Electromagnetic properties of nuclei: from few- to many-body systems

Lecture 4

Integral Transforms

Sonia Bacca

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Lecture series for SFB 1245
TU Darmstadt

Inelastic processes

Because our most ambitious goal is to calculate em inelastic processes, we need to better understand what it entails and how one can approach the problem from a theoretical point of view

Reactions to continuum

Reactions to continuum

Non-perturbative (hadronic)

$$a + b \rightarrow c + d + \ldots$$

perturbative (electro-weak)

$$\gamma^{(*)} + b \rightarrow c + d + \ldots$$

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

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

- **Linear** Response theory

$$\gamma^{(*)} + b \rightarrow c + d + \ldots$$

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$R(\omega) \sim |\langle \psi_f | \Theta | \psi_0 \rangle|^2 \; \delta(\omega - E_f - E_0)$$

$$H|\psi_f\rangle = E_f|\psi_f\rangle$$

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

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$$R(\omega) \sim \quad |\langle\psi_f|\Theta|\psi_0\rangle|^2 \ \ \delta(\omega - E_f - E_0)$$

Energy transferred by the perturbative probe

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

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$$R(\omega) \sim |\langle\psi_f|\Theta|\psi_0\rangle|^2 \; \delta(\omega - E_f - E_0)$$

Ground state of the target
A-body bound state!

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$R(\omega) \sim |\langle \psi_f | \Theta | \psi_0 \rangle|^2 \ \delta(\omega - E_f - E_0)$$

Fragmented target
A-body continuum state!

$\gamma^{(*)} + b \rightarrow c + d + \ldots$

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$R(\omega) \sim |\langle\psi_f|\Theta|\psi_0\rangle|^2 \, \delta(\omega - E_f - E_0)$$

Operator responsible of the interaction of the target with the perturbative probe

NB: now we call Θ more in general,
Could be the charge, current, dipole operator

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$R(\omega) = \sum_f |\langle\psi_f|\Theta|\psi_0\rangle|^2 \;\; \delta(\omega - E_f - E_0)$$

Inclusive: summing on all possible final states

$$\sum_f |\psi_f\rangle\langle\psi_f| = 1$$

$$H|\psi_f\rangle = E_f|\psi_f\rangle$$

$\gamma^{(*)}$ + b → c + d or e+f or …

Reactions to continuum

Perturbative Inclusive Process

Inclusive response function

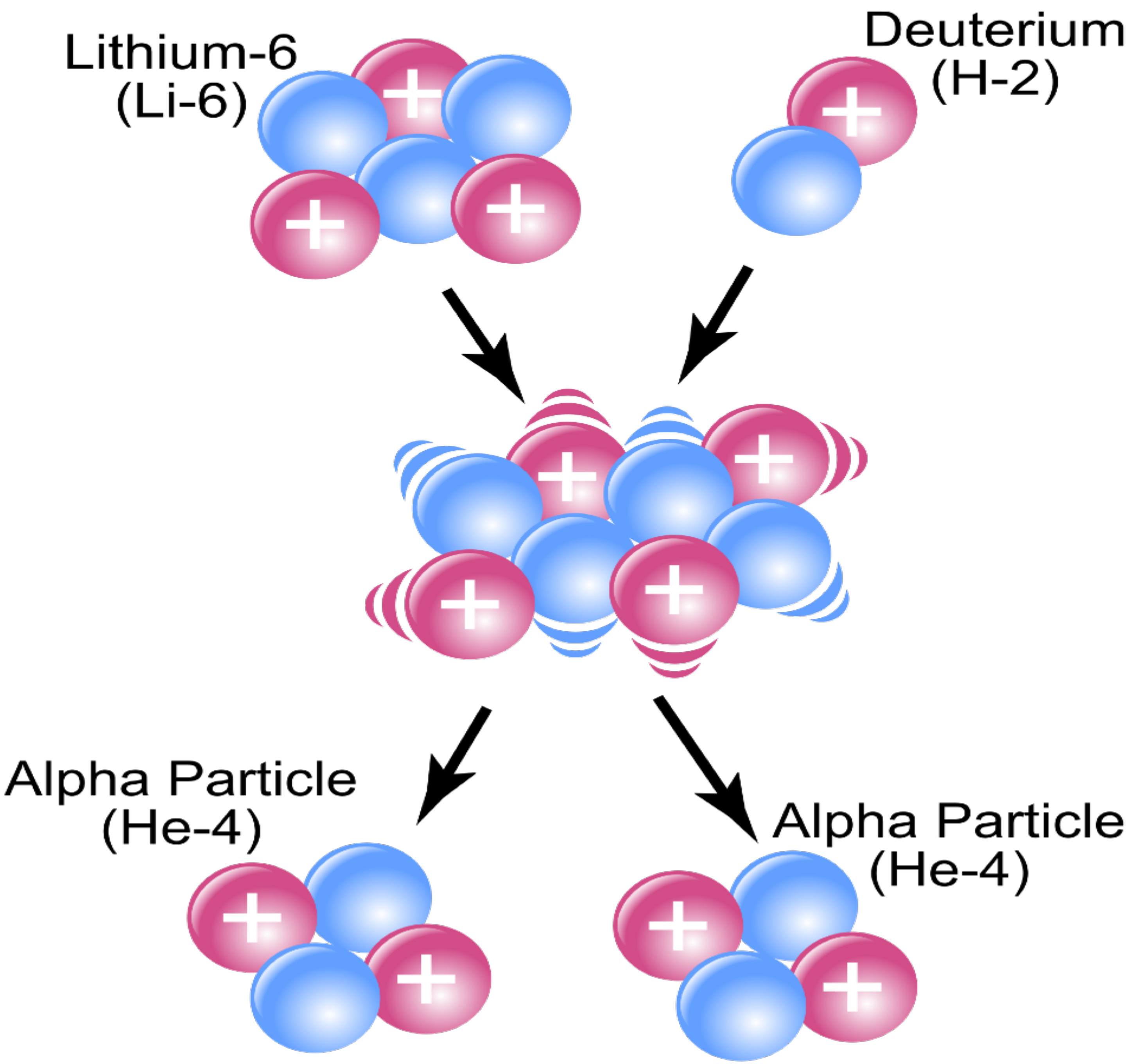
$$R(\omega) = \sum_f |\langle\psi_f|\Theta|\psi_0\rangle|^2 \; \delta(\omega - E_f - E_0)$$

