Recent Results with the Lorentz Integral Transform (LIT) Method

Outline

- Introduction
- Electron scattering off $^{3,4}He$
- Energy resolution in the LIT approach
- Role of 0^+ resonance in $^4He(e,e')$

Introduction

Consider an observable R(E) and an integral transform $\Phi(\sigma)$:

$$\Phi(\sigma) = \int dE\, K(\sigma,E)\, R(E)$$

with some kernel $K(\sigma,E)$

Often it is easier to calculate $\Phi(\sigma)$ than R(E). Then the observable R(E) can be obtained via inversion of the integral transform.

In order to make the inversion sufficiently stable the kernel $K(\sigma,E)$ should resemble a kind of energy filter (Lorentzians, Gaussians, ...); best choice would be a δ-function.

Introduction

Consider an observable R(E) and an integral transform $\Phi(\sigma)$:

$$\Phi(\sigma) = \int dE\, K(\sigma,E)\, R(E)$$

with some kernel $K(\sigma,E)$

Often it is easier to calculate $\Phi(\sigma)$ than R(E). Then the observable R(E) can be obtained via inversion of the integral transform.

In order to make the inversion sufficiently stable the kernel $K(\sigma,E)$ should resemble a kind of energy filter (Lorentzians, Gaussians, ...); best choice would be a δ-function.

For the LIT we consider Lorentzians: $K(\sigma,E) = [(E-\sigma_R)^2 + \sigma_I^2]^{-1}$

LIT - Inclusive Reactions

Cross section described by response functions R(ω)

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

1. Solve for many ω_0 and fixed Γ

$$(H - E_0 - \omega_0 + i\Gamma)\,\tilde{\Psi} = \Theta\,|0\rangle$$

LIT - Inclusive Reactions

Cross section described by response functions R(ω)

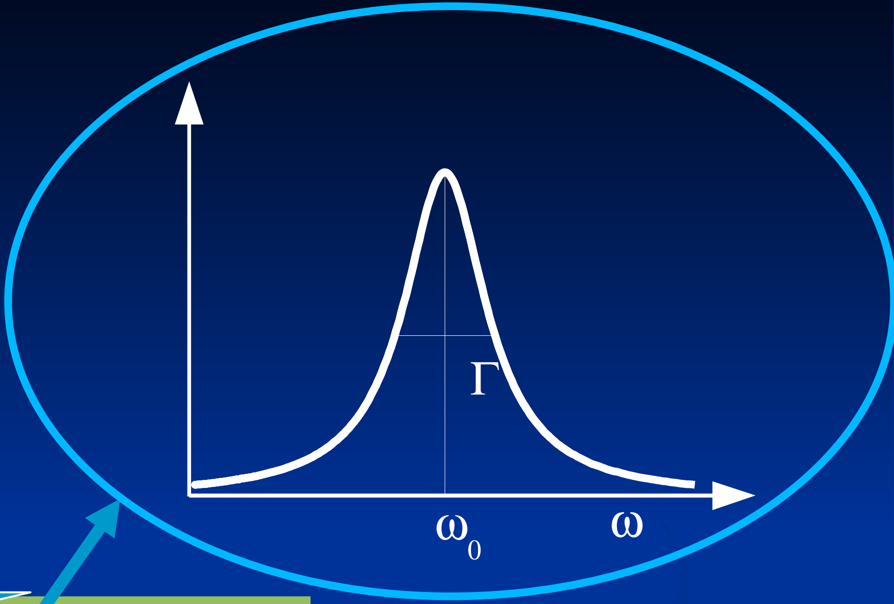
$$R(\omega) = \sum\!\!\!\!\!\!\int_n |\langle n|\Theta|0\rangle|^2 \, \delta(\omega - E_n + E_0)$$

Electron scattering: longitudinal (R_L) and transverse (R_T) responses with nuclear charge and current operators, respectively

1. Solve for many ω_0 and fixed Γ

$$(H - E_0 - \omega_0 + i\Gamma)\,\tilde{\Psi} = \Theta\,|0\rangle$$

2. Calculate



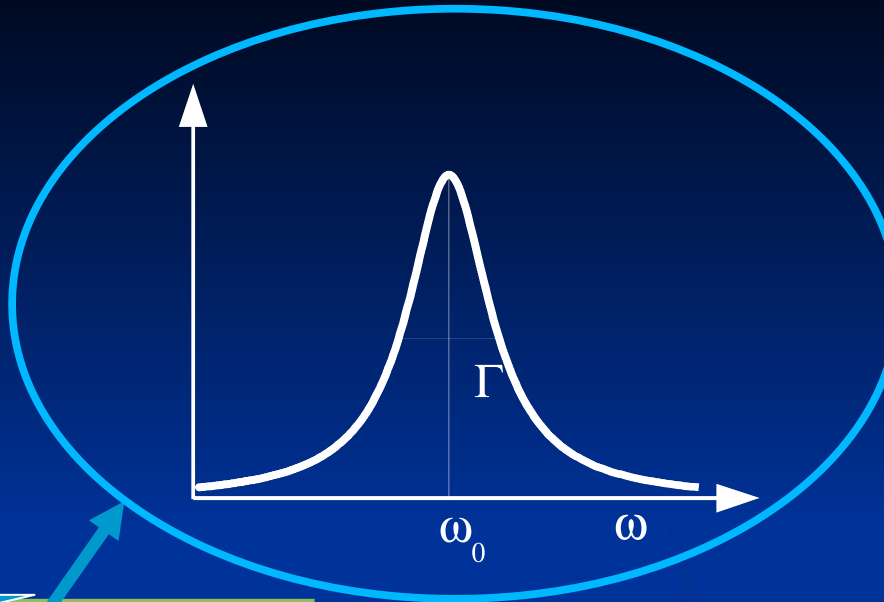
for given ω_0 and Γ

$$\left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle = \int R(\omega) L(\omega, \omega_0, \Gamma) d\omega$$

for a Theorem based on closure

3. Invert transform

2. Calculate



for given
ω_0 and Γ

$$\left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle = \int R(\omega) L(\omega, \omega_0, \Gamma) d\omega$$

for a Theorem based on closure

3. Invert transform

Normally we replace
ω_0 by σ_R and Γ by σ_I

main point of the LIT :

Schrödinger-like equation with a source

$$\left(H - E_0 - \omega_0 + i\Gamma\right)\tilde{\Psi} = S$$

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

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

Reformulation of the LIT

$$\mathrm{LIT}(\sigma_R,\sigma_I) = \mathrm{Im}\{\langle\Psi_0|\Theta^\dagger\,(\sigma_R + E_0 - H + i\,\sigma_I)^{-1}\,\Theta\,|\Psi_0\rangle\}$$

Reformulation of the LIT

$$\mathrm{LIT}(\sigma_R,\sigma_I) = \mathrm{Im}\{\langle\Psi_0|\Theta^\dagger\,(\sigma_R + E_0 - H + i\,\sigma_I)^{-1}\,\Theta\,|\Psi_0\rangle\}$$

with calculation via Lanczos algorithm

Reformulation of the LIT

$$\mathrm{LIT}(\sigma_R,\sigma_I) = \mathrm{Im}\{\langle\Psi_0|\Theta^\dagger\,(\sigma_R + E_0 - H + i\,\sigma_I)^{-1}\,\Theta\,|\Psi_0\rangle\}$$

with calculation via Lanczos algorithm

The LIT method seems to consist in a discretization of the continuum. However, this is not the proper interpretation, since the result can only be used correctly within an integral transform approach

First case: Transverse response function $R_T(q,\omega)$ of ^3He in the quasi-elastic region

First case: Transverse response function $R_T(q,\omega)$ of ^{3}He in the quasi-elastic region

Nuclear current operator includes besides the usual non-relativistic one-body currents also meson exchange currents and Δ-isobar currents as well as relativistic corrections for the one-body current

First case: Transverse response function $R_T(q,\omega)$ of ^3He in the quasi-elastic region

Nuclear current operator includes besides the usual non-relativistic one-body currents also meson exchange currents and Δ-isobar currents as well as relativistic corrections for the one-body current

Calculation in active nucleon Breit (ANB) frame ($P_T = -Aq/2$) and subsequent transformation to laboratory system

First case: Transverse response function $R_T(q,\omega)$ of ^{3}He in the quasi-elastic region

Nuclear current operator includes besides the usual non-relativistic one-body currents also meson exchange currents and Δ-isobar currents as well as relativistic corrections for the one-body current

Calculation in active nucleon Breit (ANB) frame ($P_T = -Aq/2$) and subsequent transformation to laboratory system

Calculation of bound state wave function and solution of LIT equation with the help of expansions in correlated hyperspherical harmonics

First case: Transverse response function $R_T(q,\omega)$ of ^3He in the quasi-elastic region

