Spectral densities from Euclidean-time lattice correlation functions

Matteo Saccardi
In collaboration with Mattia Bruno and Leonardo Giusti

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Based on: *Bruno, Giusti, Saccardi, arXiv:2407.04141* and *in prep.*

- ⋆ (Smeared) spectral densities play a pivotal role in particle physics
  - ⇒ Inclusive hadronic cross sections [M. T. Hansen, Meyer, and Robaina 2017; ...]
  - ⇒ Semileptonic decays [Gambino and Hashimoto 2020; ...]
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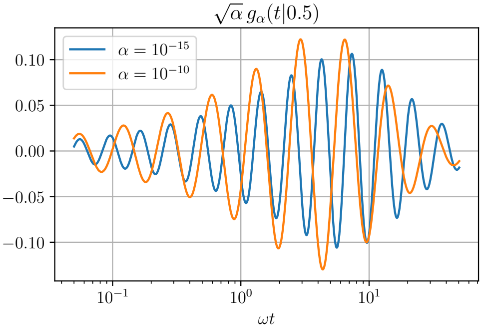
Here: explicit analytic formulae to extract $\rho(\omega)$ from $C(t)$,
both *in the continuum* and *on the lattice*

Analytic continuum solution

$$\rho(\omega) = \lim_{\alpha \to 0^+} \rho_\alpha(\omega) = \lim_{\alpha \to 0^+} \int_0^\infty dt\, g_\alpha(t|\omega) C(t)$$



- Real and computable coefficients

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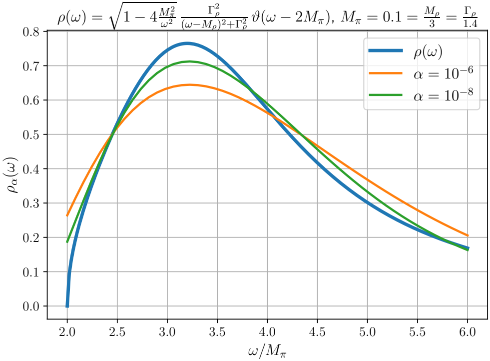

- Real and computable coefficients
- Least-square solution, minimizing

$$\int_\omega \left[\rho(\omega) - \rho_\alpha(\omega)\right]^2 \xrightarrow{\alpha\to 0} 0$$

Derivation of the continuum solution

$$C(t) = \int_0^\infty d\omega' \, \rho(\omega') \qquad e^{-\omega' t}$$

1. *Continuum* inverse problem: $t \in \mathbb{R}^+$ (Inverse Laplace Transform, ILT)

Derivation of the continuum solution

$$\int_0^\infty dt\, e^{-\omega t} C(t) = \int_0^\infty d\omega'\, \rho(\omega') \overbrace{\int_0^\infty dt\, e^{-\omega' t} e^{-\omega t}}^{\mathcal{H}(\omega,\omega')}$$

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3. Diagonalize $\mathcal{H}$ with "Mellin basis" $u_s(\omega) = \frac{\omega^{-\frac{1}{2}+is}}{\sqrt{2\pi}} = u^*_{-s}(\omega)$, $s \in \mathbb{R}$
   [McWhirter and Pike 1978; Epstein and Schotland 2008]

$$\int_{\omega'} \mathcal{H}(\omega,\omega') u_s(\omega') = \frac{\pi}{\cosh \pi s} u_s(\omega) = |\lambda_s|^2 u_s(\omega)$$

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$$g_\alpha(t|\omega) = \int_{-\infty}^{\infty} ds\, \frac{u_s^*(\omega)\lambda_s u_s^*(t)}{|\lambda_s|^2+\alpha}\,, \quad \lambda_s = \Gamma\left(\frac{1}{2} + is\right)$$

Smeared spectral densities

$$\rho_\kappa = \int_0^\infty d\omega\, \rho(\omega)\kappa(\omega)\ ,\ \rho(\omega) = \lim_{\alpha\to 0}\int_0^\infty dt\, g_\alpha(t|\omega) C(t)$$