$R(\omega)$ 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

Example



Lithium-6 – Deuterium Reaction

Reactions to continuum

Non-perturbative (hadronic)

a + b → c + d +...

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

Reactions to continuum

Non-perturbative (hadronic)

$$a + b \rightarrow c + d + \ldots$$

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

General form of the T-matrix

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

$$T_{\beta\alpha}(E) = \langle \chi_\beta V_\alpha \chi_\alpha \rangle + \langle \chi_\beta V_\beta (E - H + i\eta)^{-1} V_\alpha \chi_\alpha \rangle$$

A-body continuum energy

Reactions to continuum

Non-perturbative (hadronic)

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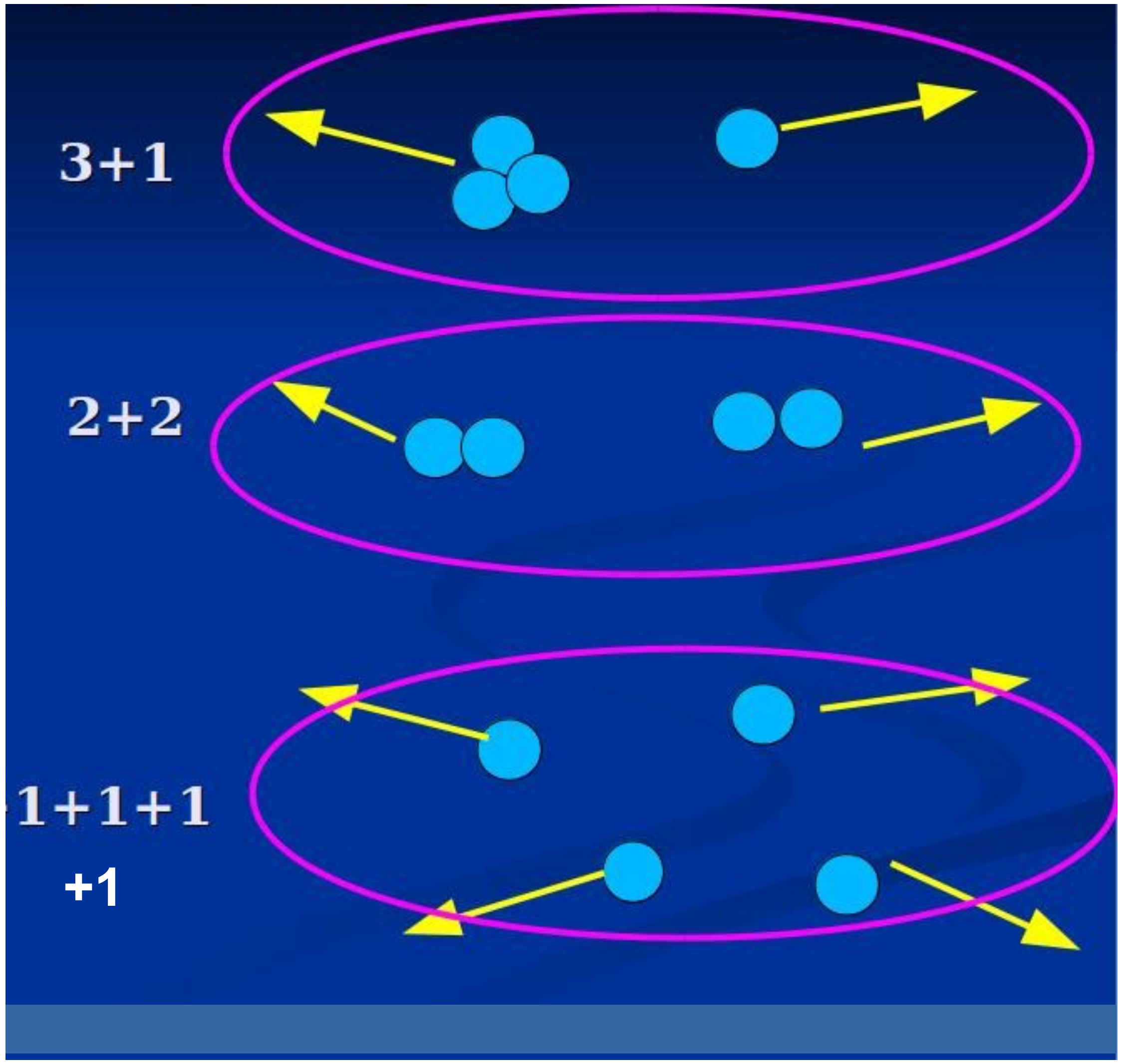
$$T_{\beta\alpha}(E) = \langle \chi_\beta V_\alpha \chi_\alpha \rangle + \langle \chi_\beta V_\beta (E - H + i\eta)^{-1} V_\alpha \chi_\alpha \rangle$$

