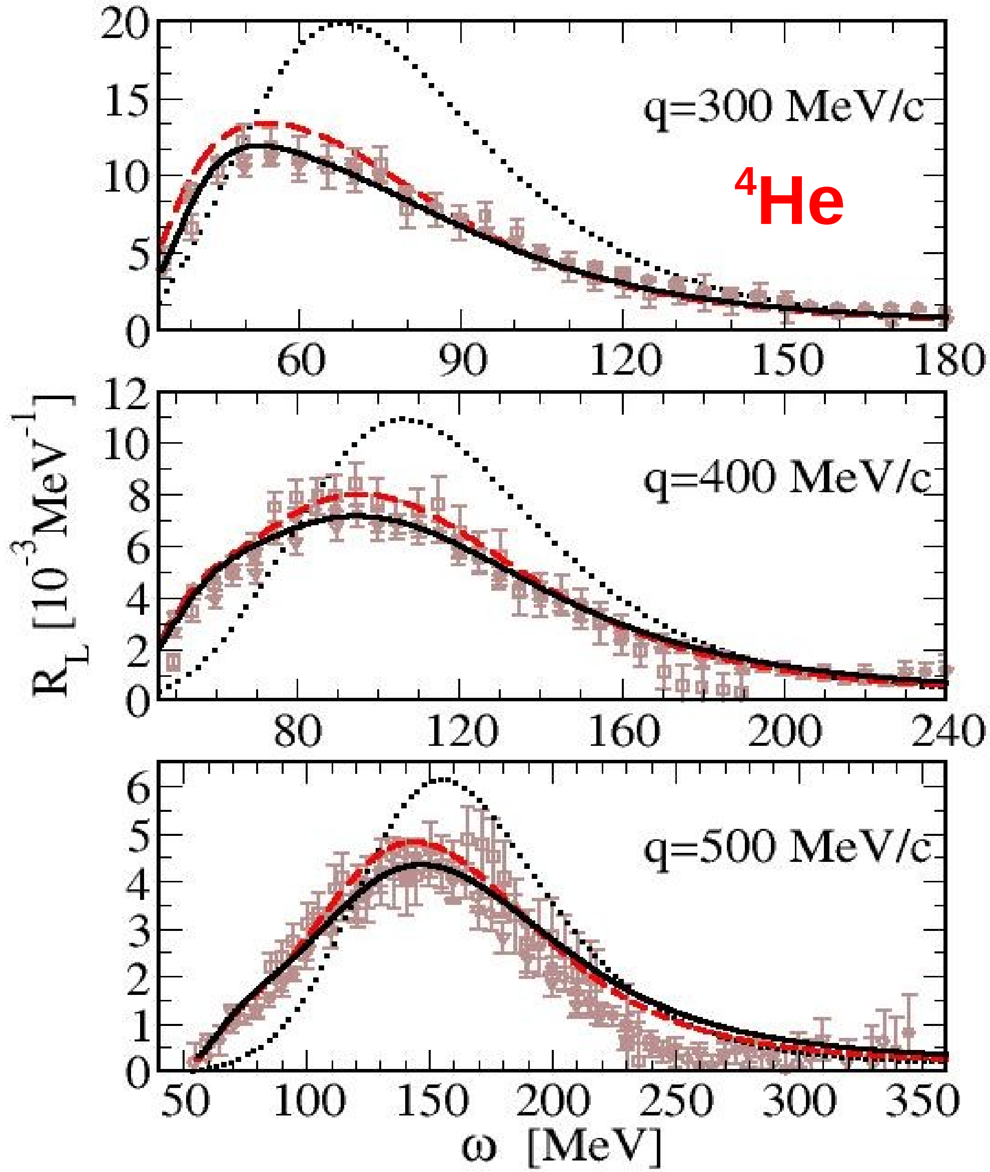
arXiv:0903.0605

Nuclear spectrum



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

Inclusive electron scattering cross section in the longitudinal channel



dotted:
Plane Wave Impulse Approximation

Dashed: 2-body force

Full: 2+3-body force

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

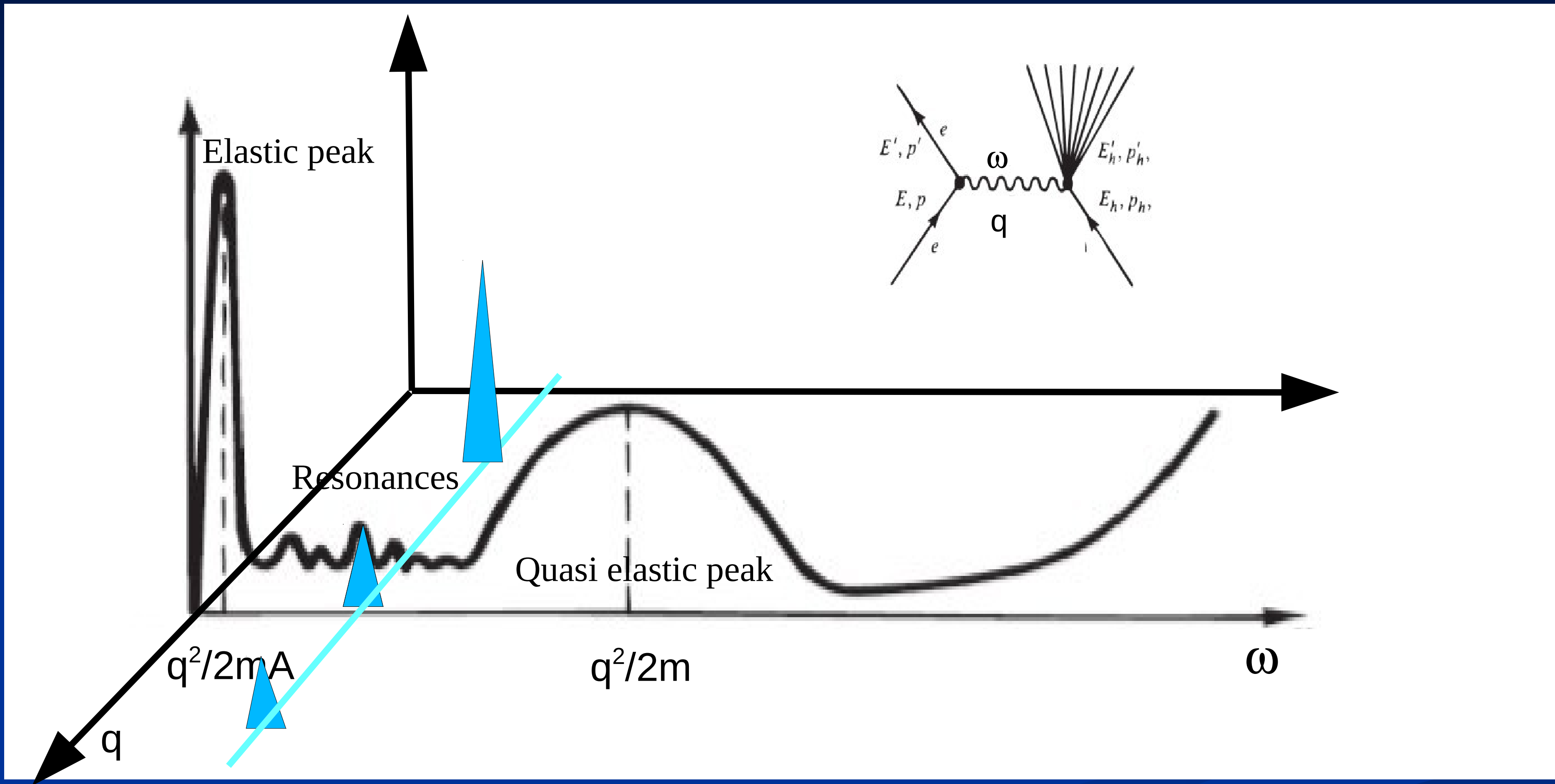
