New DoS techniques for finite density lattice QCD

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Complex action problem

- In general lattice field theories with finite chemical potential μ have actions S with an imaginary part.

- The Boltzmann factor

$$e^{-S} \in \mathbb{C}$$

  thus has a complex phase and cannot be used as a probability weight.

- Standard Monte Carlo simulation techniques are not available for a non-perturbative analysis.

  "Complex action problem" or "Sign problem"

- Generic feature of finite density field theories both, on the lattice and in the continuum, for bosonic and fermionic theories.

We discuss new DoS techniques to circumvent the problem for finite density lattice QCD.

Modern density of states approach for generic bosonic fields

- Vacuum expectation values of observables:

$$\langle \mathcal{O} \rangle \; = \; \frac{1}{Z} \int D[\Phi] \, e^{-S_R[\Phi] + i\, X[\Phi]} \, \mathcal{O}[\Phi] \qquad\qquad Z \; = \; \int D[\Phi] \, e^{-S_R[\Phi] + i\, X[\Phi]}$$

- Densities of states introduced as functions of the imaginary part $x \equiv X[\Phi]$:

$$\rho^{(\mathcal{O})}(x) \; = \; \int D[\Phi] \, e^{-S_R[\Phi]} \, \mathcal{O}[\Phi] \, \delta\Big(x - X[\Phi]\Big)$$

- Evaluation of observables:

$$\langle \mathcal{O} \rangle \; = \; \frac{1}{Z} \int dx \, \rho^{(\mathcal{O})}(x) \, e^{i\,x} \qquad , \qquad Z \; = \; \int dx \, \rho^{(\mathbb{1})}(x) \, e^{i\,x}$$

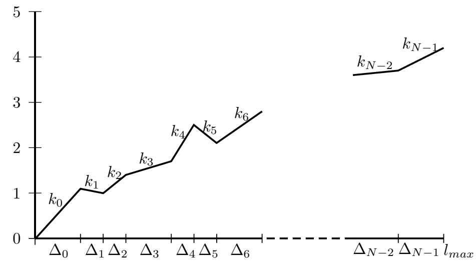
- The key challenge is to determine the densities with very high accuracy!!

Parameterization of the densities

- Divide $[0, x_{max}]$ into intervals $I_n,\ n = 0, 1 \ldots N-1$ of sizes Δ_n.

- Ansatz for the densities:

$$\rho(x) \;=\; e^{-L(x)}$$



$L(x)$: continuous and piecewise linear on the intervals I_n

- Imposing the normalization $\rho(0) = 1$ completely determines the density $\rho(x)$ in terms of the slopes k_n for the intervals I_n:

$$\rho(x) \;=\; A_n\, e^{-x\,k_n} \qquad \text{for} \quad x \in I_n \qquad\qquad \text{with} \quad A_n \;=\; e^{-\sum_{j=0}^{n-1}\left[k_j - k_n\right]\Delta_j}$$

Determination of the slopes

- To determine the slopes we use: Restricted VEVs (Langfeld, Lucini, Rago)

$$\langle X \rangle_n(\lambda) \;\equiv\; \frac{1}{Z_n(\lambda)} \int D[\Phi] \; \Theta_n(X[\Phi]) \; e^{-S_R[\Phi] \, + \, \lambda \, X[\Phi]} \; X[\Phi]$$

with

$$\Theta_n(x) \;=\; \begin{cases} 1 & \text{for} \quad x \in I_n \\ 0 & \text{for} \quad x \notin I_n \end{cases}$$

$\Longrightarrow$ exponential error suppression

- $\langle X \rangle_n(\lambda)$ is free of the complex action problem and can be computed with standard Monte Carlo simulations as a function of the parameter $\lambda \in \mathbb{R}$.

- $\langle X \rangle_n(\lambda)$ may also be computed directly using the parameterized density:

$$\langle \, X \, \rangle_n(\lambda) \;=\; \frac{d}{d\,\lambda} \, \ln \int_{x_n}^{x_{n+1}} dx \; \rho(x) \; e^{\,\lambda\, x} \;=\; \frac{d}{d\,\lambda} \, \ln \int_{x_n}^{x_{n+1}} dx \; A_n \; e^{-k_n\, x} \; e^{\,\lambda\, x}$$

