

Spectral reconstruction with a variational method

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Outline

Motivation and introduction

- Observables in a strongly-coupled QCD medium
- Inverse problem for numerical data
- Standard regularizations: linear and non-linear methods

Variational methods

- Variational methods for vacuum correlators
- A variational method in the frequency domain

Preliminary results

- Application to vacuum correlation functions from an EFT

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$\frac{\chi}{\Gamma} \epsilon$ add data

Observables in a strongly-coupled QCD medium

In-medium observables are related to the spectral function

$$\rho(\omega) \equiv \frac{1}{2\pi i} \int_{-\infty}^{\infty} dt e^{-i\omega t} (G^>(t) - G^<(t)), \quad \text{where } G^{\gtrless}(t) \equiv \begin{cases} \text{Tr}\{\hat{\rho} \mathcal{J}(t) \mathcal{J}^\dagger(0)\} \\ \text{Tr}\{\hat{\rho} \mathcal{J}^\dagger(0) \mathcal{J}(t)\} \end{cases}$$

- transport of a conserved charge, e.g.

$$\frac{\rho_L(\omega p)}{\omega} = \frac{\chi_s(p)}{\pi} \frac{D\omega^2}{\omega^2 + (Dp^2)^2}$$

[Aarts et al., 1307.6763]

- thermal production rates, e.g.

$$\left. \frac{d^4 N_{\ell^+ \ell^-}}{d\omega d^3 p} \right|_{p=0} \propto \alpha_{\text{em}}^2 n_B(\omega) \frac{\rho_V(\omega)}{\omega^2}$$

[CMS, 1208.2826]

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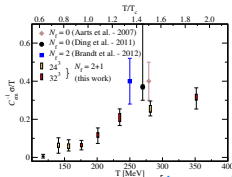
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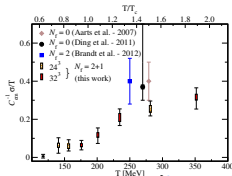
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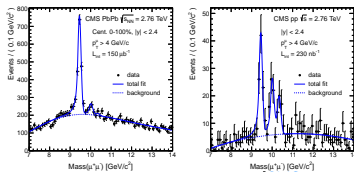
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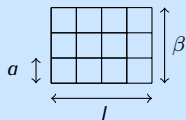
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Lattice is a non-perturbative regularization of a QFT

Many Euclidean observables can be estimated numerically in a finite time

By importance-sampling the distribution implicitly defined though

$$Z = \int_{U \text{ per. } \beta} \mathcal{D}U e^{-S_E[U]},$$

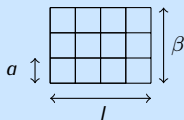
we generate $\{U_i\}_{i=1, \dots, N}$ and calculate stochastic estimator of the Euclidean correlation

$$\langle \hat{\mathcal{O}}(x_1, x_2, \dots, x_n) \rangle = \frac{1}{N} \sum_{i=1}^N \mathcal{O}(x_1, \dots, x_n)[U_i] + \mathcal{O}(1/\sqrt{N}).$$

We can access, e.g.

$$G_E(\tau) \equiv G^>(-i\tau) = \int_0^\infty d\omega K(\tau, \omega) \rho(\omega), \quad \text{where} \quad K(\tau, \omega) = \frac{\cosh(\omega\tau - \omega\beta/2)}{\sinh(\beta\omega/2)}$$

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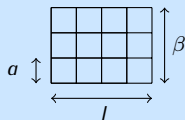
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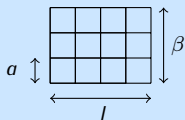
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for $G_E(\tau) = G_E(\beta - \tau)$.

Spectral decomposition in the vacuum

The Euclidean correlation admits the spectral decomposition

$$G_E(\tau) = \sum_{n=0}^{\infty} |Z^n|^2 e^{-E_n \tau}$$

in the vacuum, where $Z^{n*} \equiv \langle n | \mathcal{J}^\dagger(x) | 0 \rangle$ and $H_{\text{QCD}} | n \rangle = E_n | n \rangle$.

