# Multi-hadron observables from spectral functions

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## Recipe for strong force predictions

- 1. Lagrangian defining QCD
- 2. Formal / numerical machinery (lattice QCD)
- 3. A few experimental inputs (e.g.  $M_{\pi}, M_{K}, M_{\Omega}$ )





Wide range of precision pre-/post-dictions

Overwhelming evidence for QCD ✓

Tool for new-physics searches  $\checkmark$ 

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## QCD Fock space

☐ At low-energies QCD = hadronic degrees of freedom  $\pi \sim \overline{u}d$ ,  $K \sim \overline{s}u$ ,  $p \sim uud$ ☐ Overlaps of multi-hadron *asymptotic states* → S matrix



□ An enormous space of information

$$|\pi\pi\pi\pi\pi, \mathrm{in}\rangle |K\overline{K}, \mathrm{in}\rangle \cdot \cdot \cdot$$

## QCD resonances

 $\Box$  Roughly speaking, a bump in:  $|\mathcal{M}_{\ell}(s)|^2 \propto |e^{2i\delta_{\ell}(s)} - 1|^2 \propto \sin^2 \delta_{\ell}(s)$  scattering rate





## QCD resonances



Analyticity

Instead of  $|\mathcal{M}(s)|^2 \rightarrow$  analytically continue the **amplitude** itself For two-particle energies  $(2m)^2 < s < (4m)^2$ , what is the analytic structure?

The optical theorem tells us...

$$\rho(s)|\mathcal{M}_{\ell}(s)|^2 = \operatorname{Im} \mathcal{M}_{\ell}(s)$$

where  $\rho(s)=\frac{\sqrt{1-4m^2/s}}{32\pi}$  is the two-particle phase space

$$\Box \text{ Unique solution is...} \qquad \mathcal{M}_{\ell}(s) = \frac{1}{\mathcal{K}_{\ell}(s)^{-1} - i\rho(s)}$$

$$K \text{ matrix (short distance)} \qquad \text{ phase-space cut (long distance)}$$

Key message: The scattering amplitude has a square-root branch cut

## Cuts and sheets

$$\mathcal{M}_{\ell}(s) = \frac{1}{\mathcal{K}_{\ell}(s)^{-1} - \rho(s)} \propto \frac{1}{p \cot \delta_{\ell}(s) - ip} \propto e^{2i\delta_{\ell}(s)} - 1 \qquad \rho(s) \propto i\sqrt{s - (2m)^2}$$

 $\Box$  Each channel generates a square-root cut  $\rightarrow$  doubles the number of sheets



#### Important lessons:

Details of analyticity = important for quantitative understanding

Possible to separate... (i) long-distance kinematic singularities (ii) short-distance/microscopic physics (depending on interaction details) Microscopic physics via Lattice QCD observable =  $\int \mathcal{D}\phi \ e^{iS} \begin{bmatrix} \text{interpolator} \\ \text{for observable} \end{bmatrix}$ 



## Difficulties for multi-hadron observables

## The Euclidean signature...

- **O** Obscures real time evolution (that defines scattering)
- **O** Prevents normal LSZ (want  $p_4^2 = -(p^2 + m^2)$ , but we have only  $p_4^2 > 0$ )



## The finite volume...

- O Discretizes the spectrum
- O Eliminates the branch cuts and extra sheets
- **O** Hides the resonance poles



## Two strategies...

- Finite-volume as a tool
  - LQCD  $\rightarrow$  Energies and matrix elements

$$\langle \mathcal{O}_j(\tau)\mathcal{O}_i^{\dagger}(0)\rangle = \sum_n \langle 0|\mathcal{O}_j(\tau)|E_n\rangle\langle E_n|\mathcal{O}_i^{\dagger}(0)|0\rangle = \sum_n e^{-E_n(L)\tau} Z_{n,j} Z_{n,i}^*$$

**O** Our task is relate  $E_n(L)$  and  $\langle E_{m'}|\mathcal{J}(0)|E_m\rangle$  to experimental observables

O Applicable only in limited energy range for two- and three-hadron states

#### Spectral function method

- O Formally applies for any number of particles / any energy range
- O An answer to the question... "Can't you just analytically continue?"
- Still important challenges and limitations to consider



