Few-body Reactions

Lecture 3

Integral Transforms

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Outline of Lecture 3

- Reactions to continuum
- Integral transform
- Lanczos algorithm
- Applications

Reactions to continuum

Perturbative (e.g. electromagnetic)

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

Non-perturbative (hadronic)

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

Where a,b,c,d... are either 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)

$$\boxed{R(\omega) \quad \sim \quad |\langle \Psi_f | J^\mu | \Psi_0 \rangle|^2 \delta(\omega - E_f - E_0)}$$

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

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$\boxed{R(\omega) \sim |\langle \Psi_f | J^\mu | \Psi_0 \rangle|^2 \delta(\omega - E_f - E_0)}$$

Energy transferred by the perturbative probe

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$\boxed{R(\omega) \sim |\langle \Psi_f | J^\mu | \Psi_0 \rangle|^2 \delta(\omega - E_f - E_0)}$$

Ground state of the target
A-body bound state!

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

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$\boxed{R(\omega) \sim |\langle\Psi_f|J^\mu|\Psi_0\rangle|^2\delta(\omega - E_f - E_0)}$$

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)

$$\boxed{R(\omega) \sim |\langle \Psi_f | J^\mu | \Psi_0 \rangle|^2 \delta(\omega - E_f - E_0)}$$

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

NB: q is in the operator, but we omit it for simplicity

$\gamma^{(*)}$ + b → c + d +...

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

$$\boxed{R(\omega) = \sum_f |\langle \Psi_f | J^\mu | \Psi_0 \rangle|^2 \delta(\omega - E_f - E_0)}$$

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 …

Perturbative Reactions

Electro-weak processes (photons, electrons, neutrinos)

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

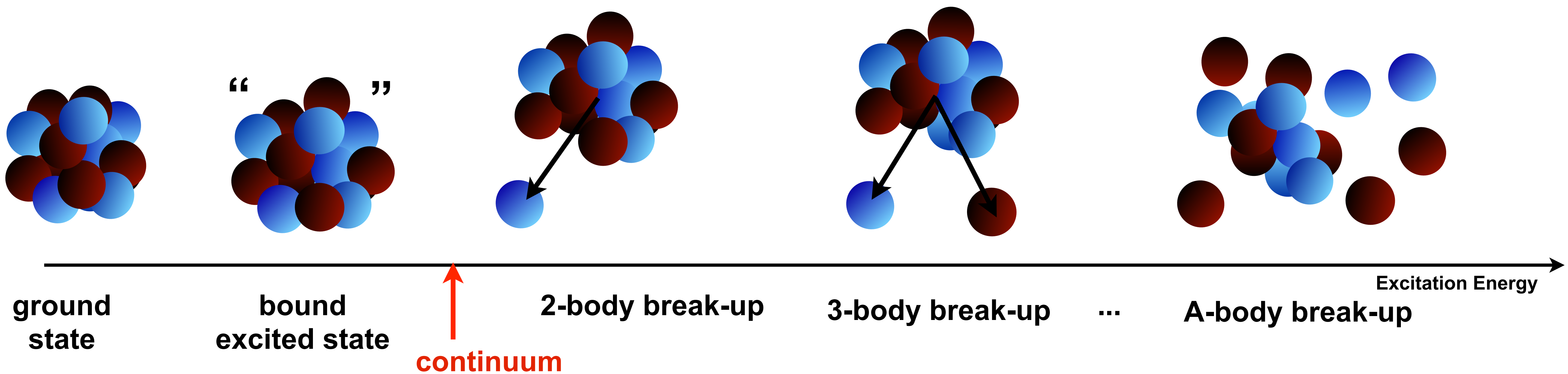
$$\boxed{R(\omega) = \sum_f |\langle\Psi_f|J^\mu|\Psi_0\rangle|^2 \delta(\omega - E_f - E_0)}$$

$R(\omega)$ represents the crucial quantity

Requires the solution of both
the bound and continuum A-body problem

Reactions to continuum

$$R(\omega) = \sum_f \left|\langle \Psi_f | J^\mu | \Psi_0 \rangle\right|^2 \delta(\omega - E_f - E_0)$$



$|\Psi_f\rangle$ Exact knowledge limited in energy and mass number

Ab-initio methods

Most representative approaches

	Few-body: A≲12	Many-body: 12≲A≲100 or more
Structure Bound states	• *Faddeev Yakubowski (FY)* • **Hyperspherical Harmonics** • **NCSM** • **SVM** • *Quantum 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)* • *Complex scaling*	

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

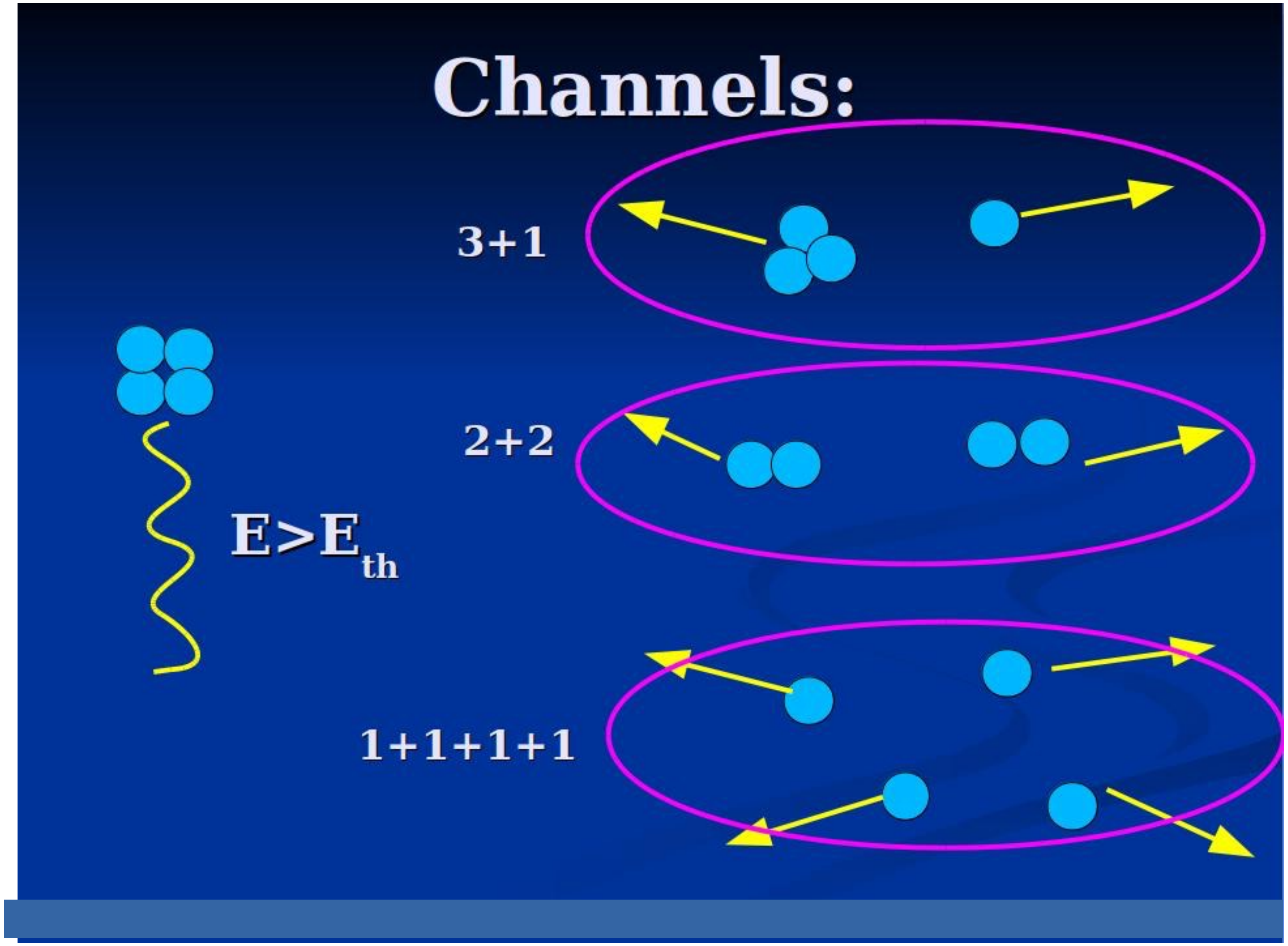
In momentum space

(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...

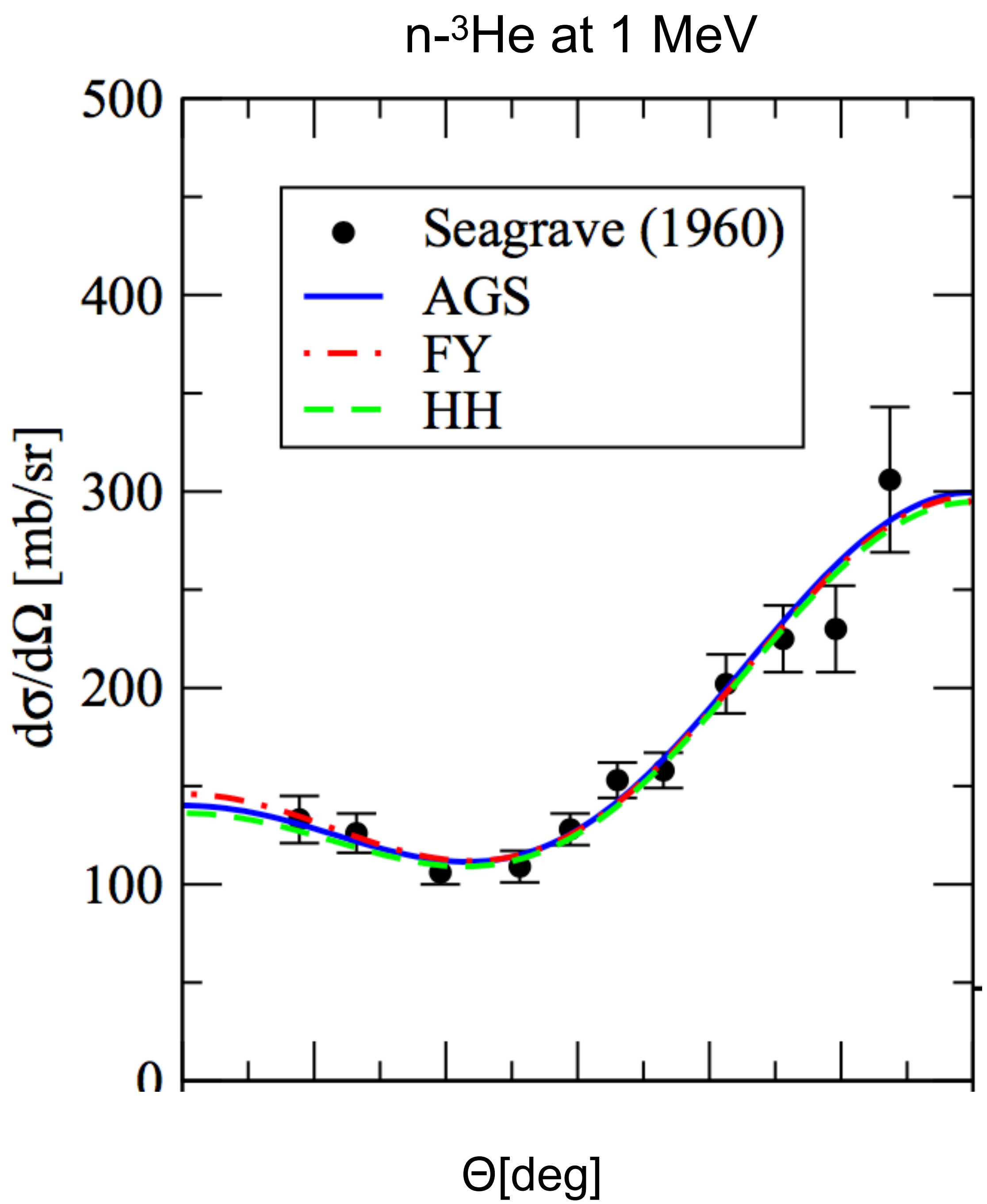
- Similar idea for (A-1) + 1 in NCSMC

TRIUMF/LLNL: Navratil, Quaglioni, et al.

Ab-initio methods

Benchmark for hadronic reaction

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



Ab-initio methods

Most representative approaches

	Few-body: A≲12	Many-body: 12≲A≲100 or more
Structure Bound states	• *Faddeev Yakubowski (FY)* • Hyperspherica … ics • NCSM • SVM • *Quantum Monte Carlo*	• *Coupled Cluster (CC)* • *Other Monte Carlo methods* • *IMSRG* • *…f consistent Green's function*
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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 $\phi(\sigma)$ may be problematic

Integral Transforms

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

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

1) integrate in dω using delta function

$$= \sum_f K(E_f - E_0, \sigma) \langle \psi_0 | J^{\mu\dagger} | \psi_f \rangle \langle \psi_f | J^\mu | \psi_0 \rangle$$

$$= \sum_f \langle \psi_0 | J^{\mu\dagger} K(H - E_0, \sigma) | \psi_f \rangle \langle \psi_f | J^\mu | \psi_0 \rangle$$

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

$$\boxed{\phi(\sigma) = \langle \psi_0 | J^{\mu\dagger} K(H - E_0, \sigma) J^\mu | \psi_0 \rangle}$$

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(ω) the inversion of the transform is equivalent to the reconstruction of R(ω) by its moments (theory of moments)

However, ϕ_n may be infinite for some n

Example: Laplace Transform

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

In condensed matter physics, QCD and nuclear physics

Example: Laplace Transform

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

In condensed matter physics, QCD and nuclear physics

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

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

and then inverted with Maximum likelyhood methods

Integral Transform

$$\Phi(\sigma) = \int R(\omega) K(\omega, \sigma) \, d\omega \;\; = \langle \psi_0 | J^{\mu\dagger} K(H - E_0, \sigma) J^{\mu} | \psi_0 \rangle$$

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 complicated operator.

