Approaches for Reactions in the Continuum

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Summary:

- General remarks on integral transform approaches
- The Lorentz kernel and the LIT method
- Selected results
- The Sumudu kernel and MonteCarlo techniques

Integral transform

Φ (σ) = ∫ dω K(ω,σ) **S(ω)**

Very useful if ONE IS NOT able to calculate $S(\omega)$, but ONE IS able to calculate Φ (σ)

Integral transform



Very useful if ONE IS NOT able to calculate $S(\omega)$, but ONE IS able to calculate Φ (σ)

One has to use the information $\Phi(\sigma)$ to achieve information on $S(\omega)$ (inversion of the transform)

a "good" Kernel has to satisfy two requirements

1) one must be able to calculate the integral transform

2) one must be able to reconstruct the function of interest (invert the transform)

A few examples:

A largely used IT In theoretical physics: $K(\omega,t) = e^{i\omega t}$ $\Phi(t) = \int e^{i\omega t} S(\omega) d\omega$ real t

the observable **S(m)** is often expressed as the imaginary part of a so called *"linear response"* or *" correlator"*

S(a) = Im
$$\left[\int \langle \Theta^{\dagger}(t) \Theta(0) \rangle \rangle e^{-i\omega t} dt \right]$$

A largely used IT In theoretical physics: $K(Q,\sigma) = e^{iQ\sigma}$ $\Phi(\sigma) = \int e^{iQ\sigma} S(Q) dQ$ real σ

the observable **S(Q)** is often expressed as the imaginary part of a so called "two-point function" or " correlator"

$$S(Q) = Im \left[\int \langle \Theta^{\dagger}(\mathbf{x}) \Theta(0) \rangle \rangle e^{-\iota \mathbf{Q} \times} d\mathbf{x} \right]$$

In 4-dimensions (field theory): $Q = (\omega, \vec{q})$

$\Phi(t) = \int e^{\iota \omega t} S(\omega) d\omega$ real t

 Φ (t) can be approached by the theory of moments:

$$\Phi(t) = \sum_{k} (-it)^{k}/k! \int d\omega \, \omega^{k} \, S(\omega) = \sum_{k} (-it)^{k}/k! \, m_{k}$$
Moments m_k

The knowledge of all moments corresponds to the knowledge of the FT of $S(\omega)$ and therefore of $S(\omega)$ itself

$\Phi(t) = \int e^{\iota \omega t} S(\omega) d\omega$ real t

 Φ (t) can be approached by the theory of moments:

$$\Phi(t) = \Sigma_k (-it)^k / k! \int d\omega \, \omega^k \, \mathbf{S}(\omega) = \Sigma_k (-it)^k / k! \, m_k$$
Moments m.

K

It may happen that one knows the $\mathbf{m}_{\mathbf{k}}$ (or at least a few of them) so one can either try to invert the (approx) Fourier Transform or parametrize **5**($\boldsymbol{\omega}$) and perform a best fit of the parameters to the few moments one knows

The moments themselves can be considered an IT: $K(\omega,\sigma) = \omega^{\sigma}$ with σ integer

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A reconstruction of $S(\omega)$ in terms of moments is equivalent to an "inversion" of this kind of IT

The cross section is proportional to

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

These states |n> are the problem !! They may be in the continuum (many-body scattering problem)

May we know the moments of $S(\omega)$ for positive σ ?

$$\mathbf{m}_{\sigma} = \mathbf{\Phi}(\sigma) = \int d\omega \, \omega^{\sigma} \, \mathbf{S}(\omega) =$$

May we know the moments of $S(\omega)$?

 $\mathbf{m}_{\sigma} = \mathbf{\Phi}(\sigma) = \int d\omega \, \omega^{\sigma} \, \mathbf{S}(\omega) =$ $= \int d\omega \, \omega^{\sigma} \, \mathbf{\Sigma}_{n} \, |\langle n| \, \Theta \, |0\rangle|^{2} \, \delta(\omega - E_{n} + E_{0})$

$$\sum_{n} |n > < n| = 1$$

$$= \int d\omega \, \omega^{\sigma} \, \Sigma_{n} \, |<\!n| \, \Theta \, |0\!>|^{2} \, \delta \, (\omega - E_{n} + E_{0})$$
$$= \sum_{n} < 0 \, | \, \Theta^{+} \, (E_{n} - E_{0})^{\sigma} \, |n\!><\!n| \Theta \, | \, 0\!>$$

$$\mathbf{m}_{\sigma} = \mathbf{\Phi}(\sigma) = \int d\omega \, \omega^{\sigma} \, \mathbf{S}(\omega) = 0$$

May we know the moments of $S(\omega)$?