χ_β 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

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

Channels

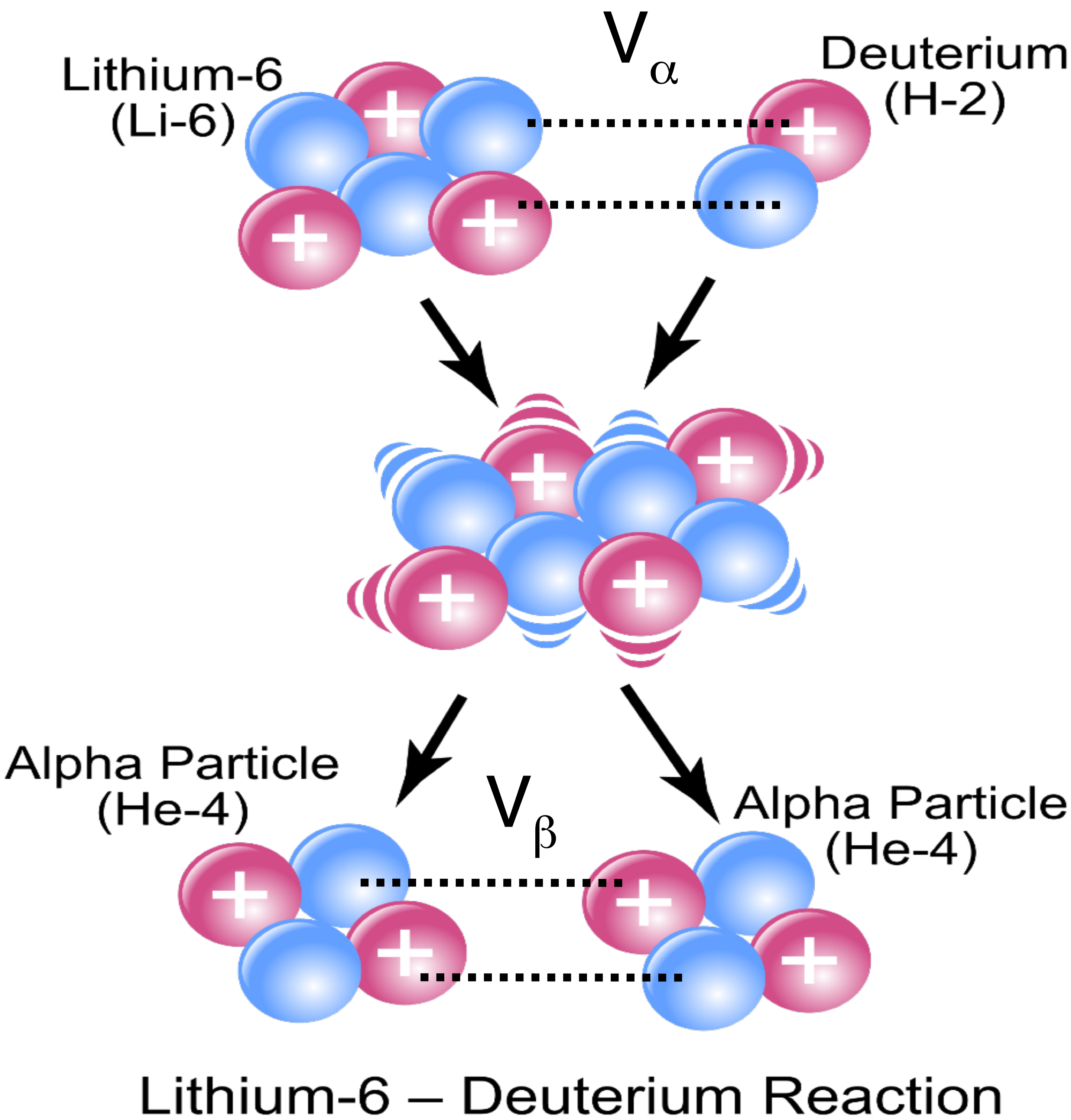
A=4



As A increases, there will be more channels…

Example

H **is the Hamiltonian of the 8-body system**



T-matrix

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

"easier" part

Very difficult part

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

If we denote $V_{\alpha,\beta} \, \chi_{\alpha,\beta} = \phi_{\alpha,\beta}$

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

Rearranging difficult part

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

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

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

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

Step 2) Insert **delta function**

$$= \int d\omega \sum_f \delta(\omega - E_f) (E - \omega + i\eta)^{-1} < \phi_\beta | f > < f | \phi_\alpha > =$$

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

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

$$F_{\beta\alpha}(\omega) = \sum_f \delta(\omega - E_f) < \phi_\beta | f > < f | \phi_\alpha >$$

Reactions to continuum

Non-perturbative (hadronic)

$$F_{\beta,\alpha}(\omega) = \sum_f \delta(\omega - E_f) \langle \phi_\beta | \psi_f \rangle \langle \psi_f | \phi_\alpha \rangle$$

perturbative (electro-weak)

$$R(\omega) = \sum_f \delta(\omega - E_f - E_0) \langle \psi_0 | \Theta^\dagger | \psi_f \rangle \langle \psi_f | \Theta | \psi_0 \rangle$$