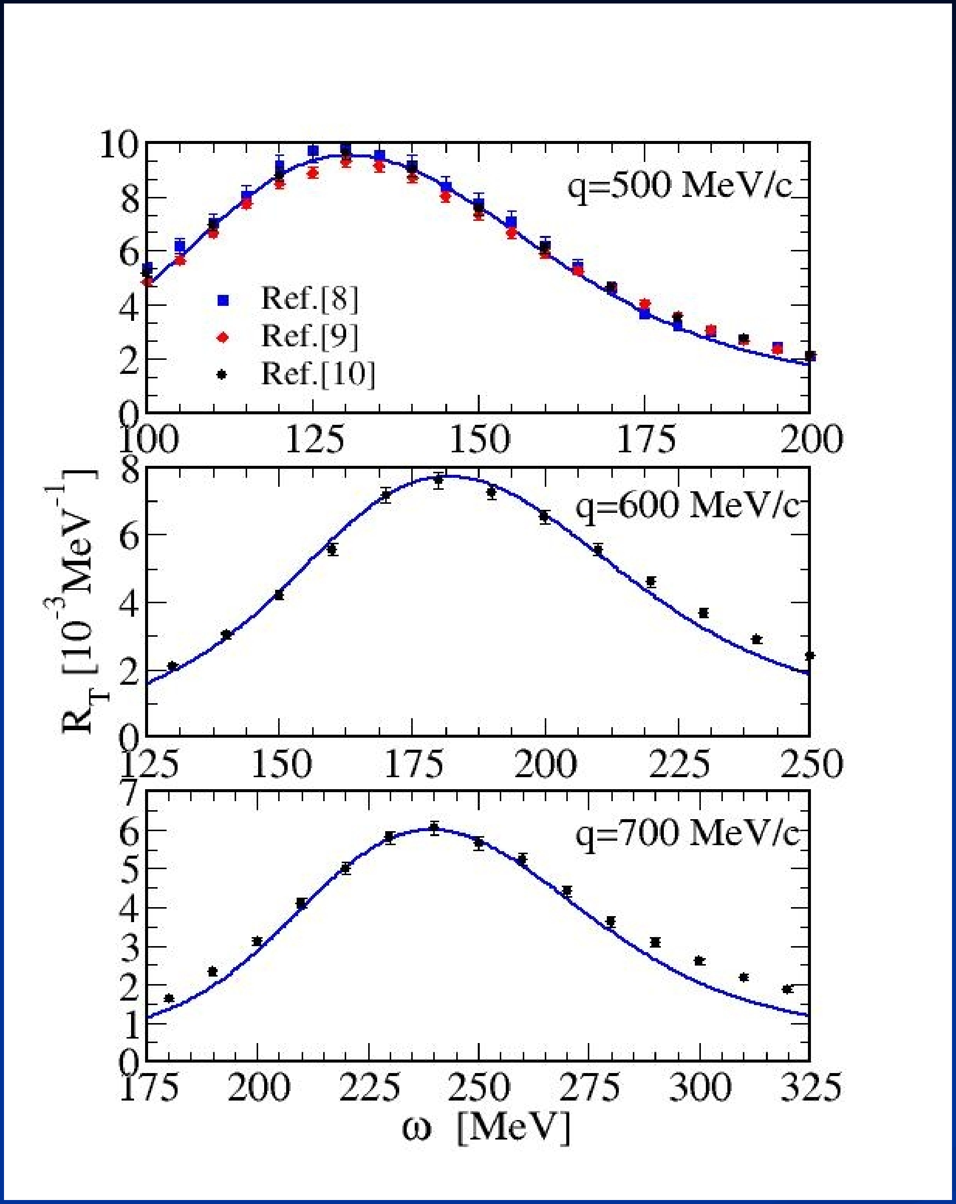
Nuclear current operator includes besides the usual non-relativistic one-body currents also meson exchange currents and Δ-isobar currents as well as relativistic corrections for the one-body current

Calculation in active nucleon Breit (ANB) frame ($P_T = -Aq/2$) and subsequent transformation to laboratory system

Calculation of bound state wave function and solution of LIT equation with the help of expansions in correlated hyperspherical harmonics

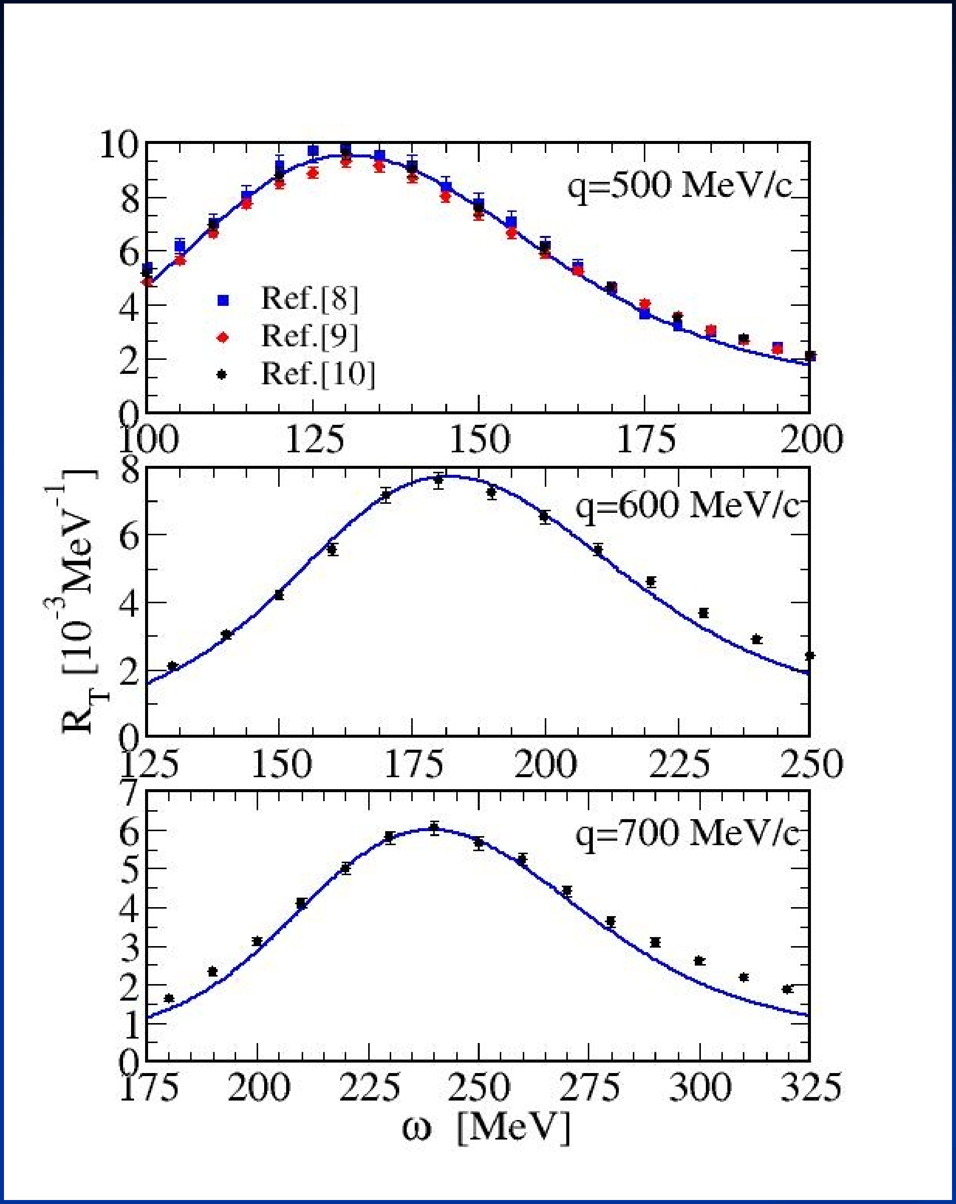
Nuclear force model: Argonne v18 NN potential and Urbana 3NF

Nuclear force model:



L. Yuan et al., PLB 706, 90 (2011)

Experimental data:
Bates, Saclay,
world data (J. Carlson et al.)