So, which kernel is suitable for the calculation?

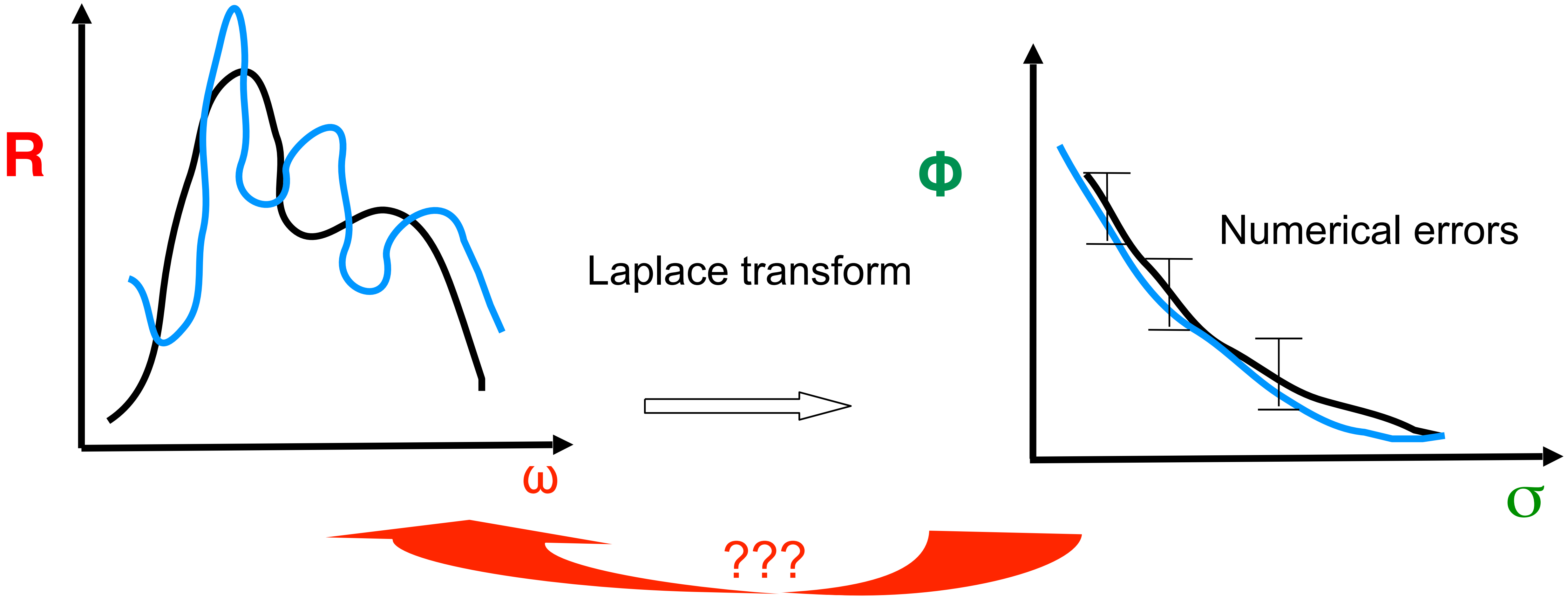
Inversion

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

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

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

$$\Delta\Phi(\nu) \xrightarrow{\text{for very large } \nu} 0$$

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?

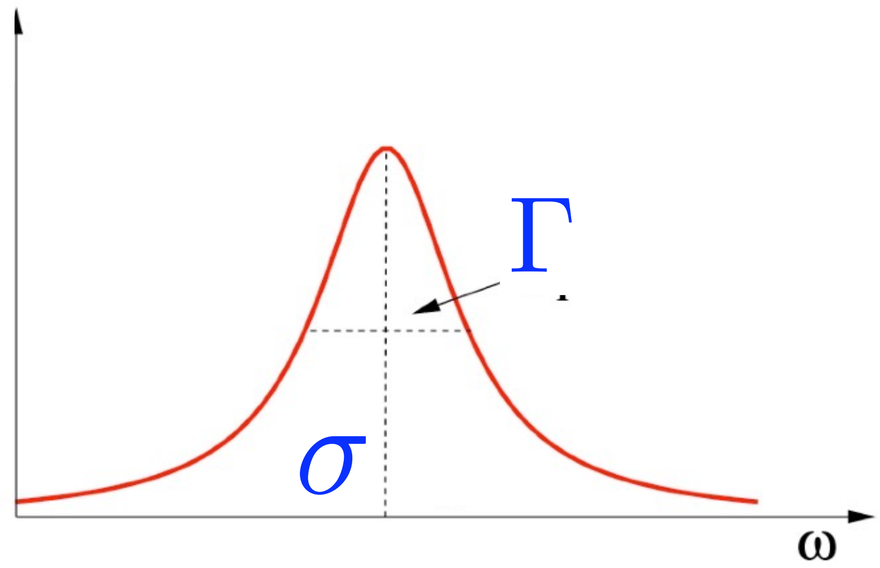
$$\boldsymbol{\Phi}(\sigma) = \int \delta(\omega - \sigma)\, R(\omega) = R(\sigma)$$

Back to the original problem ….

Best kernel

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

Lorentzian kernel



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

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

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

Lorentz Integral Transform

$$\boxed{L(\sigma,\Gamma) = \langle \psi_0 | J^{\mu\dagger} K(H-E_0,\sigma,\Gamma) J^{\mu} | \psi_0 \rangle}$$

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

$$K(\omega,\sigma,\Gamma) = \frac{\Gamma}{\pi} \frac{1}{(\omega-\sigma-i\Gamma)(\omega-\sigma+i\Gamma)}$$

$$L(\sigma,\Gamma) = \left\langle \psi_0 | J^{\mu\dagger} \frac{1}{H-E_0-\sigma-i\Gamma} \frac{1}{H-E_0-\sigma+i\Gamma} J^{\mu} | \psi_0 \right\rangle \frac{\Gamma}{\pi}$$

Lorentz Integral Transform

$$\boxed{L(\sigma,\Gamma) = \langle \psi_0 | J^{\mu\dagger} K(H-E_0,\sigma,\Gamma) J^{\mu} | \psi_0 \rangle}$$

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

$$K(\omega,\sigma,\Gamma) = \frac{\Gamma}{\pi} \frac{1}{(\omega-\sigma-i\Gamma)(\omega-\sigma+i\Gamma)}$$

$$L(\sigma,\Gamma) = \left\langle \psi_0 \left| J^{\mu\dagger} \frac{1}{H-E_0-\sigma-i\Gamma} \boxed{\underbrace{\frac{1}{H-E_0-\sigma+i\Gamma} J^{\mu} \right| \psi_0}_{= |\tilde{\psi}\rangle}} \right\rangle \frac{\Gamma}{\pi}$$

$$= \langle \tilde{\psi} | \tilde{\psi} \rangle \frac{\Gamma}{\pi}$$

Lorentz Integral Transform

main point of the LIT :

Schrödinger-like equation with a source

$$\boxed{(H - E_0 - \sigma + i\Gamma)|\tilde{\Psi}\rangle = J^\mu|\Psi_0\rangle}$$

- Due to imaginary part Γ the solution $|\tilde{\psi}\rangle$ is unique
- Since rhs is finite, $|\tilde{\psi}\rangle$ has bound state asymptotic behaviour

⇩

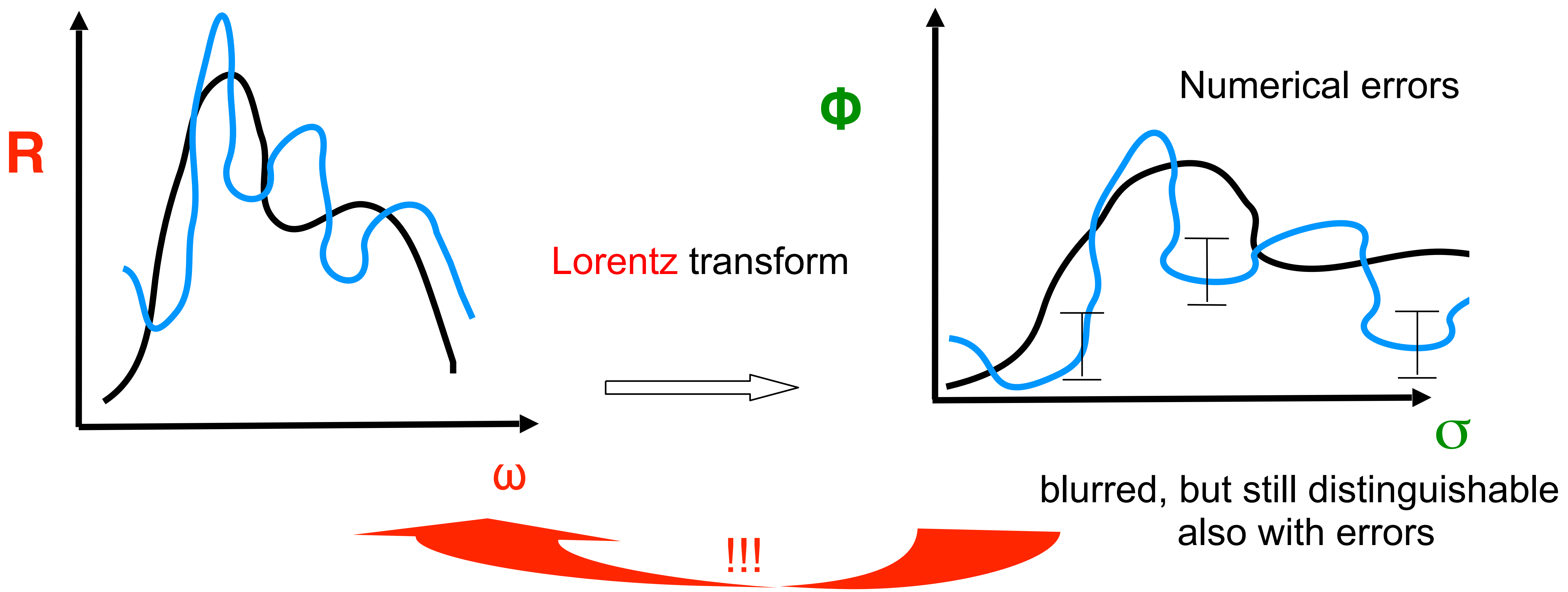
Can solve it with bound state methods

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

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

Inversion

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



Regularization method

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

Integral transform is a linear operation

$$R(\omega) = \sum_i^{\infty} c_i \chi_i(\omega, \alpha) \longrightarrow L(\sigma, \Gamma) = \sum_i^{\infty} c_i \mathcal{L}[\chi_i(\omega, \alpha)]$$

$$R(\omega) = \sum_i^{I_{\max}} c_i \chi_i(\omega, \alpha) \longrightarrow L(\sigma, \Gamma) = \sum_i^{I_{\max}} c_i \mathcal{L}[\chi_i(\omega, \alpha)]$$

