Density of states techniques for SU(2) lattice field theory with a topological term (Part I)

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Overview

- In this presentation we discuss new ideas for solving the complex action problem from θ-terms with Density of States (DoS) methods.

- Here we present a technical study of this new approach.

- The talk is divided into two parts:

  - Part 1: DoS approach to θ-terms – general formulation and tests
    Christof Gattringer

  - Part 2: First results for SU(2) LGT with a θ-term
    Oliver Orasch

C. Gattringer, O. Orasch, Nucl. Phys. B 957 (2020), 115097 [2004.03837]

Complex action problem for theories with a θ-term

- When a θ-term is coupled, the effective action $S[U]$ is generalized to

$$S[U] \; + \; i \, \theta \, Q[U]$$

- At $\theta \neq 0$ the Boltzmann factor

$$e^{- S[U] \, - \, i \, \theta \, Q[U]} \quad \in \quad \mathbb{C}$$

  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 $\Longrightarrow$ "Complex action problem"

We discuss the idea of using modern DoS techniques to circumvent the complex action problem for lattice field theory with a θ-term.

DoS formulation of the problem

- Vacuum expectation values of observables:

$$\langle \mathcal{O} \rangle_\theta \; = \; \frac{1}{Z_\theta} \int D[U] \, e^{\, - \, S[U] \, - \, i\theta \, Q[U]} \, \mathcal{O}[U] \;\; , \qquad Z_\theta \; = \int D[U] \, e^{\, - \, S[U] \, - \, i\theta \, Q[U]}$$

- Densities of states introduced as function of $Q[U]$:

$$\rho_{\mathcal{J}}(x) \; = \; \int D[U] \; e^{\, - \, S[U]} \; \mathcal{J}[U] \, \delta\Big(x - Q[U] \Big)$$

- Evaluation of observables:

$$\langle \mathcal{O} \rangle_\theta \; = \; \frac{1}{Z_\theta} \int dx \; \rho_{\mathcal{O}}(x) \; e^{\, - \, i \, \theta \, x} \;\; , \qquad Z_\theta \; = \int dx \; \rho_{\mathbb{1}}(x) \; e^{\, - \, i \, \theta \, x}$$

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

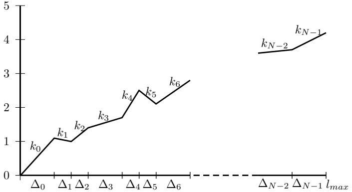
Parameterization of the densities

- Divide the x-range $[0, l_{max}]$ 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 with slopes k_n



- Normalization $\rho(0) = 1$ completely fixes densities as functions of the k_n:

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

Determination of the slopes

- Determine slopes with *Restricted VEVs* ⇒ exponential error suppression
  (Langfeld, Lucini, Rago)

$$\langle Q \rangle_{n,\lambda} \;=\; \frac{1}{Z_{n,\lambda}} \int D[U]\, e^{-S[U]}\, \mathcal{J}[U]\, e^{\lambda\, Q[U]}\; Q[U]\; \Theta_n\big(Q[U]\big)$$

with

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

- $\langle Q \rangle_{n,\lambda}$ is free of complex action problems and can be computed with standard Monte Carlo simulations as a function of the parameter $\lambda \in \mathbb{R}$.

- $\langle Q \rangle_{n,\lambda}$ may also be computed directly using the parameterized density:

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

Determination of the slopes: Functional Fit Approach (FFA)

- After suitable normalization we find

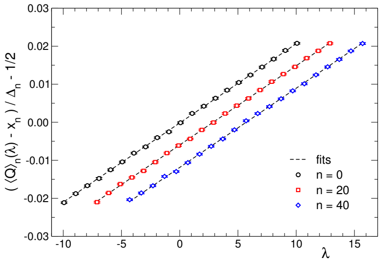
$$Y_{n,\lambda} \;\equiv\; \frac{\langle Q \rangle_{n,\lambda} - x_n}{\Delta_n} - \frac{1}{2} \;=\; h\Big(\Delta_n\big[\lambda - k_n\big]\Big)$$

where $h(s)$ is the sigmoid function

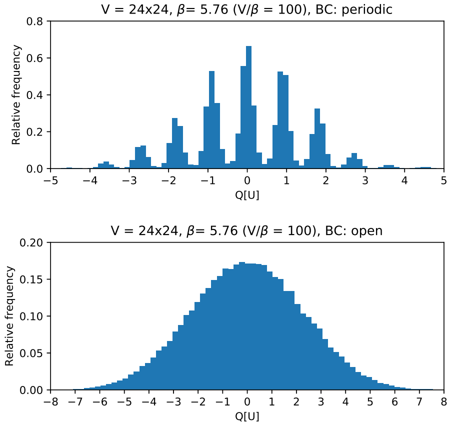
$$h(s) \equiv \frac{1}{1-e^{-s}} - \frac{1}{s} - \frac{1}{2} \qquad \text{with} \qquad h(0) = 0 \;, \quad \lim_{s\to\pm\infty} h(s) = \pm 1/2$$