Determination of the slopes

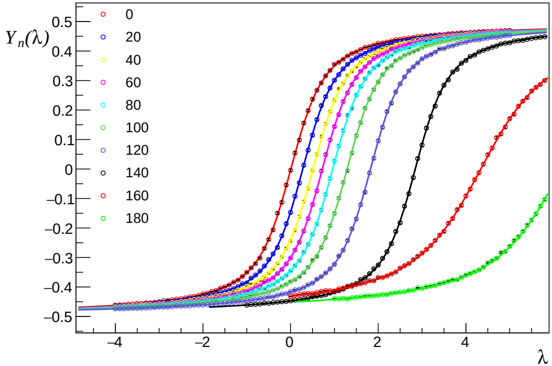
- After suitable normalization we find

$$Y_n(\lambda) \;\equiv\; \frac{\langle\, X \,\rangle_n(\lambda) - x_n}{\Delta_n} - \frac{1}{2} \;=\; h\Big(\Delta_n[\lambda - k_n]\Big)$$

where

$$h(s) \equiv \frac{1}{1-e^{-s}} - \frac{1}{s} - \frac{1}{2} \qquad \text{with} \qquad h(0) = 0 \,, \quad \lim_{s\to\pm\infty} h(s) = \pm 1/2$$

- A simple 1-parameter fit of $Y_n(\lambda)$ allows to determine k_n (Gattringer, Giuliani)



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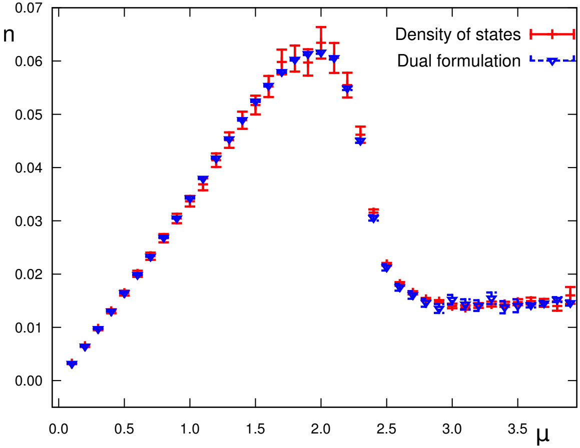
Example results

- Well tested new DoS approach. "Functional Fit Approach" (FFA)

- Here an example in the SU(3) spin model where a dual (worldline) representation without complex action problem provides reference results:



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Two proposals for implementing DoS FFA to full QCD

- Key challenge: Organize finite density lattice QCD such that the intrinsically bosonic DoS FFA formulation becomes applicable.

- Canonical DoS approach
  - Change to fixed quark number via FT with respect to imaginary $\mu = i\theta/\beta$
  - Compute the density as function of θ using DoS FFA

- Direct grand canonical DoS approach
  - Rewrite lattice QCD with a suitable pseudofermion representation
  - Isolate the imaginary part of the pseudofermion action and apply DoS FFA

- For both cases we currently conduct numerical proof of principle studies.

Elements of the canonical DoS approach

- Canonical partition sums written as Fourier moments of imaginary $\mu = i\theta/\beta$

$$Z_N \;=\; \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \int D[U]\, e^{-S_g[U]} \; \det \mathcal{D}[U,\mu] \Big|_{\mu = i\frac{\theta}{\beta}} \; e^{-i\,\theta N}$$

$$\langle \mathcal{O} \rangle_N \;=\; \frac{1}{Z_N} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \int \mathcal{D}[U]\, e^{-S_G[U]} \; \det D[U,\mu]^2 \, \mathcal{O}[U,\mu] \Big|_{\mu = i\frac{\theta}{\beta}} \; e^{-i\,\theta N}$$

- Introduce densities which we will compute with FFA:

$$\rho^{(\mathcal{O})}(\theta) \;=\; \int \mathcal{D}[U]\, e^{-S_G[U]} \; \det D[U,\mu]^2 \, \mathcal{O}[U,\mu] \Big|_{\mu = i\frac{\theta}{\beta}}$$

- Observables are obtained as Fourier transforms of the densities

$$Z_N \;=\; \int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, \rho^{(\mathbb{1})}(\theta)\, e^{-i\theta N} \quad , \qquad \langle \mathcal{O} \rangle_N \;=\; \frac{1}{Z_N} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\, \rho^{(\mathcal{O})}(\theta)\, e^{-i\theta N}$$

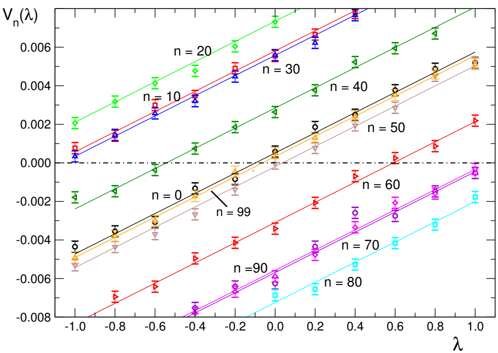
Elements of the canonical DoS approach

- Suitable restricted vacuum expectation values for determination of the slopes k_n:

$$\langle\, \theta \,\rangle_n(\lambda) \;\equiv\; \frac{1}{Z_n(\lambda)} \int_{\theta_n}^{\theta_{n+1}} d\theta \int \mathcal{D}[U]\; e^{\,-S_G[U]}\,\theta\, e^{\,\theta\lambda}\; \det D[U,\mu]^{\,2}\, \mathcal{O}[U,\mu]\,\Big|_{\mu = i\frac{\theta}{\beta}}$$