Least square fit of the coefficients c_i to reconstruct the response function

Regularization: find a range of I_{max} where results are stable

Possible basis functions to invert are:

$$\chi_i(\omega, \alpha) = \omega^{i+\frac{1}{2}} e^{-\frac{\omega}{\alpha}}$$

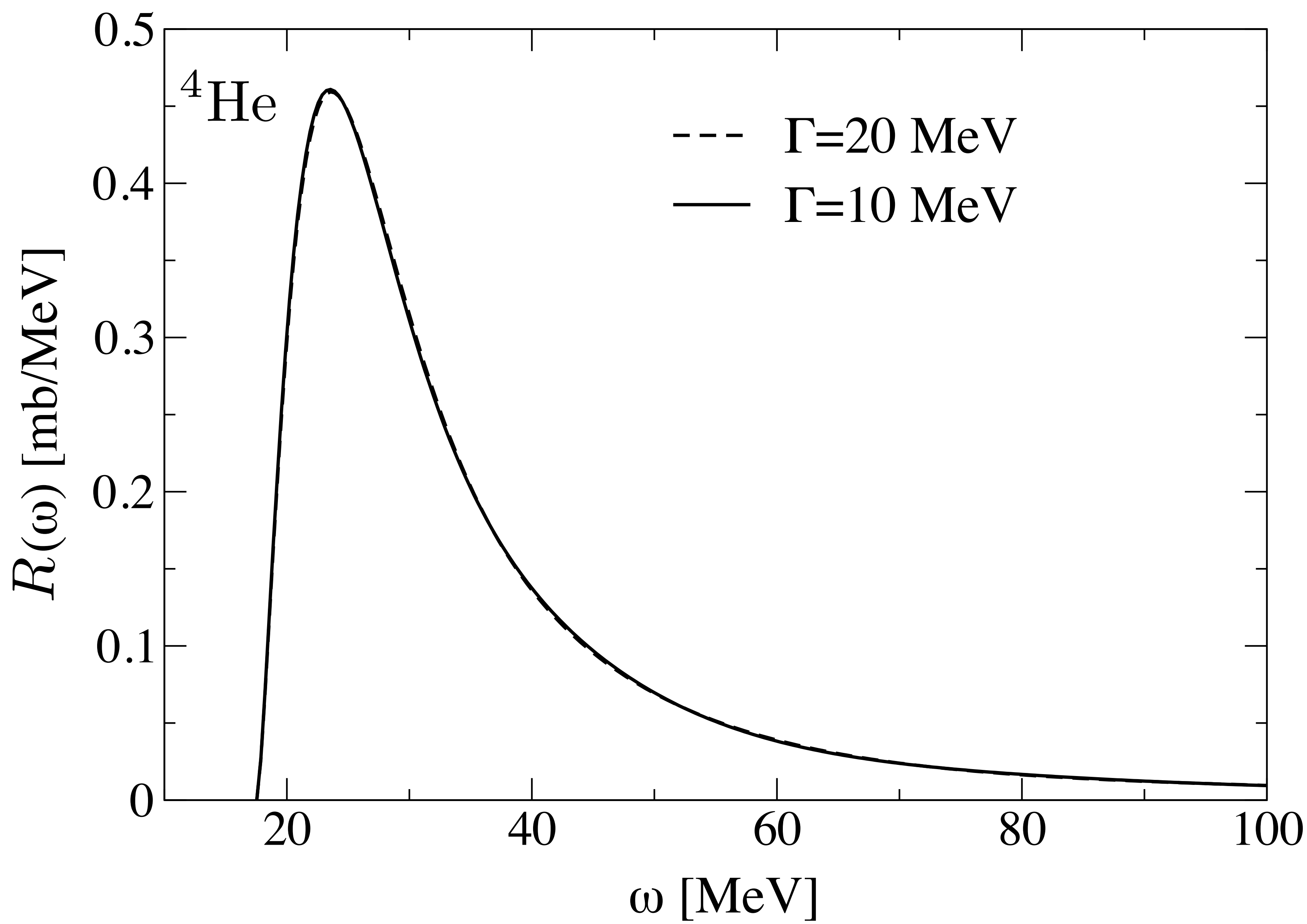
$$\chi_i(\omega, \alpha) = \omega^{n_0} e^{-\frac{\omega}{i\alpha}}, \text{with } n_0 \text{ const.}$$

Exercise

Regularization method

Strong test: different values of range of Γ and check stability

Photoabsoprtion of ^{4}He

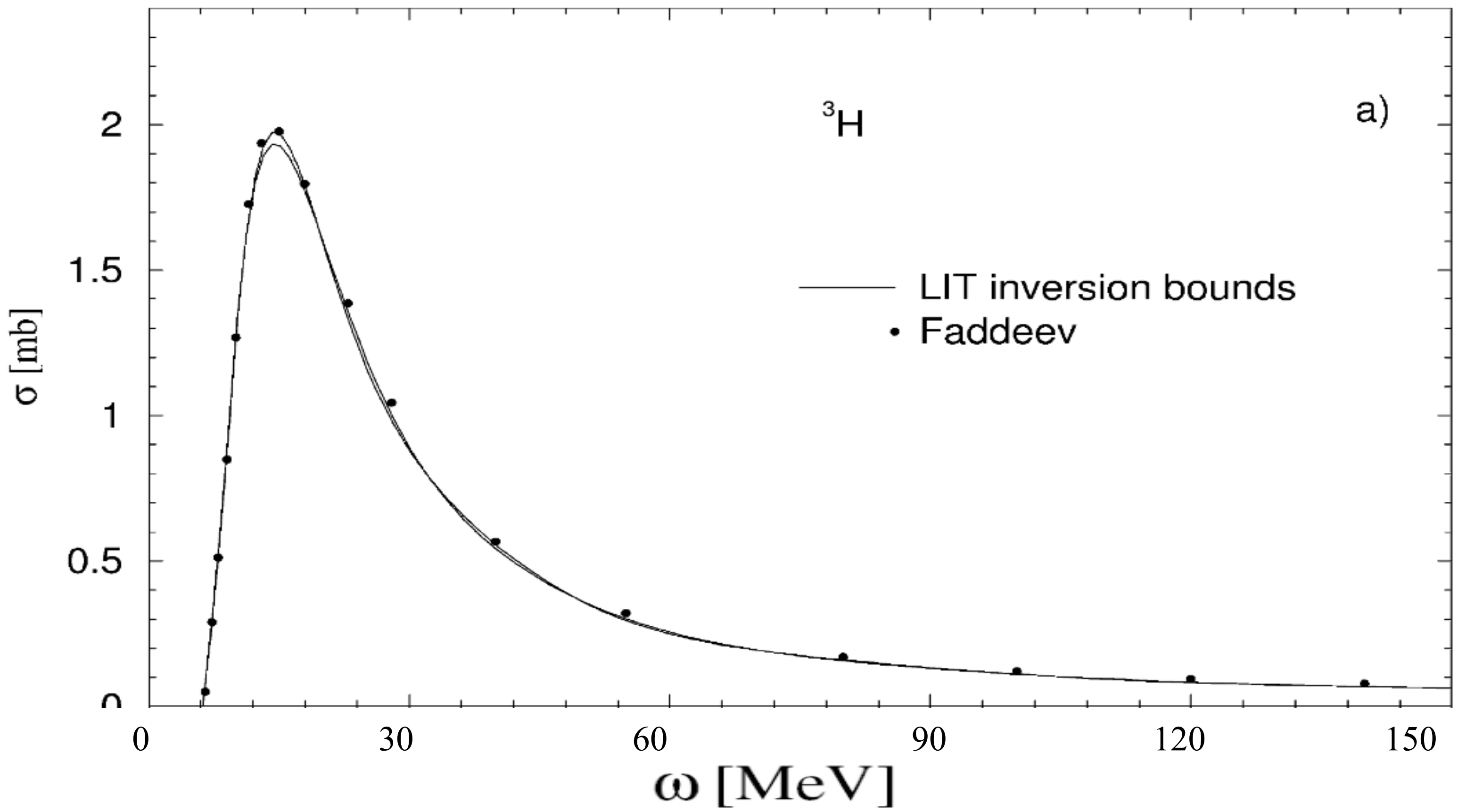


Benchmark of the LIT

The LIT method has been benchmarked with other few-body methods where $|\psi_f\rangle$ is calculated directly using same dynamical ingredients

With Fadeev approach

Nucl.Phys. A707 365 (2002)

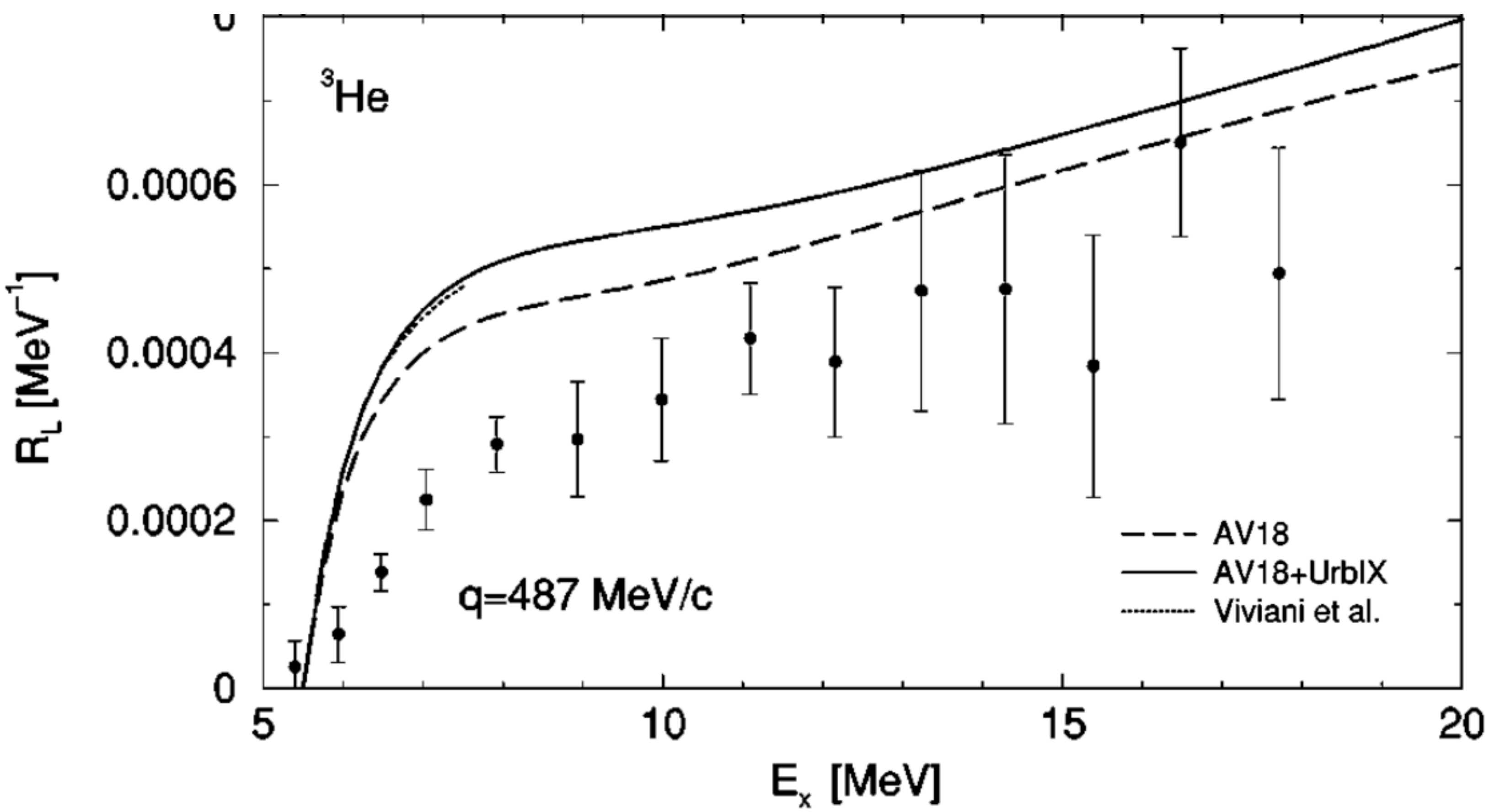


Benchmark of the LIT

The LIT method has been benchmarked with other few-body methods where $|\psi_f\rangle$ is calculated directly using same dynamical ingredients

With variational approach (HH)

Phys.Rev.C 69 (2004)



Other remarks on the LIT

Rewriting the response function

$$R(\omega) = \sum_f |\langle f|J^\mu|0\rangle|^2 \boxed{\delta(\omega - E_f - E_0)}$$

NB: Slightly simplified notation

Sokhotski formula

$$\frac{1}{x + i\epsilon} = \mathcal{P}\int dx \frac{1}{x} - i\delta(x)\pi \qquad \epsilon \to 0$$

Taking the imaginary part only

$$\mathrm{Im}\frac{1}{x + i\epsilon} = -\delta(x)\pi \quad \Rightarrow \quad \delta(x) = -\frac{1}{\pi}\mathrm{Im}\frac{1}{x + i\epsilon}$$

$$R(\omega) = \boxed{-\frac{1}{\pi}\mathrm{Im}}\left[\sum_f |\langle f|J^\mu|0\rangle|^2 \boxed{\frac{1}{\omega - E_f - E_0 + i\epsilon}}\right]$$

Rewriting the response function

$$R(\omega)=-1/\pi \ \mathrm{Im} \left[\Sigma_f \langle 0|J^+|f\rangle \langle f|\, J\, |0\rangle\right] (\omega-E_f+E_0+\iota\varepsilon)^{-1}\Big]$$

$$=-1/\pi \ \mathrm{Im} \left[\Sigma_f \langle 0|\, J^+ (\omega-E_f+E_0+\iota\varepsilon)^{-1} |f\rangle \langle f|J\, |0\rangle\right]$$

$H|f\rangle=E_f|f\rangle$

$$=-1/\pi \ \mathrm{Im} \left[\Sigma_f \langle 0|\, J^+ (\omega-H+E_0+\iota\varepsilon)^{-1} |f\rangle \langle f|J\, |0\rangle\right]$$

change sign

$$= 1/\pi \ \mathrm{Im} \left[\Sigma_f \langle 0|\, J^+(H-\omega-E_0-\iota\varepsilon)^{-1}|f\rangle \langle f|J\, |0\rangle\right]$$