- 1-parameter fits of the $Y_{n,\lambda}$ determine the slopes k_n

(Giuliani, Gattringer, Törek, NPB 2016)



The role of boundary conditions



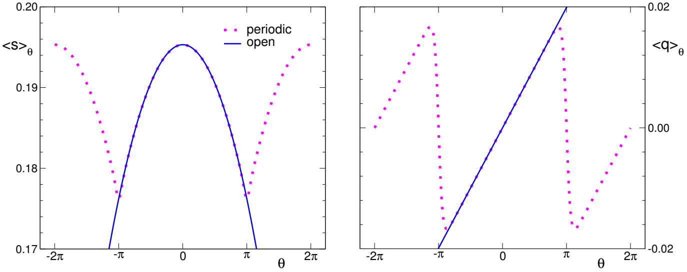
- Naive application of DoS to lattice field theories with θ-term will not work, because with periodic boundary conditions the density will approach a superposition of Dirac deltas in the continuum limit.
- Using open boundary conditions lifts the quantization of the topological charge and still gives rise to the correct continuum limit.
  Well established technique in lattice QCD. (Lüscher, Schaefer 2011, 2013; Chowdury et al 2013)
- In our project we implement DoS for lattice gauge theory with a θ-term using open boundary conditions for the topological charge.

Tests in U(1) LGT with a θ-term

- Before we discuss the results for the SU(2) case, we test the new approach in U(1) LGT with a θ-term using the Wilson and the Villain formulation.
- For both formulations one can solve the problem in closed form with dual techniques $\Longrightarrow$ Reference data for numerical tests.
- Questions to be asked:
    - Do open and periodic boundary conditions give rise to the same physics? (one expects finite volume corrections)
    - Can our new DoS techniques determine the density with sufficient accuracy?
    - Statistical and systematical errors for observables?

Open versus periodic boundary conditions

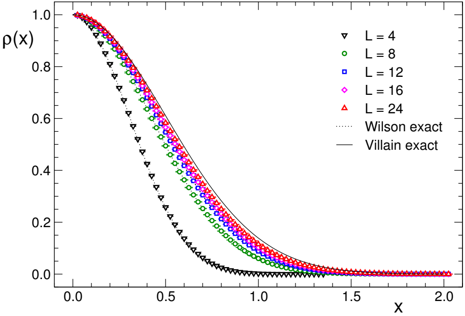
- Exact solution with dual methods allows us to compare vacuum expectation values for periodic and for open boundary conditions.
- Here we show the results for the action density $\langle s \rangle_\theta$ and the topological charge density $\langle q \rangle_\theta$ as a function of θ on 16×16 lattices.



- Good agreement with (expected) small finite size effects near $\theta = \pi$.

Results for the densities

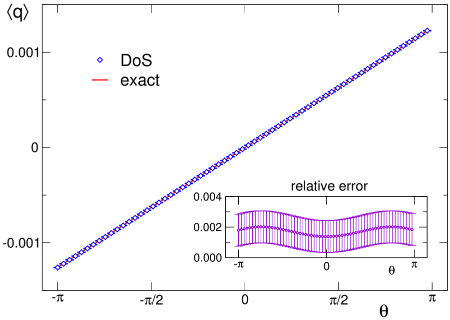
- The density of states $\rho(x)$ is computed in closed form from the k_n using the general expression from the DoS formulation.



- Numerical DoS data for $\rho(x)$ match exact results very well for all volumes.

Simple observables

- To fully judge if the achieved accuracy is sufficient, one needs to evaluate an observables by integrating the density with the respective oscillating factor.



- The exact result for $\langle q \rangle$ is reproduced with a relative error of $\sim 0.3\ \%$.

Summary and Discussion

- We explore the possibility of using modern DoS techniques for treating lattice field theories with θ-terms.
- Key ingredients are a continuous and piecewise linear parameterization of $\ln \rho(x)$ combined with restricted VEVs to compute the parameters of $\rho(x)$.
- To make theories with a θ-term accessible we need open boundary conditions to lift the integer quantization of the topological charge.
- Analytic calculation for 2-d U(1) lattice gauge theory with θ-term to check independence of b.c., and the general applicability of the DoS approach.
- Test simulations with Wilson action illustrate that accuracy is sufficient can be obtained to match of observables with exact results at the 0.3 % level.
- First results for SU(2) LGT with a θ-term $\Rightarrow$ Part II, Oliver Orasch