**G** Scattering leaves an *imprint* on finite-volume quantities



## General method

 Huang, Yang (1958)
 Lüscher (1986, 1991)
 Rummukainen, Gottlieb (1995)

 Kim, Sachrajda, Sharpe (2005)
 Christ, Kim, Yamazaki (2005)
 He, Feng, Liu (2005)

 Leskovec, Prelovsek (2012)
 Bernard et. al. (2012)
 MTH, Sharpe (2012)
 Briceño, Davoudi (2012)

 Li, Liu (2013)
 Briceño (2014)

## Using the result

□ Single-channel case (pions in a p-wave)

$$\mathcal{K}(s_n)^{-1} = \rho \cot \delta(s_n) = -F(E_n, \vec{P}, L)$$



• Dudek, Edwards, Thomas in *Phys.Rev.* D87 (2013) 034505 •



$$\begin{array}{c} \rho \rightarrow \pi\pi \\ \rho \rightarrow \pi\pi \\ \hline CP-PACS/PACS-CS 2007.2011 \\ \hline ETMC 2010 \\ \hline Lang et al.2011 \\ \hline HadSpec 2012.2016 \\ \hline Pellisier 2012 \\ \hline RQCD 2015 \\ \hline Pellisier 2012 \\ \hline Guo et al.2016 \\ \hline Fu et al. 2016 \\ \hline Bulava et al. 2016 \\ \hline Bulava et al. 2016 \\ \hline Alexandrou et al. 2017 \\ \hline Andersen et al. 2018 \\ \hline Frischer et al. 2020 \\ \hline Frien et al. 2020 \\ \hline Frelovsek et al. 2010 \\ \hline Fu cu al. 2015 \\ \hline Prelovsek et al. 2017 \\ \hline Andersen et al. 2017 \\ \hline Andersen et al. 2020 \\ \hline Frien et al. 2020 \\ \hline Frischer et al. 2010 \\ \hline Fu cu al. 2018 \\ \hline O \rightarrow \pi\pi \\ \hline Prelovsek et al. 2010 \\ \hline Howarth and Giedt 2017 \\ \hline Briteño et al. 2017 \\ \hline Briteño et al. 2018 \\ \hline O & O & O & T \\ \hline Howarth and Giedt 2017 \\ \hline Briteño et al. 2018 \\ \hline O & O & O & T \\ \hline Howarth and Giedt 2017 \\ \hline Howarth and Gied$$



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## Correlation functions $\rightarrow$ observables

 $\Box$  Lattice QCD gives finite-volume Euclidean correlators  $\langle 0 | \mathcal{O}_1(0) e^{-\hat{H}\tau} \mathcal{O}_2(0) | 0 \rangle_L$ 

have

Complete physical information is contained in...

$$\langle 0 | \, {\cal O}_1(0) \, f(\hat{H}) \, {\cal O}_2(0) \, | 0 
angle_\infty$$
 want

**]** Detailed choice of f(E) and operators determines the observable

**R-ratio** 

$$\langle 0|j_{\mu}(0)\,\delta(\hat{H}-\omega)\,j_{\mu}(0)\,|0\rangle_{\infty}$$

Meyer • Bailas, Hashimoto, Ishikawa (2020)• Alexandrou et al. (2022) •

$$\begin{aligned} \mathbf{\pi} & \mathbf{\pi} \to \mathbf{\pi} \mathbf{\pi} \text{ amplitude} \\ & \langle \pi | \, \pi(0) \, \frac{1}{E - \hat{H} + i\epsilon} \, \pi(0) \, | \pi \rangle_{\infty} \end{aligned}$$

D-meson total lifetime

$$\langle D | \mathcal{H}_W(0) \, \delta(M_D - \hat{H}) \, \mathcal{H}_W(0) \, | D \rangle_\infty$$

• MTH, Meyer, Robaina (2017) • K.F.-Liu (2016) • Hashimoto (2019-2021)

$$\mathbf{j} \rightarrow \mathbf{\pi} \mathbf{\pi} \text{ amplitude} \left\langle \pi \right| \pi(0) \frac{1}{E - \hat{H} + i\epsilon} j_{\mu}(0) \left| 0 \right\rangle_{\infty}$$