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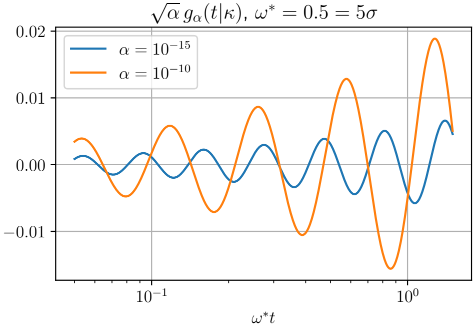


- Relevant in quantum field theories
- Straightforward generalization e.g.

$$\kappa(\omega) = \frac{1}{\pi}\frac{\sigma}{(\omega-\omega^*)^2+\sigma^2}$$

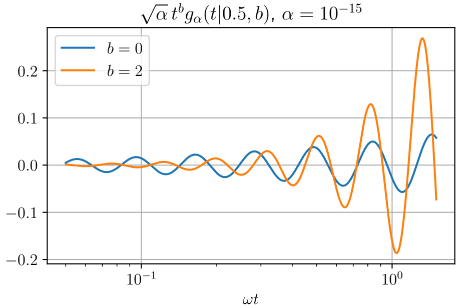
- Real and computable coefficients

Subtracted spectral densities

$$C(t) = \int_0^\infty d\omega\, \omega^b \rho_s(\omega) e^{-\omega t}\,,\; b > 0$$

e.g. isovector vector current in QCD: $b = 2 \rightarrow C(t) \sim t^{-3}$ in UV

$$\rho_s(\omega) = \lim_{\alpha\to 0} \int_0^\infty dt\, C(t)\, g_\alpha(t|\omega, b)\, t^b$$



$$g_\alpha(t|\omega, b) = \int_{-\infty}^{\infty} ds\, \frac{u_s^*(\omega)\lambda_s u_s^*(t)}{\lambda_s \lambda_{s,b}^* + \alpha}$$

$$\lambda_{s,b} = \Gamma\left(\tfrac{1}{2} + b + is\right)$$

$\Rightarrow$ Subtraction of UV divergences

$\Rightarrow$ Dispersive relations

Derivation of the discrete solution

$$\overline{C}_a(t) = \int_0^\infty d\omega' \, \rho(\omega') \qquad e^{-\omega' t}$$

1. *Discrete* inverse problem: $\frac{t}{a} \in \mathbb{N}$ (Discrete ILT), $\overline{C}_a(t) = C(t) + \mathcal{O}(a^2)$
   - ⇒ Naïve approach: discretize the continuum formula
   - ⇒ Here: exact solution at fixed a

Derivation of the discrete solution

$$a\sum_{t=a}^{\infty} e^{-\omega t}\overline{C}_a(t) = \int_0^{\infty} d\omega' \, \rho(\omega') \, \overbrace{a\sum_{t=a}^{\infty} e^{-\omega' t} e^{-\omega t}}^{\overline{\mathcal{H}}_a(\omega,\omega')}$$

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2. *Summed* inverse problem $\rightarrow$ invert $\overline{\mathcal{H}}_a$
3. Diagonalize $\overline{\mathcal{H}}_a$ with c.o.s. $v_s(\omega, a)$, $s \in \mathbb{R}^+$ [Bruno, Giusti, and MS 2024]

$$v_s(\omega, a) = \sqrt{2\pi a}\, N_s\, u_s\left(1 - e^{-a\omega}\right) e^{-a\omega}\, {}_2F_1\left(\frac{1}{2} + is, \frac{3}{2} + is; 2; e^{-a\omega}\right)$$

$$\boldsymbol{v_s(\omega, a) \xrightarrow{a\to 0} u_s(\omega) + u_{-s}(\omega) + \mathcal{O}\left((a\omega)^2\right)}$$