Strong Δ effects in T=3/2 channel beyond the peak

⇒

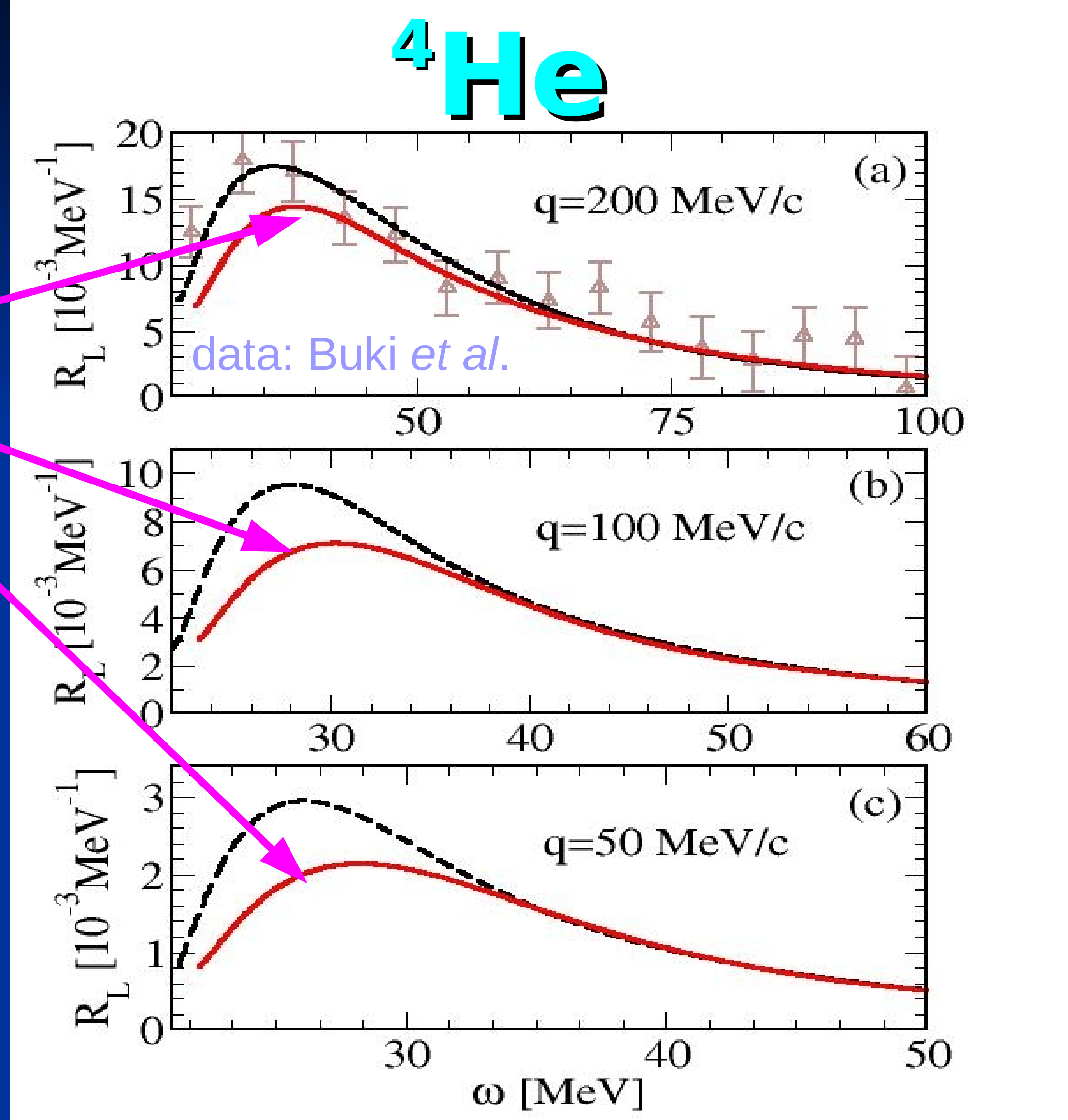
for this kinematics Δ effects are important in 3-body breakup reactions

Next case: Longitudinal response function $R_L(q,\omega)$ of ^{4}He at low q

(e,e') Longitudinal Response

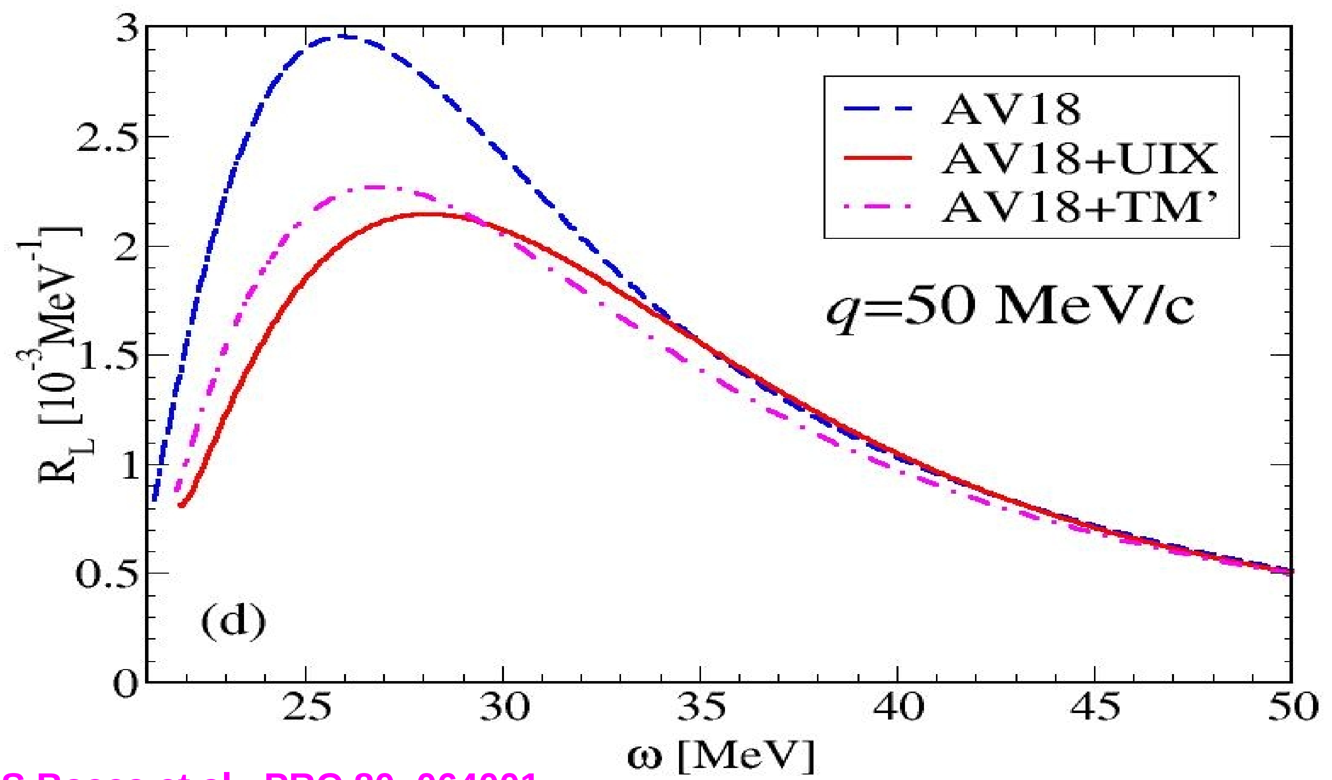
SURPRISE:
LARGE EFFECT OF 3-BODY FORCE
AT LOW q

Calculation via EIHH with force model: AV18 + UIX



S.Bacca et al., PRL 102, 162501

Dependence on different 3-nucleon forces



S.Bacca et al., PRC 80, 064001

Resolution of the LIT approach

Resolution of the LIT approach

The LIT approach is a method with a controlled resolution!

Resolution of the LIT approach

The LIT approach is a method with a controlled resolution!

Let's take deuteron photodisintegration as an example

LIT - Example

deuteron photodisintegration in unretarded dipole approximation

unretarded dipole approximation $\Rightarrow \Theta = \sum_{i=1}^{A} z_i \frac{1+\tau_{i,z}}{2}$,

z_i, $\tau_{i,z}$: 3rd componts of position and isospin coordinates

$\Rightarrow \quad \sigma_\gamma(\omega) = 4\pi^2 \alpha R(\omega)$ with $R(\omega) = \sum\!\!\!\!\!\!\int_f |\langle f| \Theta |0\rangle|^2 \delta(\omega - E_f - E_0)$

with $|0\rangle$ and E_0 bound-state wave function and energy

$|f\rangle$ and E_f final-state wave function and energy

LIT - Example

deuteron photodisintegration in unretarded dipole approximation

unretarded dipole approximation $\Rightarrow \Theta = \sum_{i=1}^{A} z_i \frac{1+\tau_{i,z}}{2}$,

z_i, $\tau_{i,z}$: 3rd componts of position and isospin coordinates

$\Rightarrow \quad \sigma_\gamma(\omega) = 4\pi^2 \alpha\, R(\omega) \quad$ with $\quad R(\omega) = \sum\!\!\!\!\!\!\int_f |\langle f|\, \Theta |0\rangle|^2\, \delta(\omega - E_f - E_0)$

with $|0\rangle$ and E_0 bound-state wave function and energy

$|f\rangle$ and E_f final-state wave function and energy

Possible np final states: $^3P_0$, $^3P_1$, $^3P_2$ - $^3F_2$

LIT - Example

deuteron photodisintegration in unretarded dipole approximation

unretarded dipole approximation $\Rightarrow \Theta = \sum_{i=1}^{A} z_i \frac{1+\tau_{i,z}}{2}$,

z_i, $\tau_{i,z}$: 3rd componts of position and isospin coordinates

$\Rightarrow \quad \sigma_\gamma(\omega) = 4\pi^2 \alpha R(\omega)$ with $R(\omega) = \sum\!\!\!\!\!\!\int_f |\langle f| \Theta |0\rangle|^2 \delta(\omega - E_f - E_0)$