- Normalizing them and fitting them with $h(\Delta_n[\lambda - k_n])$:

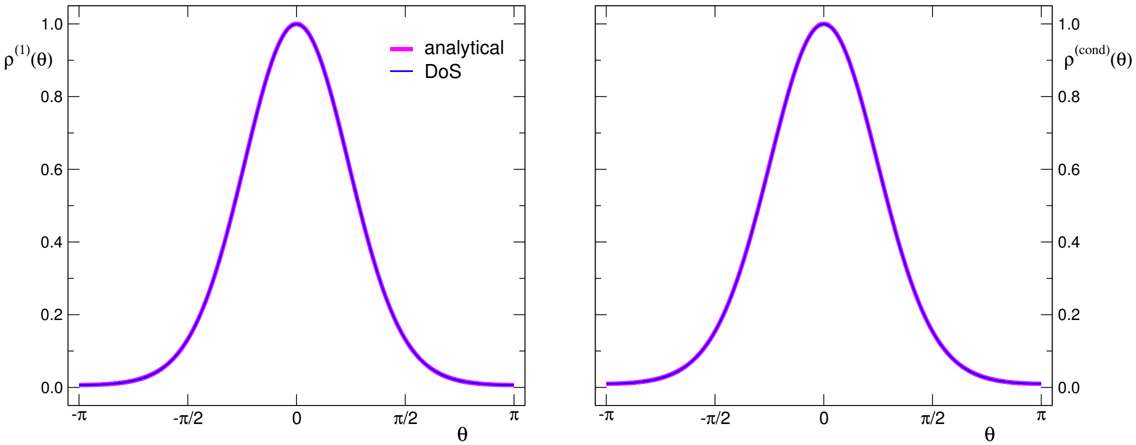
$$V_n(\lambda) \;\equiv\; \frac{\langle\, \theta \,\rangle_n(\lambda) - \theta_n}{\Delta_n} - \frac{1}{2} \;=\; h(\Delta_n[\lambda - k_n])$$



$\Rightarrow$ slopes k_n $\Rightarrow$ density $\rho(\theta)$ $\Rightarrow$ observables

Exploratory first tests of canonical DoS in the 2-d free case

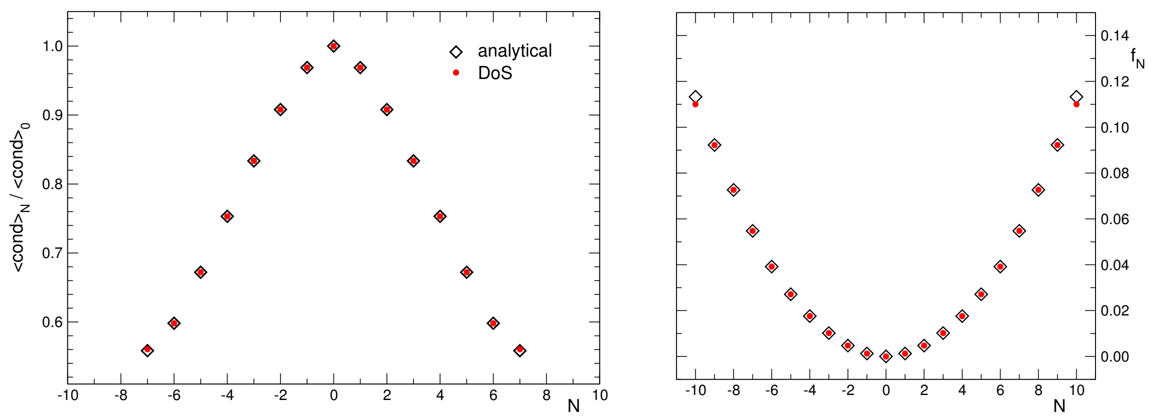
Densities for $\mathcal{O} = \mathbb{1}$ and $\mathcal{O} = \text{Tr } D^{-1}$ (staggered fermions, 16×16, $m = 0.1$):



DoS FFA data perfectly match the analytical results.

Exploratory first tests of canonical DoS in the 2-d free case

Results for observables $\langle\overline{\psi}(x)\psi(x)\rangle_N$ and $f_N = -\ln Z_N/V$:



Also for observables the canonical DoS data match the analytical results very well.

