Density of states approach for lattice field theory with topological terms

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Der Wissenschaftsfonds.

Complex action problem $\Rightarrow$ DoS formulation of the problem

- Vacuum expectation values of observables:

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

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

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

- Evaluation of observables:

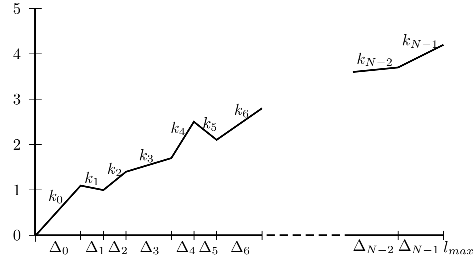
$$\langle \mathcal{O} \rangle_\theta = \frac{1}{Z_\theta} \int dx \, \rho^{(\mathcal{O})}(x) \, e^{-i\,\theta\,x} \qquad Z_\theta = \int dx \, \rho^{(\mathbb{1})}(x) \, e^{-i\,\theta\,x}$$

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

Parameterization of the densities

- Divide the (truncated) 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

- Imposing the normalization $\rho(0) = 1$ completely determines the densities $\rho(x)$ 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)

$$\langle Q \rangle_n(\lambda) \;=\; \frac{1}{Z_n(\lambda)} \int D[A]\, e^{-S[A]}\, \mathcal{J}[A]\, e^{\lambda Q[A]}\, Q[A]\, \Theta_n\Big(Q[A]\Big)$$

with

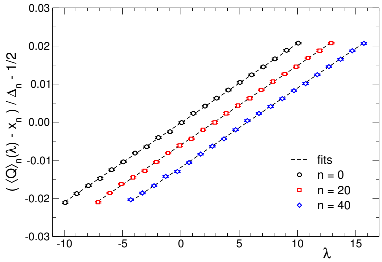
$$\Theta_n(x) \;=\; \begin{cases} 1 & \text{for} \quad x \in I_n \\ 0 & \text{for} \quad x \notin I_n \end{cases}$$

$\Longrightarrow$ exponential error suppression

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

- $\langle Q \rangle_n(\lambda)$ may also be computed from the parameterized density $\rho(x) \;=\; A_n\, e^{-x\, k_n}$:

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

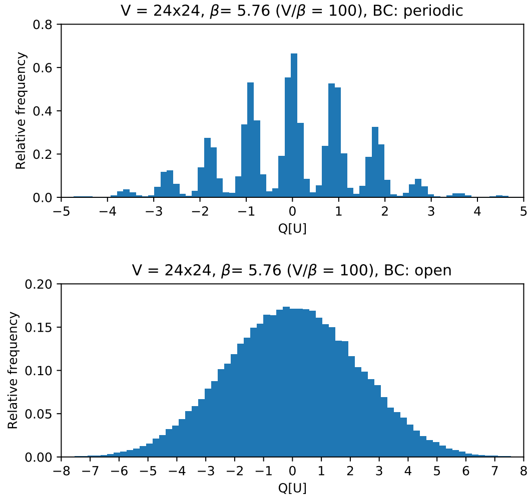


1-parameter fit with known function $\mathcal{F}_n(\lambda - k_n)$ provides k_n

(Giuliani, Gattringer, Törek, NPB 2016)

The role of boundary conditions

- A naive application of the DoS approach to lattice field theories with a theta term will not work, because in the usual formulation 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. (Lüscher, Schaefer 2011, 2013; Chowdury et al, 2013)

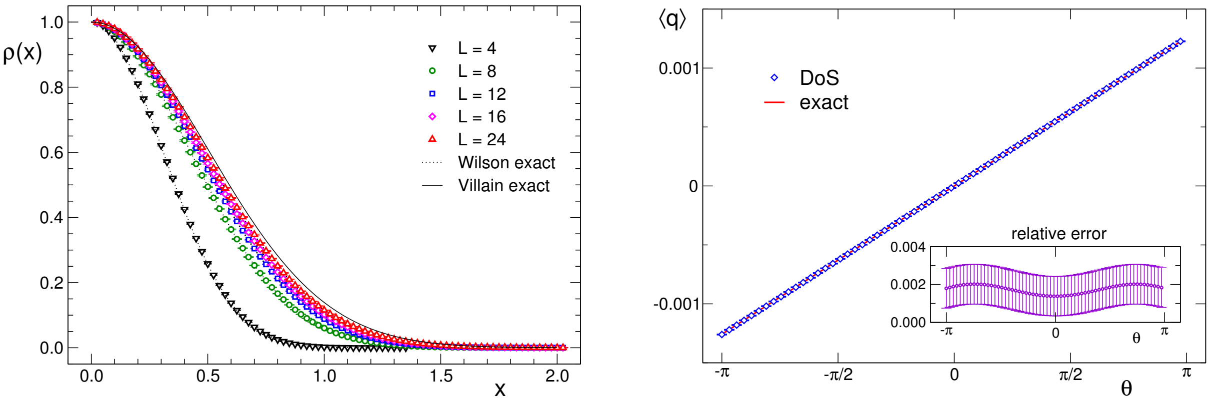
- In our project we implement DoS for lattice gauge theory with a θ-term using open boundary conditions for the topological charge.

- The concept and its implementation is tested for U(1) lattice gauge theory in 2-d where exact results can be used to assess the approach. Subsequently first results for SU(2) lattice gauge theory with a θ-term are presented.