with $|0\rangle$ and E_0 bound-state wave function and energy

$|f\rangle$ and E_f final-state wave function and energy

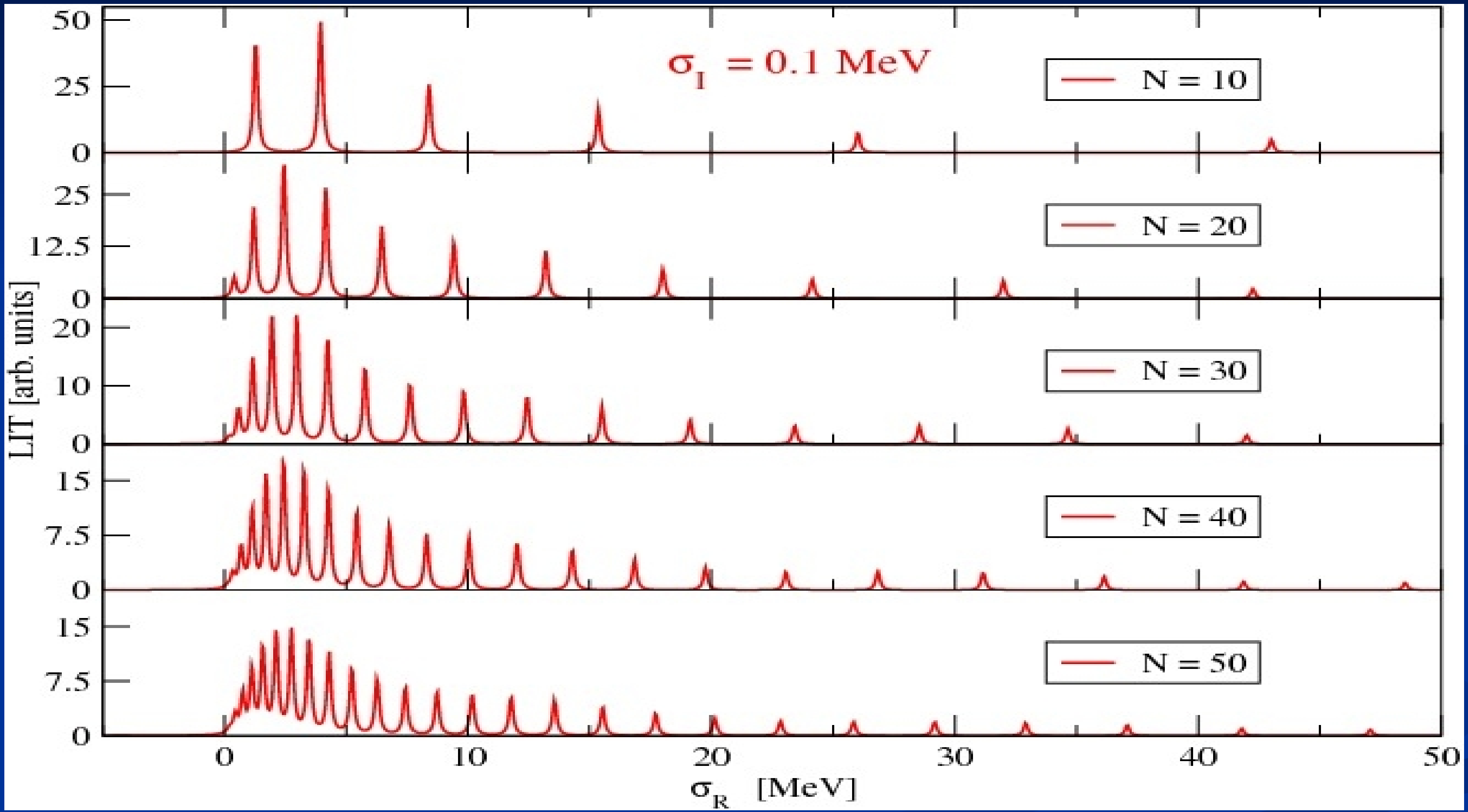
Possible np final states: $^3P_0$, $^3P_1$, $^3P_2$ - $^3F_2$

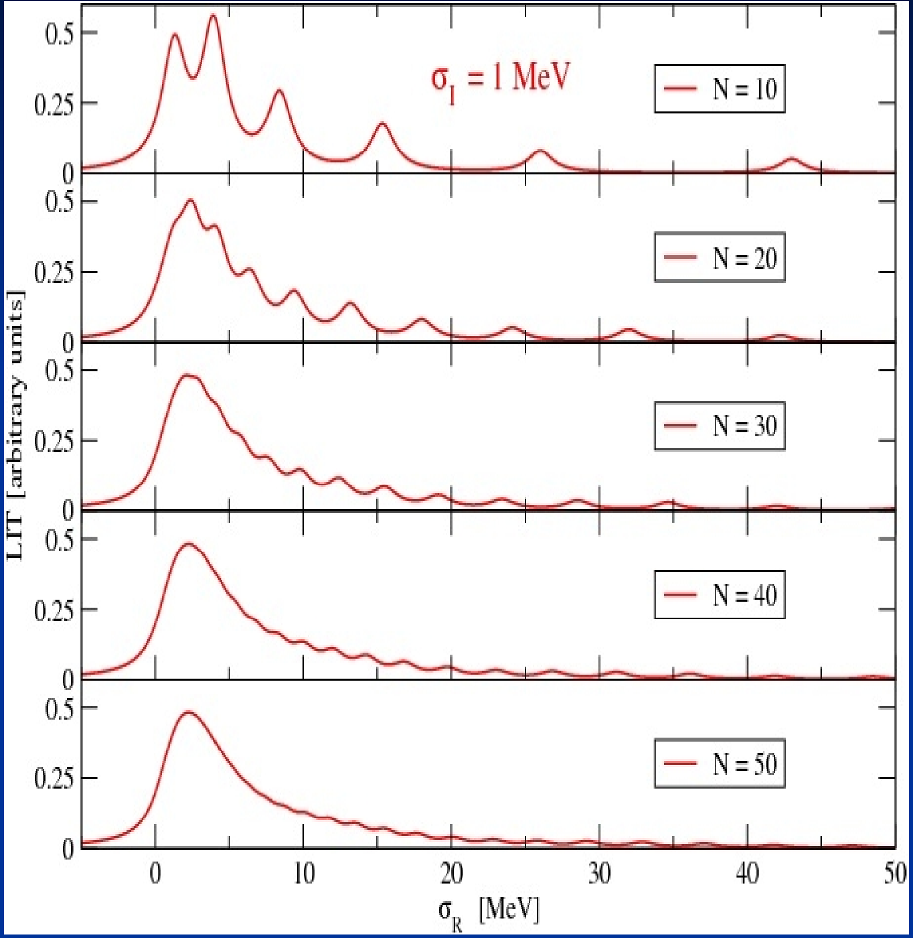
Radial part of LIT function is expanded in N Laguerre polynomials times an exponential fall-off

Consider only transitions to the $^3P_1$ np final state.

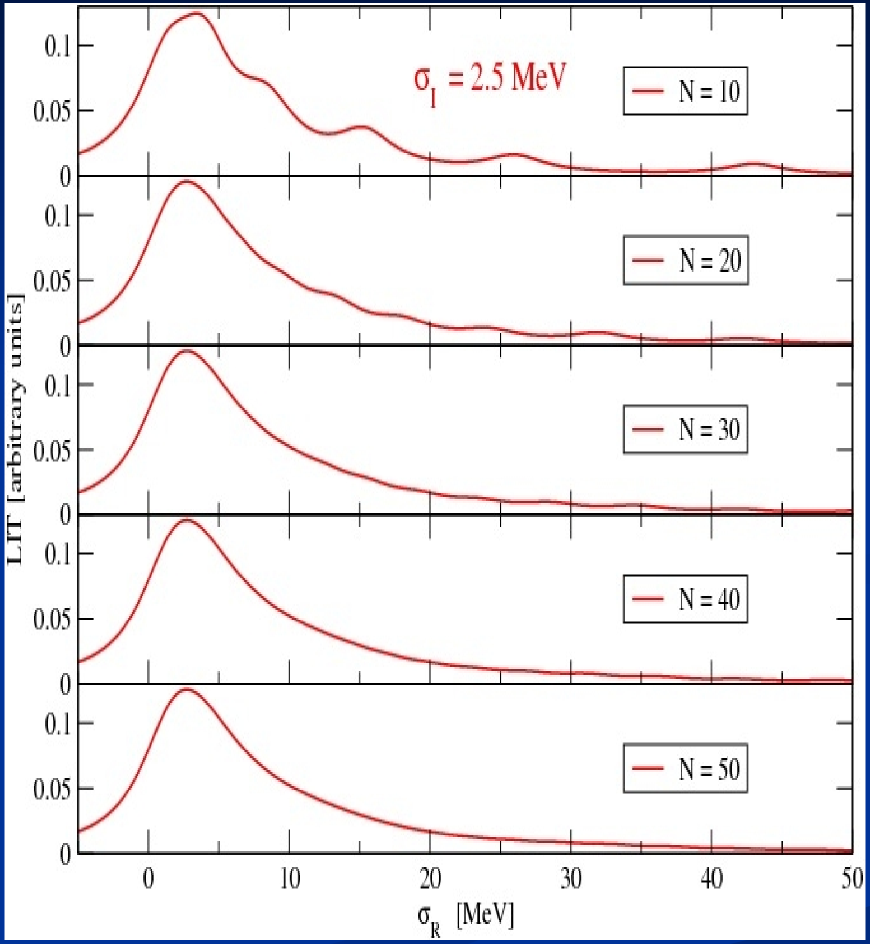
Consider only transitions to the $^3P_1$ np final state. This leads to the following LITs:

Consider only transitions to the $^3P_1$ np final state. This leads to the following LITs:

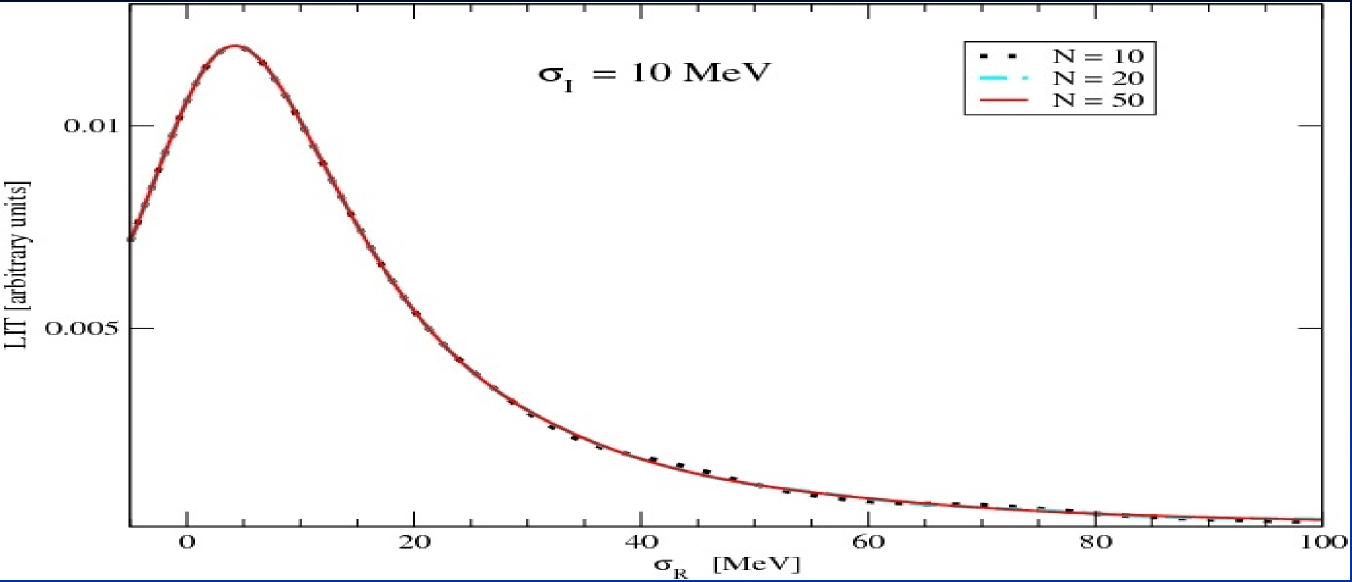


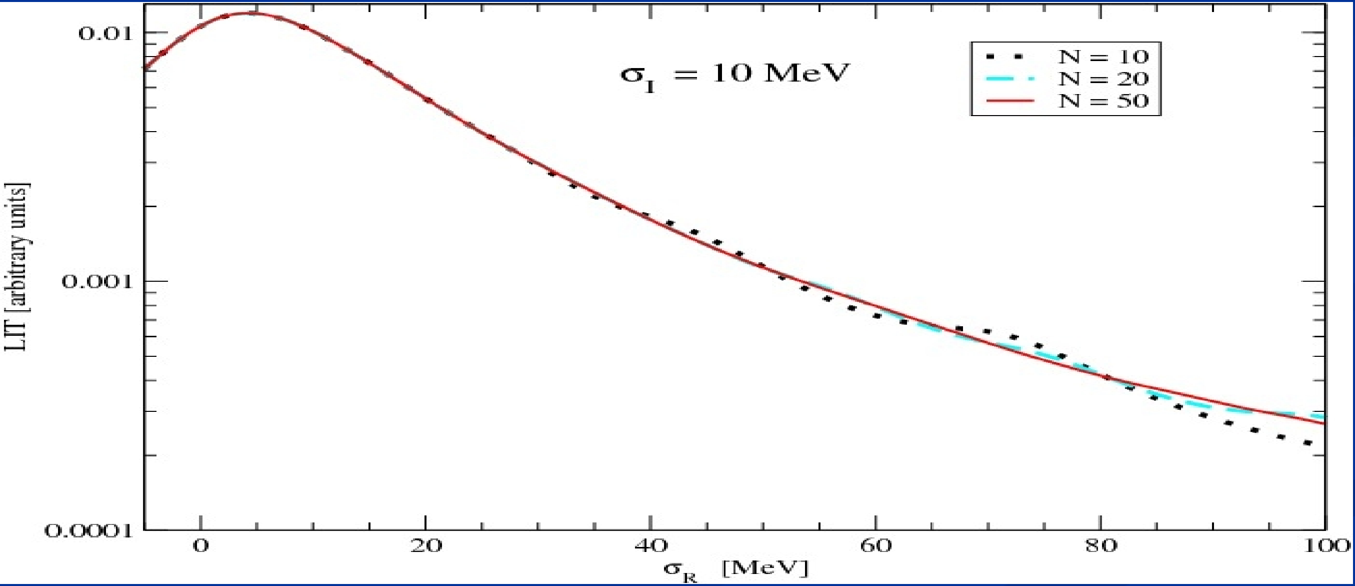


σ_I = 1 MeV
N = 10
N = 20
N = 30
N = 40
N = 50
LIT [arbitrary units]
σ_R [MeV]



σ_I = 2.5 MeV
N = 10
N = 20
N = 30
N = 40
N = 50
LIT [arbitrary units]
σ_R [MeV]


σ_I = 10 MeV
N = 10
N = 20
N = 50
0.01
0.005
LIT [arbitrary units]
0
20
40
60
80
100
σ_R [MeV]


σ_I = 10 MeV
N = 10
N = 20
N = 50
0.01
0.001
0.0001
LIT [arbitrary units]
0
20
40
60
80
100
σ_R [MeV]

Lanczos response

Since the Lorentzian function is a representation of the δ-function one could think of calculating R(ω) as the limit of $L(\omega,\sigma_R,\sigma_I)$ for $\sigma_I \longrightarrow 0$.

The extrapolation would give

$$R(\omega) = \sum_{\nu}^{N} r_{\nu}\, \delta(\omega - \varepsilon_{\nu}^{N})$$

Lanczos response

Since the Lorentzian function is a representation of the δ-function one could think of calculating R(ω) as the limit of $L(\omega,\sigma_R,\sigma_I)$ for $\sigma_I \rightarrow 0$.

The extrapolation would give

$$R(\omega) = \sum_\nu^N r_\nu \, \delta(\omega - \varepsilon_\nu^N)$$

Lanczos response: δ-function is replaced by Lorentzian with small σ_I

$$R(\omega) = \sum_\nu^N r'_\nu \, L(\omega, \varepsilon_\nu^N, \sigma_I)$$

Lanczos response

Since the Lorentzian function is a representation of the δ-function one could think of calculating R(ω) as the limit of $L(\omega,\sigma_R,\sigma_I)$ for $\sigma_I \rightarrow 0$.

The extrapolation would give

$$R(\omega) = \sum_\nu^N r_\nu \, \delta(\omega - \varepsilon_\nu^N)$$

Lanczos response: δ-function is replaced by Lorentzian with small σ_I

$$R(\omega) = \sum_\nu^N r'_\nu \, L(\omega, \varepsilon_\nu^N, \sigma_I)$$

Deuteron photodisintegration:

Consider all three transitions $^3P_0$, $^3P_1$, $^3P_2 - {}^3F_2$

now expansion of radial LIT part in HO functions

Lanczos response

Since the Lorentzian function is a representation of the δ-function one could think of calculating R(ω) as the limit of $L(\omega,\sigma_R,\sigma_I)$ for $\sigma_I \to 0$.

The extrapolation would give

$$R(\omega) = \sum_\nu^N r_\nu \, \delta(\omega - \varepsilon_\nu^N)$$

Lanczos response: δ-function is replaced by Lorentzian with small σ_I

$$R(\omega) = \sum_\nu^N r'_\nu \, L(\omega, \varepsilon_\nu^N, \sigma_I)$$

Deuteron photodisintegration:
Consider all three transitions $^3P_0$, $^3P_1$, $^3P_2 - {}^3F_2$
now expansion of radial LIT part in HO functions
NN potential: JISP6