 $\mathbf{m}_{\sigma} = \mathbf{\Phi}(\sigma) = \int d\omega \, \omega^{\sigma} \, \mathbf{S}(\omega) = 0$ $|=\int d\omega \,\omega^{\sigma} \Sigma_n |< n |\Theta| 0 > |^2 \delta (\omega - E_n + E_0)$ $= \sum_{n} < 0 | \Theta^{+} (E_{n} - E_{0})^{\sigma} | n > < n | \Theta | 0 >$ = < 0 | Θ^+ (H – E₀)^o Θ | 0> m $\Sigma_n |n > < n| = 1$ In principle, completeness of eigenstates allows to calculate moments as mean valuies on g.s. (bound state problems!)

May we know the moments of $S(\omega)$?

Unfortunately only few moments may exist.

$$\mathbf{m}_{\sigma} = \int d\omega \, \omega^{\sigma} \, \mathbf{S}(\omega) \, < \infty \, ??$$

Moreover the operator is more and more complicate as the degree of the moment σ increases

$\mathbf{m}_{\sigma} = \langle \mathbf{0} | \Theta^{+} (\mathbf{H} - \mathbf{E}_{0})^{\sigma} \Theta | \mathbf{0} \rangle$

 $\Phi(\sigma) = \int e^{\omega\sigma} S(\omega) d\omega$

real σ: Fourier Transform

Imaginary $\sigma = \iota \tau$: Laplace Transform

("IMAGINARY TIME" or "EUCLIDEAN" RESPONSES)

$$\Phi(\tau) = \int e^{-\omega \tau} S(\omega) d\omega$$

In Condensed Matter Physics: Θ = Density Operator $S(\omega)$ = "Dynamical Structure Function" $\Phi(\tau)$ is obtained with Monte Carlo Methods

In Nuclear Physics:

 Θ = Charge or current density operator $S(\omega) = R(\omega)$ "Response" Function $\Phi(\tau)$ is obtained with Monte Carlo Methods

In QCD

 Θ = quark or gluon creation operator $S(\omega)$ = Hadronic Spectral Function

 Φ (τ) is obtained by moments (OPE - QCD sum rules) or Lattice QCD

Problem: The "inversion" of Φ (τ) may be problematic ("ill posed problem")

It is well known that the numerical inversion of the **Laplace** Transform is a terribly **ill-posed** problem



What is the perfect Kernel?

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the delta-function!

What would be the "perfect" Kernel?

the delta-function!

in fact

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

The **LIT method** is based on the idea to use as kernel one of the "**representations of the delta-function**"

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The LIT Kernel is: $K(\omega,\sigma) \sim [(\omega - \sigma)(\omega + \sigma^*)]^{-1}$ with σ complex: $\sigma = \sigma_R + i \sigma_I$ $K(\omega, \sigma) = \sigma_I / \pi [(\omega - \sigma)(\omega + \sigma^*)]^{-1} = \sigma_I / \pi [(\omega - \sigma_R)^2 + \sigma_I^2]^{-1}$



The Lorentz Kernel satisfies the two requirements !

N.1. one can calculate the integral transform

N.2 one is able to invert the transform, minimizing instabilities (controlled resolution regularization)

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

THEOREM (based on completeness property of H eigenstates):



 $\Phi(\sigma_{\rm R},\sigma_{\rm I}) = \sigma_{\rm I}/\pi \int \left[(\omega - \sigma_{\rm R})^2 + \sigma_{\rm I}^2\right]^{-1} \, \mathbf{S}(\omega) \, \mathrm{d}\omega \, < \infty$

$$\Phi(\sigma_{R},\sigma_{I}) = \left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle$$

where

$$\left(H-E_{0}-\sigma_{_{\mathrm{R}}}+\mathrm{i}\;\sigma_{_{\mathrm{I}}}
ight)\tilde{\Psi}=\Theta\left|0
ight
angle$$

main point of the LIT :

Schrödinger-like equation with a source $(H - E_0 - \sigma_{\rm R} + i \sigma_{\rm I}) \tilde{\Psi} = \Theta |0\rangle$

Theorem:

The $\tilde{\Psi}$ solution is unique and has **bound state** asymptotic behavior one can apply **bound state methods**

The cross section is proportional to

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

 $\overline{\mathbf{S}(\boldsymbol{\omega})} = -1/\pi \operatorname{Im}\left[\sum_{n} <\mathbf{0} |\Theta^{+}| \mathbf{n} > <\mathbf{n}\right] \Theta |\mathbf{0} > (\boldsymbol{\omega} - \mathbf{E}_{0} + \iota \varepsilon)^{-1}]$