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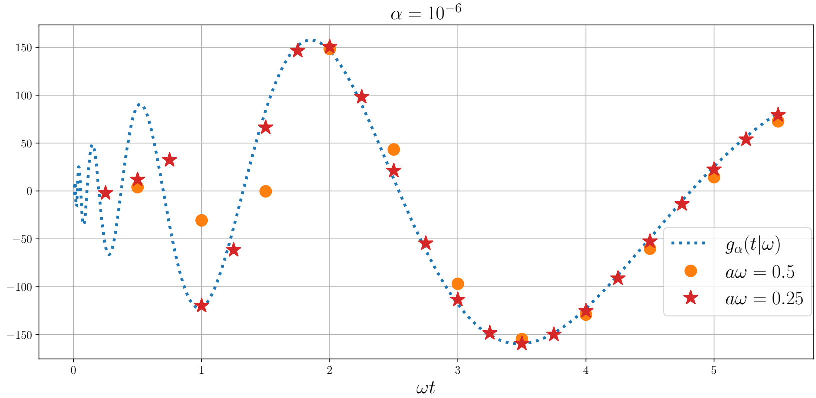

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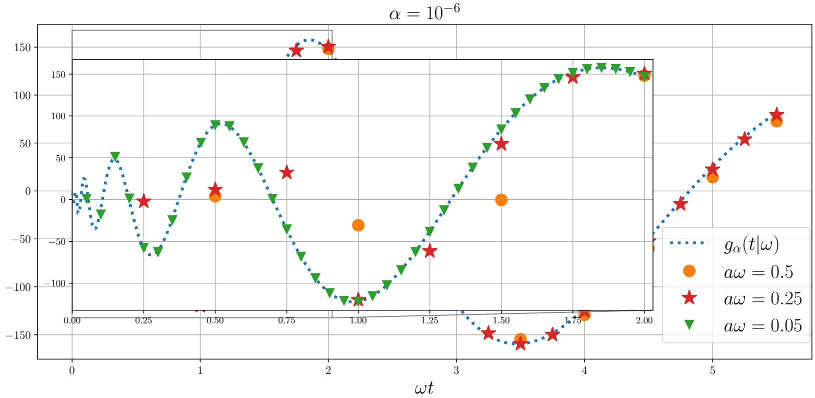


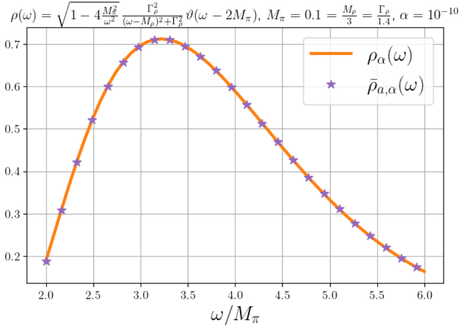
Minimize discretization errors on ρ

- $\forall\,\alpha > 0$ our solution minimizes the distance ($N = \infty$)

$$\int_0^\infty d\omega \left|\rho(\omega) - a\sum_{t=a}^{Na} g'_{a,\alpha}(t)e^{-\omega t}\right|^2 + \alpha \sum_{t=a}^{Na} g'_{a,\alpha}(t)^2$$

$\Rightarrow$ **Discretization errors on ρ are minimized as $\alpha \to 0$, even at fixed $a > 0$!**

$\Rightarrow$ Naïve discretization of continuum has large discretization errors on ρ



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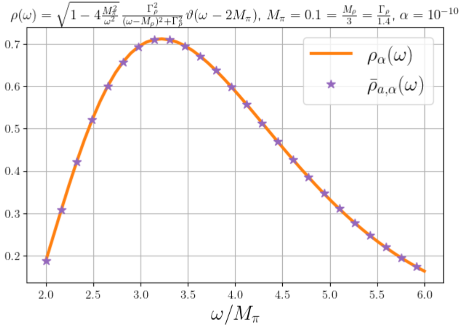
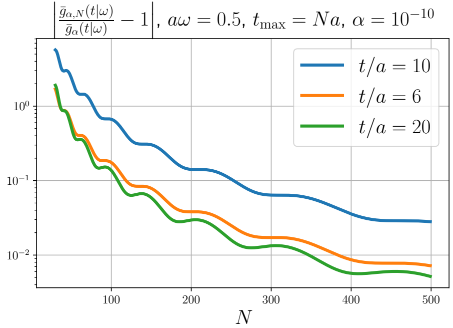
- Backus-Gilbert-like methods minimize the same functional at fixed $N < \infty$

