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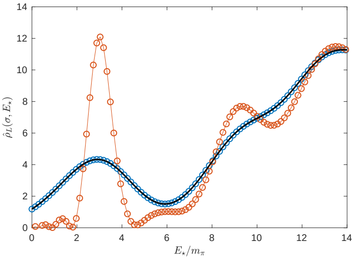
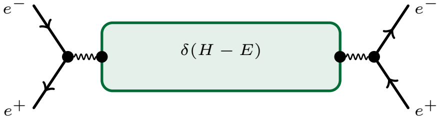
a new numerical method to cope with inverse-problems

the case of hadronic spectral densities

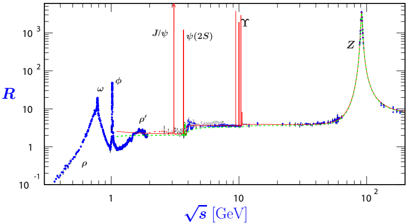
in collaboration with m.hansen and a.lupo, arXiv:1903.06476

- why hadronic spectral densities
- the problem with lattice correlators: euclidean time, finite volume, statistical and systematic errors
- recovering the physical information from smeared spectral densities
- how to extract smeared spectral densities from noisy measurements
- examples in the case of a benchmark model
- examples in the case of a true lattice data
- conclusions and outlooks



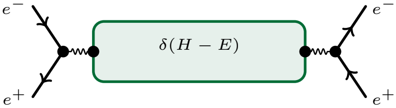


- hadronic spectral densities are central objects in the calculations of physical observables associated with the continuum spectrum of the QCD Hamiltonian



- a notable classical example is the so-called R-ratio, i.e. the ratio of the differential cross-section for $e^+e^- \mapsto hadrons$ over the corresponding quantity for $e^+e^- \mapsto \mu^+\mu^-$

$$R \propto \underbrace{\langle 0| J^k_{em}(0)\, \delta(H-E)\delta^3(\boldsymbol{P})\, J^k_{em}(0)|0\rangle}_{\rho(E)}$$



- other important examples are hadronic τ decays, the flavour–changing non–leptonic decay–rates of kaons and heavy flavoured mesons, the deep inelastic scattering cross–section, and thermodynamic observables arising in the study of QCD at finite–temperature and of the quark–gluon plasma, etc.

- first-principles model-independent calculations of hadronic spectral densities can in principle be performed by recurring to non–perturbative lattice techniques
- the primary observables in a lattice calculations are euclidean time-ordered correlators at discrete values of the coordinates and on a finite volume

$$C(t) = \frac{1}{L^3} \sum_{\boldsymbol{x}} T \langle 0 | O(x) \, \bar{O}(0) | 0 \rangle_L$$

- these can be rewritten in terms of the finite volume spectral densities

$$C(t) = \int_0^\infty dE \, \rho_L(E) \, e^{-tE} \; ,$$

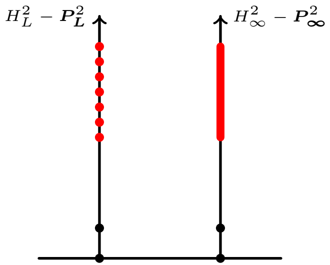
$$\rho_L(E) = \frac{1}{L^3} \sum_{\boldsymbol{x}} \langle 0 | O(0, \boldsymbol{x}) \, \delta(E - H_L) \, \bar{O}(0) | 0 \rangle_L$$

- now we see the problems:

$$C(t) = \int_0^\infty dE\, \rho_L(E)\, e^{-tE} + \delta C(t)\ ,$$

$$\rho_L(E) = \frac{1}{L^3} \sum_{\boldsymbol{x}} \langle 0 | O(0,\boldsymbol{x})\, \delta(E - H_L)\, \bar{O}(0) | 0 \rangle_L$$

$$= \sum_n w_n(L)\, \delta(E - E_n(L))$$



- lattice correlators are unavoidably affected by errors and, in this case, the inverse Laplace-transform needed to extract the spectral densities becomes an ill-posed numerical problem

- even in the ideal case in which these can be computed exactly, finite volume spectral densities cannot be associated with physical quantities