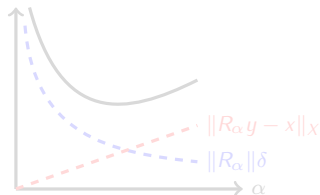
- Used to extract matrix elements of operators in the ground state in the asymptotic $\tau \rightarrow \infty$ limit for vacuum correlators.
- Spectrum is discrete in a finite volume.

Inverse problem for finite noisy numerical data

- $K : X \rightarrow Y$ is a compact linear operator between normed linear spaces, X, Y .
- Suppose we have finite noisy data, y^δ , with $\|y - y^\delta\|_Y < \delta$.
- A regularization strategy $R_\alpha : D(R_\alpha) \subseteq Y \rightarrow X$ where $R_\alpha y \xrightarrow{\alpha \rightarrow 0} K^{-1}y = x$.
- $R_{\alpha=0}$ is unbounded \Rightarrow not continuous on Y .

Let $x_\alpha^\delta \equiv R_\alpha y^\delta$, then the approximation error $\|x - x_\alpha^\delta\|_X$ satisfies

$$\|x - x_\alpha^\delta\|_X \leq \|R_\alpha\|\delta + \|R_\alpha y - x\|_X$$



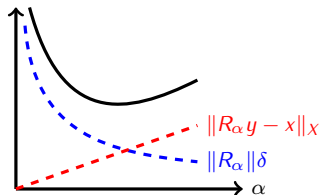
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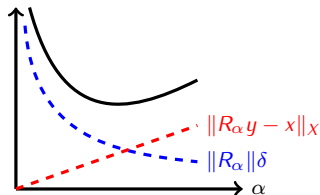
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A linear regularization – Backus–Gilbert method I

$$x_\alpha^\delta \rightarrow \hat{\rho}(\bar{\omega}), \quad \text{and} \quad y^\delta \rightarrow G_E(i\alpha) \equiv G_i,$$

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$$\hat{\rho}(\bar{\omega}) = \sum_{i=1}^{\beta/a} q_i(\bar{\omega}) G_i.$$

Choose to optimize a quadratic form in $q_i(\bar{\omega})$:

$$q_i(\bar{\omega}) = \operatorname{argmin}_{q_i(\bar{\omega})} \left\{ \alpha q_i(\bar{\omega}) \operatorname{Cov}_{ij} q_j(\bar{\omega}) + (1 - \alpha) \int_0^\infty d\omega \hat{\delta}(\bar{\omega}, \omega)^2 (\omega - \bar{\omega})^2 \right\},$$

where

$$\hat{\delta}(\bar{\omega}, \omega) \equiv \sum_{i=1}^{\beta/a} q_i(\bar{\omega}) K(i\alpha, \omega) = R_\alpha K$$

is called the *resolution function*, and is subject to the constraint $\int_0^\infty d\omega \hat{\delta}(\bar{\omega}, \omega) = 1$.

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A linear regularization – Backus-Gilbert method II

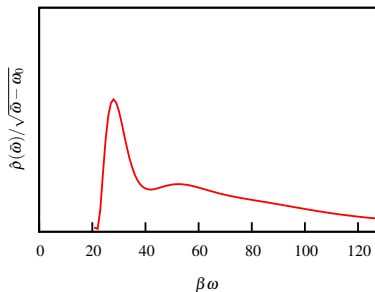
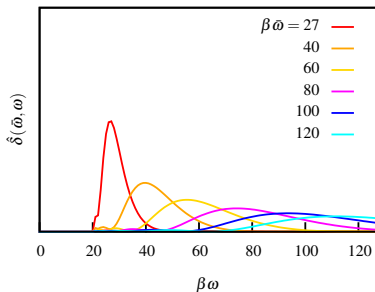
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The *estimator* $\hat{\rho}(\bar{\omega})$ is *not* the most likely solution given the data but is not misrepresenting the underlying spectrum.

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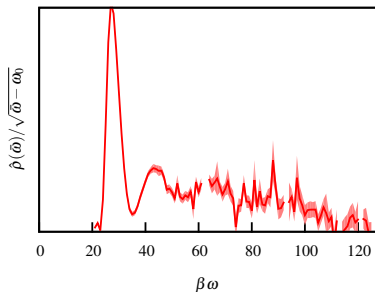
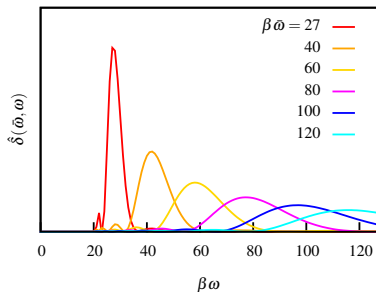


Backus-Gilbert estimator with $\alpha = 10^{-8}$ on a Euclidean correlator $\beta/a = 128$.