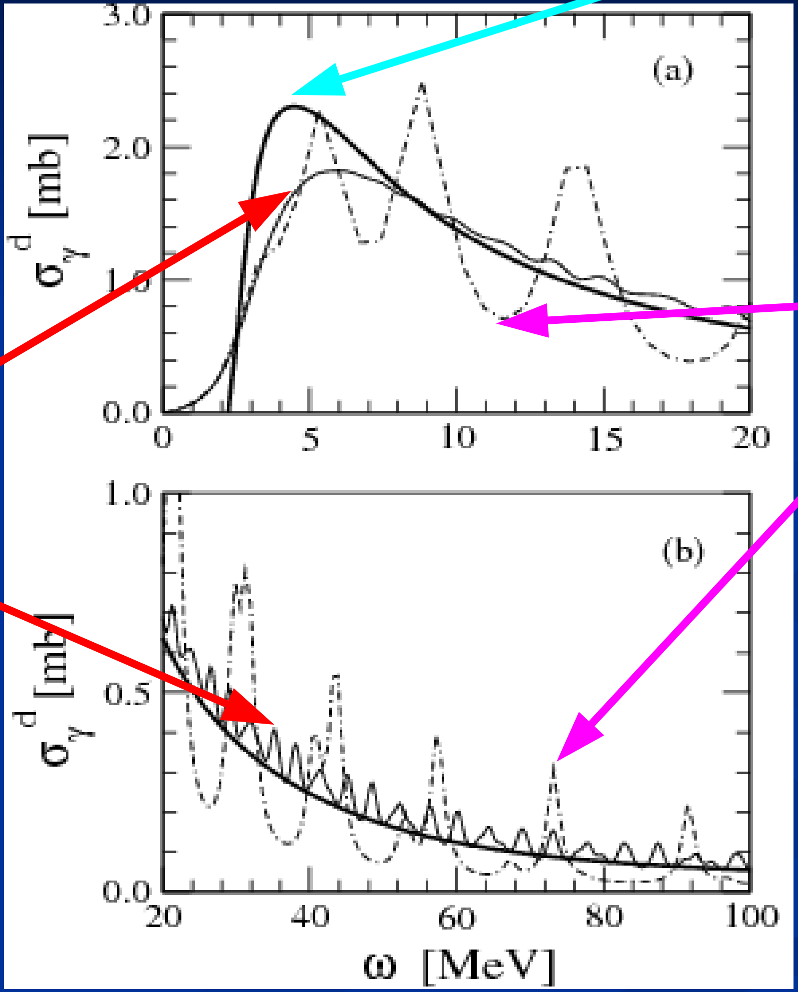
$\sigma_\gamma(\omega)$ from inversion and Lanczos response

"true"

σ_I=1 MeV

N_{ho}=2400

N_{ho}=150



$\sigma_\gamma(\omega)$ from inversion and Lanczos response

“true”

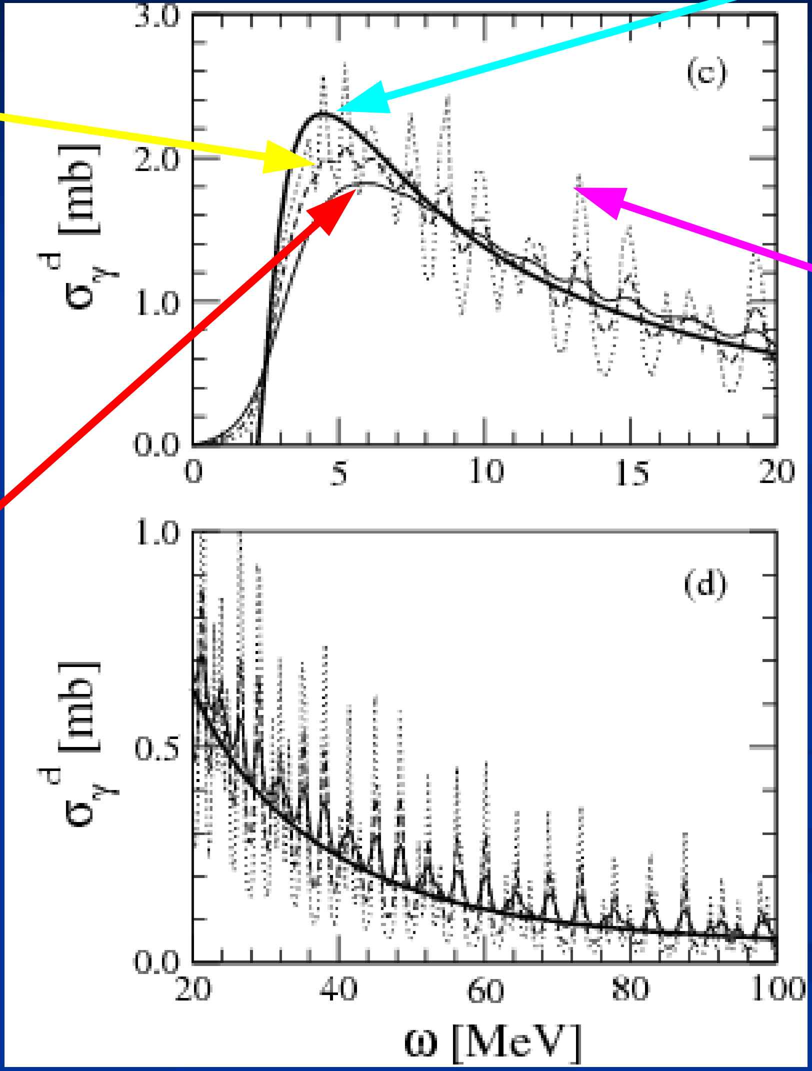
Γ= 0.5 MeV

HO basis:

fixed N_{HO}=2400

Γ=0.25 MeV

Γ=1 MeV



Conclusion

Strength for a given discrete state of energy E is not the actual strength for this energy, but can only be interpreted correctly within an integral transform approach.

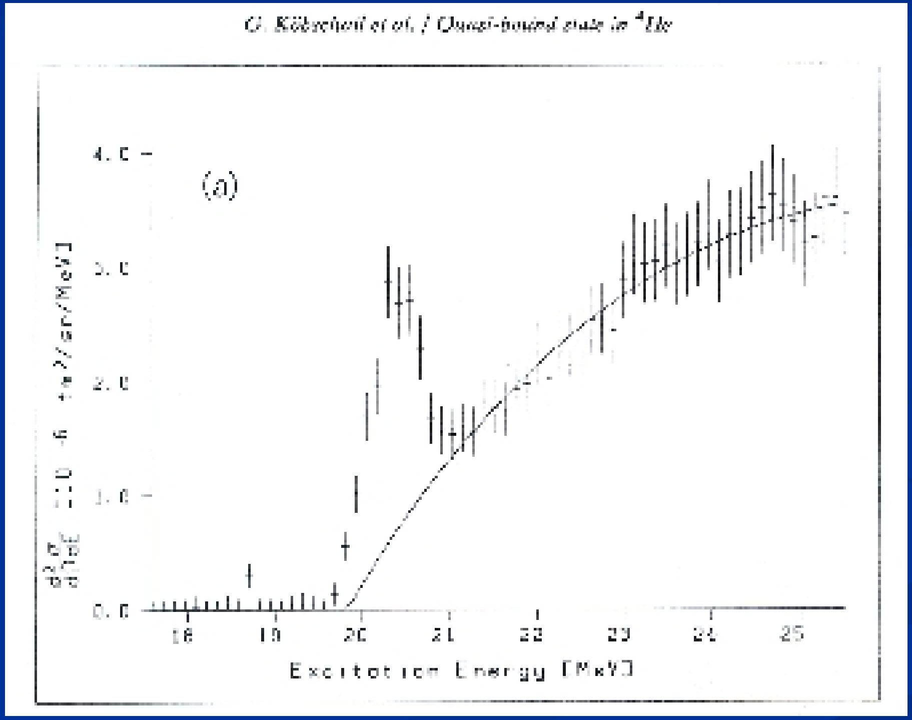
The correct distribution of strength is obtained via the inversion of the integral transform.

O$^+$ resonance in longitudinal response function R_L in ^{4}He(e,e')

S. Bacca, N. Barnea, WL, G. Orlandini, PRL 110, 042503 (2013)

0^+ Resonance in the ^{4}He compound system

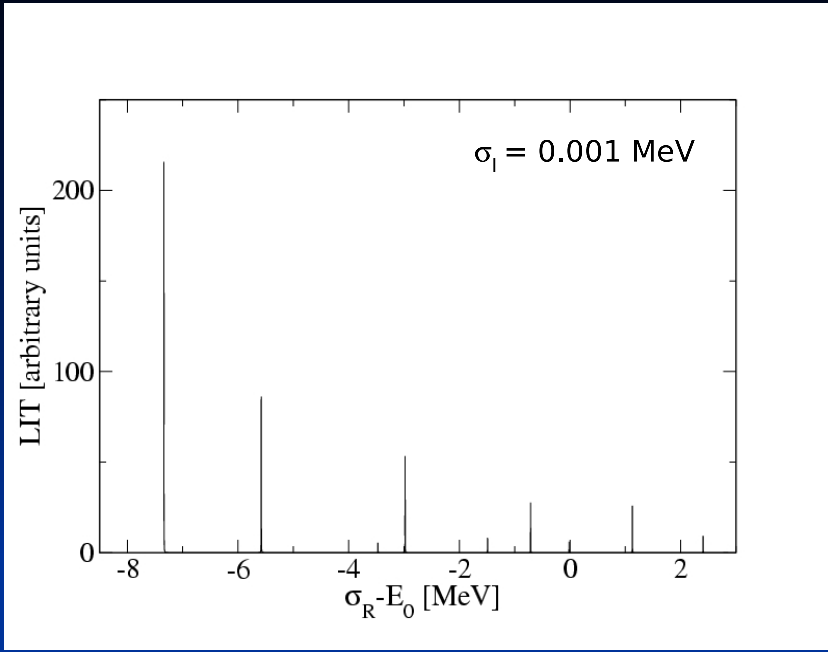
Resonance at E_R = -8.2 MeV, i.e. above the ^{3}H-p threshold. Strong evidence in electron scattering off ^{4}He