- the finite volume hamiltonian has a discrete spectrum and, consequently, the finite volume spectral densities are distributions, sums of isolated δ-function singularities

- in order to solve these problems one can conveniently consider smeared spectral densities

$$\hat{\rho}_L(\sigma, E_\star) = \int_0^\infty dE\, \Delta_\sigma(E_\star, E)\, \rho_L(E)$$

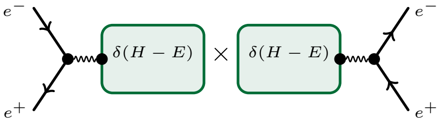
- the smearing function can be chosen to be peaked around $E_\star$ and such that it becomes a Dirac δ-function when the smearing radius parameter σ is sent to zero

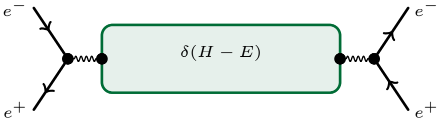
- smeared spectral densities are smooth functions of the energy and studying their infinite volume limit is a well posed problem; the physical information is recovered by taking the limits

$$\rho(E_\star) = \lim_{\sigma \to 0} \lim_{L \to \infty} \hat{\rho}_L(\sigma, E_\star)$$

in the specified order!

- notice that smeared spectral functions must be introduced in order to properly define cross-sections, this is the way we avoid the well-known issue of the square of a δ-function appearing at intermediate stages of the calculations





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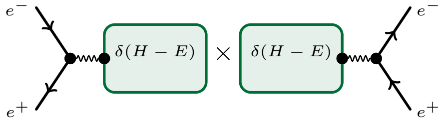
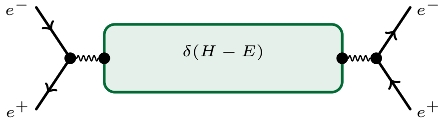
in the specified order!

- moreover, experimental data can be smeared with the same function used in the theoretical calculations





- **m.t.hansen, h.b.meyer, d.robaina, PRD96 (2017)** proposed to extract smeared spectral densities by using a classical method due to Backus and Gilbert (BG), **g.backus, f.gilbert, Geophys.J.R.Astron.Soc.16 (1968)**

- the central idea of BG is to search for a smearing function that lives in the space spanned by the basis-functions of the correlator

$$\Delta^{BG}(E_\star, E) = \sum_{t=0}^{t_{max}} g_t(E_\star)\, e^{-(t+1)E}$$

- once the coefficients $g_t(E_\star)$ are known, the smeared spectral density is given by

$$C(t+1) = \int_0^\infty dE\, \rho_L(E)\, e^{-(t+1)E}$$

$$\hat{\rho}_L^{BG}(E_\star) = \sum_{t=0}^{t_{max}} g_t(E_\star)\, C(t+1)$$

$$= \int_0^\infty dE\, \rho_L(E)\, \Delta^{BG}(E_\star, E)$$

- in absence of errors on the correlator (an idealization), the coefficients $g_t(E_\star)$ are obtained by minimizing the following functional

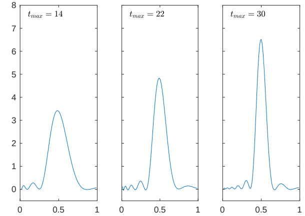
$$A_{BG}[g] = \int_0^\infty dE\,(E - E_\star)^2 \left\{\Delta^{BG}(E_\star, E)\right\}^2$$

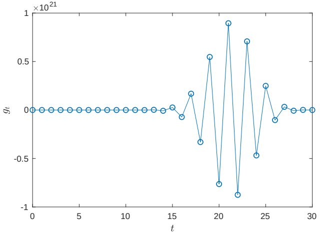
$$= \int_0^\infty dE\,(E - E_\star)^2 \left\{\sum_{t=0}^{t_{max}} g_t(E_\star)\, e^{-(t+1)E}\right\}^2$$

under the unit-area constraint

$$\int_0^\infty dE\, \Delta^{BG}(E_\star, E) = 1$$

- the width of the smearing function is optimized on the basis of the number of observations





- in the realistic case in which errors are present, the correlator has to be replaced with