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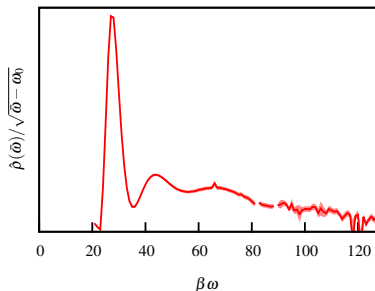
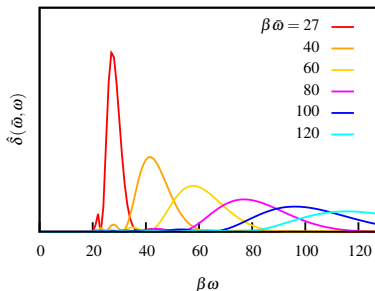


Backus-Gilbert estimator with $\alpha = 10^{-12}$ on lattice correlator $\beta/a = 128$.

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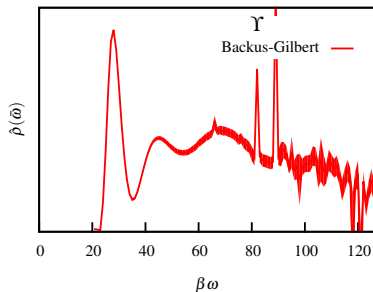
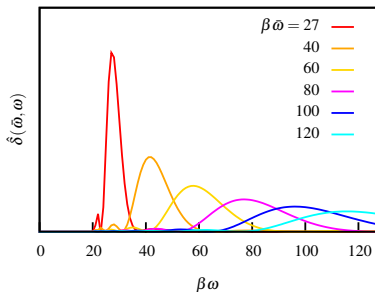


Backus-Gilbert estimator with $\alpha = 10^{-11}$ on lattice correlator $\beta/a = 128$.

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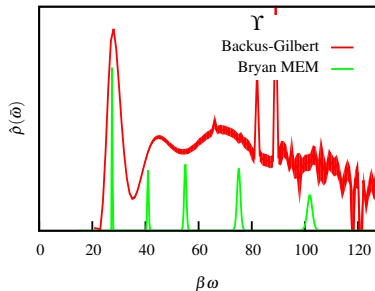
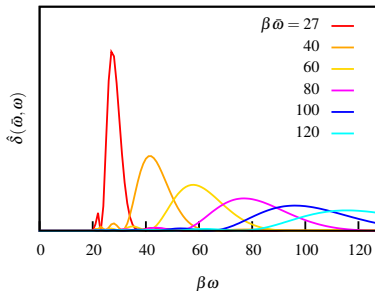


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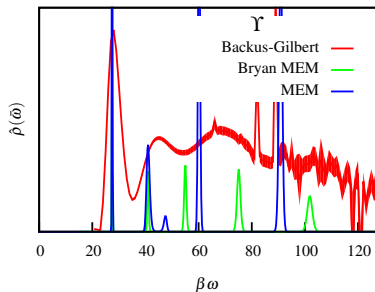
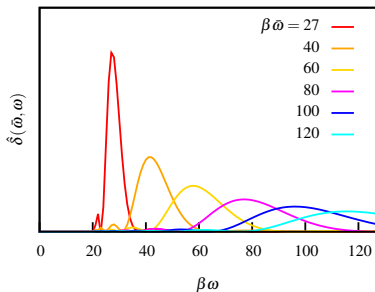


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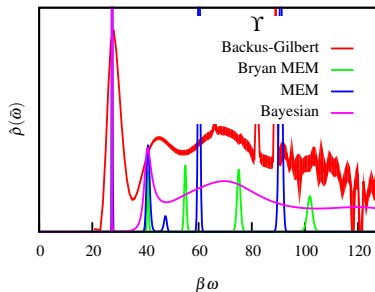
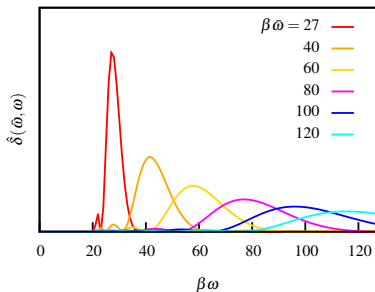