$\Sigma_f|f\rangle\langle f|=1$ and change sign

$$= -1/\pi \ \mathrm{Im} \left[\langle 0|\, J^+(H-\omega-E_0+\iota\varepsilon)^{-1} J\, |0\rangle\right]$$

Like a Green's function with poles on the real axis

Rewriting the LIT

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

$$= \Gamma/\pi \int d\omega \sum_f |\langle f| J^\mu |0\rangle|^2 \delta(\omega - E_f + E_0) \; [(\omega-\sigma)^2+\Gamma^2]^{-1}$$

Integrate delta and use $H|f\rangle = E_f|f\rangle$

Completeness

$$= \Gamma/\pi \sum_f \langle 0 | J^{\mu +} [(H-E_0-\sigma)^2+\Gamma^2]^{-1} |f\rangle\langle f| J^\mu | 0\rangle$$

$$= \Gamma/\pi \langle 0 | J^{\mu +} [(H-E_0-\sigma)^2+\Gamma^2]^{-1} \; J^\mu | 0\rangle$$

$$-\mathrm{Im}\,[(H-E_0-\sigma+i\Gamma)^{-1}] =$$

$$-\mathrm{Im}[(H-E_0-\sigma+i\Gamma)^{-1}(H-E_0-\sigma-i\Gamma)^{-1}(H-E_0-\sigma-i\Gamma)] =$$

$$=\Gamma\,[(H-E_0-\sigma)^2+\Gamma^2]^{-1}$$

Finite, not infinitesimal

$$= -1/\pi\, \mathrm{Im}\,[\langle 0 | J^{\mu +} (H-E_0-\sigma+i\Gamma)^{-1} J^\mu | 0\rangle]$$

Summarizing

$$R(\omega) = -1/\pi \; \mathrm{Im} \left[\langle 0 | J^{+} (H - \omega - E_0 + \imath\varepsilon)^{-1} J | 0 \rangle \right]$$

ε infinitesimal

$$L(\sigma, \Gamma) = -1/\pi \; \mathrm{Im} \left[\langle 0 | J^{+} (H - E_0 - \sigma_R + i\,\Gamma)^{-1} J | 0 \rangle \right]$$

Γ finite, not infinitesimal

Of course, when $\varepsilon = \Gamma$ then $R(\omega) = L(\sigma, \Gamma)$

That is indeed the case where the Kernel is the delta function

However, due to the fact that Γ is finite and $L(\sigma, \Gamma)$
is finite, one is allowed to use bound -state techniques to calculate it

Lanczos Algorithm

Algorithm used to tri-diagonalize matrices $H \longrightarrow H_{tr}$

1) Choose first Lanczos vector $|\phi_0\rangle$

2) Use recursive definition to find the other Lanczos vectors

$$b_{n+1}\,|\phi_{n+1}\rangle = H\,|\phi_n\rangle - a_n\,|\phi_n\rangle - b_n\,|\phi_{n-1}\rangle$$

With $a_n = \langle\phi_n|\, H\,|\phi_n\rangle$

$$b_n = \| b_n\,|\phi_n\rangle \|$$

3) Matrix represented on the Lanczos vectors is tridiagonal

$$H_{tr} = \begin{pmatrix} a_0 & b_1 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & \dots \\ 0 & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} .$$

Can diagonalize it using Numerical Recipes routine, e.g. TQLI

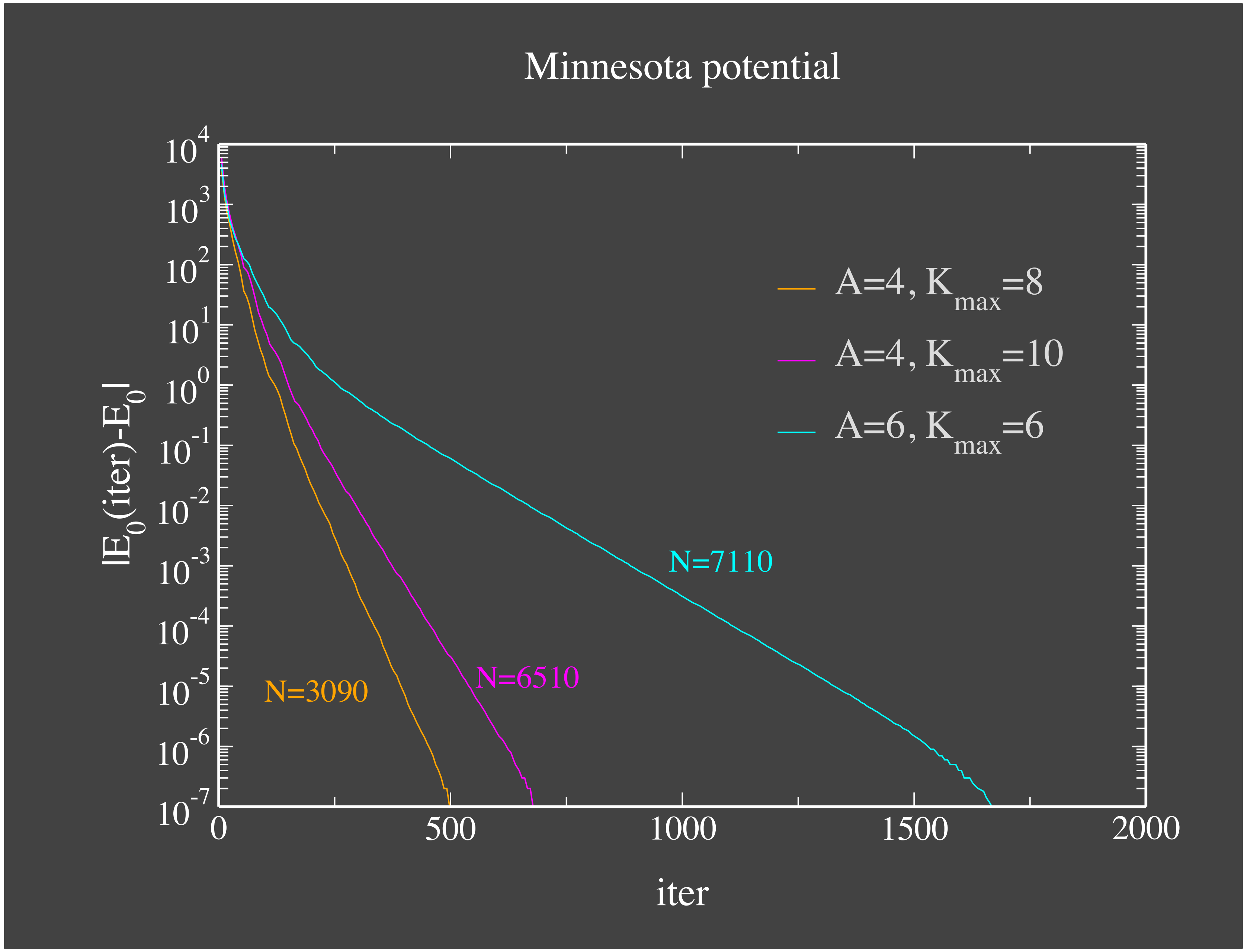
Lanczos Algorithm

For large scale eigenvalue problems, e.g. calculations with hyper-spherical harmonics

See N. Barnea's lectures

Generally, diagonalizing a matrix is a N^3 operation

With the Lanczos algorithm you can reduce it to nN^2 with n = max(iter)< N



K_{max} is here the Grandangular momentum

LIT with Lanczos Algorithm

The algorithm can be also used calculate the LIT

$$L(\sigma,\Gamma) = -\frac{1}{\pi} Im\left[\langle 0| J^\dagger (H - E_0 - \sigma_R + i\Gamma)^{-1} J|0\rangle\right]$$

Using the Lanczos algorithm one can represent
as a continuum fraction of the Lanczos coefficients $(H - E_0 - \sigma_R + i\Gamma)^{-1}$

1) Choose first Lanczos vector $|\phi_0\rangle = \dfrac{\Theta|0\rangle}{\sqrt{\langle 0|\Theta^\dagger\Theta|0\rangle}}$

2) After applying the recursive definition you obtain

$$L(\sigma) = -\frac{1}{\pi}\langle 0|\ J^\dagger J\ |0\rangle\, Im\left\{\frac{1}{(z-a_0) - \frac{b_1^2}{(z-a_1) - \frac{b_2^2}{(z-a_2) - b_3^2 \cdots}}}\right\}$$

with $z = E_0 + \sigma + i\Gamma$

Exercise

Detailed derivation

LIT with LANCZOS method

$$L(\sigma,\Gamma) = \frac{1}{\pi}\,\mathrm{Im}\left\{\langle 0|J^{\mu\dagger}\frac{1}{H-E_0-\sigma-i\Gamma}J^{\mu}|0\rangle\right\}$$

Defining $z = E_0+\sigma+i\Gamma$, we see that $L(\sigma,\Gamma)$ has the operator $\frac{1}{H-z}$;

We want $\frac{1}{z-H}$, so we change sign.

$$L(\sigma,\Gamma) = -\frac{1}{\pi}\,\mathrm{Im}\left\{\langle 0|J^{\mu\dagger}\frac{1}{z-H}J^{\mu}|0\rangle\right\}$$

Now we apply the Lanczos algorithm using the starting Lanczos vector

$$|\Phi_0\rangle = \frac{J^{\mu}|0\rangle}{\sqrt{\langle 0|J^{\mu\dagger}J^{\mu}|0\rangle}}$$

; then $H \to H_{tr}$ (tri-diagonal matrix in terms of the Lanczos coefficients)

$\Rightarrow$ we see that $L(\sigma,\Gamma) \longrightarrow \langle \Phi_0|\frac{1}{z-H_{tr}}|\Phi_0\rangle$

Detailed derivation

$$(z-H_{tr})(z-H_{tr})^{-1} = \mathbb{1}$$

$\Rightarrow$ in components $\sum_n (z-H_{tr})_{mn}(z-H_{tr})^{-1}_{np} = \delta_{mp}$

$\Rightarrow$ for the case of $p=0$: $\boxed{\sum_n (z-H_{tr})_{mn}\,(z-H_{tr})^{-1}_{n0} = \delta_{m0}}$ $(*)$

Now we define $(z-H_{tr})^{-1}_{n0} = X_n$

$\Rightarrow$ $X_0 = (z-H_{tr})^{-1}_{00} = \langle \Phi_0 | \dfrac{1}{z-H_{tr}} | \Phi_0 \rangle$ This is what we need.

Let us write $(*)$ for a 3x3 matrix:

$$\begin{pmatrix} z-a_0 & -b_1 & 0 \\ -b_1 & z-a_1 & -b_2 \\ 0 & -b_2 & z-a_2 \end{pmatrix}\begin{pmatrix} X_0 \\ X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \Rightarrow X_0 = \frac{\det\begin{pmatrix} 1 & -b_1 & 0 \\ 0 & z-a_1 & -b_2 \\ 0 & -b_2 & z-a_2 \end{pmatrix}}{\det\begin{pmatrix} z-a_0 & -b_1 & 0 \\ -b_1 & z-a_1 & -b_2 \\ 0 & -b_2 & z-a_2 \end{pmatrix}}$$

Using Cramer rule

Detailed derivation

Generalizing to $N \times N$ matrix

$$X_0 = \frac{\det(B_0)}{\det(z - H_{tr})} \quad \text{with} \quad B_0 = \begin{pmatrix} 1 & -b_1 & 0 & \cdots \\ 0 & z-a_1 & -b_2 & 0 \cdots \\ 0 & -b_2 & z-a_2 & -b_3 \cdots \\ \vdots & \vdots & & \ddots \end{pmatrix}$$

$$(z - H_{tr}) = \begin{pmatrix} z-a_0 & -b_1 & 0 & \cdots \\ -b_1 & z-a_1 & -b_2 & \cdots \\ 0 & -b_2 & z-a_2 & \cdots \\ \cdots & & \cdots & \end{pmatrix}$$

$$\Rightarrow \det(z - H_{tr}) = (z - a_0)\det D_1 - b_1^2 \det D_2$$

matrix obtained by removing first row and first column from $(z - H_{tr})$

matrix obtained by removing first two rows and first two columns from $(z - H_{tr})$

$$\det B_0 = \det D_1$$

$$\Rightarrow X_0 = \frac{\det D_1}{(z-a_0)\det D_1 - b_1^2 \det D_2} = \frac{1}{z - a_0 - b_1^2 \frac{\det D_2}{\det D_1}}$$

Detailed derivation

$$\det D_1 = (z-a_1)\det D_2 - b_2^2 \det D_2$$

$$\Rightarrow \frac{\det D_2}{\det D_1} = \frac{\det D_2}{(z-a_1)\det D_2 - b_1^2 \det D_3} = \frac{1}{(z-a_1) - b_1^2 \frac{\det D_3}{\det D_2}}$$

Putting this into our X_0 we get

$$X_0 = \left\{ \frac{1}{z-a_0 - \frac{b_1^2}{(z-a_1) - b_1^2 \ldots}} \right\}$$