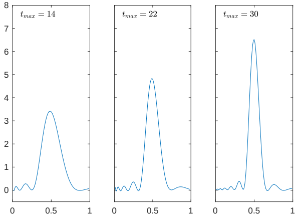
$$C_i(t) = \bar{C}(t) + \delta C_i(t) \;, \qquad i = 0, \cdots, N-1$$

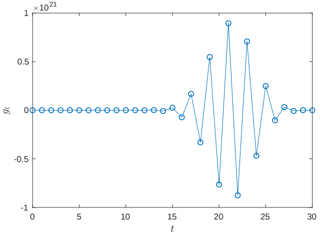
- since the coefficients are gigantic, even a tiny deviation from the average is enormously amplified

$$\sum_{t=0}^{t_{max}} g_t(E_\star)\, \delta C_i(t) \mapsto \infty$$

and statistical errors also become gigantic

- this is a manifestation of the fact that we are dealing here with a numerically ill-posed problem



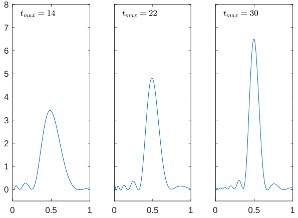


- the very smart mechanism suggested by BG to keep errors under control is to minimize the following functional

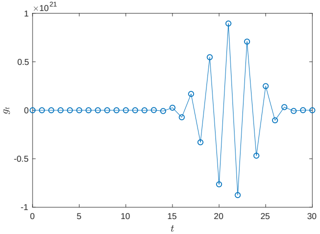
$$W[\lambda, g] = (1-\lambda) A_{BG}[g] + \lambda B[g]$$

$$B[g] = \sum_{t,r=0}^{t_{max}} \mathtt{Cov}_{tr}\, g_t(E_\star)\, g_r(E_\star)$$

$$\mathtt{Cov}_{tr} = \frac{1}{N}\sum_{i=0}^{N-1} \delta C_i(t+1)\delta C_i(r+1)$$



- the presence of the error functional $B[g]$ forbids solutions corresponding to gigantic values of the coefficients and statistical errors are thus kept under control



- on the other hand, the shape of the smearing function now depends, in addition to the number of observations, also on the associated errors: this is a particularly unpleasant feature if the method has to be used in order to take the infinite volume limit

- moreover, there is no natural way to set the trade-off parameter λ, a part from trying to balance in a subjective way between resolution and errors

m.hansen, a.lupo, n.t. arXiv:1903.06476

- we devised a method in which the target smearing function is an input of the procedure; in what follows

$$\Delta_\sigma(E_\star, E) = \frac{e^{-\frac{(E-E_\star)^2}{2\sigma^2}}}{\int_0^\infty dE\, e^{-\frac{(E-E_\star)^2}{2\sigma^2}}}$$

- the method searches for an optimal approximation of the target smearing function in the space of the basis functions

$$\bar{\Delta}_\sigma(E_\star, E) = \sum_{t=0}^{t_{max}} g_t(E_\star)\, e^{-(t+1)E}$$

- and again the coefficients are obtained by minimizing a convex combination of a deterministic and of the error functionals

$$W[\lambda, g] = (1-\lambda)A[g] + \lambda \frac{B[g]}{C(0)^2}$$

under the unit area constraint

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- but in our case the deterministic functional is a measure of the difference between the target and approximated smearing functions

$$A[g] = \int_0^\infty dE \, \left|\bar{\Delta}_\sigma(E_\star, E) - \Delta_\sigma(E_\star, E)\right|^2$$

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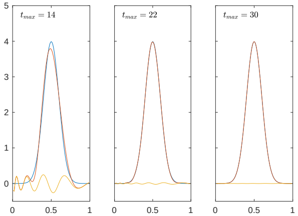
- in absence of errors, our method is just a way to find an optimal polynomial approximation to a smooth function, $x = e^{-E}$

$$A[g] = \int_0^1 dx \, \left| \sum_{t=0}^{t_{max}} g_t x^t - \frac{\Delta_\sigma(E_\star, -\log(x))}{x} \right|^2$$



