On the prediction of spectral densities from Lattice QCD: numerical aspects

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In collaboration with Mattia Bruno, Leonardo Giusti

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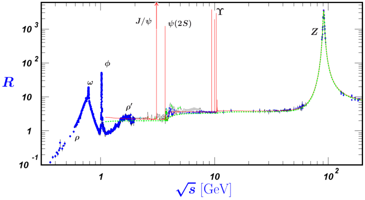
Relying on: *Dalla Brida, Giusti, Harris, Pepe, PLB 816 (2021) 136191*

- **Hadronic spectral densities** play a pivotal role in particle physics
  - R-ratio (4.2σ discrepancy in $g_\mu - 2$)
  - Inclusive semileptonic B-decay (2.7σ discrepancy in V_{cb})



[PDG 2022]

- **Lattice QCD**: model-independent non-perturbative theoretical prediction
  $\rightarrow$ numerically ill-posed inverse problem

- **Here**: vector isovector spectral density with multi-level [Dalla Brida et al. 2021]

$$C(t) = \int_{E_0}^{\infty} dE \, \rho(E) \qquad e^{-tE}$$

1. Euclidean time lattice correlation functions $C(t)$
2. Hadronic spectral densities $\rho(E)$

$$\sum_{t=1}^{t_{max}} g_t(E_*) C(t) = \int_{E_0}^{\infty} dE\, \rho(E) \sum_{t=1}^{t_{max}} \overbrace{e^{-tE}}^{b_t(E)} g_t(E_*)$$

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$$\frac{\delta \mathcal{A}[g]}{\delta g} = 0, \quad \mathcal{A}[g] = \int_{E_0}^{\infty} dE \left| \delta_\sigma(E, E_*) - \sum_{t=1}^{t_{max}} g_t(E_*) b_t(E) \right|^2$$

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1. Euclidean time lattice correlation functions $C(t)$
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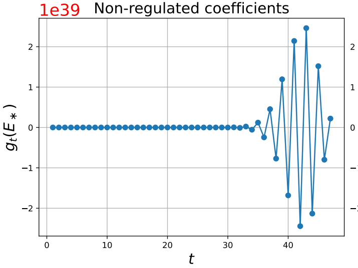
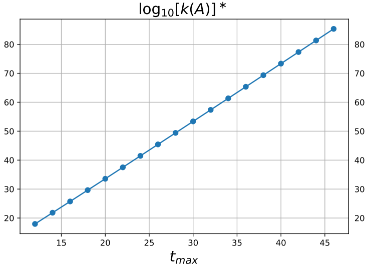
4. Combine correlators $C(t)$ with the same coefficients $g_t(E_*)$ to approximate smeared spectral densities

$$\rho_\sigma(E_*) = \int_{E_0}^{\infty} dE\, \delta_\sigma(E, E_*) \rho(E)$$

$$\frac{\delta \mathcal{A}[g]}{\delta g} = 0, \quad \mathcal{A}[g] = \int_{E_0}^{\infty} dE \left| \delta_\sigma(E, E_*) - \sum_{t=1}^{t_{max}} g_t(E_*) b_t(E) \right|^2 \to g = A^{-1} f$$

$$A_{tr} = \int_{E_0}^{\infty} dE\, b_t(E) b_r(E), \quad f_t(E_*) = \int_{E_0}^{\infty} dE\, b_t(E) \delta_\sigma(E, E_*)$$





$*k(A)$ condition number

Well-known mathematical problem: Fredholm integral equation, Hilbert and Cauchy matrices

$$\frac{\delta \mathcal{A}[g]}{\delta g} = 0, \quad \mathcal{A}[g] = \int_{E_0}^{\infty} dE \left| \delta_\sigma(E, E_*) - \sum_{t=1}^{t_{max}} g_t(E_*) b_t(E) \right|^2 \to g = A^{-1} f$$