Data: Saclay + Bates 1980's

arXiv:0903.0605

Ex. N.2: Monopole excitation of ^{4}He by (e,e') or (α,α')

- Very narrow **0^+ resonance** in the continuum
- Transition form factor $F_{tr}(q)$ has been measured by (e,e') [(α,α') has been proposed]

Nuclear spectrum

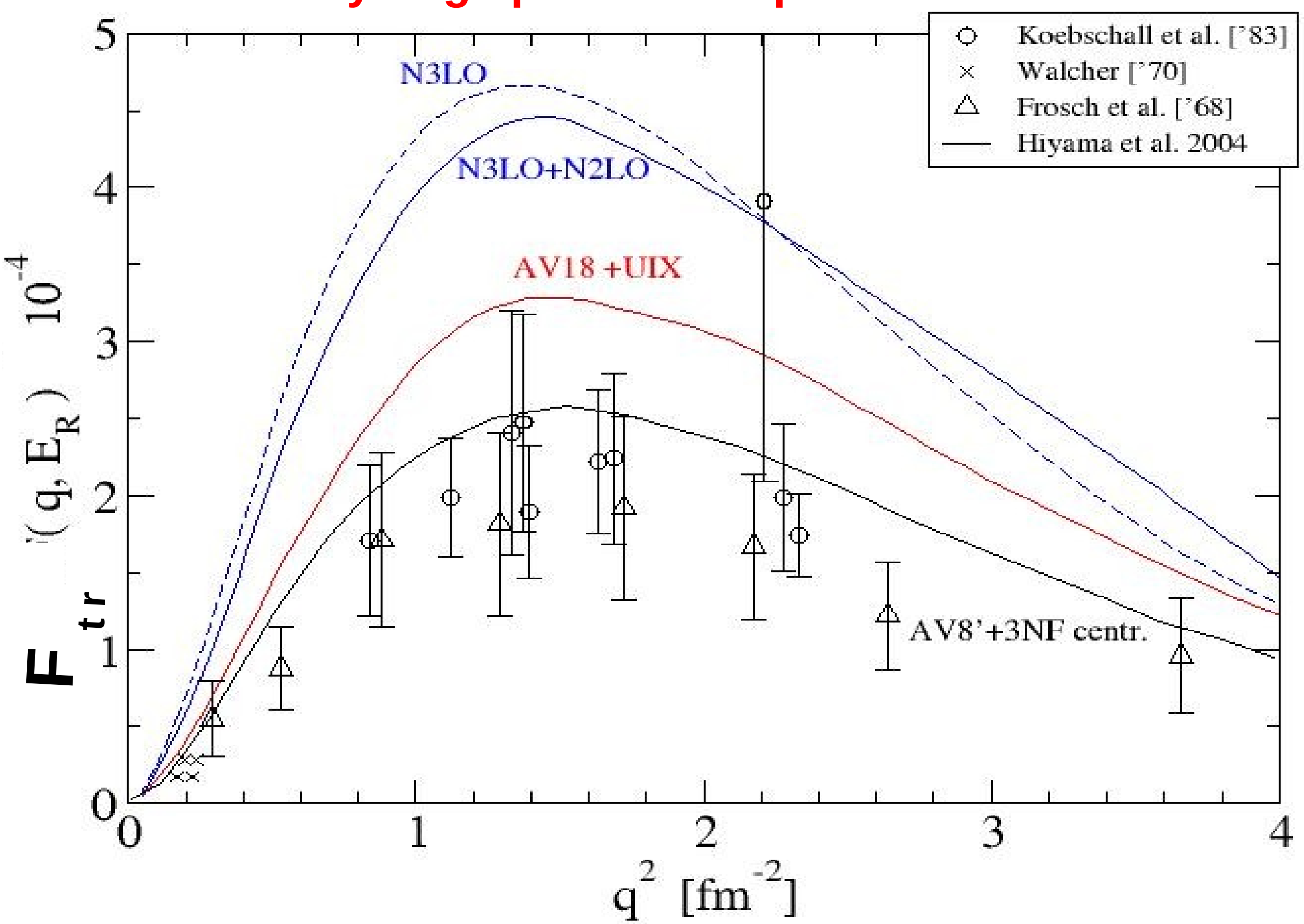


Ex. N.2: Monopole excitation of ^{4}He by (e,e') or (α,α')