$|\psi_0\rangle, |\phi_\alpha\rangle, |\phi_\beta\rangle$ A-body bound-states

$\Phi_\alpha = V_\alpha \, \chi_\alpha = V_\alpha \, \mathcal{A} \, |a\rangle \, |b\rangle \, |PW\rangle$

Reactions to continuum

Non-perturbative (hadronic)

$$F_{\beta,\alpha}(\omega) = \sum_f \delta(\omega - E_f) \langle \phi_\beta | \psi_f \rangle \langle \psi_f | \phi_\alpha \rangle$$

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$|\psi_f\rangle$ A-body bound-states and continuum states

Ab-initio methods

Most representative approaches

	Few-body: A≲12	Many-body: 12≲A≲40 or more
Structure Bound states	• *Faddeev Yakubowski (FY)* • **Diagonalization methods** *(on different basis)* • *Green Function Monte Carlo*	• *Coupled Cluster (CC)* • *Other Monte Carlo methods* • *IMSRG* • *Self consistent Green's function*
Reactions scattering states		

A=4

In the sector of the typical few-body nuclei (A up to 4) we have reached an incredible level of accuracy!

Same ingredients

m_p, m_n, T, V

Different numerical methods

Same output

PRC 64 (2001) 044001 → Important milestone ~ 200 citations

Method	$\langle T \rangle$	$\langle V \rangle$	E_0	$\sqrt{\langle r^2 \rangle}$
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

E_0 of ^{4}He (exp. -28.296 MeV); Three-nucleon forces were not used in the benchmark