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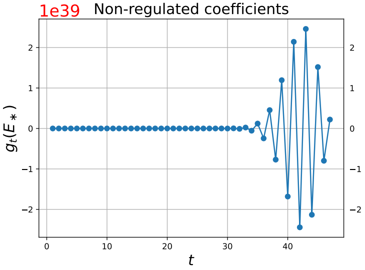
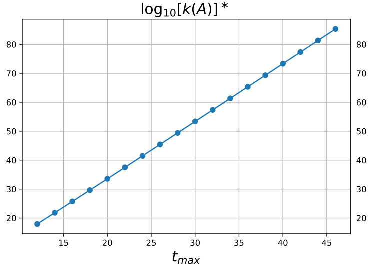


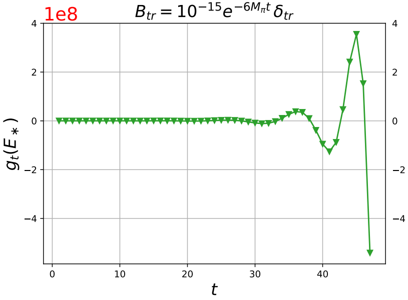


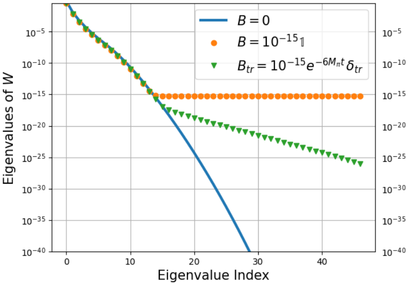
$*k(A)$ condition number

$\bar{\rho}_\sigma(E_*) = \sum_t C(t) g_t(E_*)$, but $C(t)$ are affected by statistical errors $\to$ regularization

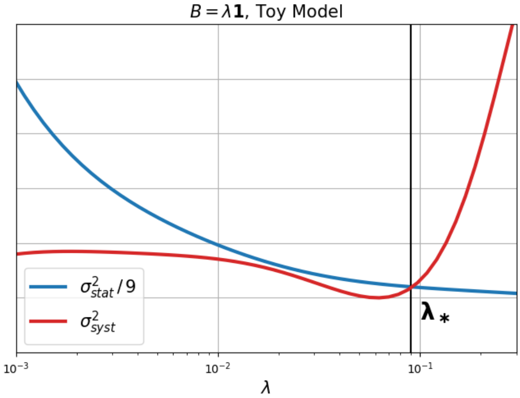
$$\frac{\delta \mathcal{W}[g]}{\delta g} = 0, \quad \mathcal{W}[g] = \mathcal{A}[g] + g^T B g \to g = W^{-1} f, \quad W = A + B$$

- $B = \lambda \frac{\text{Cov}}{C_0^2}$ [M. T. Hansen, Meyer, and Robaina 2017; M. Hansen, Lupo, and Tantalo 2019]
- $B = \lambda \mathbb{1}$ (Tikhonov)
- $B_{tr} = \lambda e^{-Mt} \delta_{tr}$





- $\sigma^2_{stat}(\lambda) = g^T \mathrm{Cov}\ g$
- $\sigma_{syst}(\lambda) = \rho_\sigma - \bar{\rho}_\sigma$ (work in progress)
- Tune λ to λ_* such that e.g. $\sigma_{stat}(\lambda_*) = 3\sigma_{syst}(\lambda_*)$



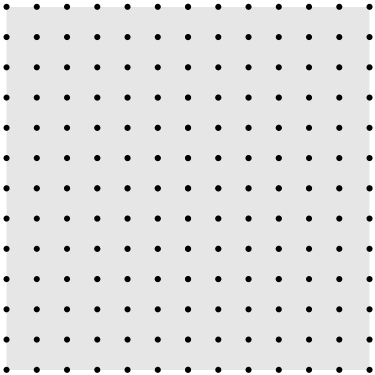
- Other strategies [M. Hansen, Lupo, and Tantalo 2019; Bulava et al. 2022]

Signal-to-Noise ratio problem [Parisi 1984; Lepage 1989], e.g. with $\boldsymbol{n}_0$ (**global**) updates of the lattice

$$C(t) = \langle V_k(t) V_k(0) \rangle$$

$$\frac{C(t)^2}{\sigma_C^2(t)} \sim \boldsymbol{n}_0 \, e^{-2(M_\rho - M_\pi)t}$$