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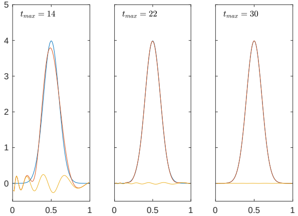

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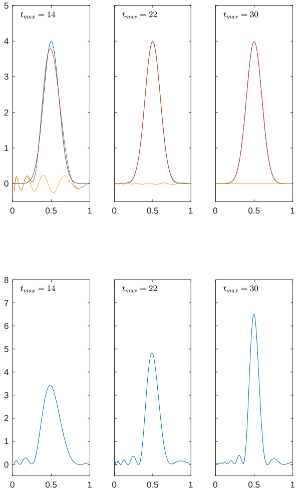
- this has to be compared with the BG method where by increasing t_{max} one gets a different (sharper) smearing function



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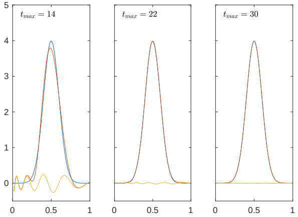
- furthermore, since at the end of the procedure the difference between the target and the approximated smearing function is known

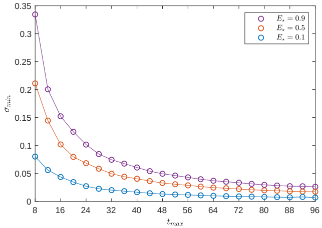
$$\delta_\sigma(E_\star, E) = 1 - \frac{\bar{\Delta}_\sigma(E_\star, E)}{\Delta_\sigma(E_\star, E)}$$

- this information can be used in our method to estimate the systematic error on the estimated smeared spectral densities induced by this difference

$$\Delta^{bias} = \int_0^\infty dE\, \delta_\sigma(E_\star, E)\, \Delta_\sigma(E_\star, E)\, \rho_L(E)$$

$$\Delta^{syst} = |\delta_\sigma(E_\star, E_\star)|\, \hat{\rho}_L(\sigma, E_\star)$$





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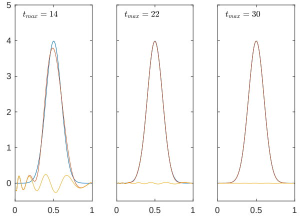
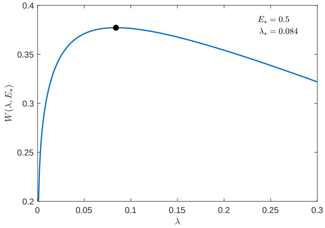
- finally, in our method there is a a natural way to set the trade-off parameter λ by studying the functional $W[\lambda, E_\star]$ evaluated at the solution $g_\star(\lambda, E_\star)$ as a function of λ

$$\max_\lambda \left\{ (1-\lambda) A[g_\star] + \lambda \frac{B[g_\star]}{C(0)^2} \right\} = W(\lambda_\star, E_\star)$$





m.t.hansen, h.b.meyer, d.robaina, PRD96 (2017)
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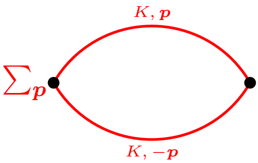
- we have decided to test our method by using the same benchmark system previously proposed to test the BG method in the context of the extraction of hadronic spectral densities

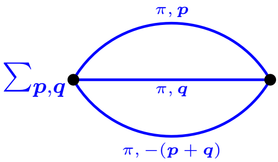
$$\mathcal{L}_{int}(x) = \frac{g_\pi}{6}\phi(x)\pi^3(x) + \frac{g_K m_\phi}{2}\phi(x)K^2(x) \ ,$$

$$3m_\pi < 2m_K < m_\phi$$



- we have considered a correlator having as finite volume spectral density

$$\rho_L(E) = \frac{g_K^2 m_\phi^2}{2(m_\pi L)^3}\sum_{\boldsymbol{p}}\frac{\delta(E-2E_K(\boldsymbol{p}))}{4E_K^2(\boldsymbol{p})}$$
$$+\ \frac{g_\pi^2}{48 m_\pi^3 L^6}\sum_{\boldsymbol{p},\boldsymbol{q}}\frac{\delta(E-E_\pi(\boldsymbol{p})-E_\pi(\boldsymbol{q})-E_\pi(\boldsymbol{p}+\boldsymbol{q}))}{E_\pi(\boldsymbol{p})E_\pi(\boldsymbol{q})E_\pi(\boldsymbol{p}+\boldsymbol{q})}$$