Some examples

No core shell model

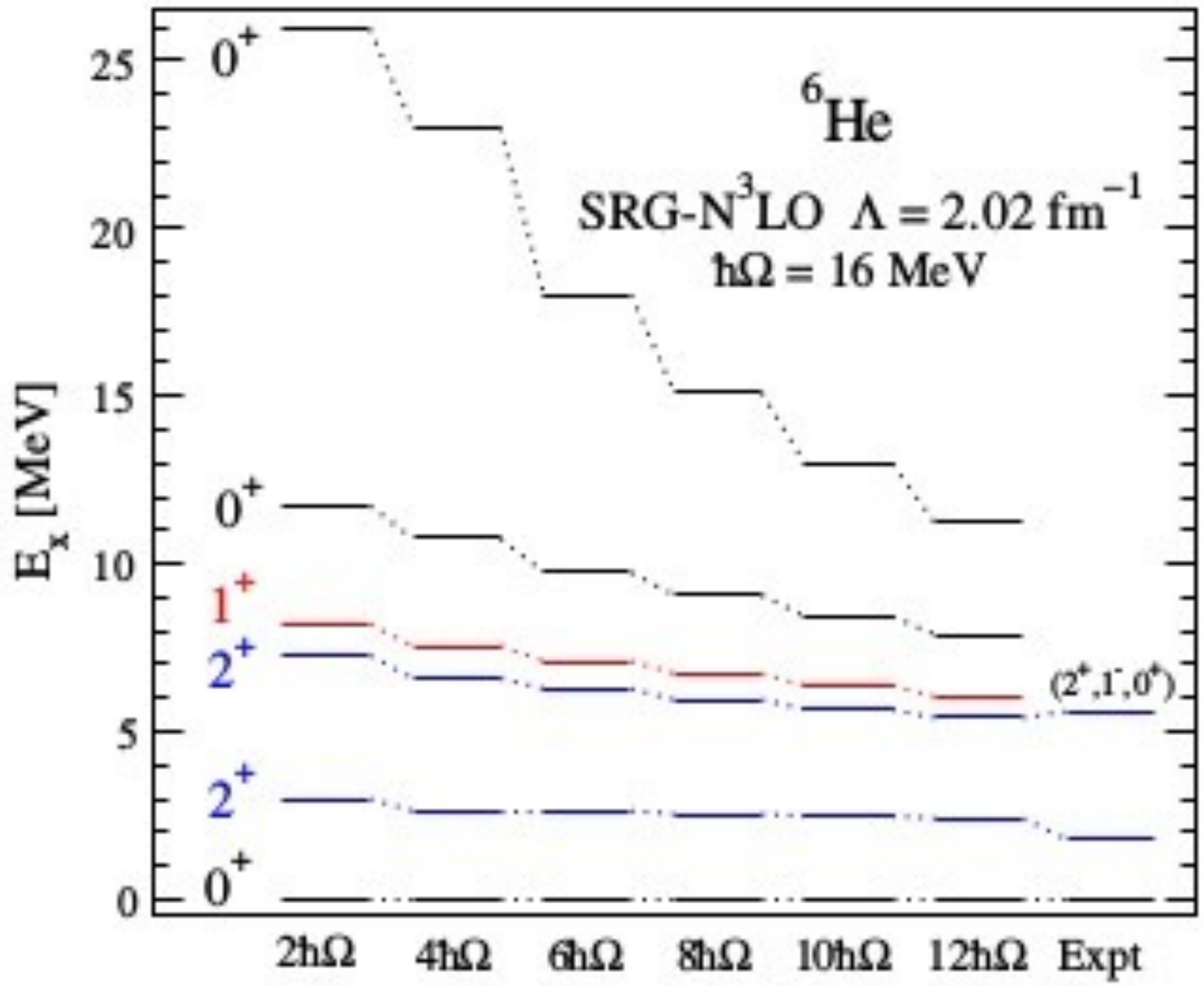
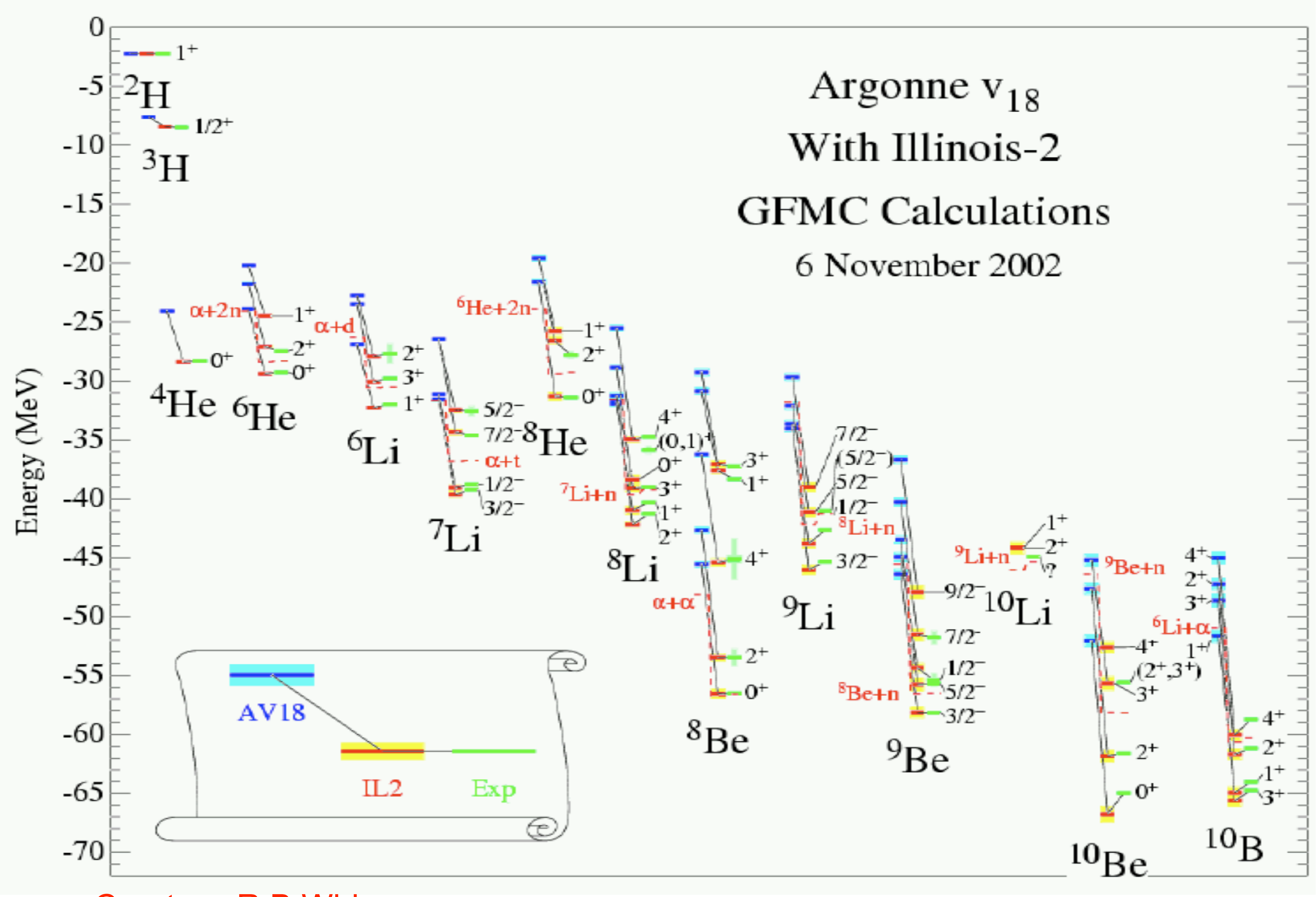


FIG. 1 (color online). Dependence of ^{6}He excitation energies on the size of the HO basis $N_{max}\hbar\Omega$.

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

Some examples

Quantum Monte Carlo Method



Courtesy R.B.Wiringa

Ab-initio methods

Most representative approaches

	Few-body: $A \lesssim 12$	Many-body: $12 \lesssim A \lesssim 40$ or more
Structure Bound states	• *Faddeev Yakubowski (FY)* • **Diagonalization methods** *(on different basis)* • *Green Function Monte Carlo*	• *Coupled Cluster (CC)* • *Other Monte Carlo methods* • *IMSRG* • *Self consistent Green's function*
Reactions scattering states	• *Faddeev Yakubowski (FY) and variations* • *HH Kohn-Variational P. (2 fragments)* • *NCSMC (only at very low energy)*	

Why are there so few methods for reactions?
Why are they limited to low-energy?