V_k zero-momentum isovector vector current



Signal-to-Noise ratio problem [Parisi 1984; Lepage 1989], e.g. with $\boldsymbol{n}_0 \cdot \boldsymbol{n}_1$ (**global** and **local**) updates of the lattice

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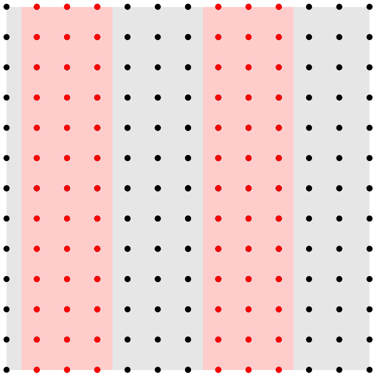
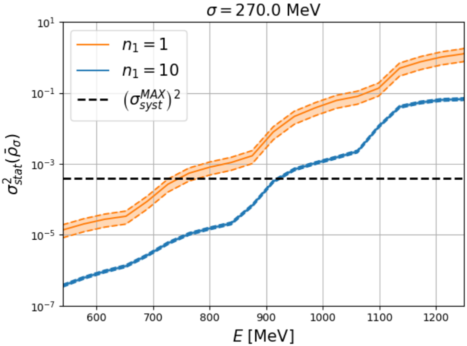


Need to factorize the fermion determinant and observables for **local** updates

- Straightforward in pure gauge theory [Lüscher and Weisz 2001]
- Recent developments for theories with dynamical fermions [Cè, Giusti, and Schaefer 2016; Cè, Giusti, and Schaefer 2017]

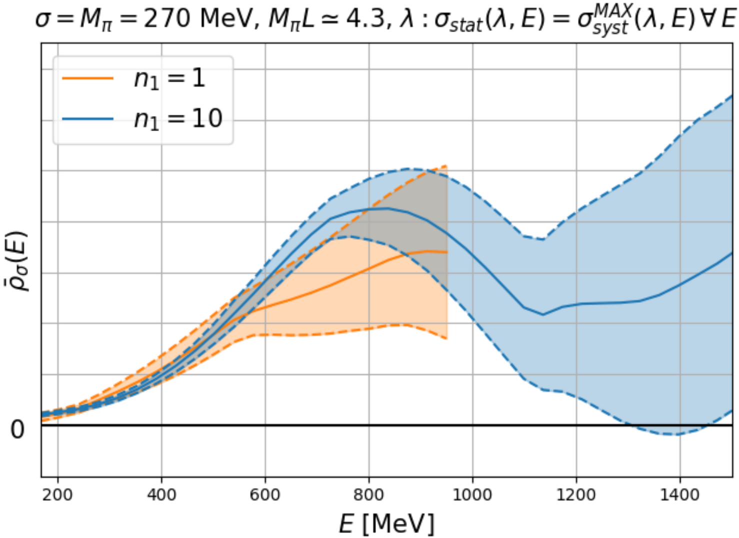
- $C(t) = \frac{1}{3}\sum_{k=1}^{3}\langle V_k(t)V_k(0)\rangle$, $\delta_\sigma(E, E_*) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(E-E_*)^2}{2\sigma^2}}$
- $N_f = 2$, $a \simeq 0.065$ fm, $M_\pi \simeq 270$ MeV, $M_\pi L \simeq 4.3$ [Dalla Brida et al. 2021]
- $\sigma_{syst} \leq \sigma_{syst}^{MAX} = \rho_{max} \int_{E_0}^{\infty} dE \, \left|\delta_\sigma(E, E_*) - \sum_t g_t(E_*) b_t(E)\right|$



- $\lambda : \sigma_{syst}^{MAX}(E)$ constant $\forall\, E$
- $Cost_{n_1=10} = 10 \cdot Cost_{n_1=1}$
- $\sigma^2_{n_1=10} = (25 \div 50) \cdot \sigma^2_{n_1=1}$

- Improving the precision on $C(t)$ at large t (Multi-Level) is beneficial for $\bar{\rho}_\sigma(E)$ at different energy scales