- Very narrow **0^+ resonance** in the continuum
- Transition form factor $F_{tr}(q)$ has been measured by (e,e') [(α,α') has been proposed]
- Using IT method (**LIT**) coupled with **EIHH** b.s. method one can calculate $F_{tr}(q)$ (*separating resonance and background contributions!*)
- We find large potential dependence
- We find hints for a "breathing mode" interpretation

S.Bacca N.Barnea,W.Leidemann and G.O.et al. PRL 110 042503 (2013)

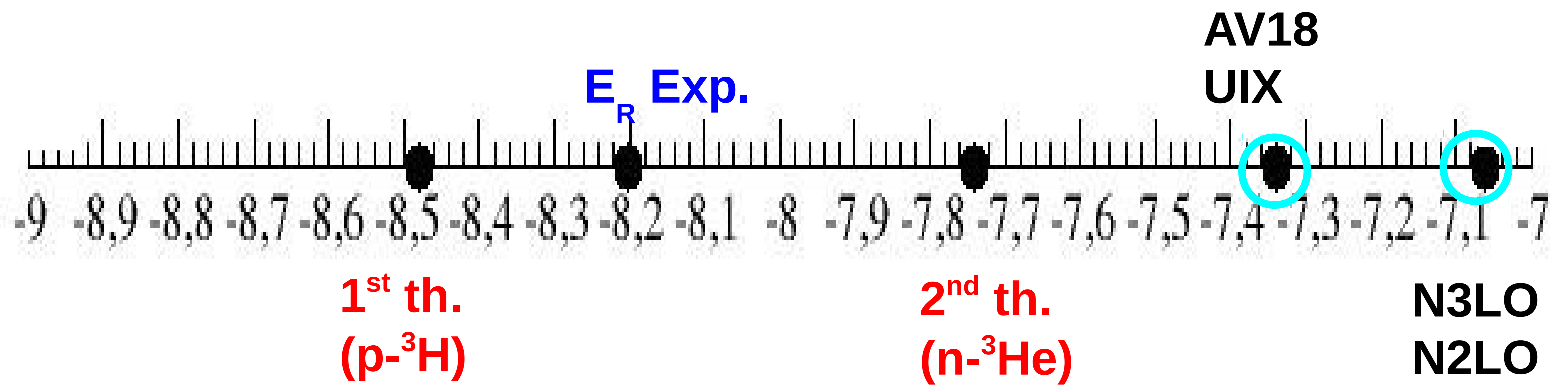
Very large potential dependence !!!



EIHH + LIT methods

Both phenomenological and EFT potentials
With and without 3-body forces

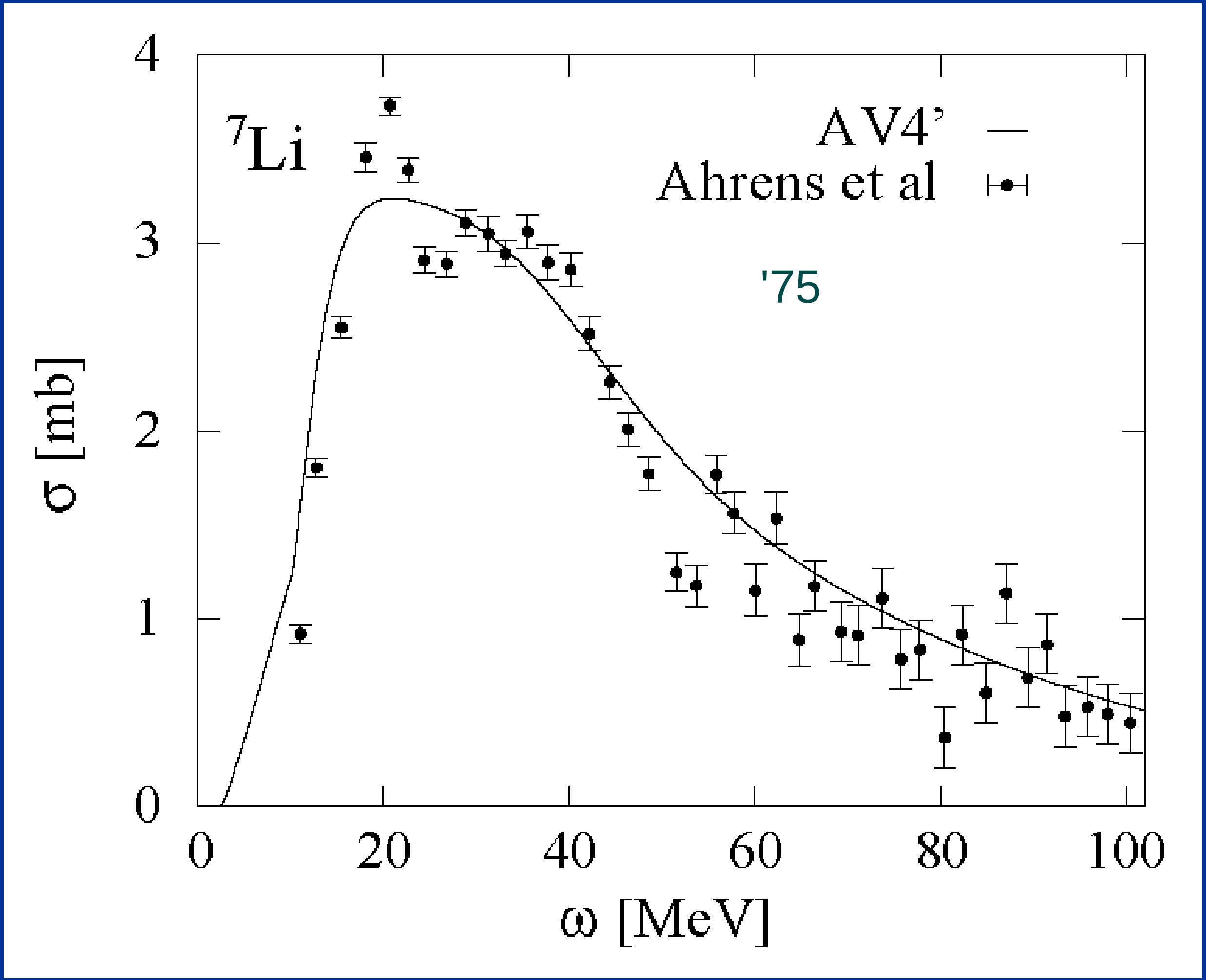
ENERGIES


AV18
UIX
E_R Exp.
-9 -8,9 -8,8 -8,7 -8,6 -8,5 -8,4 -8,3 -8,2 -8,1 -8 -7,9 -7,8 -7,7 -7,6 -7,5 -7,4 -7,3 -7,2 -7,1 -7
1st th.
(p-3H)
2nd th.
(n-3He)
N3LO
N2LO