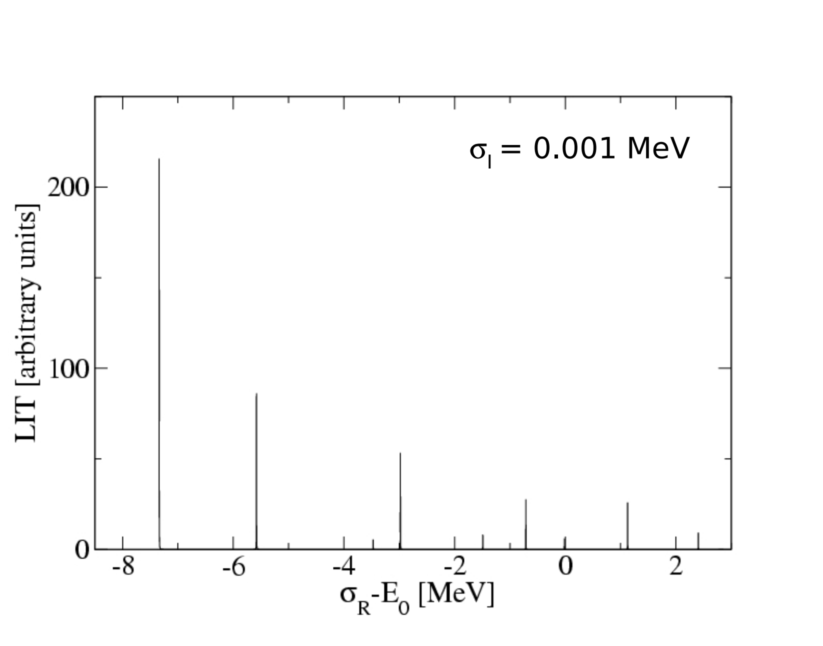


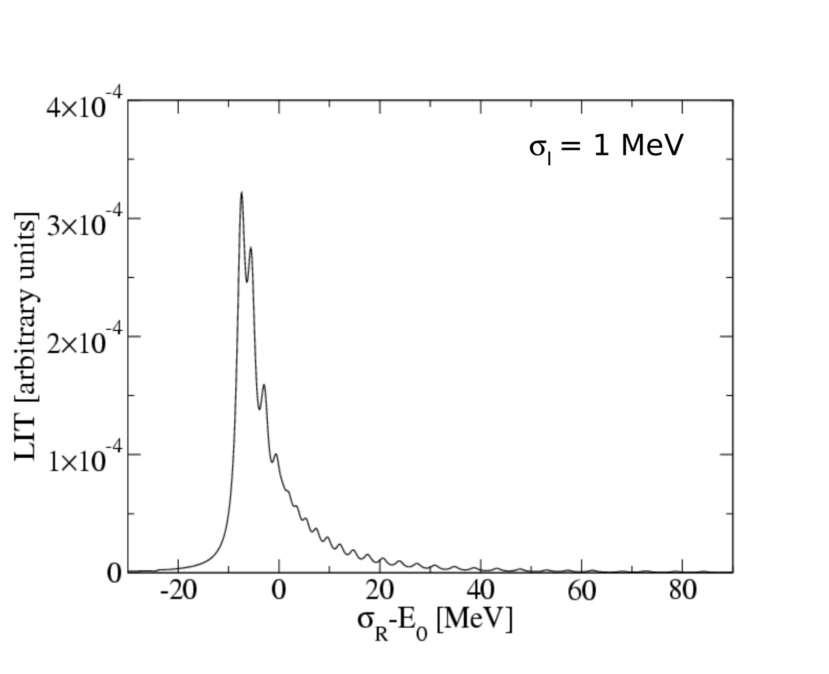
Γ = 270±70 keV

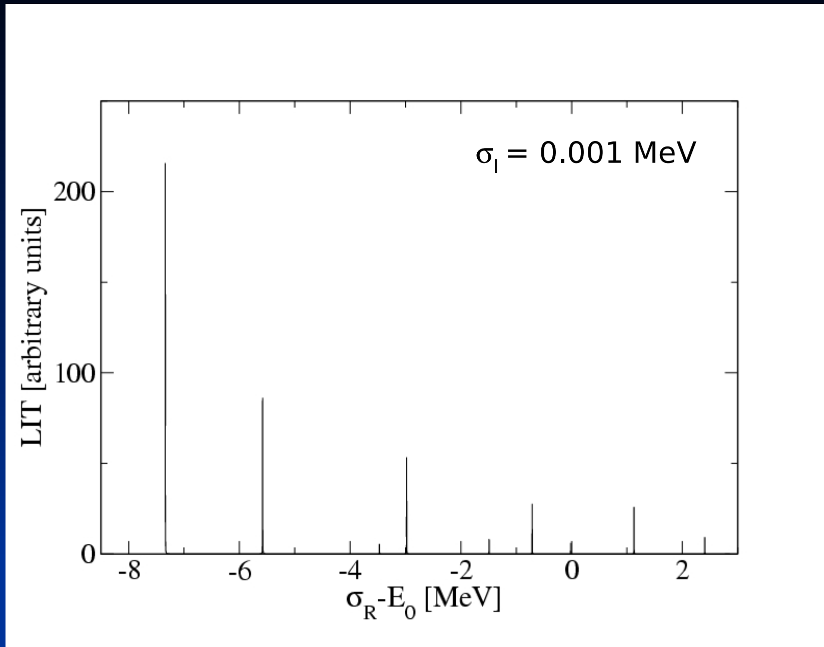
G. Köbschall et al., NPA 405, 648 (1983)

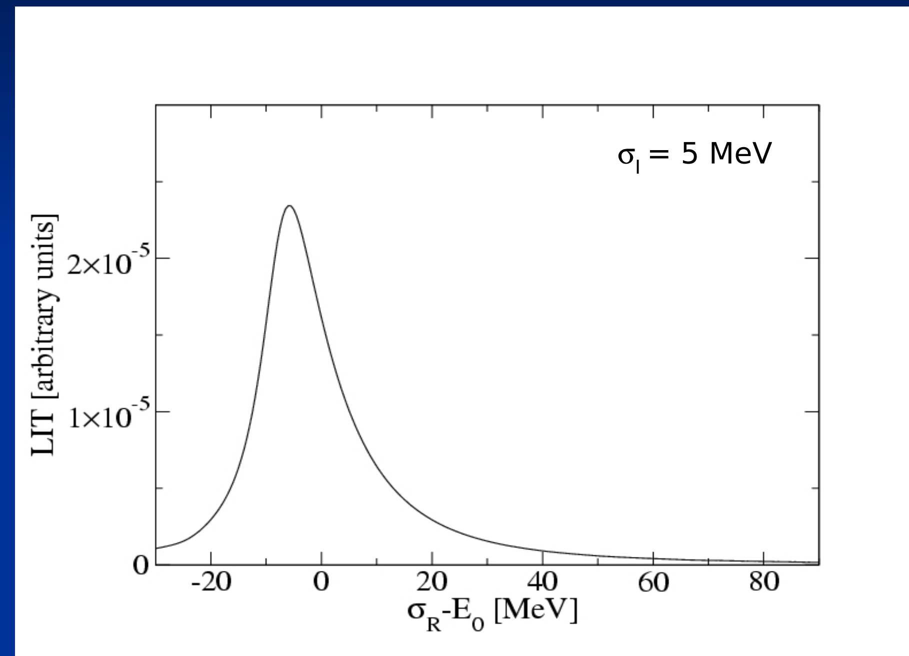
Results of our LIT calculation

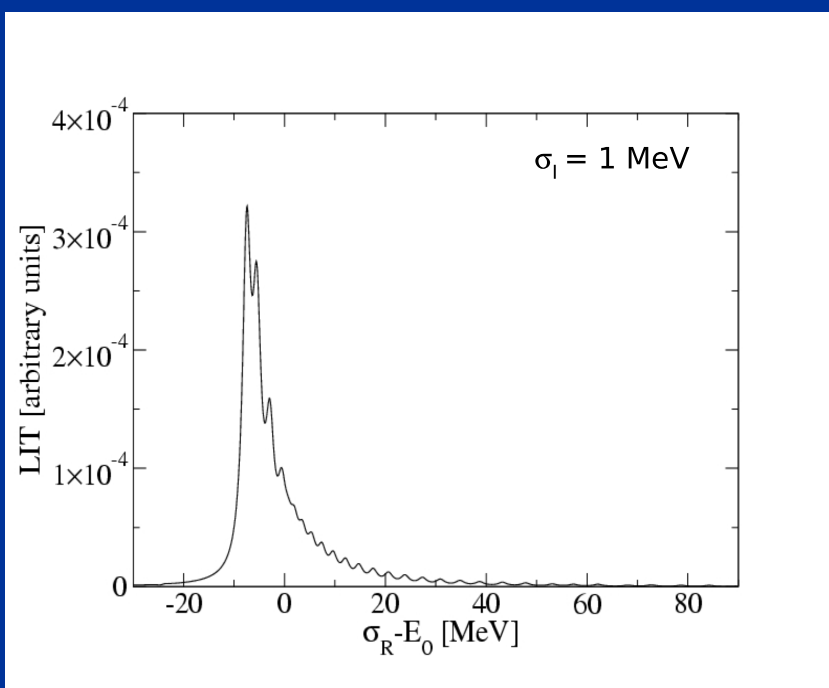

σI = 0.001 MeV
LIT [arbitrary units]
200
100
0
-8
-6
-4
-2
0
2
σR-E0 [MeV]