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Non-linear regularization strategies

Regulate the degenerate maximum-likelihood optimization with a convex functional

$$R_\alpha : y^\delta \mapsto x_\alpha^\delta = \operatorname{argmin}_{x' \in X'} \left\{ \frac{1}{2} \|y^\delta - Kx'\|_Y^2 + \alpha S[x'] \right\}$$

- MEM: family of regularizations indexed by $m \in X$

$$S[x] = \int_0^\infty d\omega \left[x - x \log \left(\frac{x}{m} \right) - m \right]$$

$\exists \frac{\mu}{h} \in$ Bryan's algorithm: the normal equation for the optimization

$$\delta_x S[x] = K^\top \operatorname{Cov}^{-1}(y^\delta - Kx) \implies \tilde{x} = V\Xi(\cdot) \implies \tilde{x} \in \operatorname{span}(\operatorname{r.s.v.}K)$$

where $K = U\Xi V^\top$ if $\tilde{x} \equiv \delta_x S[x]$ invertible.

The optimization can be given some Bayesian interpretation which also gives a prescription for integrating out α .

Variational method and the GEvP

Consider a *basis* of interpolating operators $\{\mathcal{J}_i(x)\}_{i=1,\dots,N}$ and recall the spectral decomposition

$$G_E(\tau) = \sum_{n=0}^{\infty} |Z^n|^2 e^{-E_n \tau}.$$

It can be shown (perturbatively) that the eigenvalues of the GEvP

$$G_{E,ij}(\tau)v_j^n(\tau, \tau_0) = \lambda^n(\tau, \tau_0)G_{E,ij}(\tau_0)v_j^n(\tau, \tau_0)$$

have the asymptotic behaviour

$$\lambda^n(\tau, \tau_0) = e^{-E_n \tau} + O(e^{-(E_{N+1}-E_n)\tau})$$

and the operators in the *rotated basis* satisfy

$$\mathcal{J}_i v_i^n |0\rangle = |n\rangle + O(e^{-(E_{N+1}-E_n)\tau_0}).$$

[Blossier *et al.*, 0902.1265]

Note that $G_{E,ij}$ is a **Hermitian, positive-definite bilinear form** on the space of operators, and *not* an linear map $X \rightarrow X$.

Variational method and the GEvP

Consider a *basis* of interpolating operators $\{\mathcal{J}_i(x)\}_{i=1,\dots,N}$ and recall the spectral decomposition

$$G_{E,ij}(\tau) = \sum_{n=0}^{\infty} Z_i^n Z_j^{n*} e^{-E_n \tau}.$$

It can be shown (perturbatively) that the eigenvalues of the GEvP

$$G_{E,ij}(\tau) v_j^n(\tau, \tau_0) = \lambda^n(\tau, \tau_0) G_{E,ij}(\tau_0) v_j^n(\tau, \tau_0)$$

have the asymptotic behaviour

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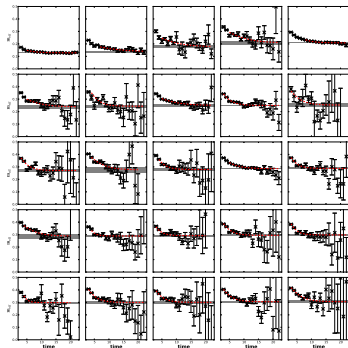
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The variational method *in vacuo*

- Used in many studies to *reliably* extract tens of energy levels in single channels.
- ≥ 100 operators used: $(\bar{\Psi}\Gamma\Psi)(x)$, $(\bar{\Psi}\Delta\Psi)(x)$, multiparticle operators with relative momentum, ...



[Morningstar *et al.*, 1510.00371]

A variational method in the frequency domain

- Ohno *et al.* applied the GEVP directly to the correlators at finite β .