PRELIMINARY PLOT



Conclusions

- **Multi-level** effective to reconstruct $\bar{\rho}_\sigma$ both at low and high energies
- Preliminary result with a conservative estimate of the systematic error
- Finite-Volume errors $\sigma_{Finite\,V}$ of order $e^{-\sigma L}$ [M. Bruno's talk]
- The general strategy is to achieve $\sigma_{syst} \ll \sigma_{stat} \simeq \sigma_{Finite\,V}$ to then increase V

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Outlooks

- Working on *accurate* spectral reconstruction for zero-momentum isovector vector spectral density at $\sigma = M_\pi = 270$ MeV
- **Systematic errors** need to be studied more in depth
- Isovector axial and isoscalar vector channels will be studied
- Compare $\bar{\rho}_\sigma$ with data by smearing experimental ρ [Alexandrou et al. 2022]

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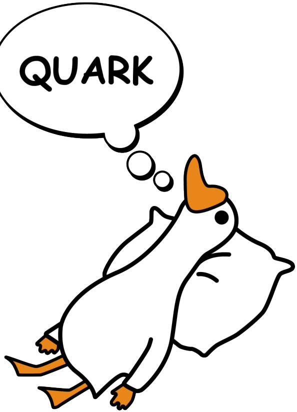
Thank you for your attention!

Backup slides



Systematic Errors (Theoretical Aspects)

- We can estimate the systematic error [MS et al. in prep]

$$\sigma^{(1)}_{syst}(E_*) = \rho_\sigma(E_*) - \bar{\rho}_\sigma(E_*) = \int_{E_0}^{\infty} dE \, \overbrace{\left[\delta_\sigma(E, E_*) - \sum_t g_t(E_*) C(t)\right]}^{\delta^{(1)}_\sigma} \rho(E)$$

by means of a new reconstruction with the smearing kernel $\delta^{(1)}_\sigma$

- We can reconstruct $\sigma^{(1)}_{syst}$ as $\bar{\sigma}^{(1)}_{syst}$ and define an improved estimator

$$\bar{\rho}^{(1)}_\sigma(E_*) = \bar{\rho}_\sigma(E_*) + \bar{\sigma}^{(1)}_{syst}(E_*)$$

- We can iterate this procedure; *if* we use the same regulator, we obtain

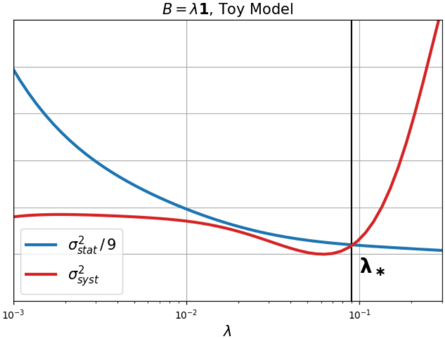
$$\bar{\sigma}^{(n)}_{syst} = C^T W^{-1} \left(\mathbb{1} - AW^{-1}\right)^n f,$$
$$\bar{\rho}^{(n)}_\sigma = C^T W^{-1} \left[\mathbb{1} - \left(\mathbb{1} - AW^{-1}\right)^{n+1}\right] WA^{-1} f$$

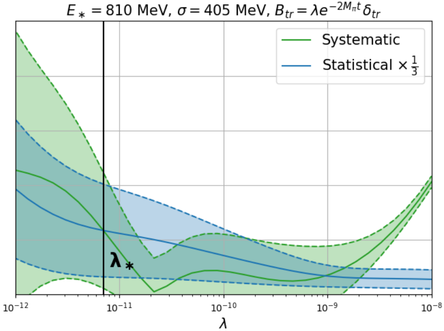
where $\left|\bar{\sigma}^{(n)}_{syst}\right| < \left|\bar{\sigma}^{(m)}_{syst}\right|$, $n < m$, but $\sigma_{stat}(\bar{\sigma}^{(n)}_{syst})$ increase with n

- We recover the non-regulated, numerically ill-defined result $\bar{\rho}^{(\infty)}_\sigma = C^T A^{-1} f$

Systematic Errors (Numerical Aspects)

Tune λ such that e.g. $\sigma_{stat} = 3\sigma_{syst}^{(1)}$ at $\lambda = \lambda_*$