Bulava, MTH (2019)

Linear reconstruction (1/2)

Linear, model-independent reconstruction (e.g. Backus-Gilbert-like, Chebyshev)

$$\begin{split} \sum_{\tau} \mathcal{K}(\bar{\omega},\tau) G(\tau) &= \sum_{\tau} \mathcal{K}(\bar{\omega},\tau) \int d\omega \, e^{-\omega\tau} \, \rho(\omega) = \int d\omega \left[ \sum_{\tau} \mathcal{K}(\bar{\omega},\tau) \, e^{-\omega\tau} \right] \rho(\omega) \\ &= \int d\omega \, \widehat{\delta}_{\Delta}(\bar{\omega},\omega) \, \rho(\omega) \longleftarrow \delta \text{ is exactly known} \end{split}$$

□ Non-linear (not discussed here...)

- Maximum Entropy Method (MEM)
- O Direct fits
- O Neural networks

I Key idea here... we aim only to construct

See multiple ECT\* and CERN workshops, work by Aarts, Allton, Amato, Brandt, Burnier, Del Debbio, Francis, Giudice, Hands, Harris, Hashimoto, Jäger, Karpie, Liu, Meyer, Monahan, Orginos, Robaina, Rothkopf, Ryan, ...

$$\widehat{\rho}(\overline{\omega}) \equiv \int_{-\infty}^{\infty} d\omega \,\widehat{\delta}_{\Delta}(\overline{\omega},\omega) \,\rho(\omega)$$

Linear reconstruction (2/2)

$$\widehat{\rho}(\bar{\omega}) = \sum_{\tau} \mathcal{K}(\bar{\omega}, \tau) G(\tau) = \int_{-\infty}^{\infty} d\omega \, \widehat{\delta}_{\Delta}(\bar{\omega}, \omega) \rho(\omega)$$
$$\widehat{\delta}_{\Delta}(\bar{\omega}, \omega) = \sum_{\tau} \mathcal{K}(\bar{\omega}, \tau) e^{-\omega\tau}$$

au

 $\Box$  Given  $\delta^{\text{target}}(\bar{\omega}, \omega)$ , best  $K(\bar{\omega}, \tau)$  = whatever minimizes combination of

$$\Delta(\mathcal{K} \,|\, \bar{\omega}, \omega) = \left| \delta^{\text{target}}(\bar{\omega}, \omega) - \sum_{\tau} \mathcal{K}(\bar{\omega}, \tau) e^{-\omega\tau} \right| \qquad + \qquad \text{statistical uncertainty on } \widehat{\rho}(\omega)$$

 $\Box \ \Delta(K \,|\, \bar{\omega}, \omega) \text{ is known}$ 

 $\Box$  If  $\Delta(K_A | \bar{\omega}, \omega) < \Delta(K_B | \bar{\omega}, \omega)$  (for similar uncertainties) ... then  $K_A$  is just better

Chebyshev polynomials and Backus-Gilbert-like approaches are some options

## Chebyshev idea

 $f \Box$  Take ar w and  $\Delta$  and 'target shape' as fixed and write...

$$\delta_{\Delta}^{\mathsf{target}}(\bar{\omega},\omega) = f(\omega) = \sum_{n} \mathcal{K}_{n} (e^{-\omega a_{t}})^{n} = \sum_{n} \mathcal{K}_{n} x^{n}$$

 $\Box$  One specific family of choices for  $K_n$  is given using Chebyshevs

$$f(\omega) = \sum_{n}^{N} c_n T_n(x)$$
 can be readily converted to  $K_n$  and compared to other methods

+

□ Any method is best if and only if it achieves combined minimization of

$$\Delta(\mathcal{K} \,|\, \bar{\omega}, \omega) = \left| \delta^{\mathsf{target}}(\bar{\omega}, \omega) - \sum_{\tau} \mathcal{K}(\bar{\omega}, \tau) e^{-\omega\tau} \right|$$

statistical uncertainty on  $\widehat{
ho}(\omega)$ 

## First examples

we want...

$$\widehat{\rho}(\bar{\omega}) \equiv \int_0^\infty d\omega \, \widehat{\delta}_{\Delta}(\bar{\omega}, \omega) \, \rho(\omega)$$

we design coefficients

we have...