Ex. N.3:
E1 cross sections & Dipole Polarizabilities

- existence of Giant Resonances of ^{4}He, ^{6}He, ^{6}Li, ^{7}Li, ^{16}O, ^{40}Ca … (recent and planned measurements of ^{22}O and ^{48}Ca)
- coupling the **LIT** method with bound state methods (**EIHH** and **CC)** one gets the results in the following slides:

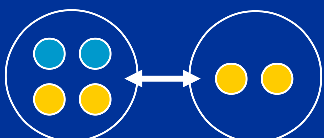
7-Body total photodisintegration with LIT method



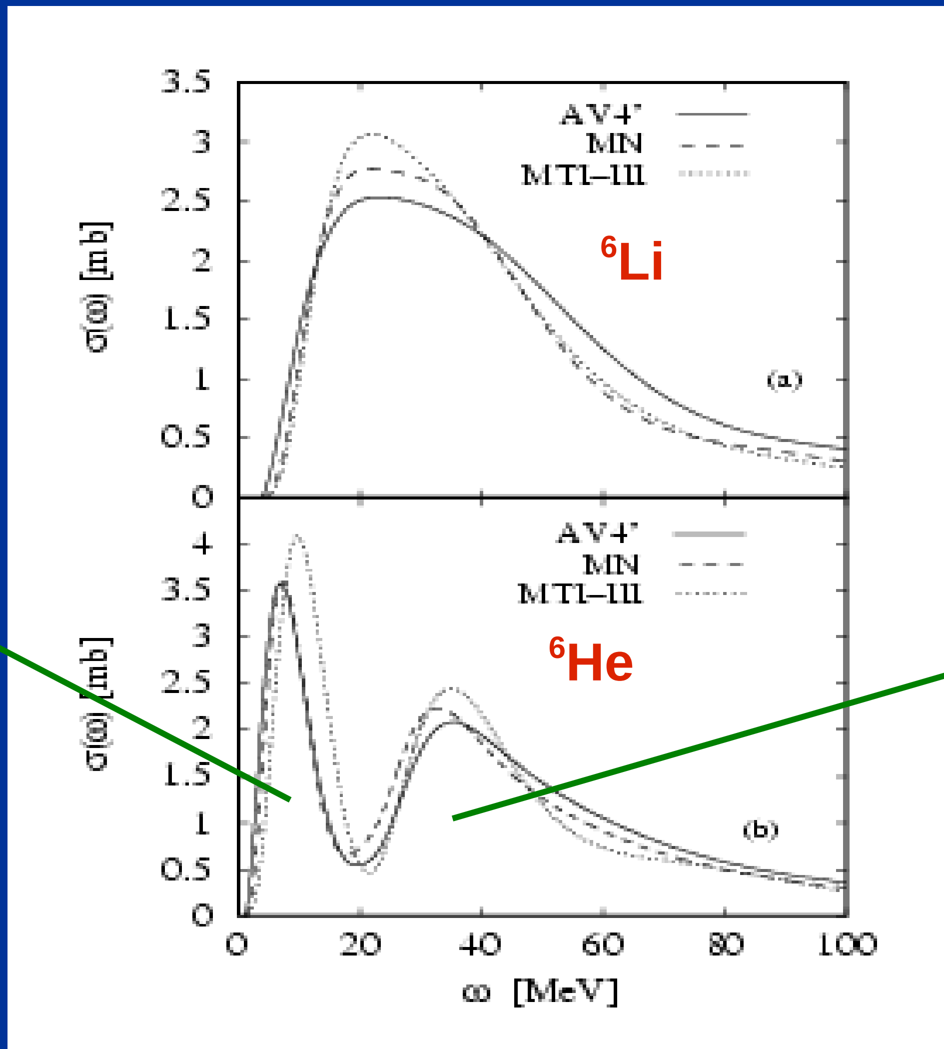
S.Bacca et al.
Phys.Lett. B603
(2004) 159-164

6-Body total photodisintegration

S.Bacca et al. PRL89(2002)052502

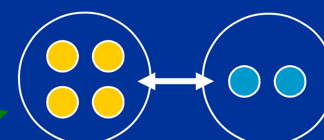


soft mode



Theory:

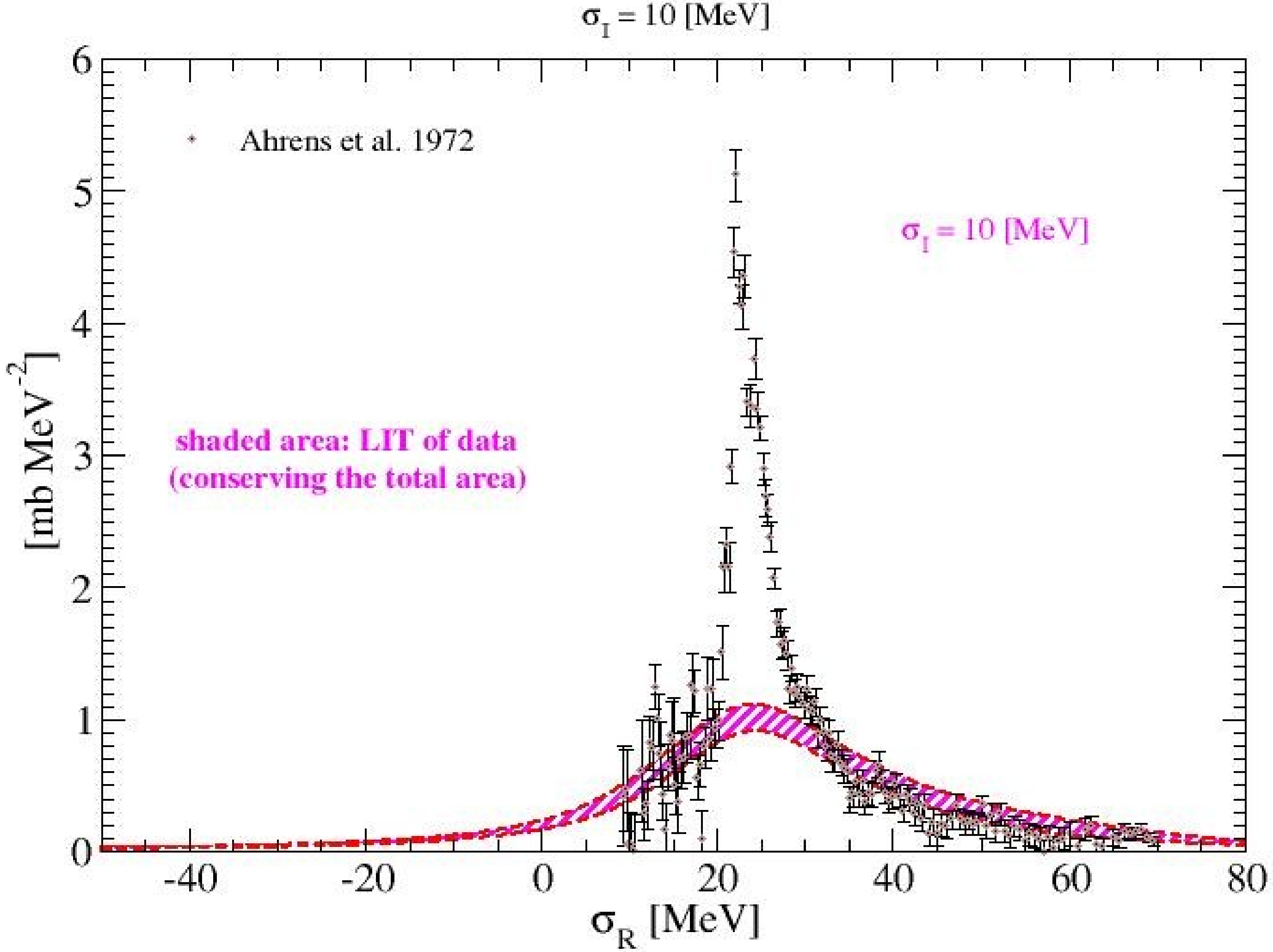
LIT+ EIHH

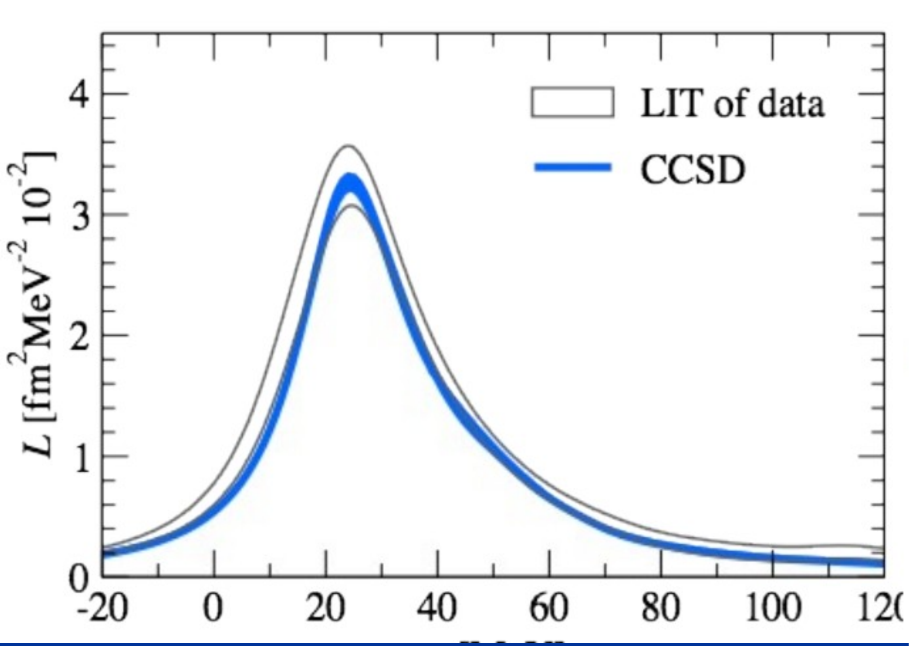


classical GT mode

Larger A?