[Ohno *et al.*, 1104.3384]

- Filtering with τ, τ_0 may not be possible when β is finite, or when the spectrum becomes dense, e.g. at $T > 0$:

$$\rho(\omega) = \frac{2 \sinh(\beta\omega/2)}{Z} \sum_{n,m} |Z^{mn}|^2 e^{-\beta(E_n + E_m)/2} \delta(\omega - E_m + E_n),$$

where $Z^{nm*} = \langle n | J^\dagger(0) | m \rangle$.

$\exists \frac{\tau}{\tau_0} \in \mathbb{C}$ solve the GEVP in the spectral function estimator $\hat{\rho}_{ij}(\bar{\omega}) = R_\alpha G_{E,ij}(\tau)$:

$$\hat{\rho}_{ij}(\bar{\omega}) v_j^n(\bar{\omega}, \tau_0) = \lambda^n(\bar{\omega}, \tau_0) G_{E,ij}(\tau_0) v_j^n(\bar{\omega}, \tau_0)$$

- the method asks for operators which couple optimally to a *local* region in frequency domain rather than at large times
- applicable even when $\tau \rightarrow \infty$ not available if good resolution is available

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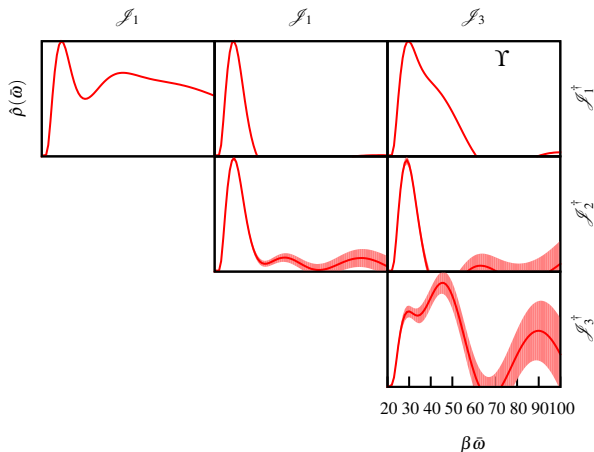
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where $Z^{nm*} = \langle n|J^\dagger(0)|m\rangle$.

$\exists \frac{\mu}{\tau} \in \mathbb{C}$ Backus-Gilbert well-suited because it resolves the spectral function *locally*.

$$\begin{array}{ccc} Y^{N^2} & \xrightarrow{R_\alpha} & X^{N^2} \\ \text{GEVP} \downarrow & & \downarrow \text{GEVP} \\ Y^{N^2} & \xrightarrow{R_\alpha} & X^{N^2} \end{array}$$

Υ channel

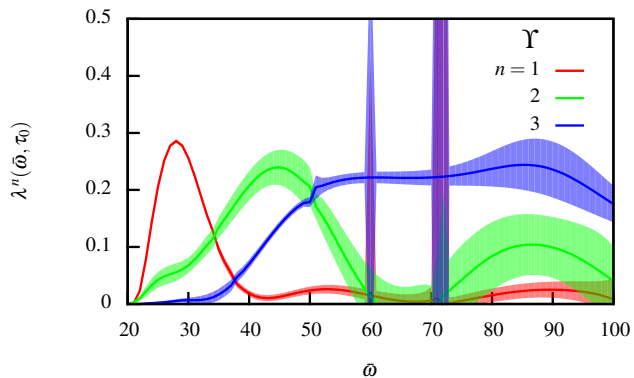


BG matrix estimator $\hat{\rho}_{ij}(\bar{\omega})$ in Υ channel for $\beta/a=128$

Operator basis $\{\mathcal{J}_i^\dagger(x) = \sum_k \chi_k^\dagger(x) \sigma_k \psi_i(x)\}$ where $\psi_1(x) \equiv \psi(x)$ and

$$\psi_2(y) \equiv \sum_x e^{-(x-y)^2/\sigma^2} \psi(x), \quad \psi_3(y) \equiv \sum_x \left(4 \frac{(x-y)^2}{\sigma^2} - 3\right) e^{-(x-y)^2/\sigma^2} \psi(x).$$