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$$\begin{aligned} \mathbf{S}(\mathbf{\omega}) &= -1/\pi \operatorname{Im} \left[\sum_{n} <0 |\Theta^{+}| n > < n | \Theta | 0 > (\omega - E_{0} + \iota \varepsilon)^{-1} \right] \\ &= -1/\pi \operatorname{Im} \left[\sum_{n} <0 | \Theta^{+}(H - E_{0} + \iota \varepsilon)^{-1} | n > < n | \Theta | 0 > \right] \\ &= -1/\pi \operatorname{Im} \left[<0 | \Theta^{+}(H - E_{0} + \iota \varepsilon)^{-1} \Theta | 0 > \right] \end{aligned}$$

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 $\begin{aligned} \mathbf{S}(\boldsymbol{\omega}) &= -1/\pi \operatorname{Im} \left[\sum_{n} <0 |\Theta^{+}| n > < n | \Theta | 0 > \right] (\boldsymbol{\omega} - \mathbf{E}_{0} + \iota \varepsilon)^{-1} \\ &= -1/\pi \operatorname{Im} \left[\sum_{n} <0 | \Theta^{+}(\mathbf{H} - \mathbf{E}_{0} + \iota \varepsilon)^{-1} | n > < n | \Theta | 0 > \right] \\ &= -1/\pi \operatorname{Im} \left[<0 | \Theta^{+}(\mathbf{H} - \mathbf{E}_{0} + \iota \varepsilon)^{-1} \Theta | 0 > \right] \\ &= -1/\pi \operatorname{Im} \left[\Pi(\boldsymbol{\omega}) \right] - \operatorname{Green} \mathbf{F}. \quad \text{poles!!} \end{aligned}$

$$\Phi(\sigma_{\rm R},\sigma_{\rm I}) = \sigma_{\rm I}/\pi \int \left[(\omega - \sigma_{\rm R})^2 + \sigma_{\rm I}^2 \right]^{-1} \mathbf{S}(\omega) \, d\omega < \infty$$

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$$\Phi(\sigma_{R},\sigma_{I}) = \sigma_{I}/\pi \int [(\omega - \sigma_{R})^{2} + \sigma_{I}^{2}]^{-1} S(\boldsymbol{\omega}) d\boldsymbol{\omega} < \infty$$

$$= \sigma_{I}/\pi \int d\boldsymbol{\omega} [(\omega - \sigma_{R})^{2} + \sigma_{I}^{2}]^{-1} \sum_{n} |\langle n| \Theta |0 \rangle|^{2} \delta(\omega - E_{n} + E_{0})$$

$$= \sigma_{I}/\pi \sum_{n} \langle 0| \Theta^{+} [(H - E_{0} - \sigma_{R})^{2} + \sigma_{I}^{2}]^{-1} |n \rangle \langle n|\Theta |0 \rangle$$

$$= Im [\langle 0| \Theta^{+} (H - E_{0} - \sigma_{R} + i\sigma_{I})^{-1} \Theta |0 \rangle]$$

$$\sigma_{I} \text{ finite!}$$

Of course, when $\sigma_{I} = \epsilon \rightarrow 0 \Phi(\sigma_{R}, \epsilon)$ coincides with $S(\omega)$!!

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$$= \operatorname{Im} [\langle 0| \Theta^{+} (H - E_{0} - \sigma_{R} + i\sigma_{I})^{-1} \Theta |0 \rangle]$$

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Of course, when $\sigma_{I} = \varepsilon \rightarrow 0 \Phi(\sigma_{R}, \varepsilon)$ coincides with $S(\omega) !!$ However, in this case since $\Phi(\sigma_{R}, \sigma_{I}) < \infty$ and σ_{I} is finite one is allowed **to use bound state approaches**, i.e. represent H on b.s.

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Of course, when $\sigma_I = \epsilon \rightarrow 0 \Phi(\sigma_R, \epsilon)$ coincides with $S(\omega) \parallel$ However, in this case since $\Phi(\sigma_R, \sigma_I) < \infty$ and σ_I is finite one is allowed **to use bound state approaches**, i.e. represent H on b.s.