$$G(\tau) = \int d\omega \, e^{-\omega\tau} \, \rho(\omega)$$

to estimate





## *R* ratio



#### PHYSICAL REVIEW D

VOLUME 13, NUMBER 7

1 APRIL 1976

#### Smearing method in the quark model\*

E. C. Poggio, H. R. Quinn,<sup>†</sup> and S. Weinberg Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138 (Received 8 December 1975)

We propose that perturbation theory in a gauge field theory of quarks and gluons can be used to calculate physical mass-shell processes, provided that both the data and the theory are smeared over a suitable energy range. This procedure is explored in detail for the process of electron-positron annihilation into hadrons. We show that a smearing range of 3  $\text{GeV}^2$  in the squared center-of-mass energy should be adequate to allow the use of lowest-order perturbation theory. The smeared data are compared with theory for a variety of models. It appears to be difficult to fit the present data with theory, unless there is a new charged lepton or quark with mass in the region 2 to 3 GeV.



## Miscellaneous comments

If correlator is indistinguishable from a single exponential, then

$$G(\tau) = c_0 e^{-E_0 \tau} \implies \rho(\omega) = c_0 \delta(\omega - E_0)$$

Ground-state-dominated time slices do not add much

 $\Box$  Systematic uncertainty on  $\hat{\rho}(\bar{\omega})$  can be challenging

$$\Delta(\mathcal{K} \,|\, \bar{\omega}, \omega) = \left| \delta^{\mathsf{target}}(\bar{\omega}, \omega) - \sum_{\tau} \mathcal{K}(\bar{\omega}, \tau) e^{-\omega\tau} \right|$$

want  $\Delta(K \mid \bar{\omega}, \omega)$  small when  $\rho(\omega)$  is large

□ A GEVP that saturates the correlator contains all relevant information

$$G(\tau) = \sum_{n} c_n e^{-E_n \tau} \implies \rho(\omega) = \sum_{n} c_n \delta(\omega - E_n)$$

## Role of the finite volume



 $\Box$  Any reconstructed spectral function that  $\neq$  forest of deltas...

contains implicit smearing (or else  $L \rightarrow \infty$ )



MTH, Meyer, Robaina (2017)

# Backus-Gilbert (*Numerical Recipes* version) Un-stabilized inverse



Without uncertainties, minimize the functional...

$$A[\mathcal{K}] \equiv \int_0^\infty d\omega \, (\bar{\omega} - \omega)^2 \, \widehat{\delta}_\Delta(\bar{\omega}, \omega)^2 = \int_0^\infty d\omega \, (\bar{\omega} - \omega)^2 \left[ \sum_{\tau} \mathcal{K}_\tau e^{-\omega\tau} \right]^2$$

with unit area constraint on  $\boldsymbol{\delta}$ 

#### □ Stabilized inverse

With uncertainties, instead minimize...

$$W_{\lambda}[\mathcal{K}] \equiv (1 - \lambda)A[\mathcal{K}] + \lambda \frac{\mathcal{K} \cdot \text{COV} \cdot \mathcal{K}}{\mathcal{N}}$$
wants oscillating K  $\mathcal{K}$  wants well-behaved K

 $\lambda$  parametrizes the tradeoff between *final resolution* and *final uncertainty* 

## Backus-Gilbert example

#### Un-stabilized inverse



#### □ Stabilized inverse



## Backus-Gilbert example

#### Un-stabilized inverse



#### □ Stabilized inverse



## Extended Backus Gilbert

Important generalization from Martin Hansen, Lupo, Tantalo

Addressed two limitations...



Hansen, Lupo, Tantalo (2019)

## Extended Backus Gilbert example

🔲 e.g. target a Breit-Wigner





Method will fail if one tries to...