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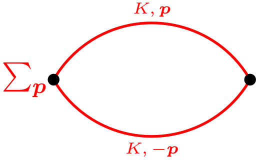
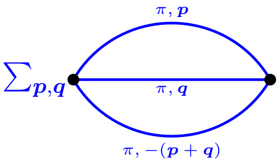


- that in the infinite volume limit becomes

$$\rho(E) = \frac{g_K^2 m_\phi^2}{32\pi^2 m_\pi^3}\sqrt{1-\frac{4m_K^2}{m_\phi^2}}\,\theta(E-2m_K)$$

$$+ \frac{g_\pi^2}{3072\pi^4\, m_\pi}\left(\frac{E}{m_\pi}\right)^2 \mathcal{F}\left(\frac{E}{m_\pi}\right)\,\theta(E-3m_\pi)$$

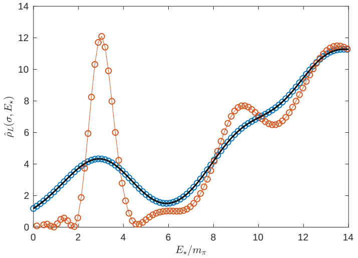


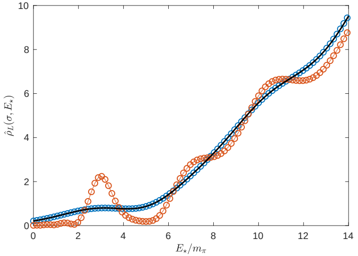
$$\mathcal{F}(x) =$$

$$\frac{2}{x^4}\int_4^{(x-1)^2} dy\sqrt{(y-4)\left[\frac{(x^2-1)^2}{y} - 2(x^2+1) + y\right]}$$

m.hansen, a.lupo, n.t. arXiv:1903.06476

- the plots show the results obtained by using our method and the ones obtained by using the BG method
- both plots have been obtained by setting $\sigma = 0.1$ and $t_{max} = 30$; the one on the top corresponds to $L = 24$ while the one on the bottom to $L = 32$
- the blue points, obtained with our method, are in perfect agreement with the expected result that in this case is known exactly
- in the case of the BG (orange points) the smearing function is an output of the procedure, it can only be controlled by changing t_{max} and, moreover, it is different at different values of $E_\star$





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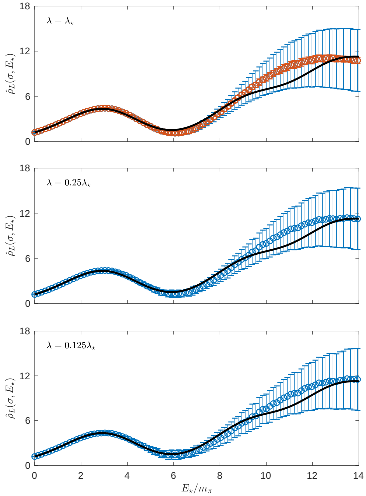
- the plots have been obtained by using our method on the volume $L = 24$ with $t_{max} = 30$ and $\sigma = 0.1$

- having a reliable estimate of the systematic errors, the results must be compatible at different values of λ within the total uncertainties