NO DISCRETIZATION OF THE CONTINUUM

 $\Phi (\sigma_{R}, \sigma_{I}) = \operatorname{Im} [< 0 | \Theta^{+} (H - E_{0} - \sigma_{R} + i\sigma_{I})^{-1} \Theta | 0>]$ $\sigma_{I} \text{ finite!}$

One can use the Lanczos algorithm to represent $(\mathbf{H} - \mathbf{E}_0 - \boldsymbol{\sigma}_{\mathbf{R}} + i\boldsymbol{\sigma}_{\mathbf{I}})^{-1}$ as a continuum fraction

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

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

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

The LIT method

- reduces the continuum problem to a bound state-like problem
- needs only a "good" method for bound state calculations (FY, HH, NCSM, ???)
- has been benchmarked in "directly solvable" systems (A=2,3)

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

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

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

results

Schroedinger-like equation (bound state problem) with the source has been solved with HH, FY, NCSM, EIHH methods

Only few-body methods!

What about many-body methods! Can one access larger A?

Try with Coupled Cluster

S. Bacca, N. Barnea, G. Hagen, G.O., T. Papenbrock arXiv:1303.7446 [nucl-th]

We have applied it to ¹⁶O total photoabsorption cross section GDR



NN forces derived from χ EFT (N³LO)



Validation of the method on ⁴He



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The width of the GDR is around 6 MeV Our width is 10 MeV We can try to invert the LIT

S. Bacca, N. Barnea, G. Hagen, G.O., T. Papenbrock First principles description of the giant dipole resonance in 16O arXiv:1303.7446 [nucl-th]

Blue band: result of the inversion with uncertainties



(A.Roggero, F. Pederiva, G.Orlandini arXiv-1209.5638)

combination of Sumudu kernels: $K_{p}(\omega, \sigma) = N \sigma \left(\underbrace{e^{-\mu \omega/\sigma}}_{\sigma} - \underbrace{e^{-\nu \omega/\sigma}}_{\sigma} \right)^{p}$ $v/\mu = b/a \qquad v - \mu = \ln [b] - \ln [a] \qquad b > a > 0$ integer

(A.Roggero, F. Pederiva, G.Orlandini arXiv-1209.5638)

combination of Sumudu kernels:

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

$$K_{P}(\omega, \sigma) \longrightarrow \delta(\omega - \sigma)$$

(A.Roggero, F. Pederiva, G.Orlandini arXiv-1209.5638)

combination of Sumudu kernels:

$$\begin{split} \mathsf{K}_{\mathsf{P}}(\boldsymbol{\omega},\,\boldsymbol{\sigma}) &= \operatorname{N}\boldsymbol{\sigma}\left(\frac{\mathbf{e}^{-\mu\,\boldsymbol{\omega}/\boldsymbol{\sigma}}}{\boldsymbol{\sigma}} - \frac{\mathbf{e}^{-\nu\,\boldsymbol{\omega}/\boldsymbol{\sigma}}}{\boldsymbol{\sigma}}\right)^{\mathsf{P}} \\ &= \operatorname{N}\boldsymbol{\Sigma}_{\mathsf{k}}^{\mathsf{P}}\left(-1\right)^{\mathsf{k}}\binom{\mathsf{k}}{\mathsf{P}} \mathbf{e}^{-\tau(\mathsf{P},\mathsf{k},\boldsymbol{\sigma})\,\boldsymbol{\omega}} \end{split}$$

(A.Roggero, F. Pederiva, G.Orlandini arXiv-1209.5638)

combination of Sumudu kernels:

$$\begin{split} \mathsf{K}_{\mathsf{P}}(\omega,\sigma) &= \operatorname{N}\sigma\left(\frac{e^{-\mu\,\omega/\sigma}}{\sigma} - \frac{e^{-\nu\,\omega/\sigma}}{\sigma}\right)^{\mathsf{P}} \\ &= \operatorname{N}\Sigma_{\mathsf{k}}^{\mathsf{P}}\left(-1\right)^{\mathsf{k}}\binom{\mathsf{k}}{\mathsf{P}} e^{-\tau(\mathsf{P},\mathsf{k},\sigma)\,\omega} \end{split}$$

The smaller the width ---> the larger P ---> large τ !!!

First application for bosons (no sign problem) The transform is calculated with Reptation MC and then inverted

Bosonic system: Liquid Helium



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Bosonic system: Liquid Helium



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conclusions

1) Integral transform approaches are very powerful ab initio methods for cross sections in the continuum

2) Good kernels are representations of the delta-functions (provided that one can calculate the integral transform !)

The work presented here has been done in collaboration with

- Victor Efros (Moscow)
- Nir Barnea (Jerusalem)
- Sonia Bacca (TRIUMF)
- Gaute Hagen (ORNL)
- Thomas Papenbrock (ORNL)

- Winfried Leidemann (Trento)
- Francesco Pederiva (Trento)
- Alessandro Roggero (Trento)