Continued fraction in terms of the Lanczos coefficients

$\Rightarrow$ Alltogether you obtain that

$$L(\sigma,\Gamma) = -\frac{1}{\pi} \langle 0 | J^{\mu\dagger} J^{\mu} | 0 \rangle \, \mathrm{Im} \left\{ \frac{1}{z-a_0 - \frac{b_1^2}{(z-a_1) - \frac{b_2^2}{(z-a_2) \ldots}}} \right\}.$$

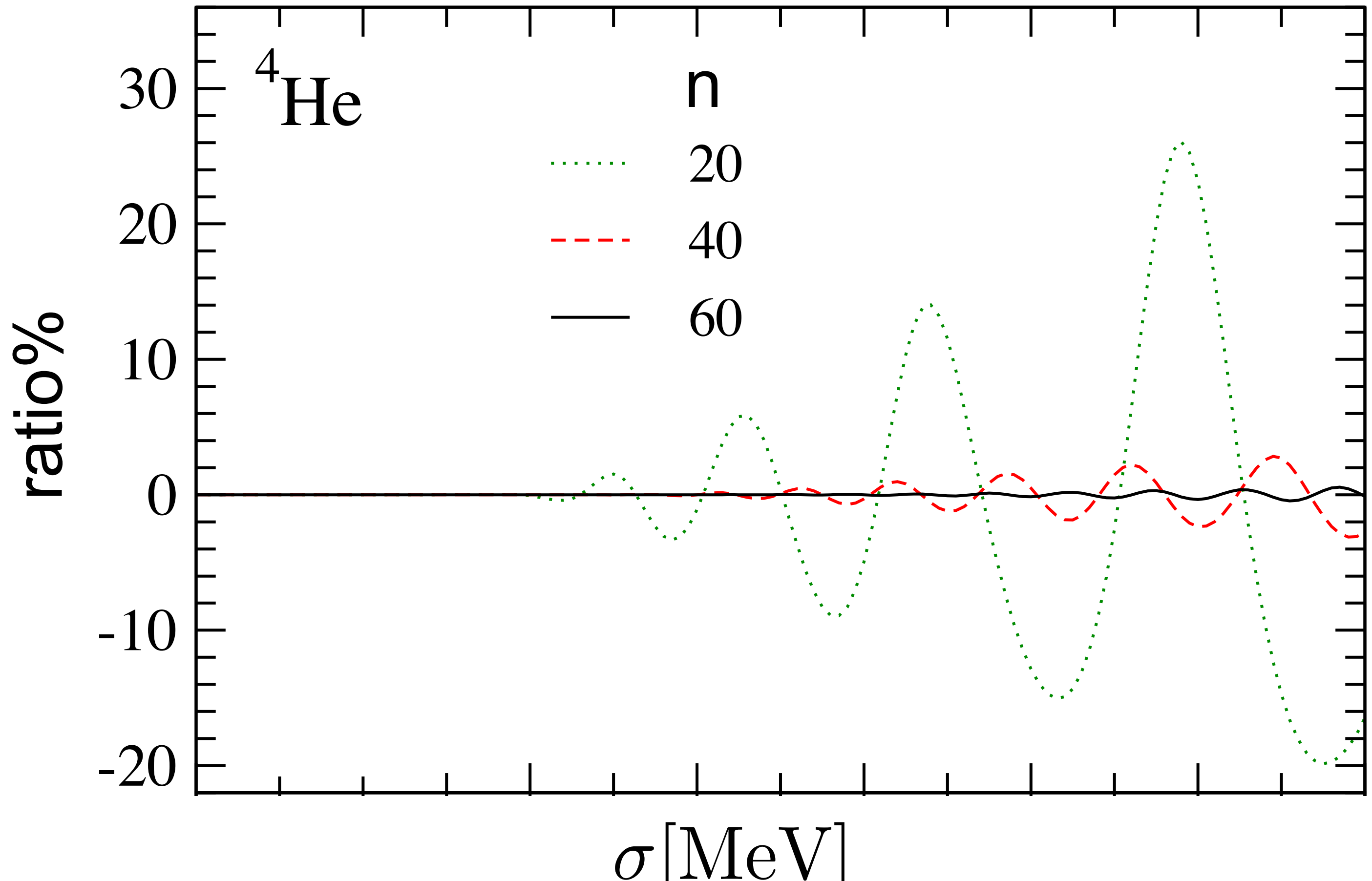
LIT with Lanczos Algorithm

Advantages

The Lanczos algorithm involves just a matrix-vector multiplication (N^2)

Continues fractions converge fast

Again, with the Lanczos algorithm the computational load is becoming nN^2 with $n = \max(iter) < N$

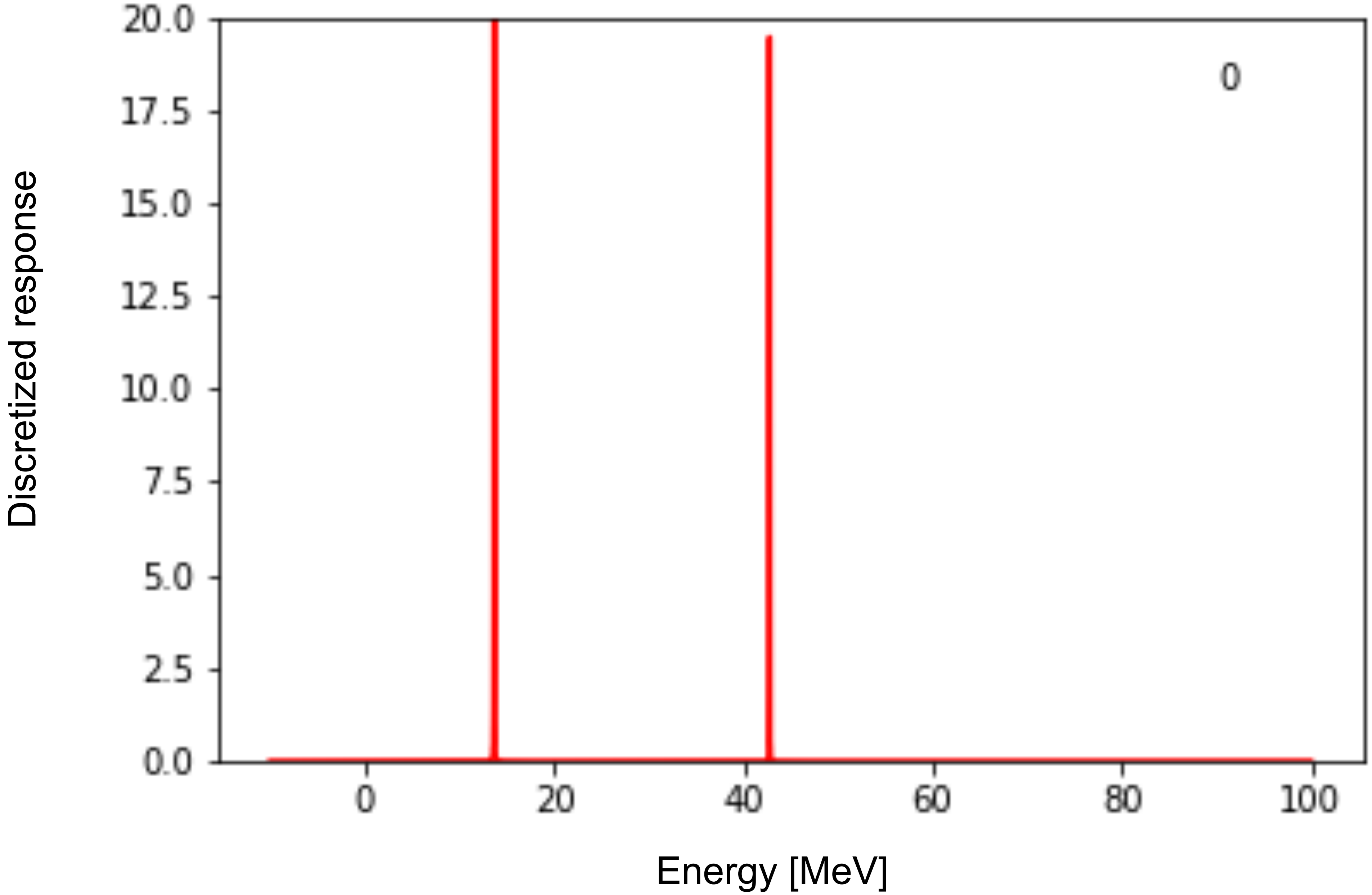


See that as an exercise

LIT with Lanczos Algorithm

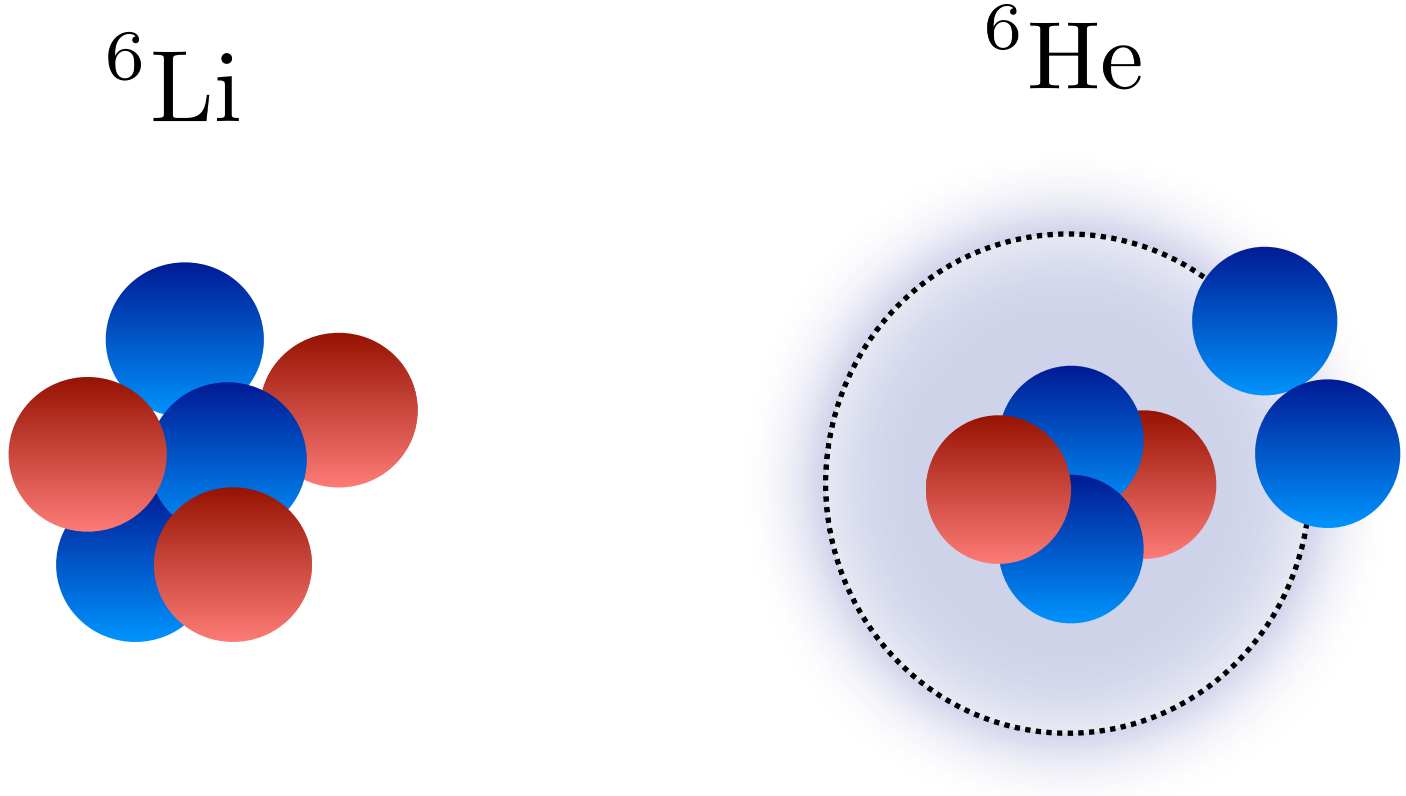
Strength building up from Lanczos vectors (LIT with small Γ)

Movie from M.Miorelli



Some more applications

Do these nuclei respond differently to em probes?

