Theoretical aspects on the prediction of spectral densities from Lattice QCD

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work in collab. with Maxwell T. Hansen

Turin Lattice Meeting 2023
Torino, IT, December 20th

On the N_f-dependence of gluonic observables

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SFB TR9

December 19, 2013, Torino

Advances in simulations with dynamical fermions

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WEAK DECAYS BEYOND NLO

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December 23[th], 2016

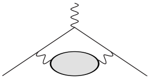
Motivations

Predictions of hadronic amplitudes, decay rates, spectral densities

- important tests of the Standard Model
  - $(g-2)_\mu$ based e.g. on $\gamma \to \pi^+\pi^-$, $\pi^0 \to \gamma\gamma$
  - test of CP violation in K, D decays
- improve our understanding of strong interactions
  - properties of resonances like ρ^0

$(g-2)_\mu$: Dispersive approach

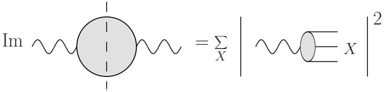
Method



$$a_\mu = \frac{\alpha}{\pi} \int \frac{ds}{s} K(s, m_\mu) \frac{\mathrm{Im}\Pi(s)}{\pi}$$ [Brodsky, de Rafael '68]

analyticity $\hat{\Pi}(k^2) = \Pi(k^2) - \Pi(0) = \frac{k^2}{\pi} \int_0^\infty ds \frac{\mathrm{Im}\Pi(s)}{s(s-k^2-i\varepsilon)}$

unitarity



$$\frac{4\pi^2\alpha}{s} \frac{\mathrm{Im}\Pi(s)}{\pi} = \sigma_{e^+e^- \to \gamma^\star \to \mathrm{had}}$$

At present $O(30)$ channels: $\pi^0\gamma, \pi^+\pi^-, 3\pi, 4\pi, K^+K^-, \cdots$

$K(s, m_\mu) \to \pi^+\pi^-$ dominates due to ρ resonance

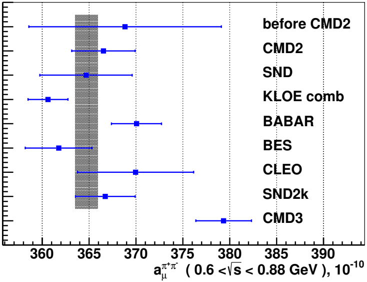
$\pi\pi$ channel is $\sim 70\%$ of signal and $\sim 70\%$ of error

$(g-2)_\mu$: Dispersive approach

Tensions in $\pi^+\pi^-$ channel

Large tensions among experiments: BaBar, KLOE, now CMD3

[CMD3 2302.08834]



very difficult to combine different experiments

- what is the error of $\pi\pi$ contribution to a_μ?
- motivates even more first-principles Lattice QCD calculations

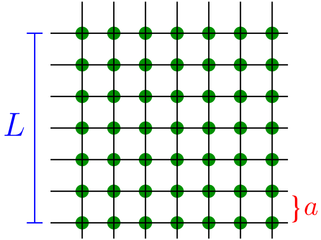
Lattice field theories

lattice spacing $a \to$ regulate UV divergences

finite size $L \to$ infrared regulator

Continuum theory $a \to 0$, $L \to \infty$

Euclidean metric $\to$ Boltzman interpretation of path integral



$$\langle O \rangle = \mathcal{Z}^{-1} \int [DU] e^{-S[U]} O(U) \approx \frac{1}{N} \sum_{i=1}^{N} O[U_i]$$

Very high dimensional integral $\to$ Monte-Carlo methods

Markov Chain of gauge field configs $U_0 \to U_1 \to \cdots \to U_N$

1. Inverse problems and smeared spectral densities
2. Finite-volume effects on smeared spectral densities
3. Θ correlators and the Maiani-Testa problem

Analytic continuation

Time-momentum representation very natural for Lattice QCD
project operator $\mathcal{O}$ to definite spatial momentum
evaluate $C(t) = \langle \mathcal{O}(t)\mathcal{O}(0)\rangle$

$+$ Physical observables as integrals of spectral densities
$P = \int d\omega\, \kappa(\omega)\, \rho(\omega)$
e.g. inclusive diff. decay rate semileptonic [Gambino, Hashimoto '20]

$+$ Correlator is integral of spectral density $C(t) = \int d\omega e^{-\omega|t|}\rho(\omega)$

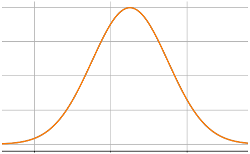
$=$ Solve $P = \int dt\, f(t)\, C(t)$ for unknown f?

