Solving the complex action problem of the finite density Z_3 spin model with the density of states approach using FFA

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[C. Gattringer, P. Törek, PLB (2015), arXiv:1503.04947]

[Y. Mercado, C. Gattringer, P. Törek, PoS (2014), arXiv:1410.1645]

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Motivation

- MC simulations of finite density field theories: Sign problem
- Possible way out: Density of states (DoS) method
- Challenges of DoS:
  - Density ρ varies over many orders of magnitude
  - Finite-μ problem $\rightarrow$ ρ integrated over highly oscillating factor
  - Need precise determination of ρ
- Based on idea of Wang-Landau algorithm:
  [K. Langfeld, B. Lucini, A. Rago, PRD (2014)]
  - Simulation in small intervals of density argument
  - Restricted MC in intervals $\rightarrow$ determine ρ
  - Exponential error suppression
- Here: Further development of DoS method
  $\rightarrow$ Functional Fit Approach (FFA)
  Compare with dual approach (no sign problem) in Z_3 spin model

Action and partition sum

Effective action for Polyakov loop in QCD at $g \to \infty$ and $m \to \infty$
$\Rightarrow$ action of the Z_3 spin model at $\mu \neq 0$ and $T \neq 0$

$$S[P] = -\sum_{x\in\Lambda}\left[\tau\sum_{\nu=1}^{3}\left(P_x\,P^\star_{x+\hat\nu} + c.c.\right) + \kappa\,e^{+\mu}\,P_x + \kappa\,e^{-\mu}\,P^\star_x\right]$$

$\mu \leftarrow \mu\beta$

with (Polyakov loops) $P_x \in Z_3 = \left\{1, e^{i\,2\pi/3}, e^{-i\,2\pi/3}\right\}$ and Λ a 3D lattice

Partition sum

$$Z = \sum_{\{P\}} e^{-S[P]} = \prod_{x\in\Lambda}\sum_{P_x} e^{-S[P]}$$

Rewriting the action and the partition sum

N_0, $N_\pm$ is the number of spins equal to 1, $e^{\pm i\,2\pi/3}$ and
$\Delta N = N_+ - N_- \in [-V, V]$

$$S = -\,\tau \sum_{x,\nu} \left(P_x\, P^\star_{x+\hat\nu} + c.c. \right) - (3\,N_0 - V)\,\kappa \cosh \mu - i\,\sqrt{3}\;\Delta N\,\kappa\,\sinh \mu$$
$$\equiv\; S_R + i\,S_I$$

Symmetry: $P \to P^\star \Rightarrow\; \Delta N \to -\,\Delta N,\, N_0 \to N_0$

$$\Rightarrow Z = \sum_{\{P\}} e^{-S_R}\;\cos(S_I)$$

The density of states

Definition of a weighted density of states: q net particle number

$$\rho(q) = \sum_{\{P\}} e^{-S_R} \, \delta(q - \Delta N) \, , \; q \in [-V, V]$$

One can write the partition sum as (use $\rho(q) = \rho(-q)$)

$$Z = \rho(0) + 2 \sum_{q=1}^{V} \rho(q) \, \cos\left(\sqrt{3}\, q\, \kappa \sinh \mu\right)$$

Observables can be computed with

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{q=-V}^{V} \rho(q) \, e^{i\sqrt{3}\, q\, \kappa \sinh \mu} \, \mathcal{O}(q)$$

Key features of the FFA

- Parametrize ρ as a piecewise constant function in q (exact!)
- Compute $\langle q \rangle$ with restricted MC simulations on small intervals for q
- Populate regions of low density with a auxiliary Boltzmann factor $e^{-\lambda q}$
- Parameters of $\rho(q)$ are obtained by fitting the restricted MC data with a known function of λ

Computation of $\rho(q)$: functional fit approach (FFA)

- Parametrize the density of states $\rho(q) = \rho(-q)$

$$\rho(q) = \exp\left(-\sum_{i=0}^{|q|} a_i\right) \quad , \quad a_i \in \mathbb{R}$$

- Compute the coefficients a_i using restricted expectation values

$$\langle\langle \Delta N \rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \sum_{\{P\}} \theta_n(\Delta N)\, e^{-S_R - \lambda\,\Delta N}\, \Delta N, \; \theta_n(q) = \begin{cases} 1, & |q-n| \leq 1 \\ 0, & \text{otherwise} \end{cases}$$