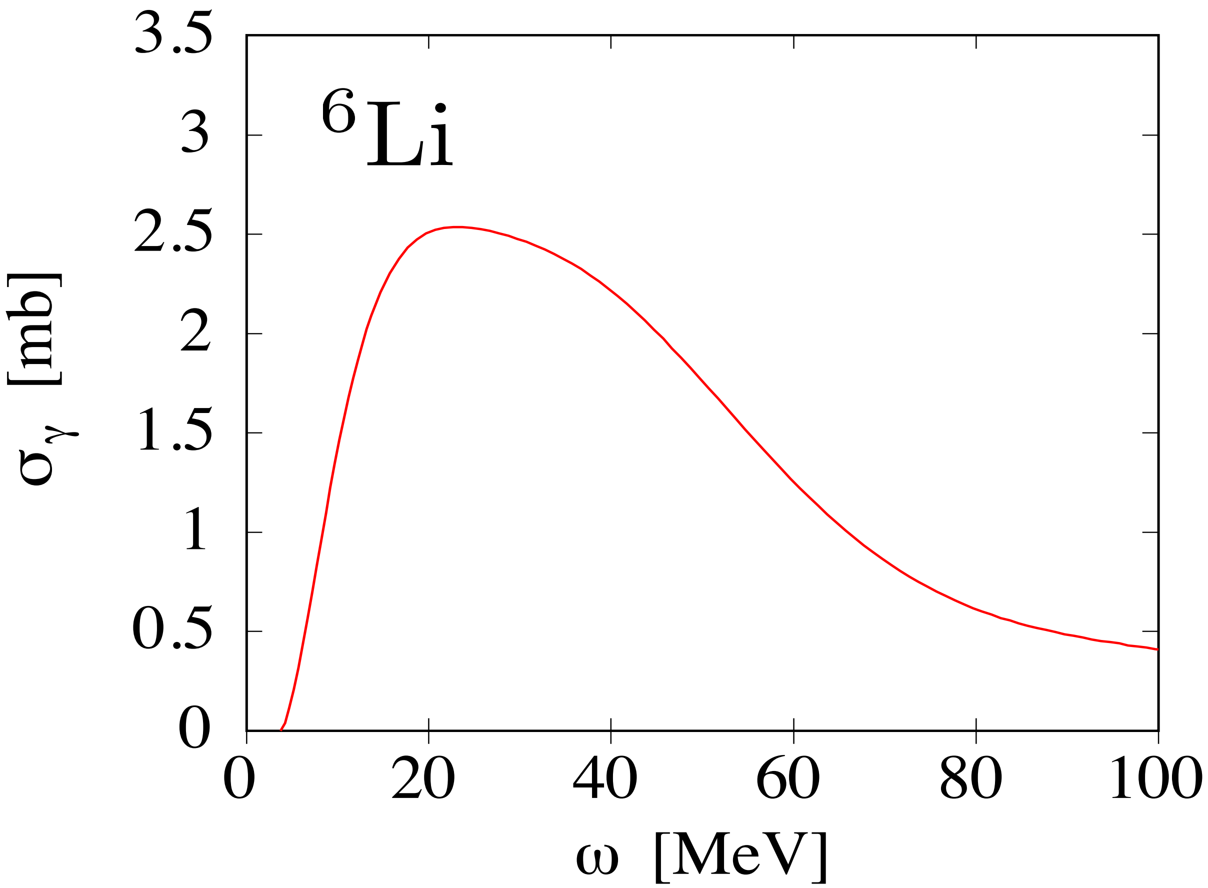


We did calculate them with Hyper-spherical Harmonics and the LIT

Photo-absorption reaction

S.Bacca et al, PRL **89** 052502 (2002)

$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega R^{E1}(\omega)$$ AV4' potential



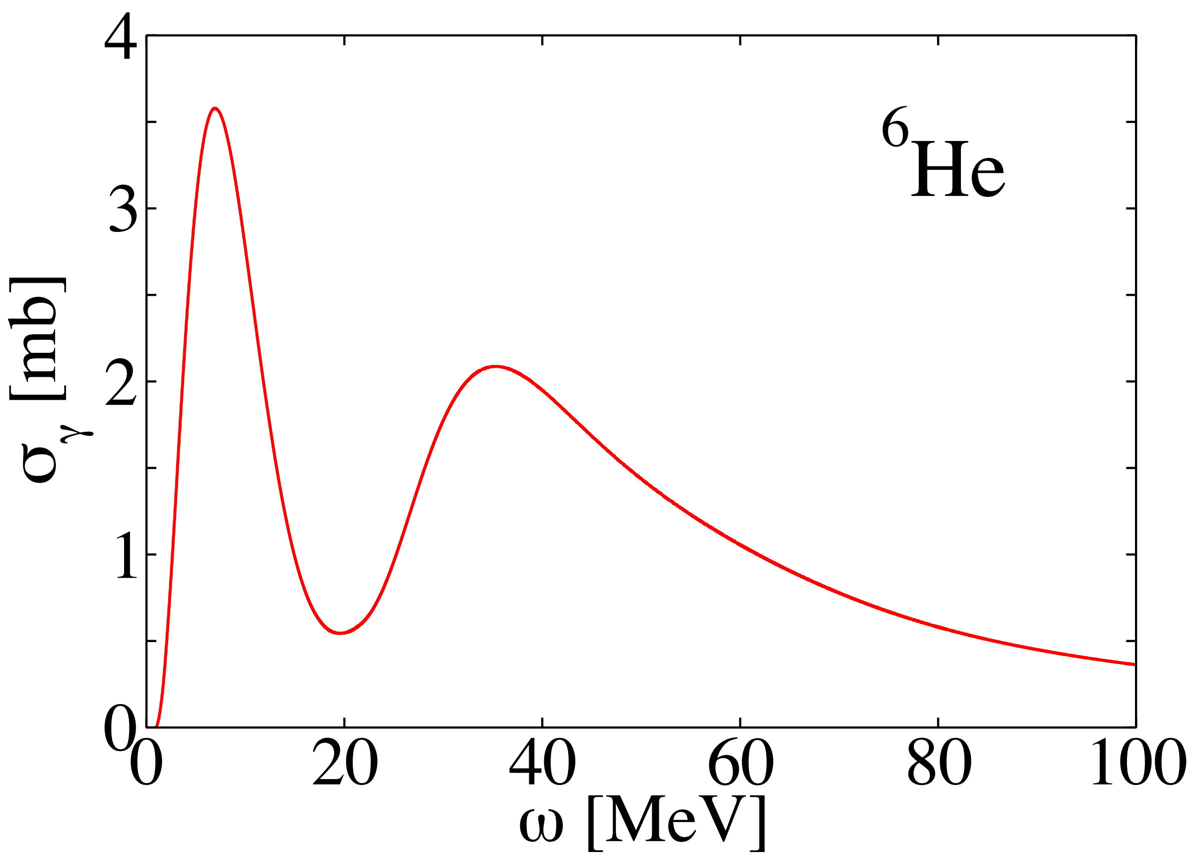


Photo-absorption reaction

S.Bacca et al, PRL **89** 052502 (2002)

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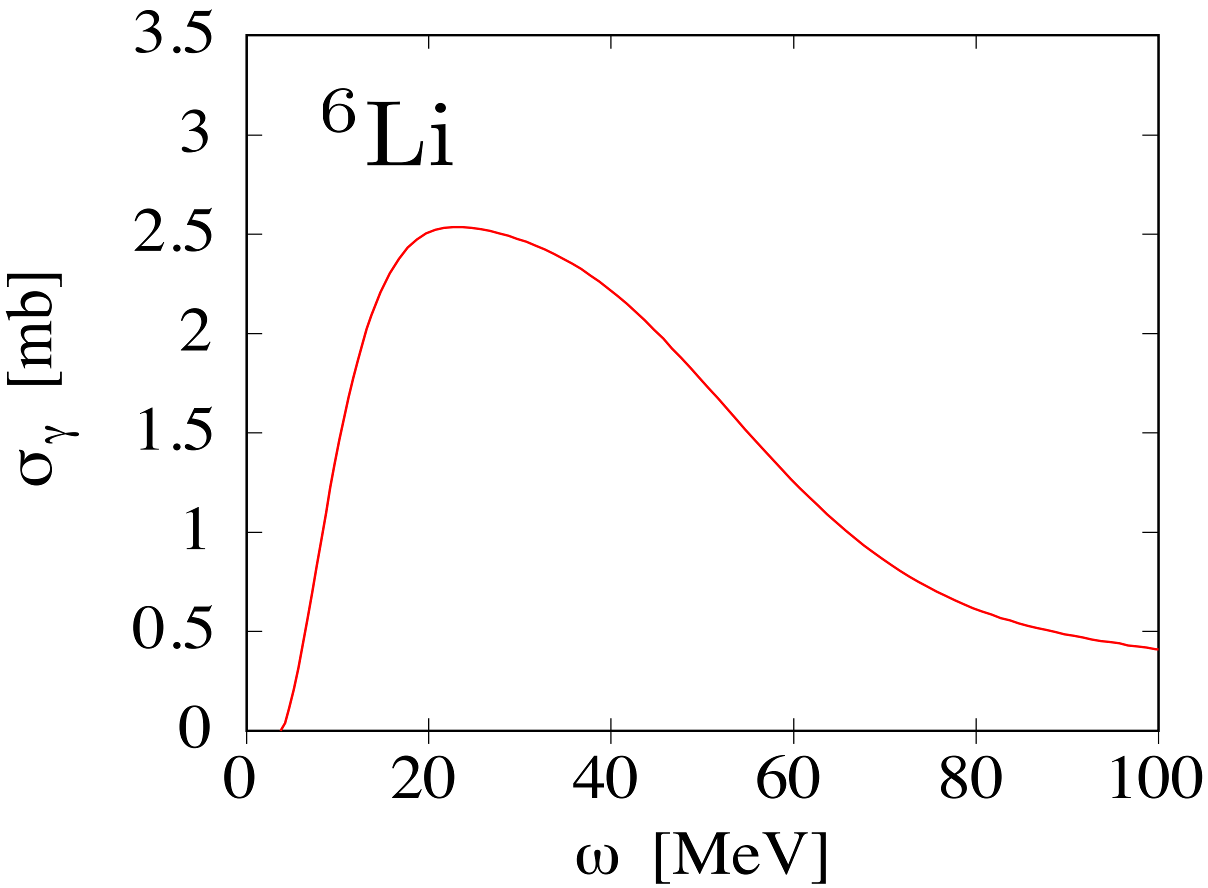
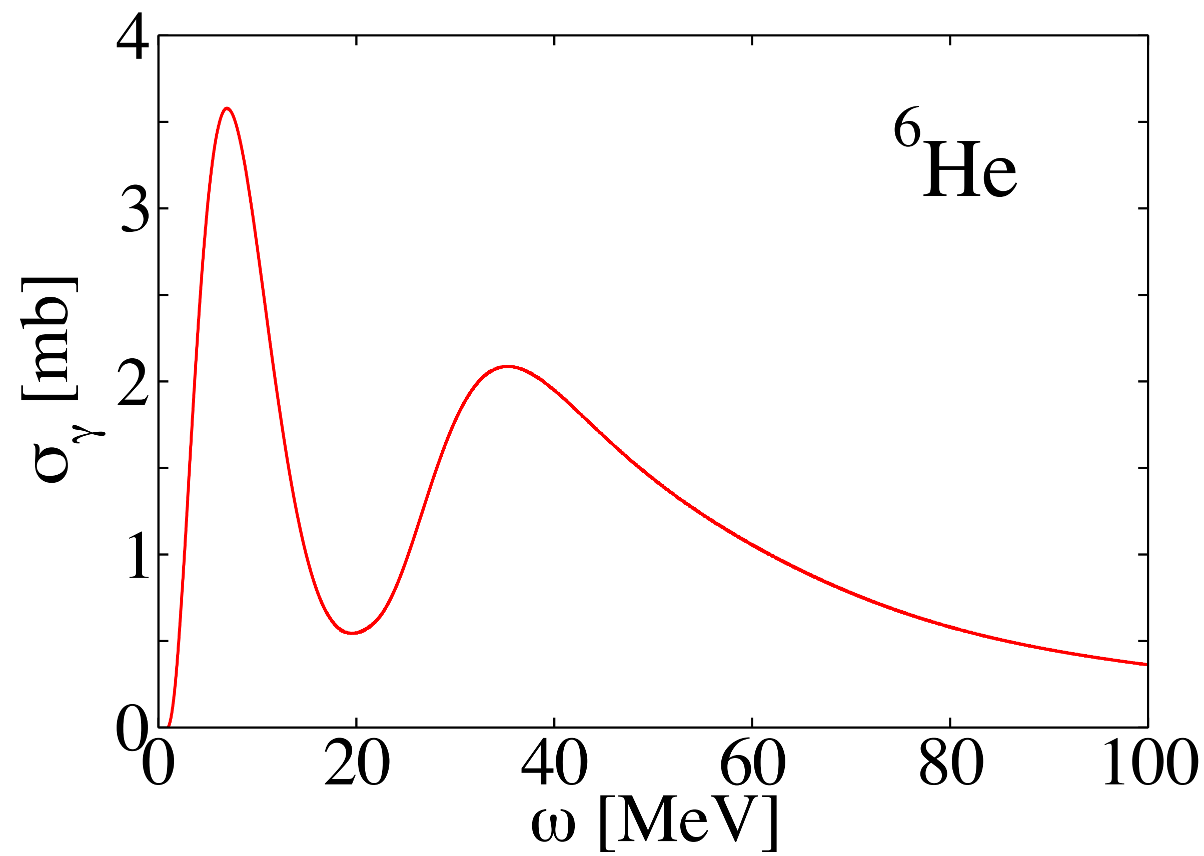
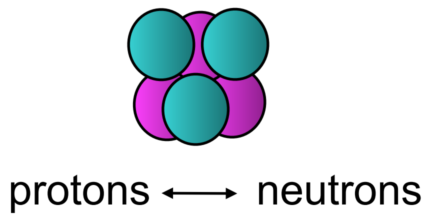
AV4' potential