Inverse problems

Take $L = \infty$, $a = 0$ but $C(t)$ only known on set $\{t_1, t_2 \cdots\}$
is it possible $\rho(\omega) = \sum_t g_t C(t)$?

$C(t)$ finite discrete Euclidean times
cannot extract continuous $\rho(\omega)$
$\rho_\sigma(\omega) = \int d\omega' \, \rho(\omega') \, \delta_\sigma(\omega' - \omega)$
$\delta_\sigma(x) = \frac{\sigma/\pi}{x^2+\sigma^2}$

smooth Dirac δ_σ



let's reformulate the question ... is it possible $\rho_\sigma(\omega) = \sum_t g_t C(t)$?
problem remains ill-posed, but solution admitted

Ansatz $\sum_t g_t e^{-\omega t} = \kappa'(\omega) \quad \rightarrow \quad \sum_t g_t C(t) = \int d\omega \, \kappa'(\omega) \, \rho(\omega)$
minimize $\int d\omega [\kappa'(\omega) - \kappa(\omega)]^2$ w.r.t. g_t
for finite set of time slices $\kappa' \neq \kappa$
but not always a problem [Boito et al]

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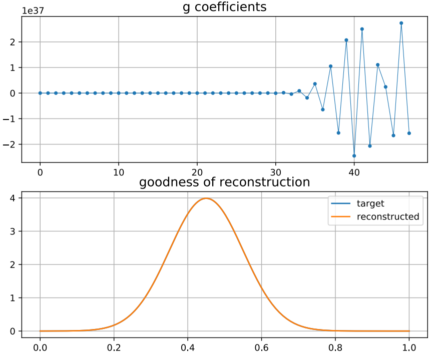
Approximate solutions

Sketch

Ansatz $\sum_t g_t e^{-\omega t} = \kappa(\omega) \quad \to \quad \sum_t g_t C(t) = \int d\omega\, \kappa(\omega)\, \rho(\omega)$

1. minimize L^2 norm $\int d\omega \left[\sum_t g_t e^{-\omega t} - \kappa(\omega) \right]^2$
2. define $A(t,t') = \int d\omega e^{-\omega(t+t')}$, $\quad f(t) = \int d\omega \kappa(\omega) e^{-\omega t}$
3. solution is $g_t = \sum_{t'} [A^{-1}]_{t,t'} f(t')$

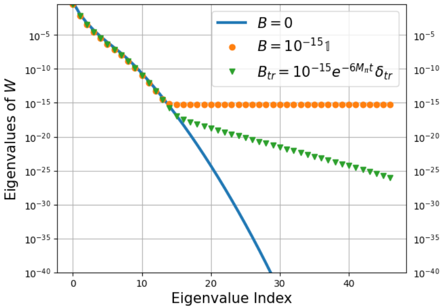


A^{-1} ill-conditioned matrix
$\to$ 1e32 y-axis

coefficients useless in practice $\leftrightarrow$ stat. errors

Regulators

[MB, Giusti, Saccardi Hadron23]



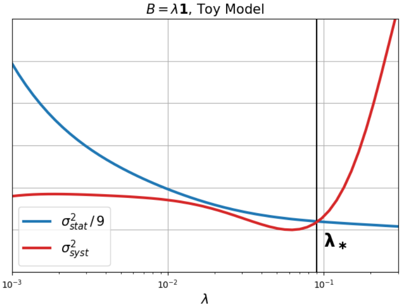
Regularization by suppressing small eigenvalues of A

$W = A + B$

$B_{tt'} = \lambda \delta_{tt'}$ [Tikhonov]

$B_{tt'} \propto \mathrm{cov}_{tt'}$ [HLT '19]

sparsening of A [Boito et al]



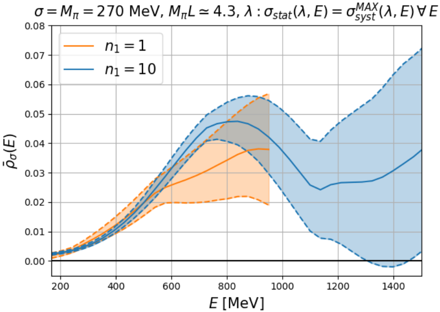
stat. errs down

syst. errs up

tuning required...