  $\Rightarrow$ As $N \to \infty$, numerical solution approaches our coefficients

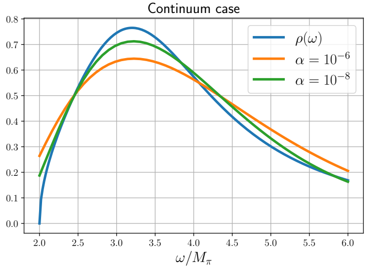




Continuum case

$$\rho(\omega) = \lim_{\alpha \to 0} \int_0^\infty dt \, g_\alpha(t|\omega) C(t)$$

- ⇒ Symanzik and Lüscher FV analysis
- ⇒ Analytic study of errors:
  statistical, $\alpha > 0$, $t_{\max} < \infty$
- ⇒ Quantifiable error estimates/bounds



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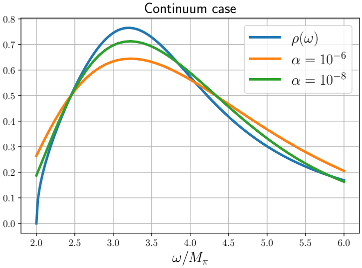

Discrete case

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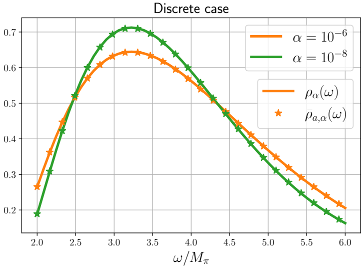
- ⇒ Only discretization errors due to $\overline{C}_a$
- ⇒ Clear continuum limit scaling



An outlook: computation of integrals in time (1/2)

$$I = \int_0^\infty dt\, C(t) K(t)$$

- $C(t)$ sampled at $t \in \{a, 2a, \ldots, t_{\max} = Na\} \to \overline{C}_a(t)$
- $K(t)$ analytically known e.g. $g_\alpha(t|\omega)$, $g_\alpha(t|\kappa)$, TMR for $a_\mu^{\mathrm{HVP,LO}}$, ...

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1. Discrete sums (trapezoidal rule):

$$I_1 = a \sum_{n=1}^{N} \overline{C}_a(na) K(na)$$

An outlook: computation of integrals in time (1/2)

$$I = \int_0^\infty dt\, C(t) K(t) = \int_0^\infty d\omega\, \rho(\omega)\kappa(\omega)$$

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1. Discrete sums (trapezoidal rule):

$$I_1 = a \sum_{n=1}^{N} \overline{C}_a(na) K(na)$$

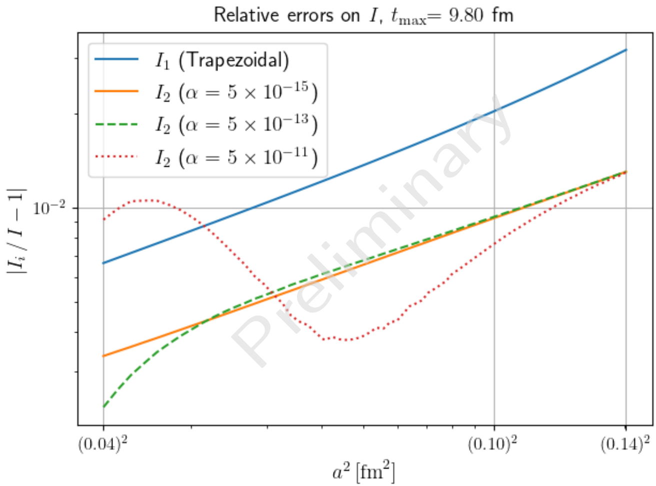
2. Interpret I as ρ_κ, $\kappa(\omega) = \int_0^\infty dt\, e^{-\omega t} K(t)$:

$$I_2 = a \sum_{n=1}^{N} \overline{C}_a(na) \overline{g}_{a,\alpha}(na|\kappa)\,, \quad \overline{g}_{a,\alpha}(t|\kappa) = \int_\omega \overline{g}_{a,\alpha}(t|\omega)\kappa(\omega)$$