$$W[\lambda, g] = (1 - \lambda)A[g] + \lambda \frac{B[g]}{C(0)^2}$$



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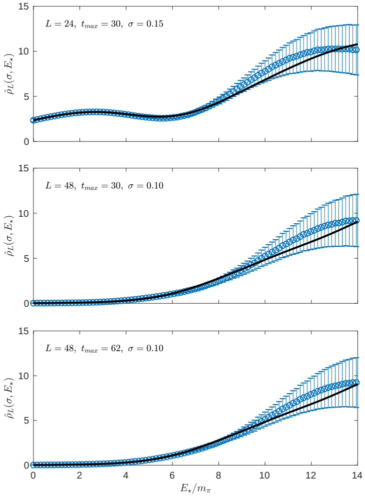
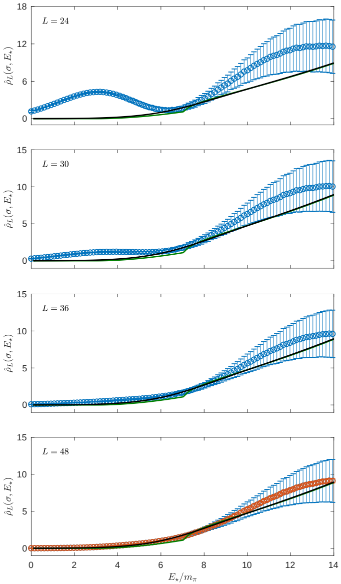


- when the smeared spectral density is smoother, either because the smearing radius is larger or because the volume is larger, the reconstruction works much better
- in these cases using

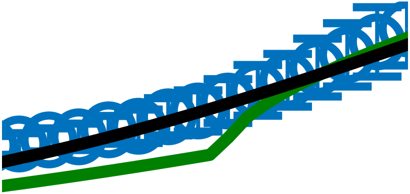
$$\Delta^{syst} = |\delta_\sigma(E_\star, E_\star)|\, \hat{\rho}_L(\sigma, E_\star)$$

provides a very conservative estimate of the systematic errors

- the plots, obtained with $\sigma = 0.1$ and $t_{max} = 31$, show the approach to the infinite volume limit of the estimated smeared spectral functions



- the plots, obtained with $\sigma = 0.1$ and $t_{max} = 31$, show the approach to the infinite volume limit of the estimated smeared spectral functions
- the green curve is the exact infinite volume spectral density: this is a continuous function of the energy but has a cusp in correspondence of the two-kaons threshold
- in the infinite volume limit the data have to reproduce the black curve, the exact infinite volume smeared spectral density: this is a smooth curve



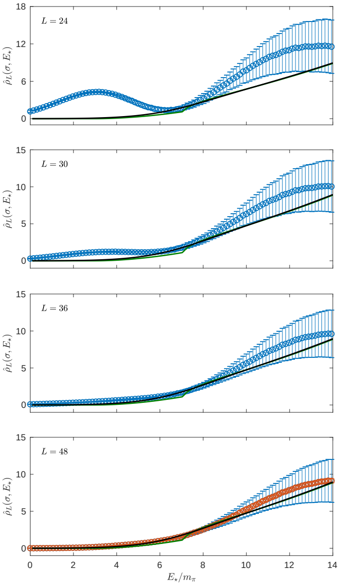
- the plots, obtained with $\sigma = 0.1$ and $t_{max} = 31$, show the approach to the infinite volume limit of the estimated smeared spectral functions

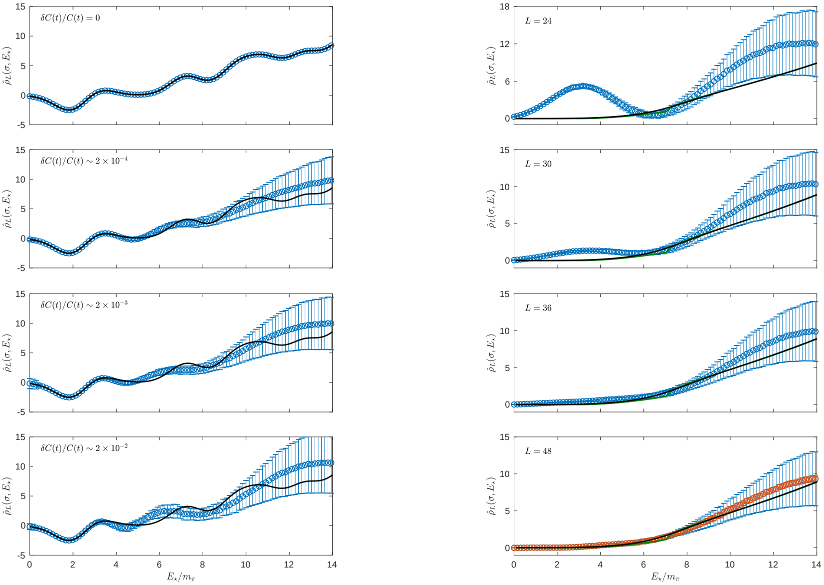
- the green curve is the exact infinite volume spectral density: this is a continuous function of the energy but has a cusp in correspondence of the two-kaons threshold