σ_I = 0.001 MeV
LIT [arbitrary units]
200
100
0
-8
-6
-4
-2
0
2
σ_R-E_0 [MeV]


σ_I = 1 MeV
LIT [arbitrary units]
4×10^-4
3×10^-4
2×10^-4
1×10^-4
0
-20
0
20
40
60
80
σ_R-E_0 [MeV]


σ_I = 0.001 MeV
LIT [arbitrary units]
200
100
0
-8
-6
-4
-2
0
2
σ_R-E_0 [MeV]


σ_I = 5 MeV
LIT [arbitrary units]
2×10^{-5}
1×10^{-5}
0
-20
0
20
40
60
80
σ_R-E_0 [MeV]


σ_I = 1 MeV
LIT [arbitrary units]
4×10^{-4}
3×10^{-4}
2×10^{-4}
1×10^{-4}
0
-20
0
20
40
60
80
σ_R-E_0 [MeV]

The present precision of the calculation does not allow to resolve the shape of the resonance, therefore the width cannot be determined.

The present precision of the calculation does not allow to resolve the shape of the resonance, therefore the width cannot be determined.

However, the strength of the resonance can be determined!

The present precision of the calculation does not allow to resolve the shape of the resonance, therefore the width cannot be determined.

However, the strength of the resonance can be determined!

Of course not by taking the strength to the discretized state, but by rearranging the inversion in a suitable way:

The present precision of the calculation does not allow to resolve the shape of the resonance, therefore the width cannot be determined.

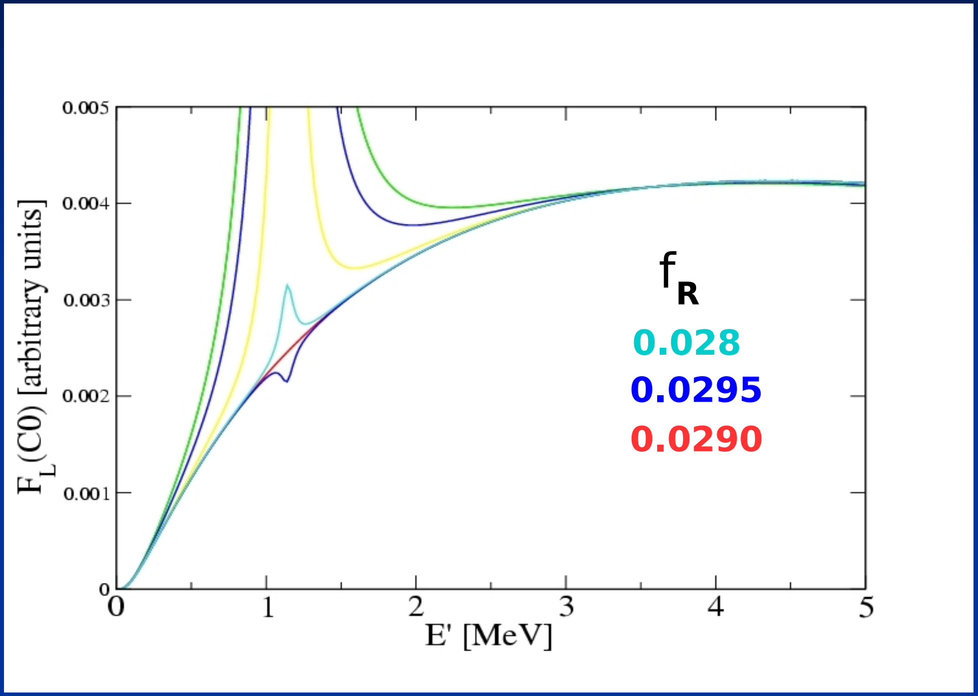
However, the strength of the resonance can be determined!

Of course not by taking the strength to the discretized state, but by rearranging the inversion in a suitable way:

Reduce strength to the state up to the point that the inversion does not show any resonant structure at the resonance energy $E_{\mathbf{R}}$:

$$\mathrm{LIT}(\sigma_R, \sigma_I) \rightarrow \mathrm{LIT}(\sigma_R, \sigma_I) - f_R \,/\, [(E_{\mathbf{R}} - \sigma_R)^2 + \sigma_I^2] \equiv \mathrm{LIT}(\sigma_R, \sigma_I, f_R)$$

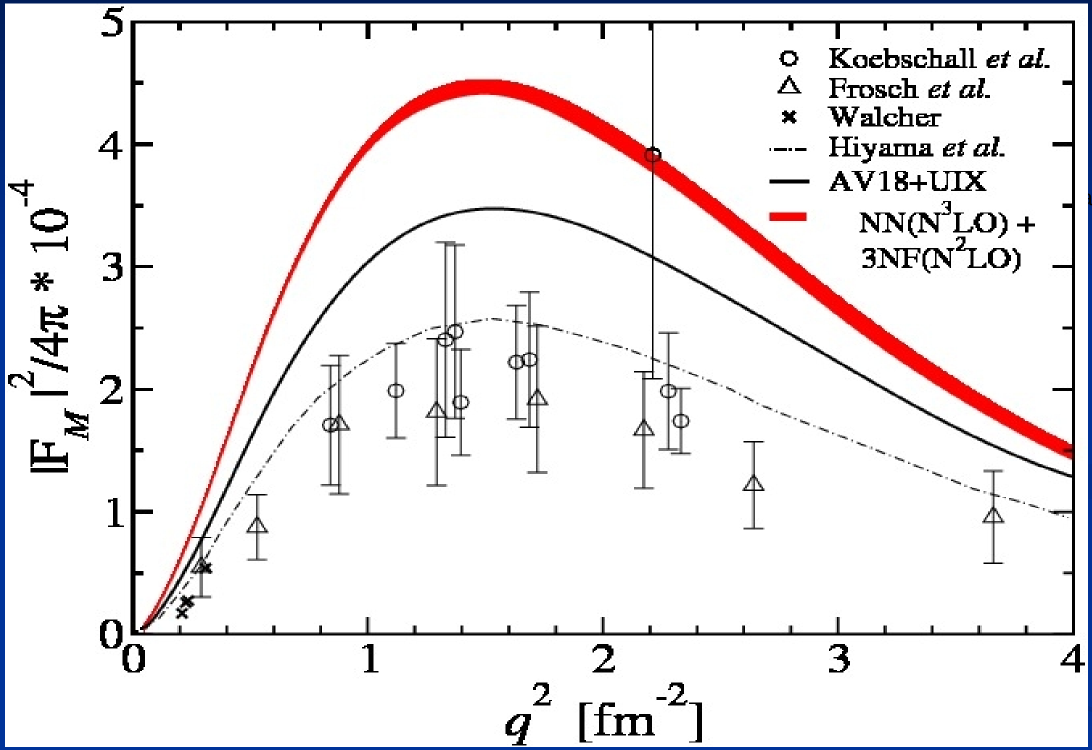
with resonance strength f_R



Inversion results with different f_R values

AV18+UIX, q=300 MeV/c

Comparison to experimental results



LIT/EIHH Calculation for AV18+UIX and Idaho-N3LO+N2LO

Dotted: AV8' + central 3NF (Hiyama et al.)

Summary

Ab initio calculations of reactions far into the continuum can be made with the LIT approach

Important: It is a method with a controlled resolution

LIT - Inversion

Standard LIT inversion method

Take the following ansatz for the response function $R(\omega)$ (or $F_{fi}(E,E')$)

$$R(\omega') = \sum_{m=1}^{M_{max}} c_m \, \chi_m(\omega',\alpha_i)$$

with $\omega'=\omega-\omega_{th}$, given set of functions χ_m , and unknown coefficients c_m

Define: $$\tilde{\chi}_m(\sigma_R,\sigma_I,\alpha_i) = \int_0^\infty d\omega' \, \frac{\chi_m(\omega',\alpha_i)}{(\omega'-\sigma_R)^2+\sigma_I^2}$$

Take calculated LIT $L(\sigma_R,\sigma_I) = \langle\tilde{\psi}|\tilde{\psi}\rangle$ for many σ_R and fixed σ_I

and expand in set $\tilde{\chi}_m$: $L(\sigma_R,\sigma_I) = \sum_{m=1}^{M_{max}} c_m \, \tilde{\chi}_m(\omega',\alpha_i)$

Determine c_m via best fit

Increase M_{max} up to the point that stable result is obtained for $R(\omega)$. Even further increase of M_{max} might lead to oscillations in $R(\omega)$

As basis set χ_m we normally use

$$\chi_m(\omega',\alpha_i) = (\omega')^{\alpha_1}\exp(-\alpha_2\omega'/m)$$

Determination of resonance strength f_R

Include in the inversion a basis function with resonant structure

$$\chi_1(E') = 1 \Big/ \left[(E_R - E')^2 + \Gamma^2 / 4 \right]$$

and check inversion result.