$\Rightarrow$ minimize discretization errors, but $\alpha > 0$ systematic errors

An outlook: computation of integrals in time (2/2)

$$\rho(\omega) = \sqrt{1 - 4\frac{M_\pi^2}{\omega^2}} \left[\frac{\Gamma_\rho^2}{(M_\rho - \omega)^2 + \Gamma_\rho^2} + \left(\frac{\omega}{3M_\rho} \right)^2 \right] , \; K(t) = t^3 , \; \{M_\pi , M_\rho , \Gamma_\rho\} \text{ physical}$$



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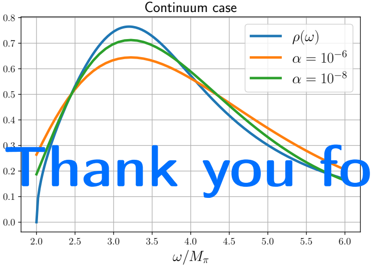
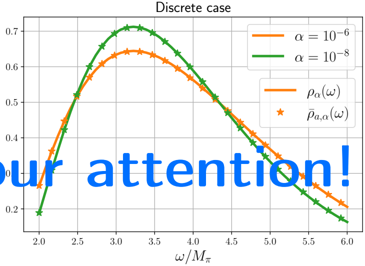




Thank you for your attention!

⇒ Application to computation of $\int_0^\infty dt\, C(t)K(t)$

Backup slides

Continuum basis

[Bruno, Giusti, and MS 2024 and in prep]

$$u_s(x) = \frac{x^{-\frac{1}{2}+is}}{\sqrt{2\pi}} = \frac{e^{is\log x}}{\sqrt{2\pi x}} = u^*_{-s}(x)\,, \quad s \in \mathbb{R}\,, x \in \mathbb{R}^+$$

- Orthogonality: $\int_0^\infty dx\, u^*_s(x) u_{s'}(x) \overset{y=\log x}{=} \int_{-\infty}^\infty \frac{dy}{2\pi}\, e^{iy(s'-s)} = \delta(s-s')$
- Completeness: $\int_{-\infty}^\infty ds\, u^*_s(x) u_s(y) = \frac{1}{\sqrt{xy}}\delta(\log x - \log y) = \delta(x-y)$
- Diagonalize simultaneously $\mathcal{H}$ and $\mathcal{A}$ with eigenvalues $|\lambda_s|^2 = \frac{\pi}{\cosh \pi s}$

$$\mathcal{H}(\omega,\omega') = \int_t e^{-(\omega+\omega')t} = \frac{1}{\omega+\omega'} \;\;,\;\; \mathcal{A}(t,t') = \int_\omega e^{-(t+t')\omega} = \frac{1}{t+t'}$$

- ILT can be written as

$$C(t) = \int_\omega \rho(\omega) e^{-\omega t} \xrightarrow{\int_t e^{-\omega t}} \int_t C(t) e^{-\omega t} = \int_{\omega'} \mathcal{H}(\omega,\omega')\rho(\omega')$$

$$\rho = \lim_{\alpha\to 0} \rho_\alpha = \lim_{\alpha \to 0} \int_{\omega'} \delta_\alpha(\omega,\omega')\rho(\omega')$$

$$\delta_\alpha(\omega,\omega') = \int_{-\infty}^\infty ds \frac{u^*_s(\omega)|\lambda_s|^2 u_s(\omega')}{|\lambda_s|^2+\alpha} \xrightarrow{\alpha\to 0} \delta(\omega-\omega')$$

Discrete basis

[Bruno, Giusti, and MS 2024 and in prep]

$$v_s(\omega, a) = \sqrt{2\pi a}\,|\lambda_s|^2\,|N_s|\;u_s\left(1-e^{-a\omega}\right)e^{-a\omega}\,{}_2F_1\left(\frac{1}{2}+is, \frac{3}{2}+is; 2; e^{-a\omega}\right)$$

$$v_s(\omega, a) = a\sum_{t=a}^{\infty} e^{-\omega t}\overline{v}_s(t, a)\,,\, N_s = \sqrt{2\pi}\frac{\left(\frac{1}{2}+is\right)\lambda_s^*}{\Gamma(-2is)\lambda_s}\,, s\in\mathbb{R}^+$$