Outlooks

[MB, Giusti, Saccardi Hadron23]



Open questions I am working on

- syst. errors from regularization of inverse problem
- signal-to-noise problem in ρ_σ? multi-level useful?

1. Inverse problems and smeared spectral densities
2. Finite-volume effects on smeared spectral densities
3. Θ correlators and the Maiani-Testa problem

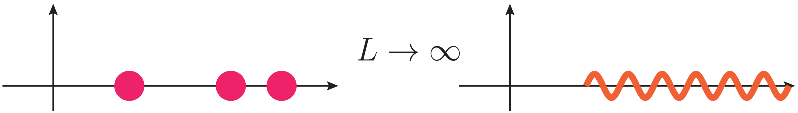
Finite volume

Quantization of spectrum

Lattice Simulations performed in finite box $L^3 \times T$ (T large)

periodic BC $\vec{p} = \frac{2\pi}{L}\vec{n}$, $\vec{n} \in \mathbb{Z}^3$

$\rightarrow$ spectrum quantized



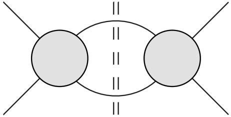
Hamiltonian $\hat{H}_L$ (on slice L^3), momentum operator $\hat{P}_i$

Hilbert space $\hat{H}_L|n, \vec{p}\rangle_L = E_n(\vec{p}, L)|n, \vec{p}\rangle_L$

scattering? decay rates?

what is meaning of $|n, \vec{p}\rangle_L$ and $E_n(\vec{p}, L)$?

1. s-channel one-loop diagram



$$\int \frac{dk_0}{2\pi} \int \frac{d\vec{k}}{(2\pi)^3} \frac{iz(k)}{k^2-m^2+i\epsilon} \frac{iz(P-k)}{(P-k)^2-m^2+i\epsilon}$$
$$\int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} \frac{iz(k)}{k^2-m^2+i\epsilon} \frac{iz(P-k)}{(P-k)^2-m^2+i\epsilon}$$

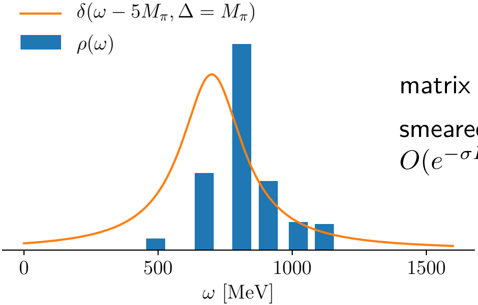
2. evaluate integral-sum difference w/ Poisson's formula
   non-analytic function $\to 1/L^n$ corrections, i.e. loop legs on-shell
   analytic function $\to e^{-mL}$ corrections, i.e. loop legs off-shell

3. re-sum all $2 \to 2$ diagrams
   $2 \to 4$ diagrams $1/L^k$ correction if $\sqrt{s} > 4m$
   quantization condition $Q(E_n) = n\pi$

Spectral decomposition

EM current J_μ, projected to momentum $\vec{p}$

$$\langle J_\mu(t,\vec{p}) J_\mu(0,\vec{p})\rangle = \sum_n |\langle 0|J_\mu(0)|n,\vec{p}\rangle_L|^2 e^{-E_n(L)t}$$



matrix elements $1/L^k$ finite vol. effects

smeared $\delta_\sigma \to$ smeared ρ_σ FV $O(e^{-\sigma L})$?

Smeared spectral densities

Finite volume effects

Scalar current J projected to zero-momentum
$$\rho(\omega) = \langle 0|\hat{J}\,\delta(\hat{H}-\omega)\,\delta^3(\vec{P})\,\hat{J}|0\rangle\,, \quad \rho(\omega|L) = \sum_n \delta(\omega - E_n)|\langle 0|\hat{J}|n\rangle_L|^2$$

Goal: finite volume effects of $\rho_\kappa = \int d\omega\,\rho(\omega)\,\kappa(\omega)$ [MB, Hansen in prep]

- $\kappa(\omega) = e^{-\omega t}$: correlator (checks w/ literature)
- $\kappa(\omega) = \delta_\sigma(\omega - E)$: smeared ρ_σ
- $\kappa(\omega) = \Theta(\omega - E, \Delta)e^{-(\omega-E)t}$: Θ correlators [MB, Hansen '20]

Setup of our derivation:

1. restrict to two-particle form factor $F_\pi = \langle 0|\hat{J}|\pi\pi\rangle$
2. lowest partial wave $Q(E,L) = \delta_0(E) + \varphi(E,L)$
3. applicable to $I=1$ vector-vector channel

Our work builds upon [Lellouch-Lüscher '00][Hansen-Sharpe '12][...]
[Bulava, Hansen, Hansen, Patella, Tantalo '21]

Sketch of derivation

MB, Hansen 23xx.yyyy

Quant. condition function $Q(E,L)$ s.t. $Q(E_n,L) = n\pi$

1. $\rho(E_n|L) = |\langle 0|\hat{J}|n\rangle_L| = \dfrac{\rho(E_n)}{Q^{(1,0)}(E_n,L)}$ Lellouch-Lüscher factor
2. $$\int dE\, \rho(E|L)\, \kappa(E) = \sum_n \int dE\, \frac{\rho(E)}{Q^{(1,0)}} \delta(E-E_n)\, \kappa(E) = \sum_n \int dE\, \delta(n\pi - Q(E,L))\rho(E)\, \kappa(E)$$
3. Poisson's summation formula $\sum_n \delta(n\pi - Q) \to \sum_k e^{2iQk}$
   - 3.1 perform change of variables $E = 2\sqrt{m_\pi^2 + p^2}$
4. Analytically continue p to $p + i\mu$ in complex plane
   4D proof that $e^{2i\phi} \simeq e^{ipL}$

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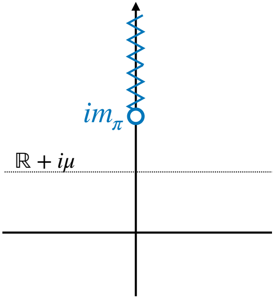
Finite volume effects

MB, Hansen 23xx.yyyy

$$\rho_\kappa(L) - \rho_\kappa \to \int_{\mathbb{R}+i\mu} dp \frac{p^2}{p^2+m_\pi^2}\, e^{2iQ(\omega)}\, e^{-E(p)t}$$



$$E(p) = 2\sqrt{m_\pi^2+p^2}$$

$$e^{2iQ(\omega)} \simeq e^{ipL} \to e^{-\mu L}$$

how large μ?

Finite-vol effects driven by analytic structure of

$E(p)$

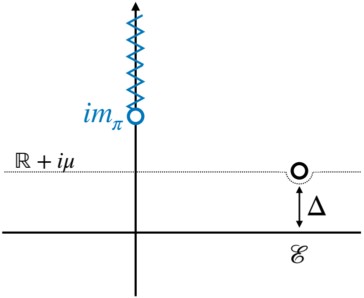
$|F_\pi(\omega(p))|^2$

$\kappa(\omega(p))$

Finite volume effects

MB, Hansen 23xx.yyyy

$$\rho_\kappa(L) - \rho_\kappa \to \int_{\mathbb{R}+i\mu} dp \frac{p^2}{p^2+m_\pi^2}\, e^{2iQ(\omega)}\, \kappa(E(p))$$



$$E(p) = 2\sqrt{m_\pi^2+p^2}$$

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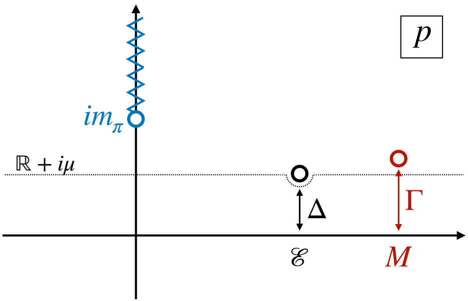
Finite volume effects

MB, Hansen 23xx.yyyy

$$\rho_\kappa(L) - \rho_\kappa \to \int_{\mathbb{R}+i\mu} dp \frac{p^2}{p^2 + m_\pi^2} \, e^{2iQ(\omega)} \, \kappa(E(p)) \, |F_\pi(E)|^2$$



$$E(p) = 2\sqrt{m_\pi^2 + p^2}$$

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how large μ?