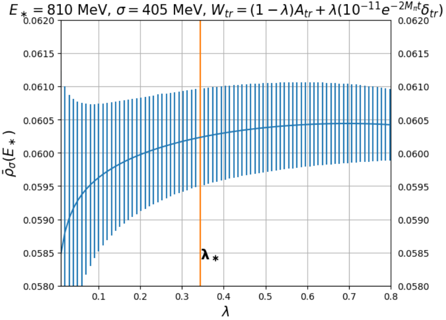


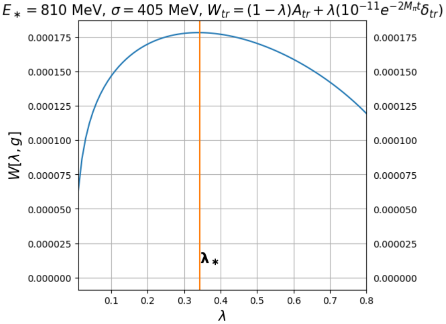
Systematic Errors (Other Strategies)

Tune λ such that [M. Hansen, Lupo, and Tantalo 2019]

$$\mathcal{W}[\lambda, g] = (1-\lambda)\mathcal{A}[g] + \lambda\mathcal{B}[g]$$

$$\max_{\lambda} \mathcal{W}[\lambda, g(\lambda, E_*)] = \mathcal{W}[\lambda_*, g(\lambda_*, E_*)] \equiv \mathcal{W}[\lambda_*, E_*]$$

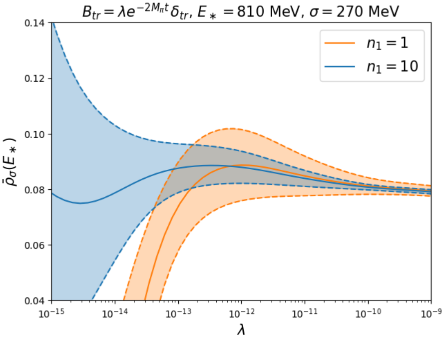


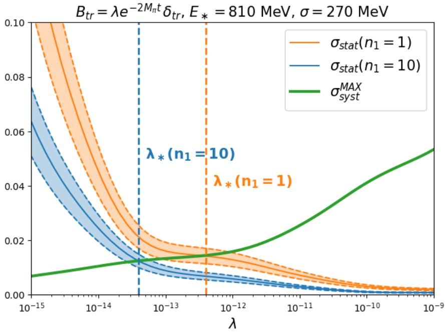


Systematic Errors (Upper Bound)

$$\sigma_{syst}(E_*) = \left| \int dE\, \rho(E) \left[\delta_\sigma(E, E_*) - \sum_t g_t(E_*) b_t(E) \right] \right| \qquad [\rho(E) \geq 0]$$

$$\leq \underbrace{\rho_{max}}_{\simeq 1 \text{ in our units}} \int dE \left| \delta_\sigma(E, E_*) - \sum_t g_t(E_*) b_t(E) \right| \equiv \sigma^{MAX}_{syst}(E_*)$$





Vector Correlator: Multi-Level

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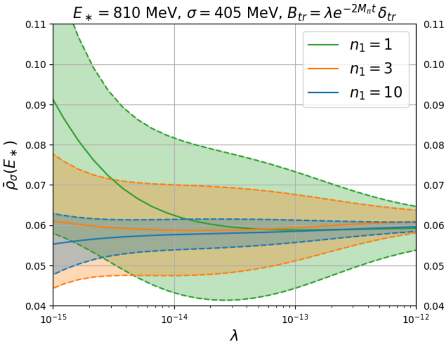

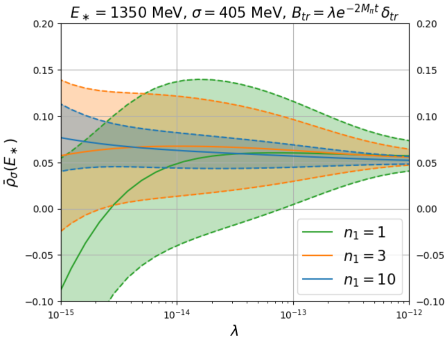

- At fixed regulator (and σ_{syst}), smaller σ_{stat} for larger n_1