- Continuum limit: $v_s(\omega, a) \xrightarrow{a\to 0} \sqrt{a}\left(u_s(a\omega)\frac{N_s}{|N_s|} + u_s^*(a\omega)\frac{(N_s)^*}{|N_s|}\right)$ restoring continuum orthogonality and completeness relations
- $\overline{\mathcal{H}}_a$ and $\overline{\mathcal{A}}_a$ are diagonalized by v_s and $\bar{v}_s$ with eigenvalues $|\lambda_s|^2$

$$\overline{\mathcal{H}}_a(\omega, \omega') = a\sum_{t=a}^{\infty} e^{-(\omega+\omega')t} = \frac{ae^{-a(\omega+\omega')}}{1-e^{-a(\omega+\omega')}}\,, \quad \overline{\mathcal{A}}_a(t, t') = \frac{1}{t+t'}$$

$$\int_{\omega'}\overline{\mathcal{H}}_a(\omega, \omega')e^{-\omega' t} = a\sum_{t'=a}^{\infty} e^{-\omega t'}\overline{A}_a(t', t)$$

- Discrete ILT can be written as

$$\rho = \lim_{\alpha\to 0}\bar{\rho}_{a,\alpha} = \lim_{\alpha\to 0}\int_{\omega'}\bar{\delta}_{a,\alpha}(\omega, \omega')\rho(\omega')$$

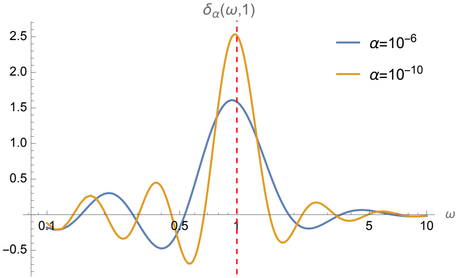
$$\bar{\delta}_{a,\alpha}(\omega, \omega') = \int_0^{\infty} ds\,\frac{v_s(\omega, a)|\lambda_s|^2 v_s(\omega', a)}{|\lambda_s|^2+\alpha} \xrightarrow{\alpha\to 0} \delta(\omega-\omega')\,\forall\, a$$

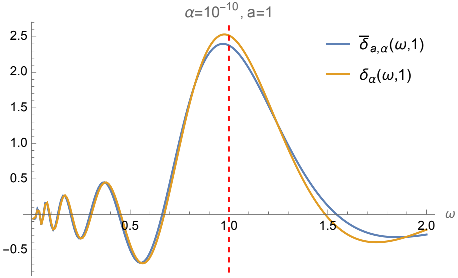
Smearing at $\alpha > 0$

[Bruno, Giusti, and MS 2024 and in prep]

$$\rho_\alpha(\omega) = \int_{\omega'} \delta_\alpha(\omega,\omega')\rho(\omega') \qquad \bar{\rho}_{a,\alpha}(\omega) = \int_{\omega'} \bar{\delta}_{a,\alpha}(\omega,\omega')\rho(\omega')$$

$$\delta_\alpha(\omega,\omega') = \int_{-\infty}^{\infty} ds\, \frac{u_s^*(\omega)|\lambda_s|^2 u_s(\omega')}{|\lambda_s|^2+\alpha} \qquad \bar{\delta}_{a,\alpha}(\omega,\omega') = \int_0^{\infty} ds\, \frac{v_s(\omega,a)|\lambda_s|^2 v_s(\omega',a)}{|\lambda_s|^2+\alpha}$$



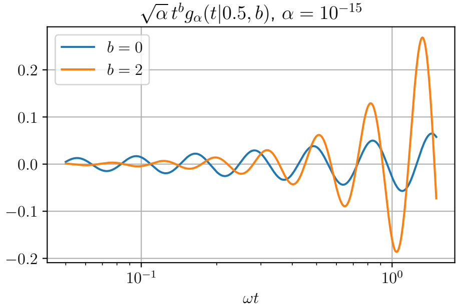


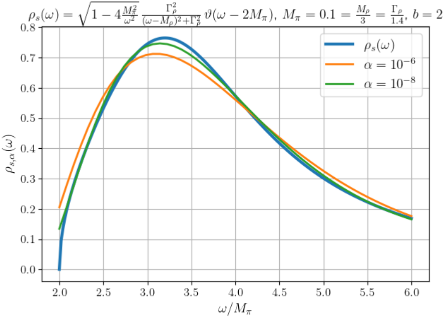
Subtracted spectral densities

Subtraction of UV divergences $\Rightarrow$ $C(t) = \int_0^\infty d\omega\, \omega^b \rho_s(\omega) e^{-\omega t}$, $b > 0$