Scattering many-body problem

In configuration space
(Schrödinger equation)

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

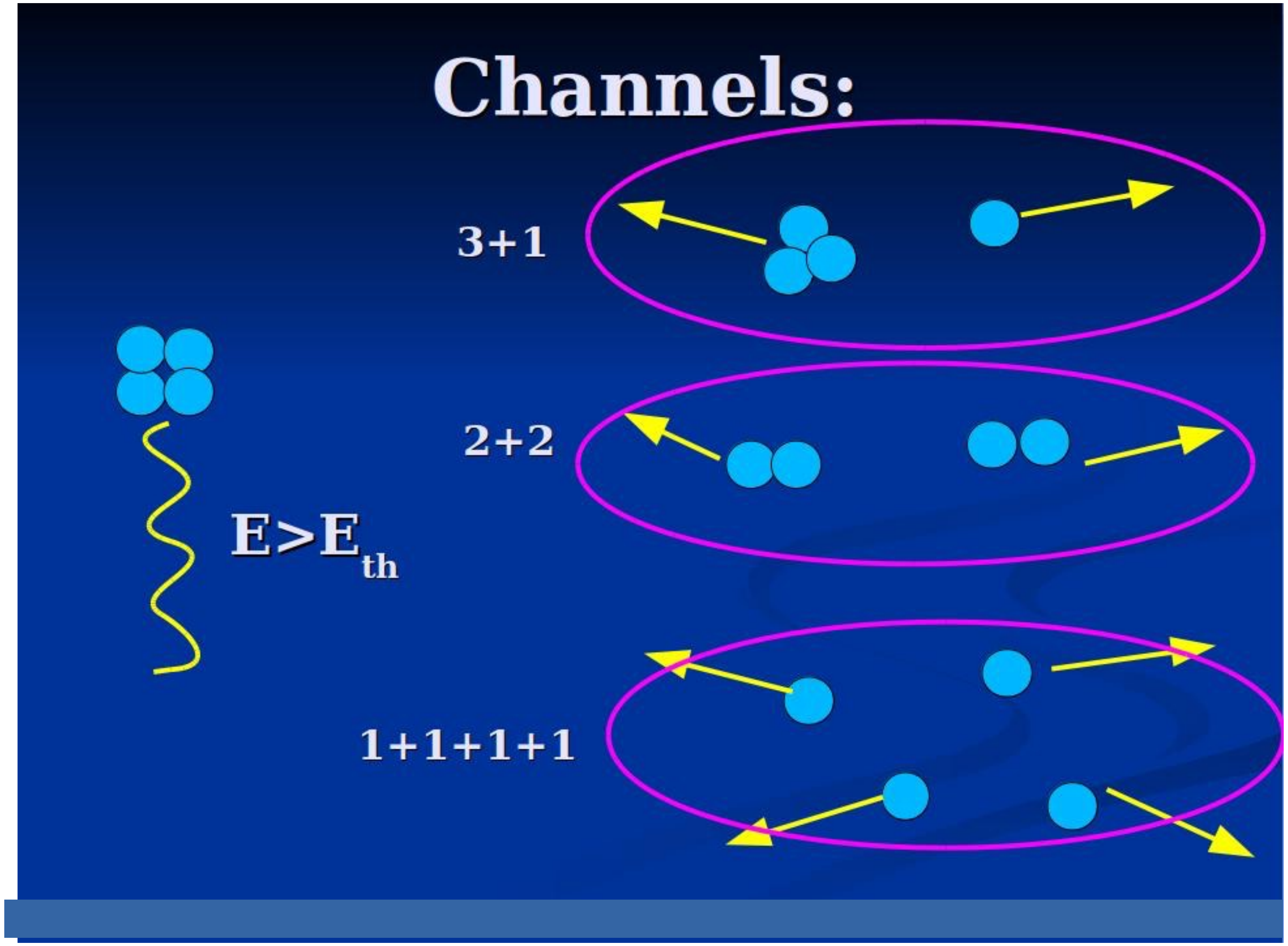
Scattering many-body problem

In momentum space
(Lippmann-Schwinger equation)

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

Scattering many-body problem

Even before reaching the asymptotic condition all channels are coupled



Today

- Faddeev: solved for scattering states for A=3 (1+2, 1+1+1)
- Faddeev-Yakubovsky: 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)
- Also some first results on A=5 (Lazauskas)

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

- Alternative approach to 2+1, 3+1 scattering based on Kohn variational principle and correct asymptotic conditions

Pisa School: Kievsky, Viviani, Marcucci...