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





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

LIT +CC(SD) methods

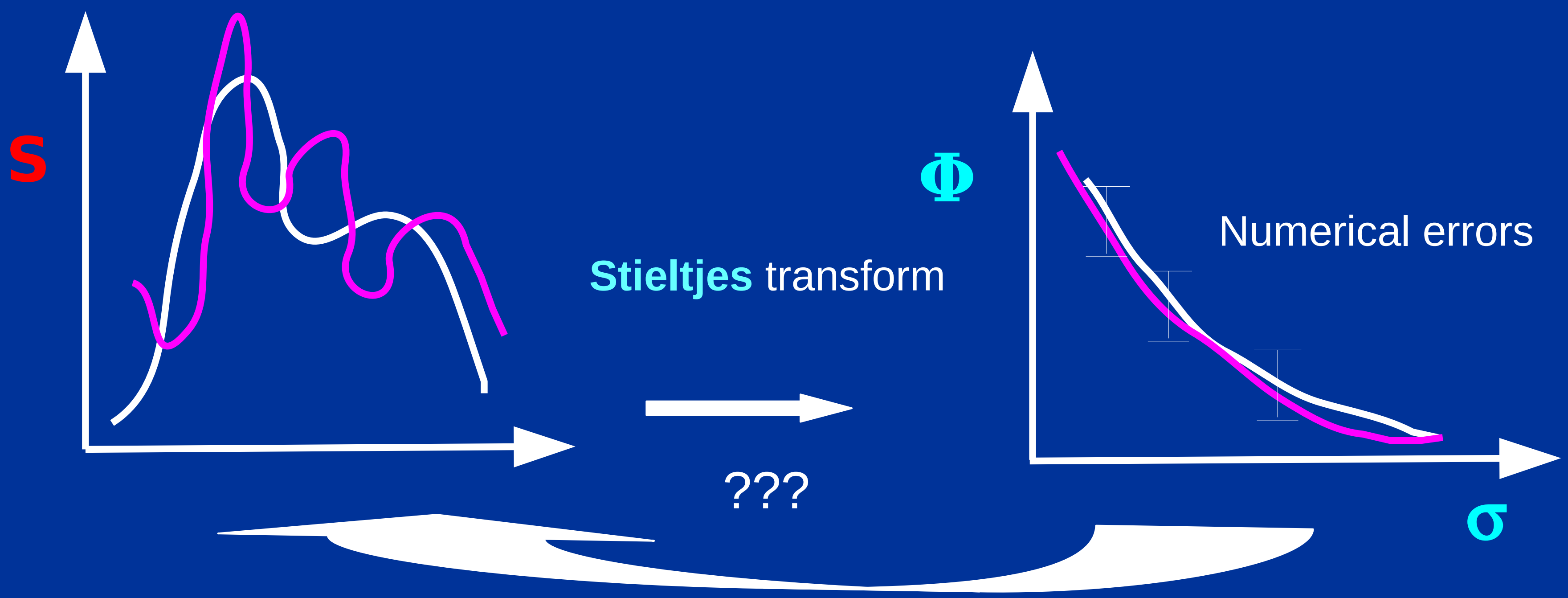
N3LO EFT 2-body potential only

Other Kernels?

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:

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

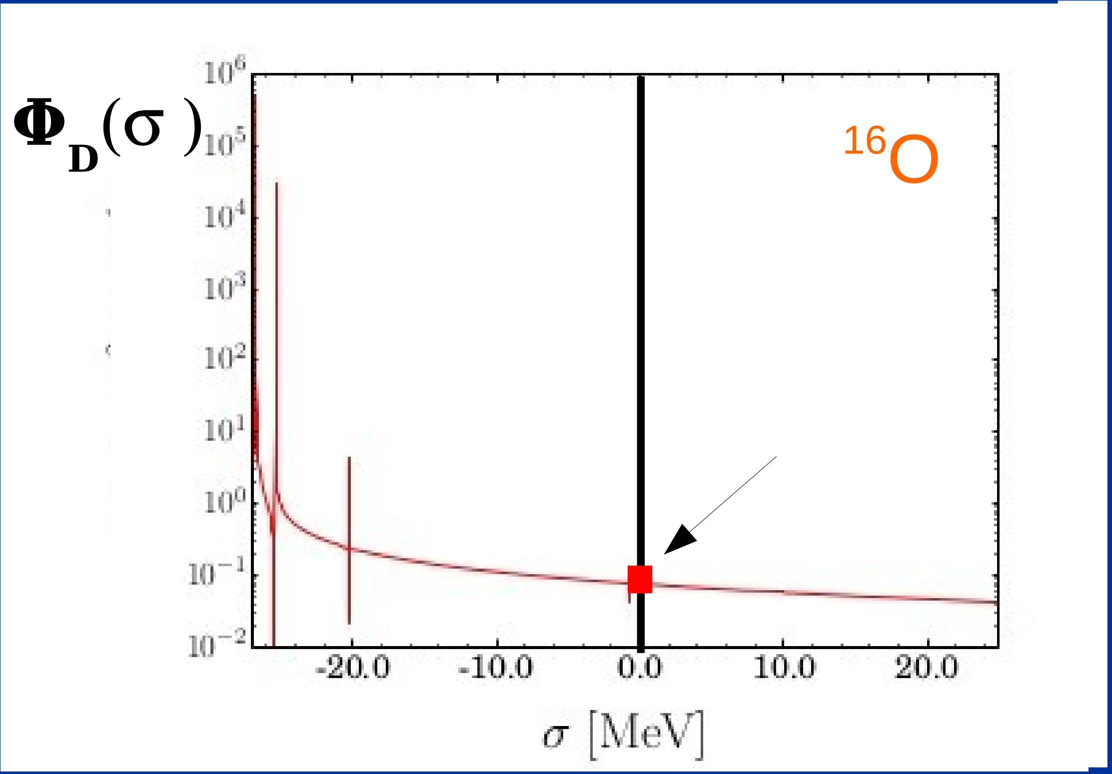
"generalized polarizability"

e.g. electric polarizability, magnetic susceptibility,

compressibility etc... depending on Θ

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

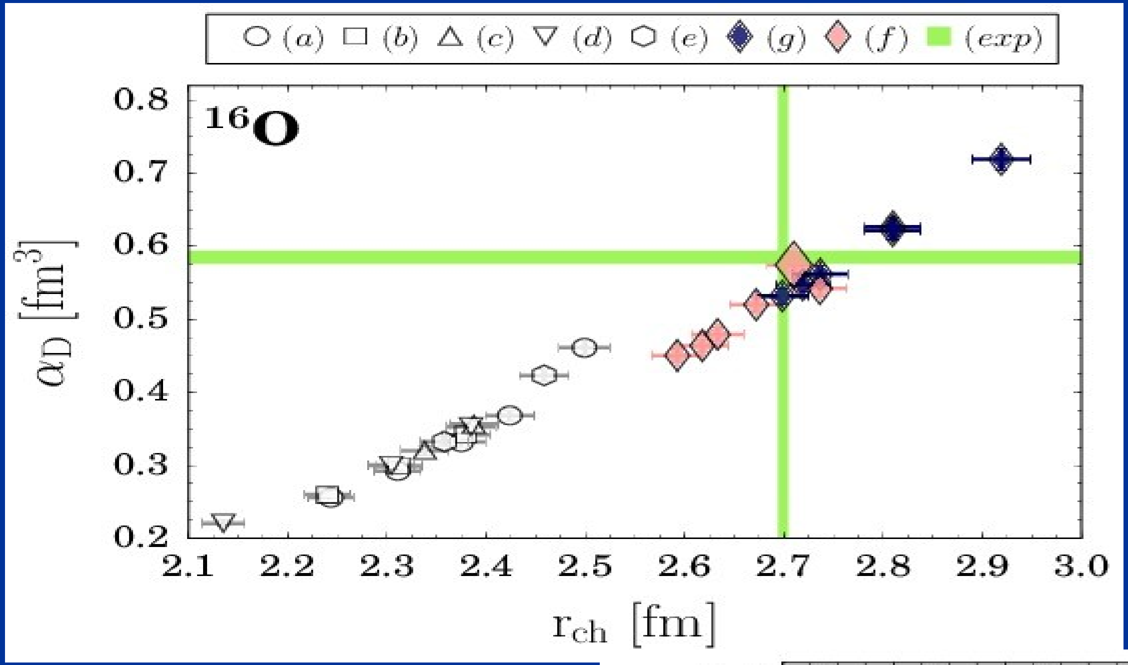
Electric Dipole Polarizability as limit of the Stieltjes transform for σ ---> 0