$$\rho_s(\omega) = \lim_{\alpha\to 0} \int_0^\infty dt\, t^b g_\alpha(t|\omega, b) C(t)\,, g_\alpha(t|\omega, b) = \int_{-\infty}^\infty ds\, \frac{u_s^*(\omega)\lambda_s u_s^*(t)}{\lambda_s \lambda_{s,b}^* + \alpha}$$

$$\lambda_{s,b} = \Gamma\left(\frac{1}{2} + b + is\right)$$





Least-square solutions (coefficients)

[Bruno, Giusti, and MS 2024 and in prep]

- The coefficients $g_\alpha(t|\omega)$ can be defined from minimizing

$$\frac{\delta}{\delta g}\left\{\int_{\omega'}\left[\delta(\omega-\omega')-\int_t e^{-\omega' t} g_\alpha(t|\omega)\right]^2+\alpha\int_t g_\alpha(t|\omega)\right\}=0$$

$$g_\alpha(t|\omega)=\int_{t'} e^{-\omega t'}\mathcal{A}_\alpha^{-1}(t,t')\,,\ \mathcal{A}_\alpha=\mathcal{A}+\alpha\mathcal{I}$$

- The coefficients $\overline{g}_{a,\alpha}(t|\omega)$ can be defined from minimizing

$$\frac{\delta}{\delta\overline{g}}\left\{\int_{\omega'}\left[\delta(\omega-\omega')-a\sum_{t=a}^{\infty} e^{-\omega' t}\overline{g}_{a,\alpha}(t|\omega)\right]^2+\alpha a\sum_{t=a}^{\infty}\overline{g}_{a,\alpha}(t|\omega)\right\}=0$$

$$\overline{g}_{a,\alpha}(t|\omega)=a\sum_{t'=a}^{\infty} e^{-\omega t'}\overline{\mathcal{A}}_{a,\alpha}^{-1}(t,t')\,,\ \overline{\mathcal{A}}_{a,\alpha}=\overline{\mathcal{A}}_a+\alpha\mathcal{I}$$

Least-square solutions (spectral density)

[Bruno, Giusti, and MS 2024 and in prep]

- $\rho_\alpha(\omega) = \int_t e^{-\omega t} g'_\alpha(t) \xrightarrow{\alpha\to 0} \rho(\omega)$ can be defined from minimizing

$$\frac{\delta}{\delta g}\left\{\int_\omega \left[\rho(\omega) - \int_t e^{-\omega t} g'_\alpha(t)\right]^2 + \alpha \int_t g'_\alpha(t)^2\right\} = 0$$
$$g'_\alpha(t) = \int_{t'} \mathcal{A}_\alpha^{-1}(t,t') C(t') \Rightarrow \rho_\alpha(\omega) = \int_{t,t'} e^{-\omega t} \mathcal{A}_\alpha^{-1}(t,t') C(t')$$
$$\Rightarrow \rho_\alpha(\omega) = \int_t g_\alpha(t|\omega) C(t) \ , \ \ g_\alpha(t|\omega) = \int_{t'} e^{-\omega t'} \mathcal{A}_\alpha^{-1}(t',t)$$

- $\overline{\rho}_{a,\alpha}(\omega) = a \sum_{t=a}^{\infty} e^{-\omega t} \overline{g}'_{a,\alpha} \xrightarrow{\alpha\to 0} \rho(\omega)\ \forall\, a$ can be defined from minimizing