- Similar idea for (A-1) + 1 in NCSMC

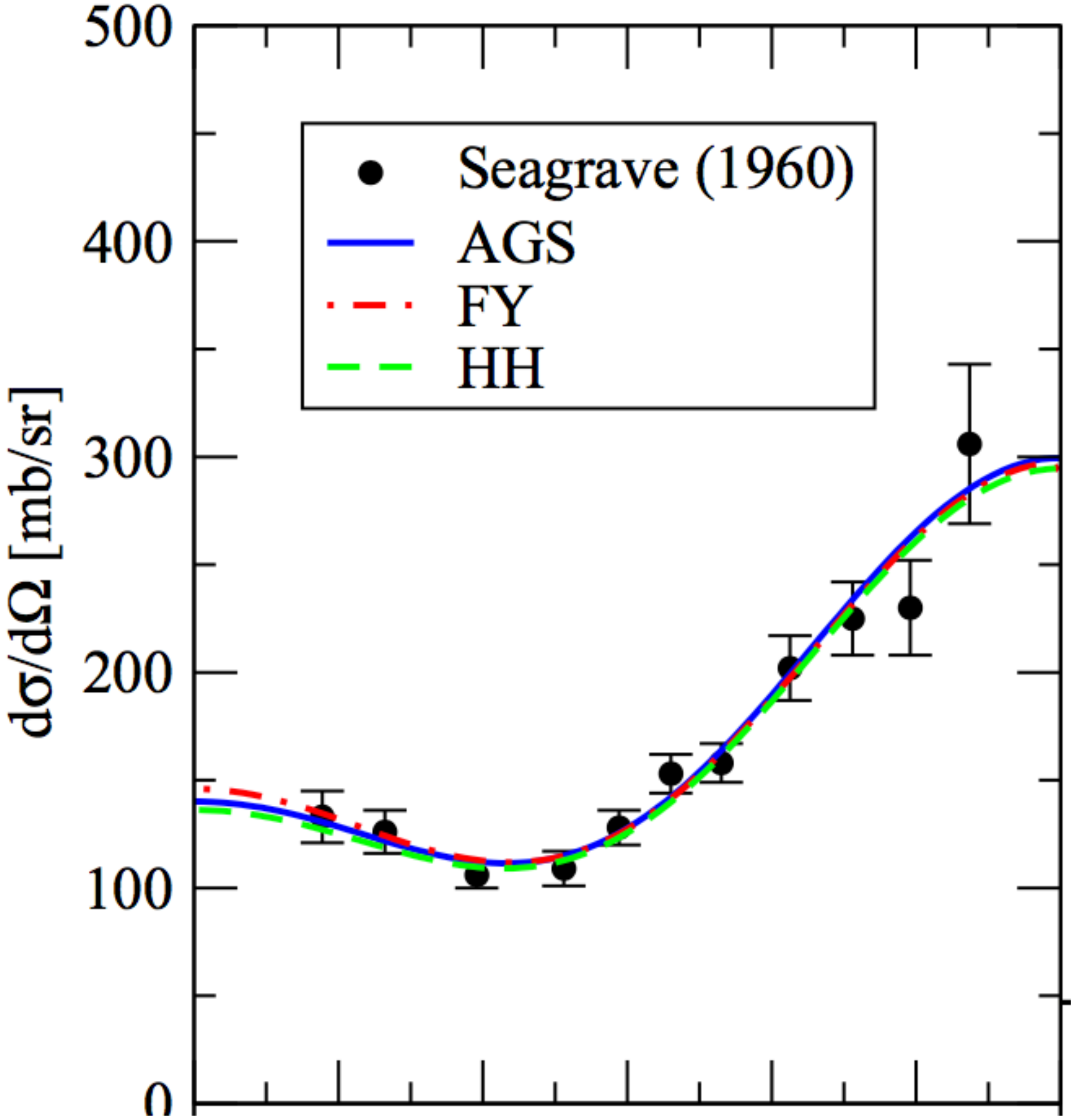
TRIUMF/LLNL/Da: Navratil, Quaglioni, Roth…

Ab-initio methods

Benchmark

Phys. Rev. C **95**, 034003 (2017)

n-^{3}He at 1 MeV



Θ[deg]

Ab-initio methods

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Integral Transforms Methods

Integral Transforms

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

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

(the quantity of direct physical meaning)

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

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

Problem:

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

Integral Transforms

Suppose we want a response function R(ω)

$$R(\omega) = \sum_f |\langle \psi_f | \Theta | \psi_0 \rangle|^2 \; \delta(\omega - E_f - E_0)$$

Scattering states

Energies in the continum

Integral Transforms

$$R(\omega) = \sum_f |\langle \psi_f | \Theta | \psi_0 \rangle|^2 \; \delta(\omega - E_f - E_0)$$

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

1) integrate in dω using delta function

$$= \sum_f K(E_f - E_0, \sigma) \langle \psi_0 | \Theta^\dagger | \psi_f \rangle \langle \psi_f | \Theta | \psi_0 \rangle$$

$$= \sum_f \langle \psi_0 | \Theta^\dagger K(H - E_0, \sigma) | \psi_f \rangle \langle \psi_f | \Theta | \psi_0 \rangle$$

2) Use $\sum_f |\psi_f\rangle\langle\psi_f| = 1$

$$\phi(\sigma) = \langle \psi_0 | \Theta^\dagger K(H - E_0, \sigma) \Theta | \psi_0 \rangle$$

Example: sum rules

$$\Phi_n = \int d\omega \;\; \omega^n R(\omega)$$

Sum rules are a kind of “Moment transform”

$K(\omega,\sigma) = \omega^n$ with n integer

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

However, $\Phi(\sigma)$ may be infinite for some n

Example: Laplace Transform

$$\phi(\sigma) = \int e^{-\omega\sigma} R(\omega) d\omega = \langle \psi_0 | \Theta^\dagger e^{-(H-E_0)\sigma} \Theta | \psi_0 \rangle$$

In condensed matter physics, QCD and nuclear physics

Example: Laplace Transform

$$\phi(\sigma) = \int e^{-\omega\sigma} R(\omega) d\omega = \langle\psi_0|\Theta^\dagger e^{-(H-E_0)\sigma}\Theta|\psi_0\rangle$$

In condensed matter physics, QCD and nuclear physics

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

Φ (τ) is calculated with **Monte Carlo Methods**

and then inverted with Bayesian methods

Integral Transform

$$\Phi(\sigma) = \int R(\omega) K(\omega, \sigma)\ d\omega \ = \langle \psi_0 | \Theta^\dagger K(H - E_0, \sigma) \Theta | \psi_0 \rangle$$

Matrix element on the ground state

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 the calculation?