Elements of the direct grand canonical DoS with FFA

- Grand canonical partition sum:

$$Z(\mu) \;=\; \int D[U]\, e^{-S_g[U]}\, \det \mathcal{D}[U,\mu]$$

- Introduction of pseudo-fermions:

$$\det \mathcal{D}[U,\mu] \;=\; \frac{\det \mathcal{D}[U,\mu]^\dagger \;\det \mathcal{D}[U,\mu]}{\det \mathcal{D}[U,\mu]^\dagger} \;\propto\; \det\big(\mathcal{D}[U,\mu]^\dagger\, \mathcal{D}[U,\mu]\big) \int D[\Phi]\, e^{-\,\Phi^\dagger \mathcal{D}[U,\mu]^\dagger \Phi}$$

- Real factor $\det\big(\mathcal{D}[U,\mu]^\dagger\, \mathcal{D}[U,\mu]\big)$ can be handled with conventional techniques.

- The pseudo-fermion integral is treated with DoS FFA.

$$\begin{aligned} \int D[\Phi]\, e^{-\,\Phi^\dagger \mathcal{D}[U]^\dagger \Phi} \;&=\; \int D[\Phi]\, e^{-\,\frac{1}{2}\Phi^\dagger\left(\mathcal{D}[U] + \mathcal{D}[U]^\dagger\right)\Phi \;+\; \frac{1}{2}\Phi^\dagger\left(\mathcal{D}[U] - \mathcal{D}[U]^\dagger\right)\Phi} \\ &=\; \int D[\Phi]\, e^{-\,S_R[\Phi,U] \;+\; i\,X[\Phi,U]} \end{aligned}$$

Elements of the direct grand canonical DoS with FFA

- Definition of the densities:

$$\rho(x) \;=\; \int D[U]\, e^{-S_{eff}[U]} \int D[\Phi]\, e^{-\,S_R[\Phi,U]}\, \delta\left(x \,-\, X[\Phi,U]\right)$$

$$e^{-S_{eff}[U]} \;=\; e^{-S_g[U]}\; \det\!\big(\mathcal{D}[U,\mu]^\dagger\, \mathcal{D}[U,\mu]\big)$$

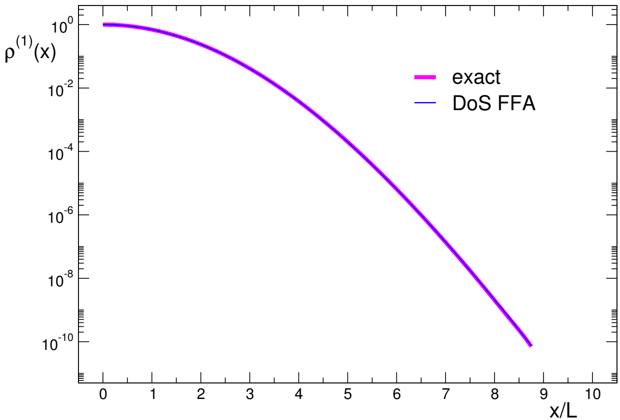
- Necessary restricted VEVs are directly accessible with MC:

$$\langle X \rangle_n(\lambda) \;=\; \frac{1}{Z_n(\lambda)} \int D[U]\, e^{-S_{eff}[U]} \int D[\Phi]\, e^{-\,S_R[\Phi,U] \,+\, \lambda\, X[\Phi,U]}\; X[\Phi,U]\; \Theta_n(X[\Phi,U])$$

Fits with $h(\Delta_n[\lambda - k_n])$ $\Rightarrow$ slopes k_n $\Rightarrow$ density $\rho(x)$ $\Rightarrow$ observables

Exploratory first tests of the direct approach in the 2-d free case

Comparison of $\rho(x)$ to analytical results (Wilson fermions, 16×16, $m = 0.1$, $\mu = 0.05$):



- Here the range of x is unbounded. $\rho(x)$ decreases quickly $\Rightarrow$ truncation is possible.
- The density from DoS FFA matches the analytic result.

Summary

- The functional fit approach FFA was established as a new powerful DoS approach for dealing with complex action problems in bosonic theories.
- The key ingredients are a continuous and piecewise linear parameterization of $\ln\,\rho(x)$ combined with restricted VEVs for computing the parameters of $\ln\,\rho(x)$.
- The challenge for applying DoS FFA to finite density lattice QCD is finding a suitable representation such that the bosonic DoS FFA approach can be used.
- Canonical DoS: Switch to canonical formulation using FT with respect to imaginary chemical potential $\mu = i\theta/\beta$. Use FFA to determine $\rho(\theta)$.
- Direct grand canonical approach: Use pseudo-fermions to convert the problem into a bosonic one. Identify the imaginary part and directly apply DoS FFA.
- Both approaches have been worked out and tested in small simulations using the free case as reference. The preliminary results are encouraging and we started larger tests.