Giant Dipole Resonance



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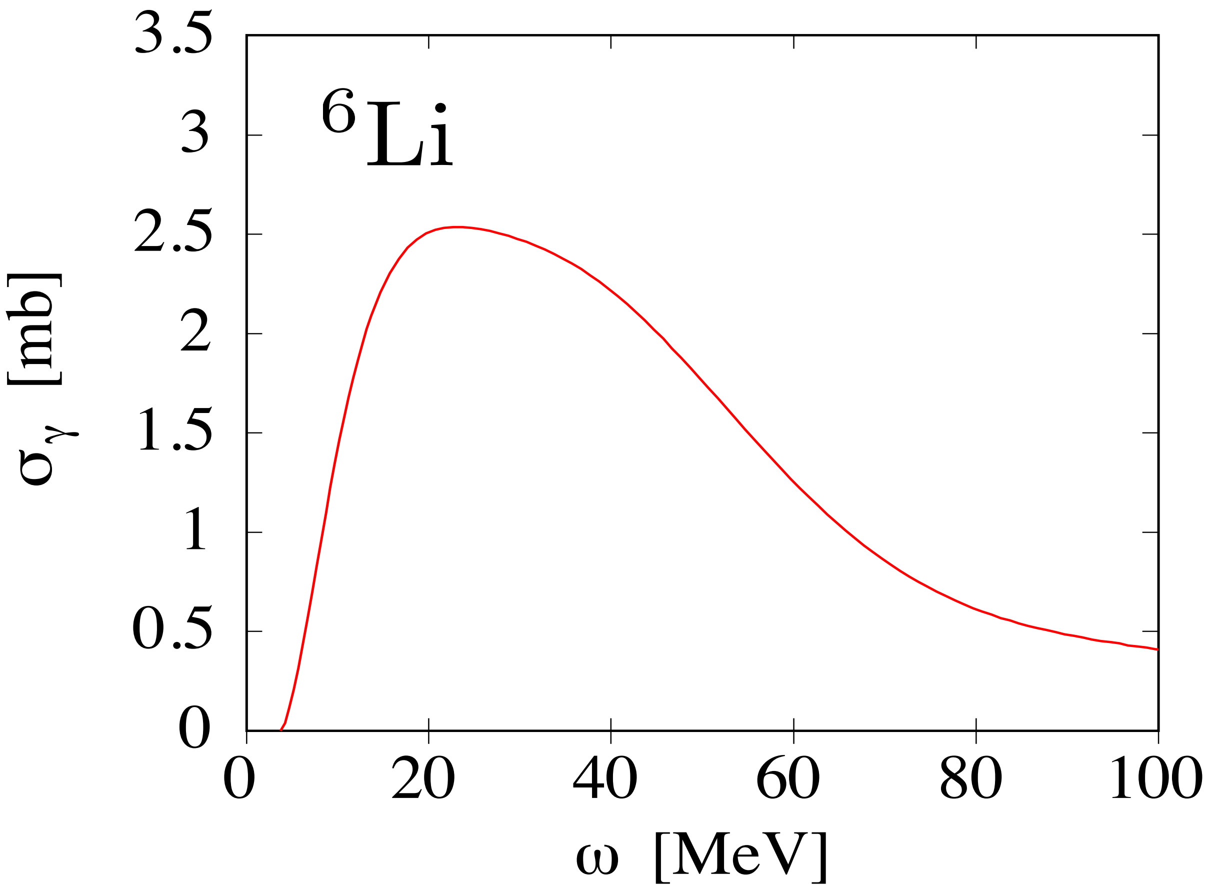
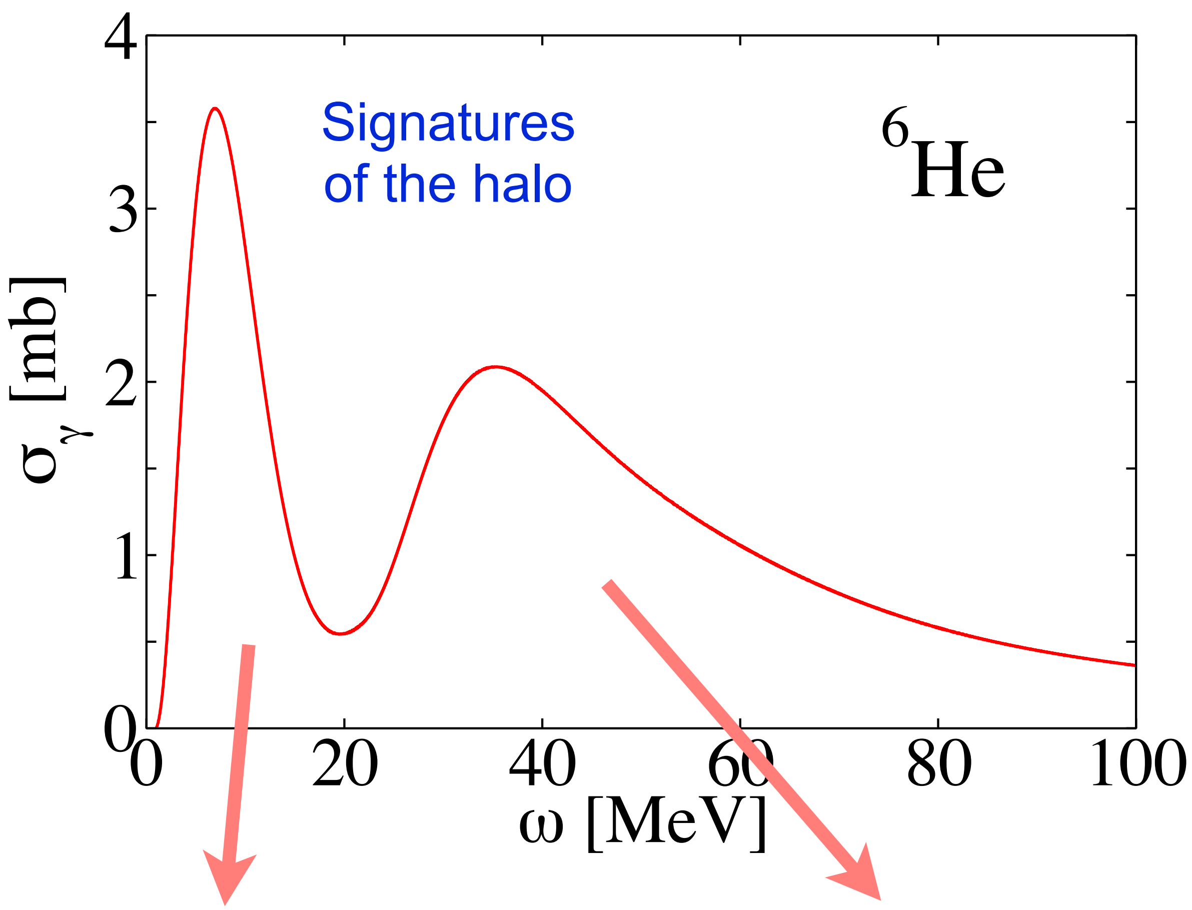
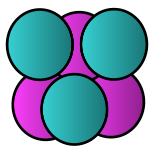
AV4' potential

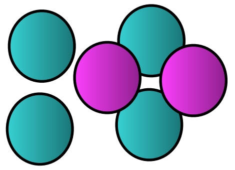




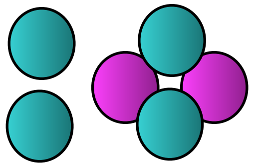
Giant Dipole Resonance



Soft-dipole Mode



Giant Dipole Mode



Inelastic Electron Scattering

$$R_L(\omega, \mathbf{q}) = \sum\!\!\!\!\!\!\!\int_f |\langle \Psi_f | \rho(\mathbf{q}) | \Psi_0 \rangle|^2 \, \delta\left(E_f - E_0 - \omega + \frac{\mathbf{q}^2}{2M} \right)$$

$$\rho(\mathbf{q}) = \sum_k^A e^{i\mathbf{q}\cdot\mathbf{r}'_k} \frac{1+\tau_k^3}{2} = \sum_J^{\infty} C_J^S(\mathbf{q}) + C_J^V(\mathbf{q})$$

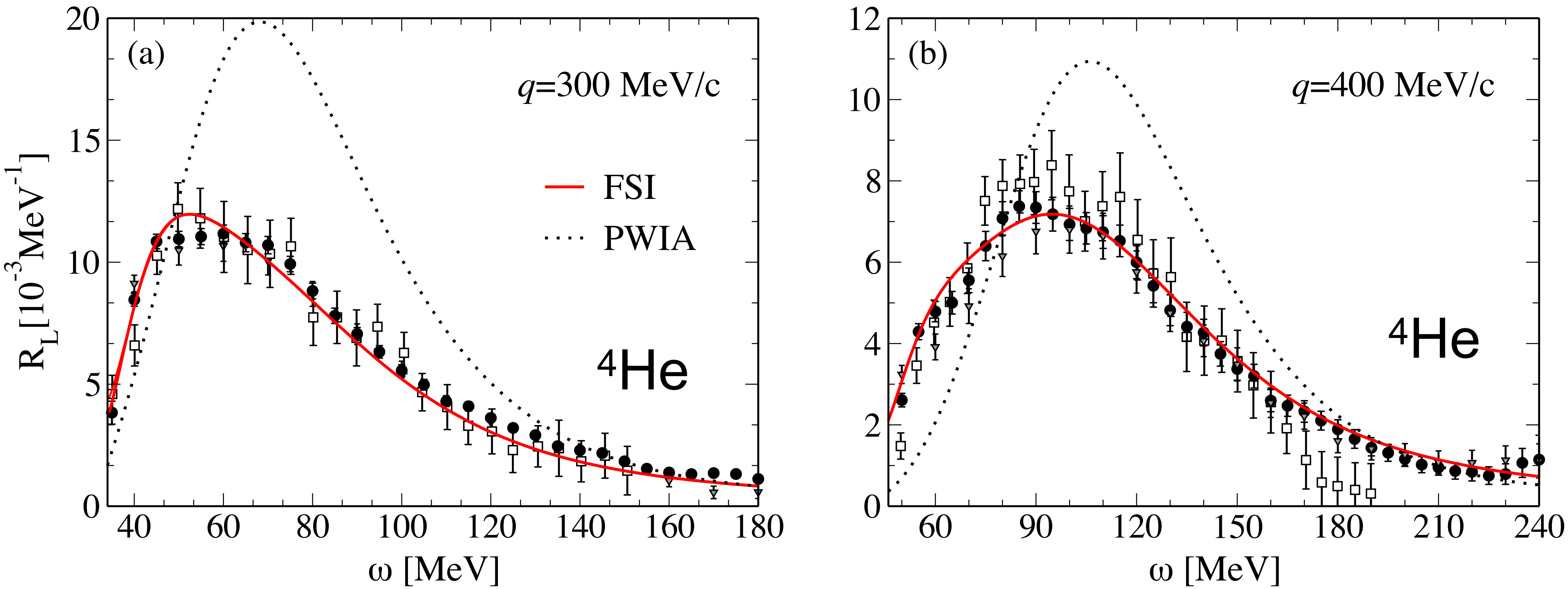
- Calculate every multipole on a grid of q
- Multipole expansion converges with finite number of multipoles
- Solve LIT equation for every multipole
- Invert LIT for every multipole and sum equiv to invert sum of LITs

Inelastic Electron Scattering

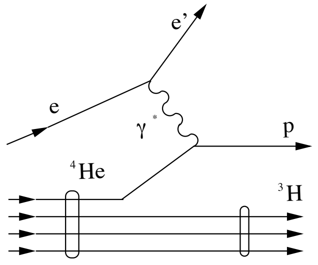
^{4}He with Hyper-spherical Harmonics

Final state interaction

SB *et al.*, PRL **102**, 162501 (2009)



PWIA



Full FSI:

AV18+UIX

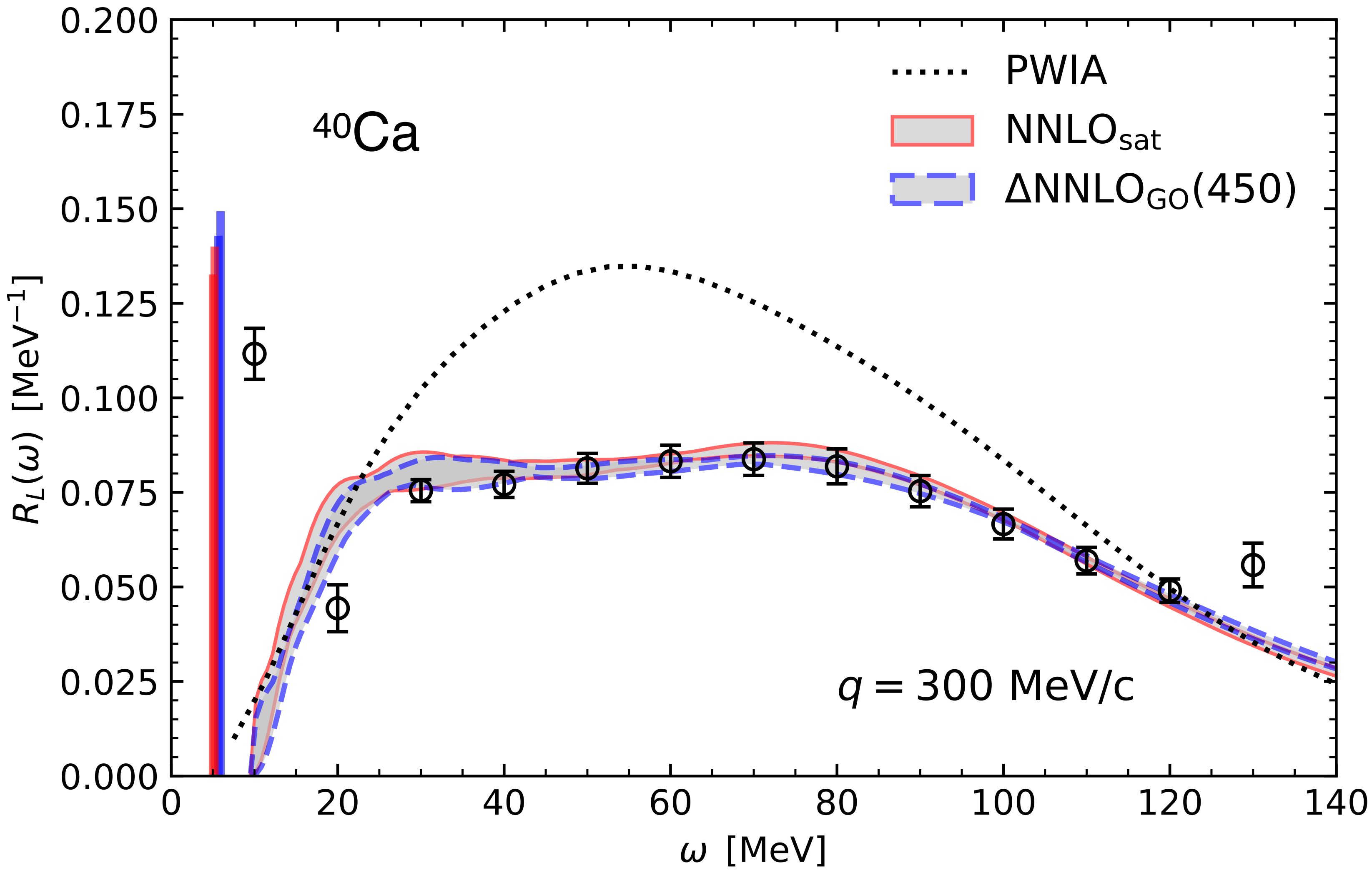
Strong effect of FSI: known form Carlson and Schiavilla PRL 68 (1992) and PRC 49 R2880 (1994) but now we can look at the energy dependence of FSI

Inelastic Electron Scattering

^{40}Ca with coupled-cluster theory

Final state interaction

Sobczyk, Acharya, SB, Hagen, PRL **127**, 072501 (2021)



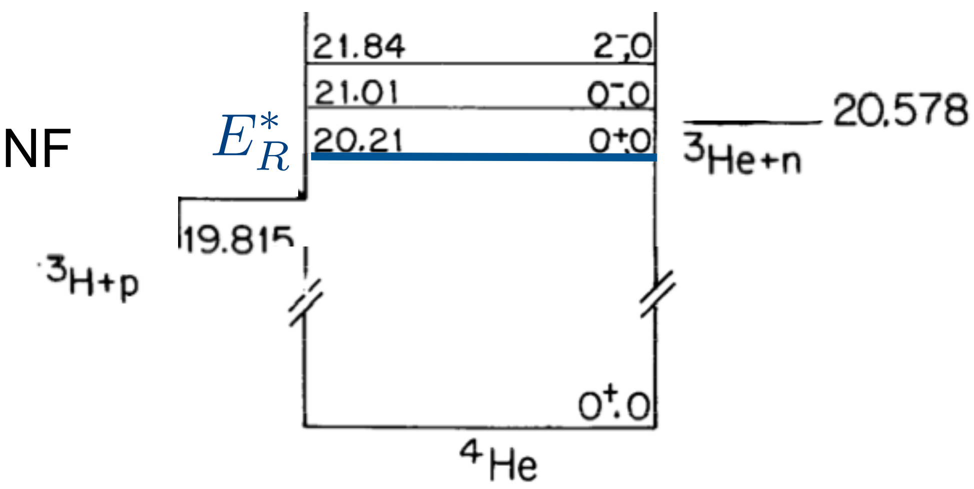
Monopole Resonance $^4He(e,e')0^+$

Resonant Transition Form Factor

$0_1^+ \longrightarrow 0_2^+$

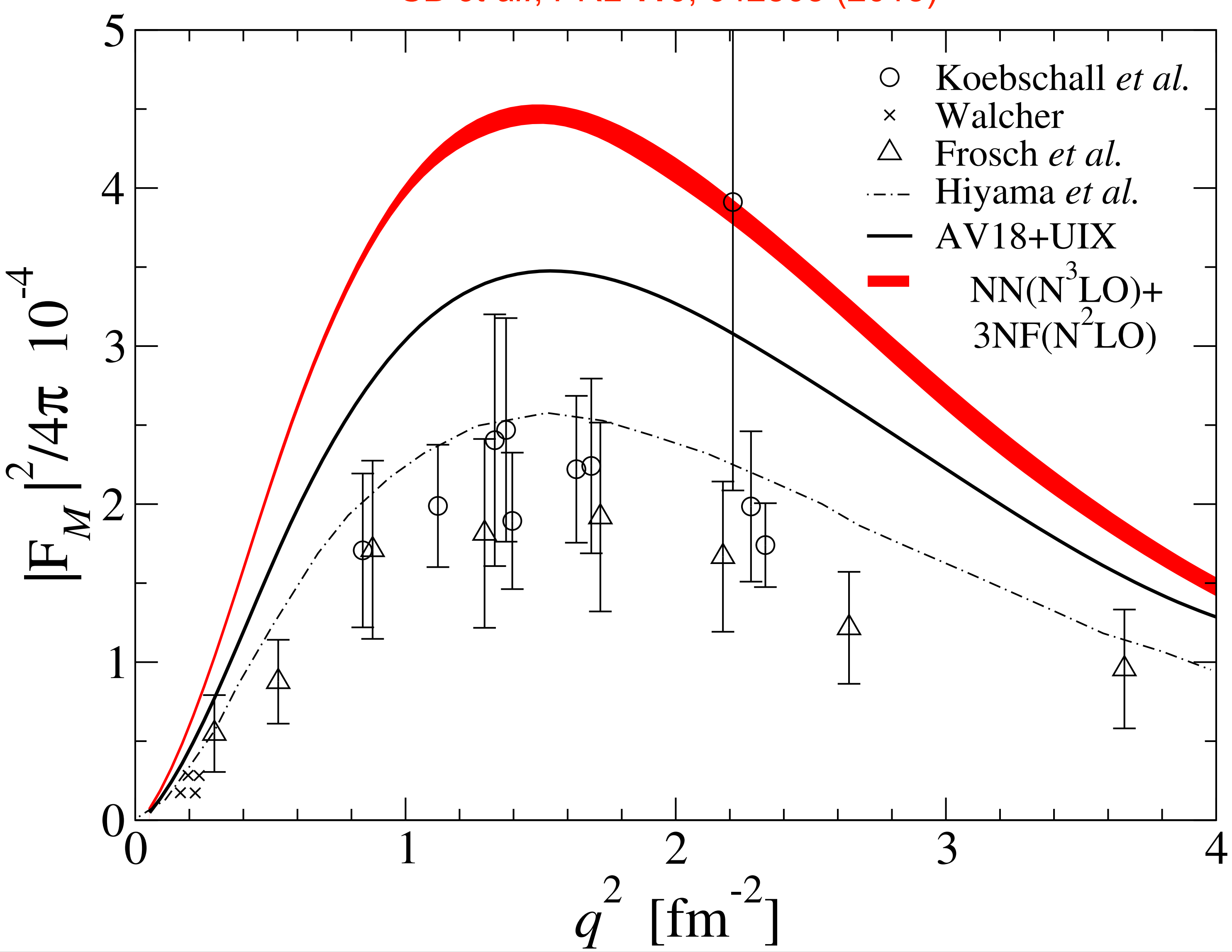
$$|F_{\mathcal{M}}(q)|^2 = \frac{1}{Z^2}\int d\omega R_{\mathcal{M}}^{\mathrm{res}}(q,\omega)$$

First ab-initio calculation: Hiyama *et al.*, PRC **70** 031001 (2004) obtained good description of data with phenomenological central 3NF but not with realistic forces



$\Gamma_R = 270 \pm 70$ keV

SB *et al.*, PRL **110**, 042503 (2013)



conventional forces

EFT forces

Central 3N force

Pronounced sensitivity to the input Hamiltonian

Monopole Resonance $^4He(e,e')0^+$

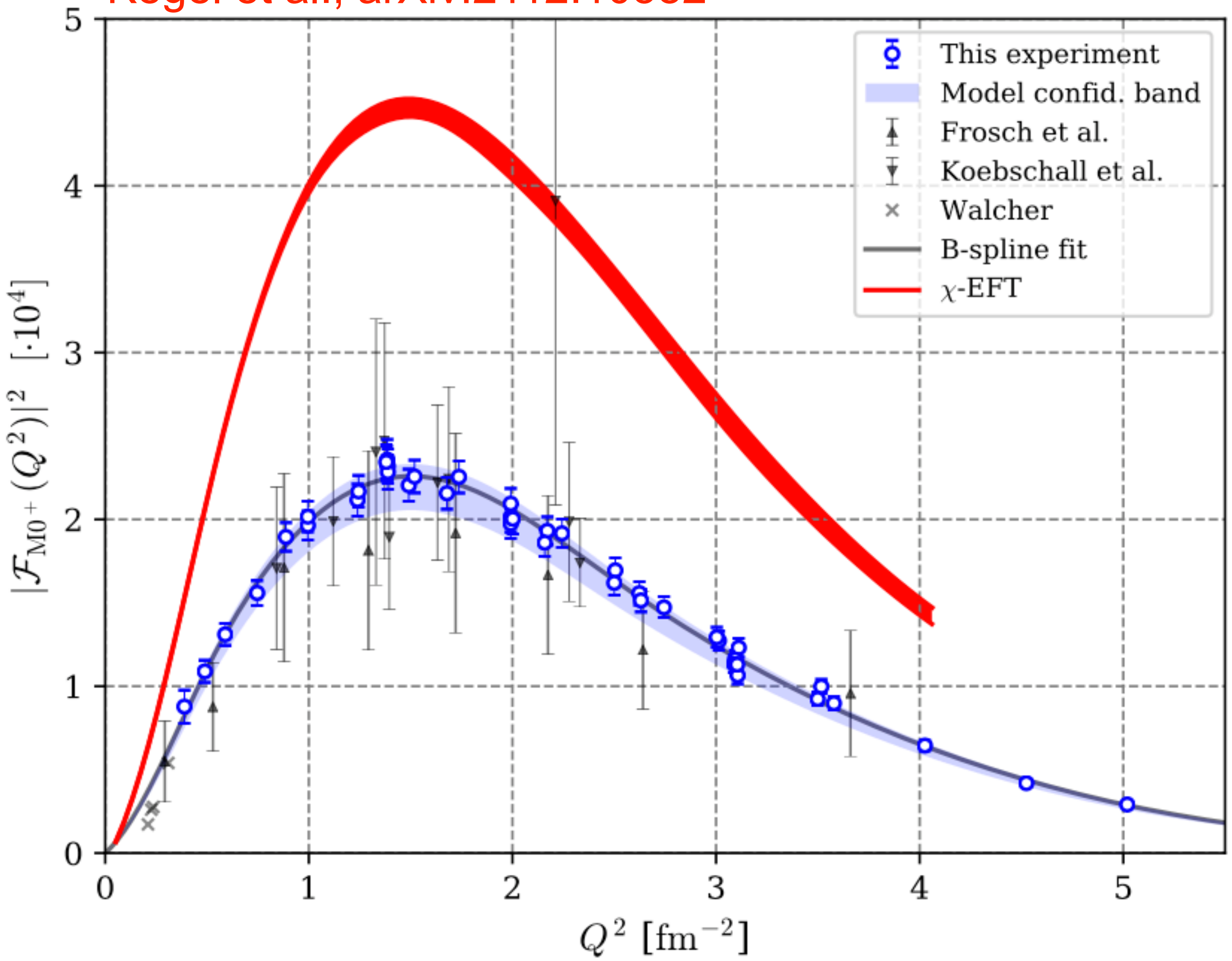
Resonant Transition Form Factor

$0_1^+ \longrightarrow 0_2^+$

$$|F_{\mathcal{M}}(q)|^2 = \frac{1}{Z^2}\int d\omega R_{\mathcal{M}}^{\text{res}}(q,\omega)$$

New electron scattering experiment was performed at MAMI in Mainz

Kegel et al., arXiv:2112.10582



Disagreement now is even stronger!
Probably a problem of the Hamiltonian

Thank you for your attention