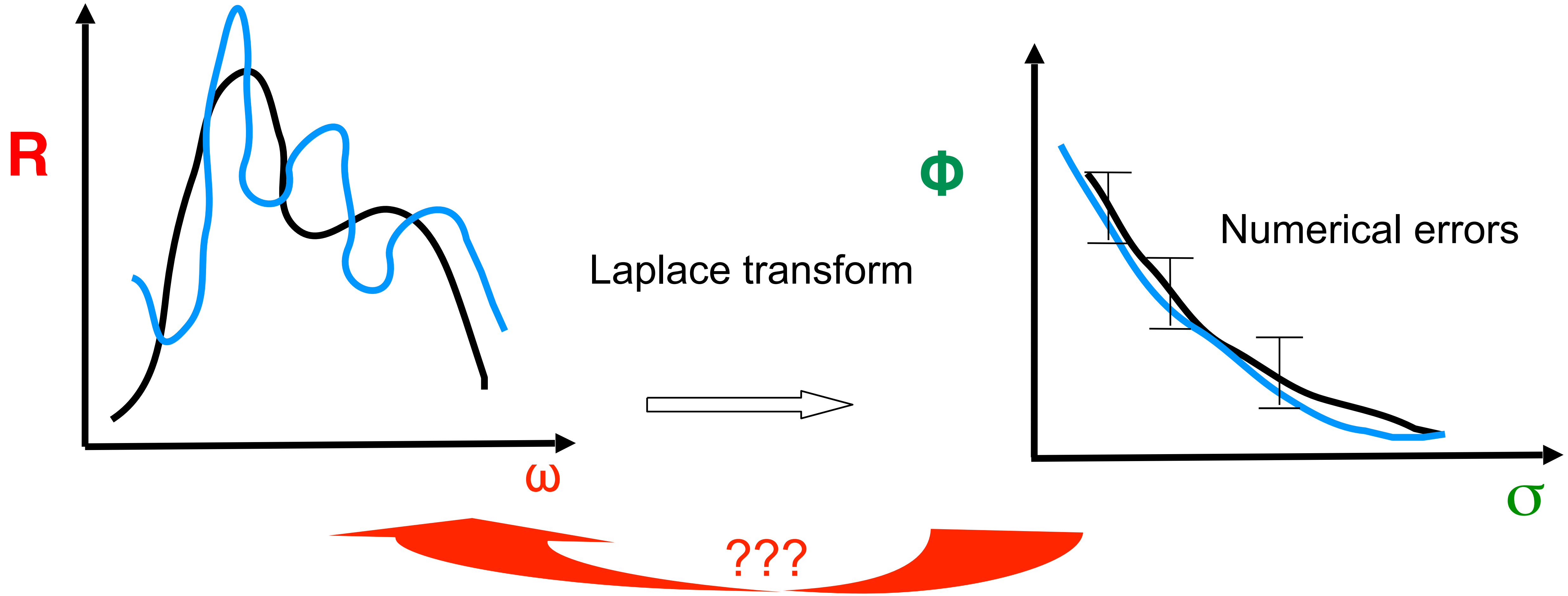
Inversion

$$\phi(\sigma) = \int e^{-\omega\sigma} R(\omega) d\omega$$

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

Inversion

Illustration of the problem:



Inversion

Illustration of the problem:

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

If there is a numerical noise

↓

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

Inversion

Illustration of the problem:

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

If there is a numerical noise

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

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

independently on the amplitude A of the error!

Best kernel

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?

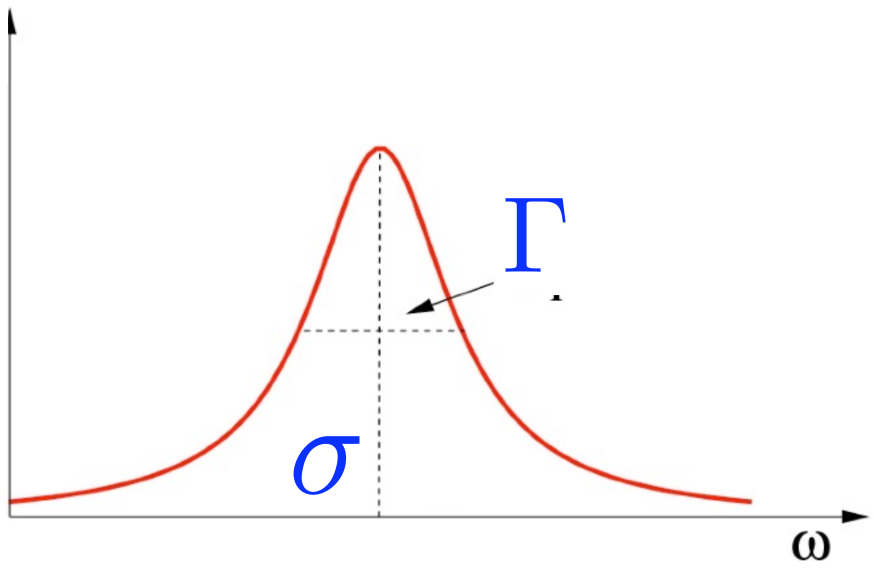
$$\Phi(\sigma) = \int \delta(\omega - \sigma)\, R(\omega) = R(\sigma)$$

Back to square zero….

Best kernel

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

Lorentzian kernel



$$K(\omega, \sigma, \Gamma) = \Gamma/\pi \, [(\omega - \sigma)^2 + \Gamma^2]^{-1}$$

It is a representation of the δ-function

$$L(\sigma, \Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2}$$

Lorentz Integral Transform (LIT) Efros, *et al.*, JPG.: Nucl.Part.Phys. **34** (2007) R459

Lorentzian kernel

See inversion procedures in Mirko's talk

In the next lecture we will make further theoretical considerations on the LIT