Hansen, Lupo, Tantalo (2019)

## Total rate based applications

Hadronic tensor, heavy flavor lifetimes

$$W_{\mu\nu}(p,q) \equiv \int d^4x \ e^{iqx} \langle \pi, p | \mathcal{J}^{\dagger}_{\mu}(x) \mathcal{J}_{\nu}(0) | \pi, p \rangle \quad \propto \langle \pi, p | \widetilde{\mathcal{J}}^{\dagger}_{q,\mu}(0) \delta(\hat{H} - \omega) \mathcal{J}_{\nu}(0) | \pi, p \rangle$$

$$\propto \int d\Phi \Big| \underbrace{\mathcal{M}}_{\bullet} \underbrace{\mathcal{J}}_{\bullet} \Big|^2 + \int d\Phi \Big| \underbrace{\mathcal{M}}_{\bullet} \underbrace{\mathcal{J}}_{\bullet} \Big|^2 + \int d\Phi \Big| \underbrace{\mathcal{M}}_{\bullet} \underbrace{\mathcal{J}}_{\bullet} \Big|^2 + \dots$$

$$W_{\mu\nu} = \lim_{\Delta \to 0} \lim_{L \to \infty} W_{\mu\nu;\Delta,L}$$

Inclusive and semi-inclusive, importance of smearing/volume/kinematics

What about scattering and transition amplitudes?

MTH, Meyer, Robaina (2017), see also K.F.-Liu (2016), Hashimoto (2019-2021)

## Amplitudes from spectral functions

First define the Euclidean correlator

$$G_L(\tau) = \langle \pi_{\mathbf{p}_4} | \pi(\tau_3, \mathbf{p}_3) \pi(0) | \pi_{\mathbf{p}_1} \rangle_L = \int_0^\infty dE_3 \, \rho(E_3) e^{-E_3 \tau_3}$$

and the smeared spectral function

$$\widehat{\rho}_{\boldsymbol{p}_{4}\boldsymbol{p}_{1}}^{L,\epsilon}(q_{3}) = \int_{0}^{\infty} dE_{3} \, \frac{1}{q_{3}^{0} - E_{3} + i\epsilon} \, \rho(E_{3}) = \int_{0}^{\infty} dE_{3} \, \widehat{\delta}_{\epsilon}(q_{3}^{0}, E_{2}) \, \rho(E_{3})$$



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 $\Box$  Next project on shell at finite  $\varepsilon$ 

$$\mathcal{M}_{c}^{L,\epsilon}(p_{4}p_{3}|p_{2}p_{1}) \equiv \frac{2E(\boldsymbol{p}_{3})}{Z^{1/2}(\boldsymbol{p}_{3})} \frac{2E(\boldsymbol{p}_{2})}{Z^{1/2}(\boldsymbol{p}_{2})} \epsilon^{2} \,\widehat{\rho}_{\boldsymbol{p}_{4}\boldsymbol{p}_{1}}^{L,\epsilon}(E(\boldsymbol{p}_{3}),\boldsymbol{p}_{3})$$

**G** Finally project out the scattering amplitude

$$\mathcal{M}_{c}(p_{4}p_{3}|p_{2}p_{1}) = \lim_{\epsilon \to 0^{+}} \lim_{L \to \infty} \mathcal{M}_{c}^{L,\epsilon}(p_{4}p_{3}|p_{2}p_{1})$$

Bulava, MTH (2019)

## Some comments

 $\Box$  Derivation based in modified LSZ + signature-independence of  $\rho(E)$ 

Holds when LSZ holds

 $\langle m, \operatorname{out}|n, \operatorname{in} \rangle \qquad \quad \langle m, \operatorname{out}|\mathcal{J}(0)|n, \operatorname{in} \rangle$ 

#### □ Some nice features...

GEVP-like operator freedom

$$G_L^{[ab]}(\tau) = \langle \pi_{\boldsymbol{p}_4} | \pi^a(\tau_3, \boldsymbol{p}_3) \pi^b(0) | \pi_{\boldsymbol{p}_1} \rangle_L \longrightarrow \mathcal{M}^{[ab], \epsilon, L}$$

Finite range of analyticity in E



Bulava, MTH (2019)

## Perturbative study...

Calculate in PT  $G_L(\tau) = \langle \pi_{p_4} | \pi(\tau_3, p_3) \pi(0) | \pi_{p_1} \rangle_L$ 