Υ channel



Eigenvalues in Υ channel for $\beta/a=128$

Note the local *rank-1* (in the operator space) property of the spectral function:

$$\rho_{ij}(\omega) = \frac{2 \sinh(\beta\omega/2)}{Z} \sum_{n,m} Z_i^{mn} Z_j^{mn*} e^{-\beta(E_n+E_m)/2} \delta(\omega - E_m + E_n)$$

Identifying quasiparticle poles:

- A large hierarchy between in the eigenvalues is the approximate rank

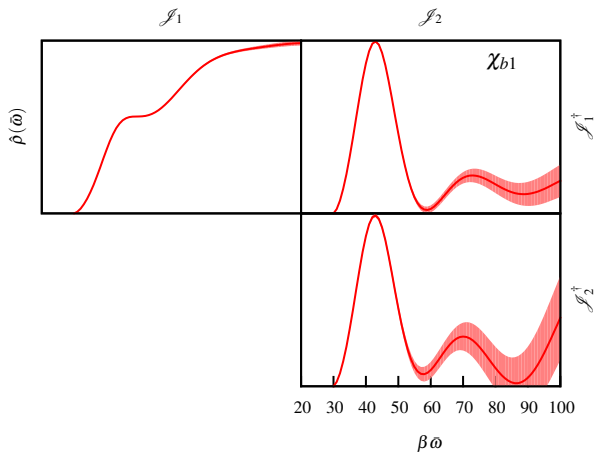
$$\lambda^n(\bar{\omega}, \tau_0) \gg \lambda^{m \neq n}(\bar{\omega}, \tau_0).$$

Estimating the contribution to a spectral function from a local frequency region:

- Define an optimal operator $\sum_i \mathcal{J}(x)_i^\dagger v_i^n(\bar{\omega}^n)$

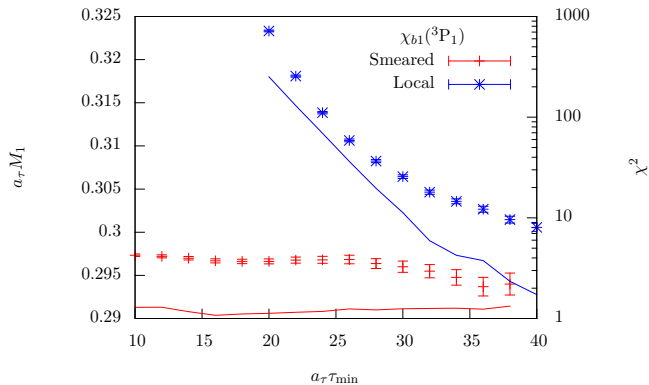
$$\bar{\omega}^n \equiv \operatorname{argmax}_{\bar{\omega}} \{ \lambda^n(\bar{\omega}, \tau_0) \}$$

χ_{b1} channel



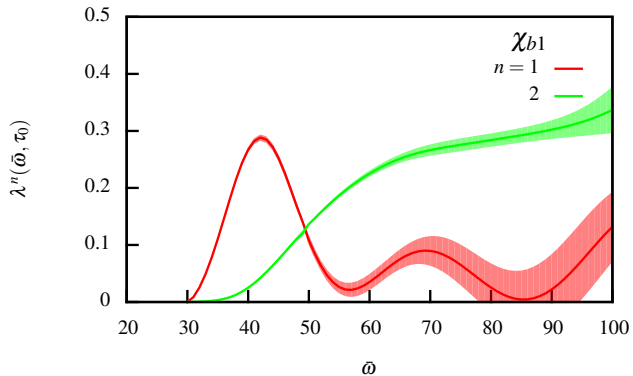
BG matrix estimator $\hat{\rho}_{ij}(\bar{\omega})$ in χ_{b1} channel for $\beta/a=128$

χ_{b1} channel



Sliding-window plot for χ_{b1} effective energy showing slow convergence on the ground state.

χ_{b1} channel



Eigenvalues in χ_{b1} channel for $\beta/a=128$

Conclusions

- Regulation easily controlled with linear methods
 - ↪ Backus-Gilbert transforms kernel to a smoothing one
- GEVP can focus on *local* regions of a spectral function
 - ◁ define *optimal* operators with compact-enough support in the frequency domain
 - ▷ identify quasiparticles
 - ▷ applying other (non-linear) inverse methods using *optimal* basis
- Application to finite- β relativistic and non-relativistic channels underway

Conclusions