Finite-vol effects driven by analytic structure of

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1. Inverse problems and smeared spectral densities
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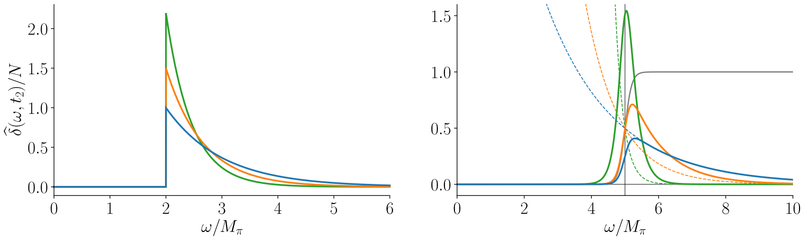
A simple observation

Maiani-Testa theorem

$\langle \pi, \vec{q}_1 | \widetilde{\pi}_{\vec{q}_2}(0) \quad e^{-(\hat{H}-2\omega_{\vec{q}})t_2} J(0)|0\rangle$ [Maiani-Testa '90]

$\langle \pi, \vec{q}_1 | \widetilde{\pi}_{\vec{q}_2}(0)\, \Theta(\hat{H}-2\omega_{\vec{q}}, \Delta) e^{-(\hat{H}-2\omega_{\vec{q}})t_2} J(0)|0\rangle$ [Bruno-Hansen, '20]



smooth Θ, smearing width Δ

tames growing exponentials in $2M_\pi < E < 2\omega_{\vec{q}}$

combination of Θ and exponential $\rightarrow$ localization in energy ω

like Maiani and Testa we want analytic control by expanding t_2

Spectral densities

Preliminary

$$G(t) = \int d^3\vec{x}\,\langle J(t,\vec{x})J(0)\rangle = \langle \widetilde{J}_{\vec{q}}(t)J(0)\rangle = \int_{2m}^{\infty} d\omega\, e^{-\omega t}\,\rho(\omega^2)$$

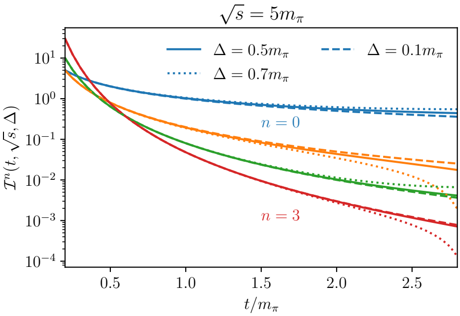
1. smooth Θ function

$$G^{\Theta}(t|\mathcal{E}) = \langle \widetilde{J}_{\vec{0}}(0)\, e^{-(\hat{H}-\mathcal{E})t}\, \Theta(\hat{H}-\mathcal{E},\Delta)\, J(0)\rangle$$

2. large t expansion: localize "right shoulder"

$$G^{\Theta}(t|\mathcal{E}) = \sum_n r_n \mathcal{I}_n(t,\mathcal{E},\Delta)$$

[MB APLAT'21]



$\mathcal{I}_n$ analytic functions
asymptotic series

r_n free fit parameters

$r_0 \equiv \rho(s = \mathcal{E}^2)$

r_n all physical $\leftrightarrow \partial_s^n \rho$

Proposed numerical strategy

[MB, Hansen '20][MB APLAT '21]

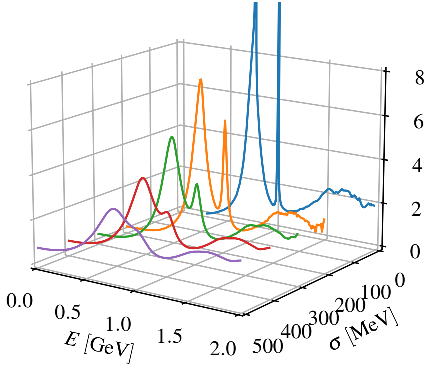
In a finite-volume $G^\Theta(t) = \sum_n \Theta(E_n - \omega, \Delta) c_n e^{-E_n t}$

1. build G^Θ from original G
   1. GEVP large set of operators $\to$ first N states
      $G^\Theta(t) = G(t) - \sum_{n=0}^{N} c_n \Theta(\omega - E_n, \Delta)\, e^{-E_n t}$
   2. numerical reconstruction of G^Θ a lá Backus-Gilbert
2. fit G^Θ, $t \in [t_{\min}, t_{\max}]$ using $\mathcal{I}_n$ basis functions

   similar numerical complexity of syst. error from excited states
3. fixed t $G^\Theta(t)$ is a smeared spectral density

Smeared spectral densities ρ_σ have physical meaning

- $\sigma \gg 0$ needed to control finite-vol effects
- is $\sigma \simeq 0$ really needed for physics?
  - e.g. CMD3 vs BaBar vs KLOE $\sigma \simeq m_\pi$ likely sufficient!



Thanks for the attention