- Relation between MC data and the a_i

$$\langle\langle \Delta N \rangle\rangle_n(\lambda) - n = \frac{e^{2\lambda - a_n - a_{n+1}} - 1}{e^{2\lambda - a_n - a_{n+1}} + e^{\lambda - a_n} + 1}$$

Restricted Monte Carlo

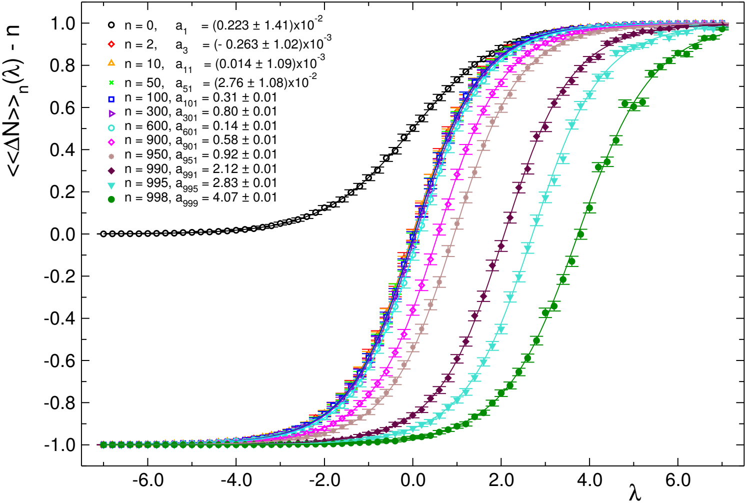
- Generate initial configurations P such that $\Delta N[P] \in \{n-1, n, n+1\}$
- Modified Metropolis steps: If $\Delta N[P] \notin \{n-1, n, n+1\} \Rightarrow$ reject trial configuration (additional rejection step)

Strategy for obtaining the coefficients a_i

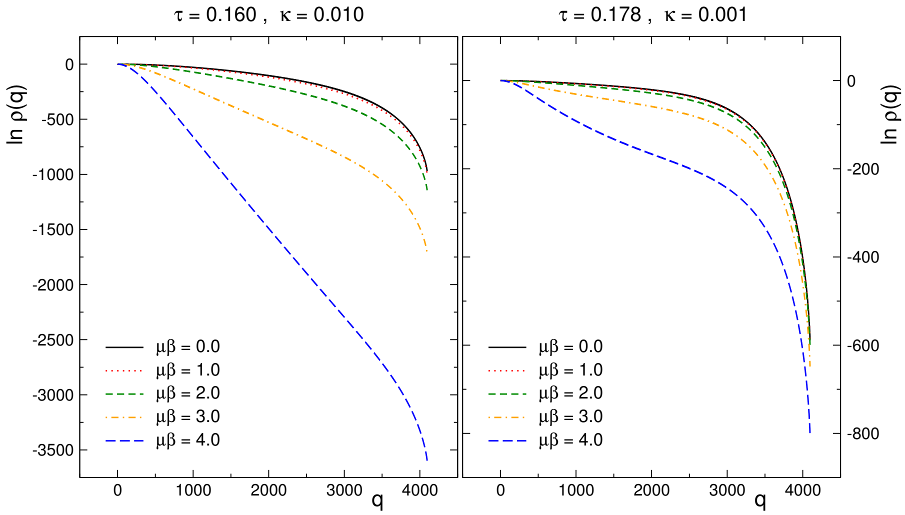
- Restricted Monte Carlo for λ_i, $i = 1, \ldots, N_\lambda \Rightarrow \langle\langle \Delta N \rangle\rangle_n(\lambda_i) - n$
- Fit the results (χ^2-minimization) $\Rightarrow$ recursive sequence:

  $n = 0 : \; a_1 \rightarrow n = 1 : \; a_2 \rightarrow \cdots \rightarrow n = V - 1 : \; a_V$

Examples for $\langle\langle \Delta N \rangle\rangle_n(\lambda) - n$: $V = 10^3$ $\tau = 0.16$, $\kappa = 0.01$, $\mu = 1.0$