- in the infinite volume limit the data have to reproduce the black curve, the exact infinite volume smeared spectral density: this is a smooth curve

- this already happens at $L = 36$ and the agreement is remarkably good (at the level of the statistical errors) at $L = 48$

- as already noticed, experimental data can be smeared with the same smearing function used in the theoretical calculations so that the results can directly be compared with measurements





$\delta C(t)/C(t) = 0$
$\delta C(t)/C(t) \sim 2 \times 10^{-4}$
$\delta C(t)/C(t) \sim 2 \times 10^{-3}$
$\delta C(t)/C(t) \sim 2 \times 10^{-2}$
$L = 24$
$L = 30$
$L = 36$
$L = 48$
$\hat{\rho}_L(\sigma, E_\star)$
$E_\star/m_\pi$

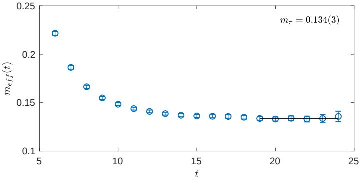
- we have applied our method to true lattice data in the case of a QCD pseudoscalar-pseudoscalar correlator

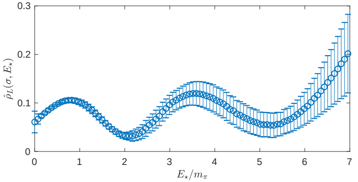
$$C_{\text{QCD}}(t) = \frac{1}{2L^3} \sum_{\boldsymbol{x}} T \langle 0 | \, P(0) \, P(x) \, | 0 \rangle \ ,$$

$$P(x) = \{ \bar{d}\gamma_5 u + \bar{u}\gamma_5 d \} \, (x)$$

- the simulation has been performed on a lattice volume $L^3 \times T = 24^3 \times 48$ with equal (unphysical) masses for the dynamical up, down and strange quarks

- in this channel we expect a peak in correspondence of m_π and the next contribution to be at $E_\star \simeq 3m_\pi$

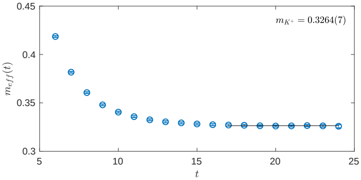




- we have applied our method to true lattice data also in the case of a QCD+QED pseudoscalar-pseudoscalar correlator

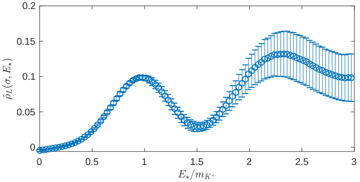
$$C_{\text{QCD+QED}}(t) = \frac{1}{2L^3} \sum_{\boldsymbol{x}} T \langle 0|\, P(0)\, P(x)\, |0\rangle \ ,$$

$$P(x) = \left\{ \bar{S}\gamma_5 U + \bar{U}\gamma_5 S \right\}(x)$$



- the simulation has been performed on a lattice volume $L^3 \times T = 24^3 \times 48$, at the unphysical value $\alpha_{em} = 0.05$ with dynamical up, down and strange quarks

- in this channel we expect a peak in correspondence of m_{K^+} and the next contribution to be at $E_{3K}/m_{K^+} \simeq 2.6$



- we have devised a new numerical method to cope with inverse problems
- the method inherits from the classical BG approach the very smart mechanism that allows to keep statistical errors under control
- in our method the smearing function is an input of the procedure and there is a natural way to chose the trade-off parameter λ
- by comparing results at sub-optimal values of λ one can asses the reliability of the estimated errors
- the method is general and can be applied to inverse problems arising in different research fields
- we look forward to many interesting applications: the R-ratio, hadronic τ decays, exotic spectroscopy, etc.