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

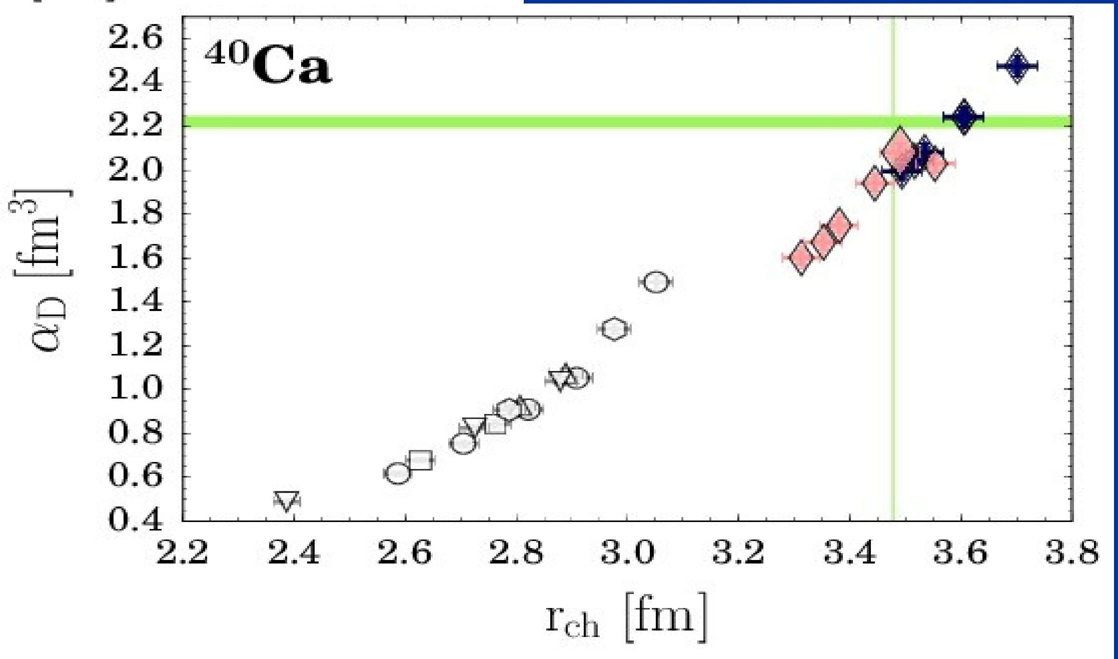
b.s. expansion: Coupled Cluster

(non hermitian) Lanczos diagonalization



Interesting correlation with the proton charge radius

Role of 3b-force



G. Hagen et al.
Nature Phys. 2016

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:

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

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

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:

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

$\nu/\mu = b/a$ $\quad\quad$ $\nu - \mu = \dfrac{\mathit{ln}\,[b] - \mathit{ln}\,[a]}{b - a}$ $\quad\quad$ $b > a > 0$ integer

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

A Transform with a kernel suitable for Monte Carlo methods:

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

combination of Sumudu kernels:

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

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

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)]

combination of Sumudu kernels:

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

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

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

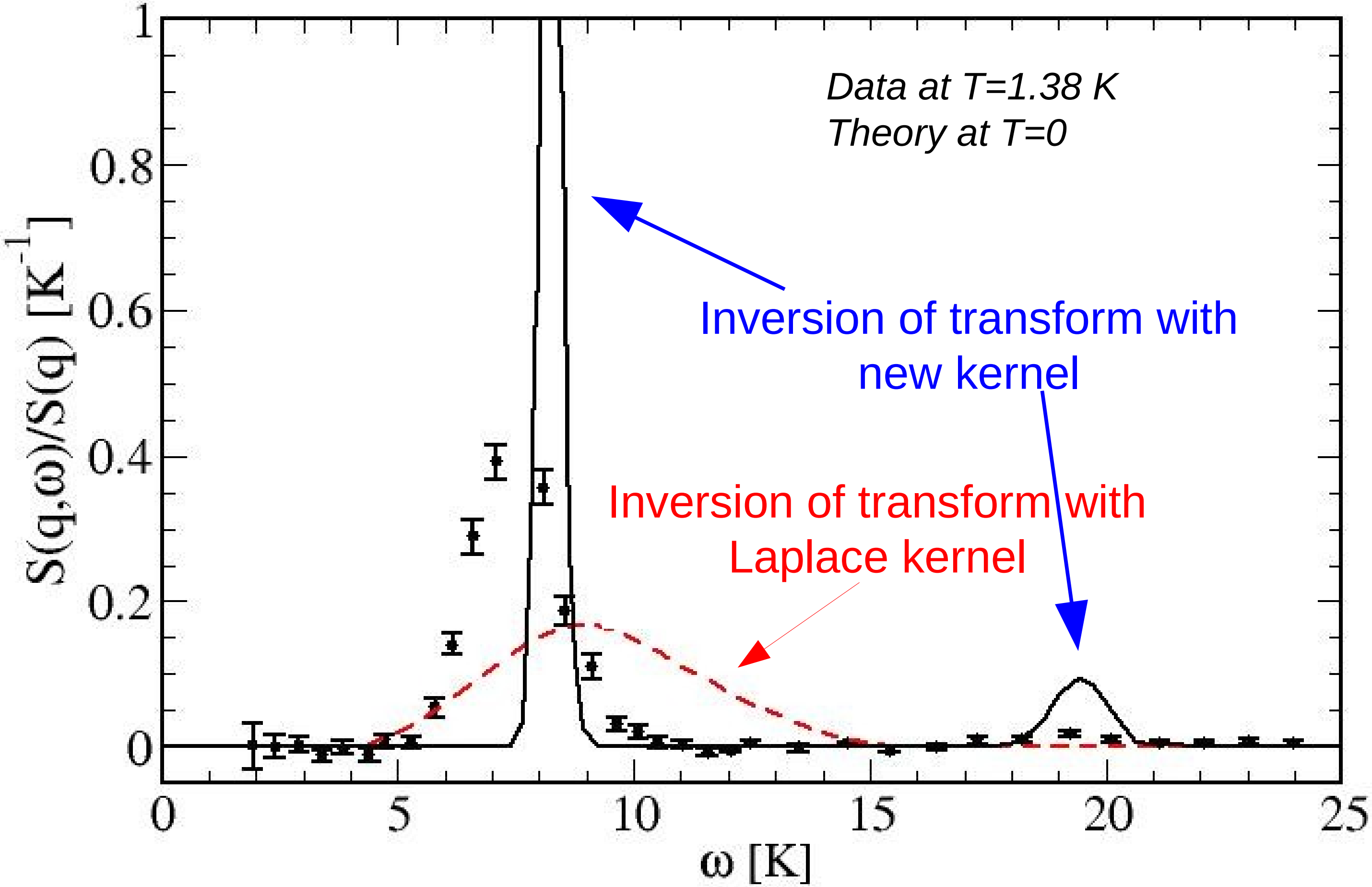
Small width ---> large P ---> **large** imaginary time

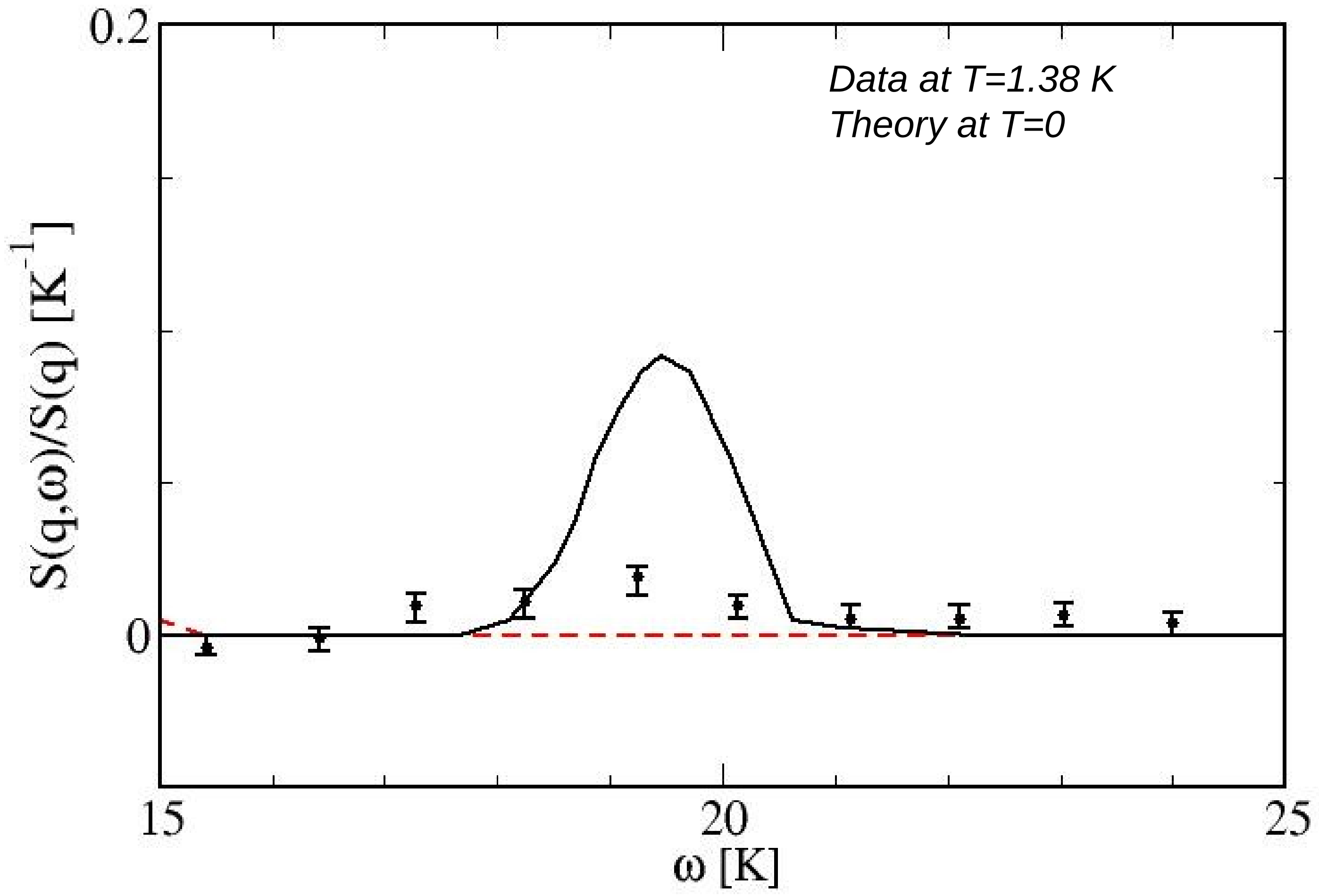
Bosonic system: Liquid Helium

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]

Summary:

- Ab initio few-body methods help building the bridge between QCD and nuclear phenomena
- They are moving from the traditional A=2,3 regime to larger systems
- IT methods are alternative approaches to overcome the many-body scattering problem

THANK YOU!