Convert to this $\mathcal{M}^{L,\epsilon}_{ ext{c}}(p_4p_3|p_2p_1)$ 

$$\operatorname{Im} \mathcal{M}_{c}^{L,\epsilon}(p_{4}p_{3}|p_{2}p_{1}) = \frac{\lambda^{2}}{2} \frac{1}{L^{3}} \sum_{\boldsymbol{k}'}^{\Lambda} \frac{1}{(2E(\boldsymbol{k}'))^{2}} \operatorname{Im} \left\{ \frac{1}{(E_{cm} - 2E(\boldsymbol{k}') + i\epsilon)} \left[ 1 - \frac{\epsilon^{2}}{4E(\boldsymbol{k}')^{2}} - \frac{\epsilon(\epsilon + 2iE(\boldsymbol{k}'))}{E_{cm}E(\boldsymbol{k}')} \right] \right\}$$



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## Monte-Carlo test

□ Full lattice calculation in two-dimensional O(3) non-linear sigma model

Demonstrating the modified Backus-Gilbert (HLT) method for the "R-ratio"

$$C(t) \equiv \int d\boldsymbol{x} \left\langle \Omega \right| \hat{j}_{1}^{a}(0,\boldsymbol{x}) e^{-\hat{H}t} \hat{j}_{1}^{a}(0) \left| \Omega \right\rangle = \int_{0}^{\infty} d\omega \, e^{-\omega t} \, \rho(\omega)$$

Data + theory driven analysis of finite-L and -T effects and discretization

ID	$(L/a) \times (T/a)$	eta	$am_{\star}$	$m_{\star}L$	$m_{\star}T$
A1	640  imes 320	1.63	0.0447989(62)	29	14
A2	$1280 \times 640$	1.72	0.0257695(31)	33	17
A3	$1920 \times 960$	1.78	0.0176104(31)	34	17
A4	$2880\times1440$	1.85	0.0112608(29)	32	16
B1	$5760 \times 1440$	1.85	0.0112607(73)	65	16
B2	$2880\times 2880$	1.85	0.0112462(72)	32	32

Bulava, MTH, Hansen, Patella, Tantalo (2021)







## Monte-Carlo test

 $\square$  Construct different smearings of  $\rho(\omega)$ 

$$\rho_{\epsilon}^{\lambda}(E) = \int_{0}^{\infty} d\omega \, \delta_{\epsilon}^{\lambda}(E,\omega) \, \rho(\omega)$$

$$\begin{split} \delta^{\mathsf{g}}_{\epsilon}(x) &= \frac{1}{\sqrt{2\pi\epsilon}} \exp\left[-\frac{x^2}{2\epsilon^2}\right], \qquad \delta^{\mathsf{c0}}_{\epsilon}(x) = \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}, \\ \delta^{\mathsf{c1}}_{\epsilon}(x) &= \frac{2}{\pi} \frac{\epsilon^3}{(x^2 + \epsilon^2)^2}, \qquad \qquad \delta^{\mathsf{c2}}_{\epsilon}(x) = \frac{8}{3\pi} \frac{\epsilon^5}{(x^2 + \epsilon^2)^3}. \end{split}$$



Bulava, MTH, Hansen, Patella, Tantalo (2021)

## Extrapolation





Use known relations between different smearing kernels

Bulava, MTH, Hansen, Patella, Tantalo (2021)

Result



Bulava, MTH, Hansen, Patella, Tantalo (2021)

## Spectral summary

 $\Box \text{ Cannot solve the inverse problem, we can get } \widehat{\rho}_{L,\Delta}(\bar{\omega}) \equiv \int_0^\infty d\omega \,\widehat{\delta}_{\Delta}(\bar{\omega},\omega) \,\rho_L(\omega)$ 

Smearing is needed anyway to suppress volume effects





Generalized Backus-Gilbert takes

 $\widehat{\delta}^{\mathrm{target}}_{\Delta}(ar{\omega},\omega)$  as input

Succesful implementation in O(3) model



## Two strategies... Conclusion

- Finite-volume as a tool
  - **O** Relate energies and matrix elements
  - **O** Tested and highly successful approach
  - Limitations:
    - modeling/parametrizing in order to fit need formalism for all open channels at a given energy

## Spectral function method

- O More direct/natural in a sense (my opinion)
- No new formalism needed for any energies, channels
- O Limitations:
  - Tricky volume effects Difficult inverse problem

Thanks for listening!... questions?



4.5