$$\frac{\delta}{\delta \overline{g}_{a,\alpha}}\left\{\int_\omega \left[\rho(\omega) - a\sum_{t=a}^{\infty} e^{-\omega' t} \overline{g}'_{a,\alpha}(t)\right]^2 + \alpha a \sum_{t=a}^{\infty} \overline{g}'_{a,\alpha}(t)^2\right\} = 0$$
$$\overline{g}'_{a,\alpha}(t) = a\sum_{t'=a}^{\infty} \overline{\mathcal{A}}_{a,\alpha}^{-1}(t,t') \overline{C}_a(t') \Rightarrow \overline{\rho}_{a,\alpha}(\omega) = a^2 \sum_{t,t'=a}^{\infty} e^{-\omega t} \overline{\mathcal{A}}_{a,\alpha}^{-1}(t,t') \overline{C}_a(t')$$
$$\Rightarrow \overline{\rho}_{a,\alpha}(\omega) = a\sum_{t=a}^{\infty} \overline{g}_{a,\alpha}(t|\omega) \overline{C}_a(t) \ , \ \ \overline{g}_{a,\alpha}(t|\omega) = a\sum_{t'=a}^{\infty} e^{-\omega t'} \overline{\mathcal{A}}_{a,\alpha}^{-1}(t',t)$$

Errors: finite t_{max}

[Bruno, Giusti, and MS 2024 and in prep]

- Systematic error due to $t \in (0, t_{\mathrm{max}})$

$$\rho_\alpha(\omega) - \rho_{\alpha,t_{\mathrm{max}}}(\omega) = \int_{-\infty}^{\infty} ds \, \frac{u_s^*(\omega)\lambda_s}{|\lambda_s|^2 + \alpha} \int_{t_{\mathrm{max}}}^{\infty} dt \, u_s^*(t) C(t)$$

- If $\exists$ mass gap, $C(t) = c\, e^{-Mt}$ at $t \geq t_{\mathrm{max}}$

$$\int_{t_{\mathrm{max}}}^{\infty} dt \, u_s^*(t) C(t) = c \, u_s(M) \, \Gamma\left(\frac{1}{2} - is, M\, t_{\mathrm{max}}\right)$$

$$\Gamma\left(\frac{1}{2} - is, M\, t_{\mathrm{max}}\right) = \sqrt{2\pi} e^{-M\, t_{\mathrm{max}}} u_s^*(M\, t_{\mathrm{max}}) \left[1 + \mathcal{O}\left(\frac{1}{M\, t_{\mathrm{max}}}\right)\right]$$

- Bounded systematic error as $\alpha > 0$, exponentially suppressed in $M\, t_{\mathrm{max}}$

$$\rho_\alpha(\omega) - \rho_{\alpha,t_{\mathrm{max}}}(\omega) = c \int_{-\infty}^{\infty} ds \, \frac{u_s^*(\omega)\lambda_s u_s(M)}{|\lambda_s|^2 + \alpha} \, \Gamma\left(\frac{1}{2} - is, M\, t_{\mathrm{max}}\right)$$

Errors: $\alpha > 0$

[Bruno, Giusti, and MS 2024 and in prep]

- Error on $\rho(\omega)$ can be estimated from a separate reconstruction ($\beta > 0$)
  [Bruno, Giusti, and MS, IL NUOVO CIMENTO **47 C** (2024) 197]

$$\rho(\omega) - \rho_\alpha(\omega) = \int_0^\infty dt\, g^{(1)}_{\alpha,0}(t|\omega) C(t)$$

$$g^{(1)}_{\alpha,\beta}(t|\omega) = \alpha \int_{-\infty}^{\infty} ds\, \frac{u_s^*(\omega)\lambda_s u_s^*(t)}{(|\lambda_s|^2 + \beta)(|\lambda_s|^2 + \alpha)}$$

- A similar double reconstruction works also for ρ_κ. In this case, we can interpret κ as being smeared with ρ to estimate a computable bound

$$|\rho_\kappa - \rho_{\kappa,\alpha}|^2 = \left| \int_\omega \rho(\omega)[\kappa(\omega) - \kappa_\alpha(\omega)] \right|^2$$
$$\leq \alpha^2 \left[\int_\omega \rho(\omega)^2 \right] \int_{\omega,\omega'} \kappa(\omega)\kappa(\omega') \int_{-\infty}^{\infty} ds\, \frac{u_s^*(\omega) u_s(\omega')}{(|\lambda_s|^2 + \alpha)^2}$$

and $\int_\omega \rho(\omega)^2$ can be modeled/estimated from another inverse problem