Examples for $ln\,\rho$: $V = 16^3$



Fitting the density

Fit the density of states

$$ln\,\rho(q) = \sum_{n=1}^{N} c_n\, q^{2n}$$

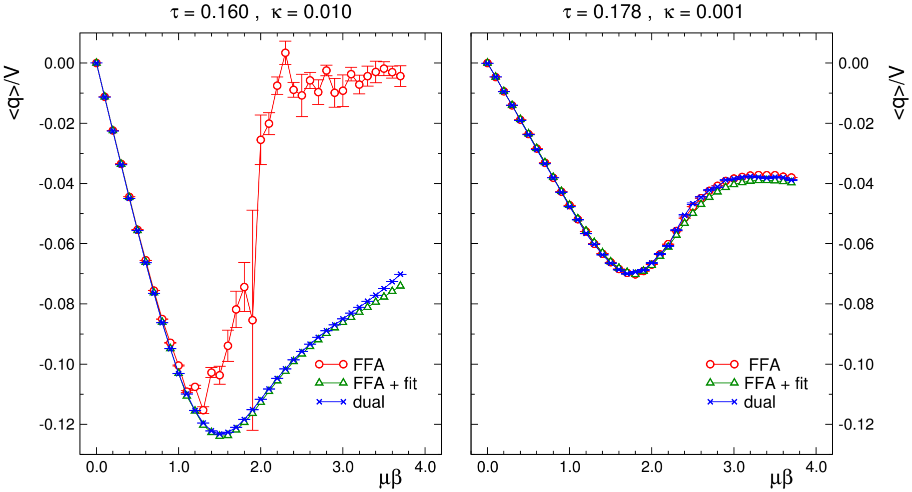
and compute the convolution integral numerically

$$Z = 2\int_0^V dq\,\rho(q)\cos\left(\sqrt{3}\,q\,\kappa\,\sinh\mu\right)$$

$\rho(q)$ is a smooth function $\Rightarrow$ fit is numerically less expensive than a drastic increase of the statistics

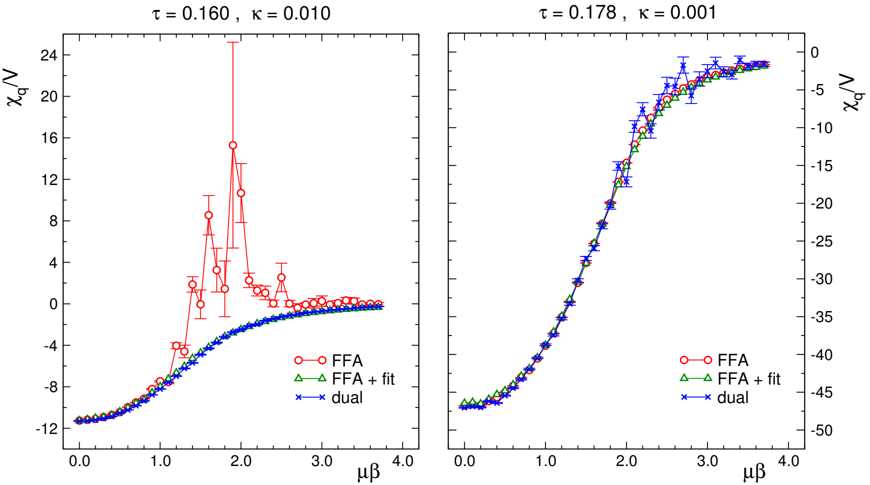
Not a fundamental ingredient of the DoS method

Particle number density $\langle q \rangle$: $V = 16^3$



Dual results: [Y. Mercado, H. G. Evertz, C. Gattringer, PRL (2012) & CPC (2012)]

Susceptibility χ_q: $V = 16^3$



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Conclusions

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- We have developed further the density of states method using the Z_3 spin model
- The density of states has been calculated with restricted Monte Carlo updates and the functional fit approach (FFA)
- We compared our results with results obtained form a dual approach (free of complex action problem)
- At very large $\mu\beta$ the rapidly oscillating factor $\cos\left(\sqrt{3}\, q\, \kappa \sinh \mu\beta\right)$ limits the accuracy of DoS
- Future projects: FFA for the $SU(3)$ spin model

  $\Rightarrow$ Talk by Mario Giuliani