Results for 2-d U(1) gauge theory with a θ-term

Gattringer, Orasch, NPB 957 (2020)

Wilson and Villain action, field theoretical Q, comparison to exact results



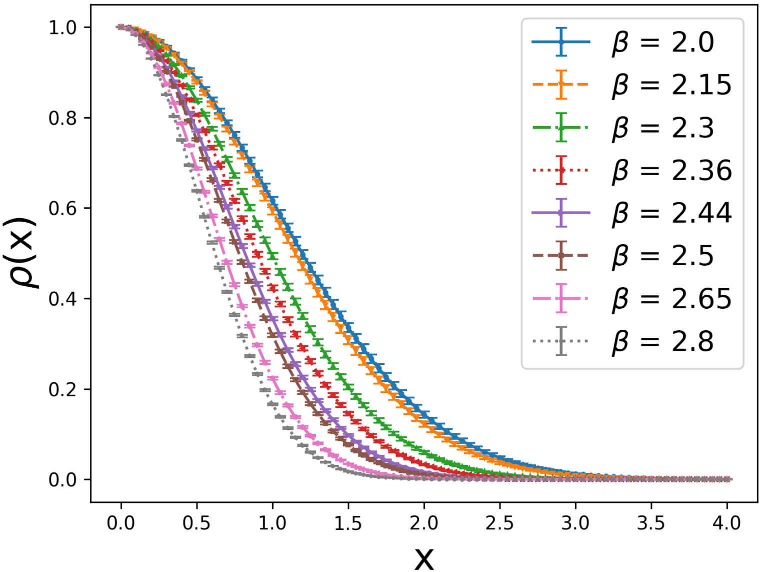
- The numerical DoS calculations of $\rho(x)$ match the exact results very well for all volumes.
- The exact result for $\langle q \rangle = \langle Q \rangle / V$ is reproduced with a relative error of $\sim$ 0.3 % .
- $1/\mathrm{V}$ corrections between open and periodic b.c. are understood analytically.

4-d SU(2) gauge theory with a θ-term

- Wilson action with field theoretical definition of Q.
- Mixed boudary conditions: Open b.c. for one spatial direction. All other b.c. periodic.
- Test study for comparison of finite volume effects for fully periodic and mixed periodic b.c. suggests that the direction with the open b.c. should be larger.
- Here: Results for $16^3 \times 4$ lattices to study temperature behavior of θ-dependence.
- Fit of the exponent $L(x)$ of the density with an even polynomial in x.
- Cross-check of the DoS results for $\langle Q^2 \rangle$ and $\langle Q^4 \rangle$ at $\theta = 0$ with conventional simulation.
- Results for $\langle Q \rangle$ as a function of θ for different temperatures.

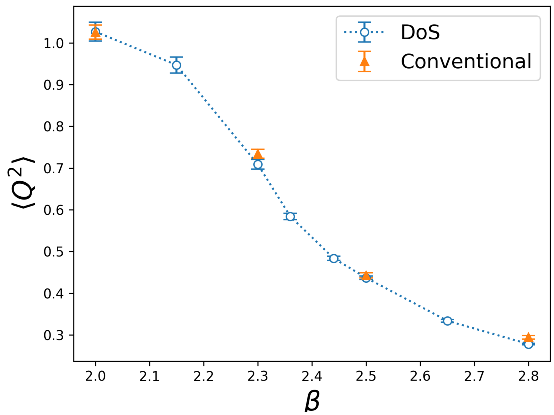
Results for 4-d SU(2) gauge theory with a θ-term – I

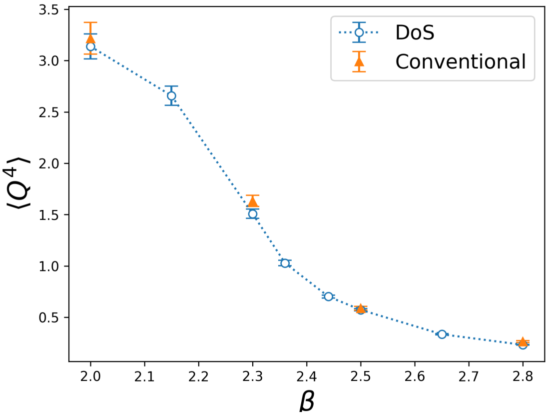
Density of states for different inverse gauge couplings β (i.e. different temperatures):



Results for 4-d SU(2) gauge theory with a θ-term – II

Consistency / accuracy check at $\theta = 0$:

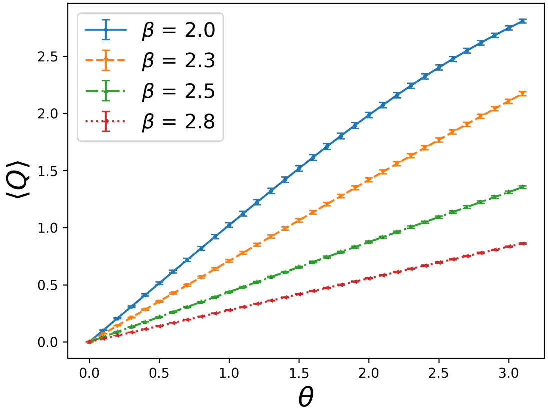


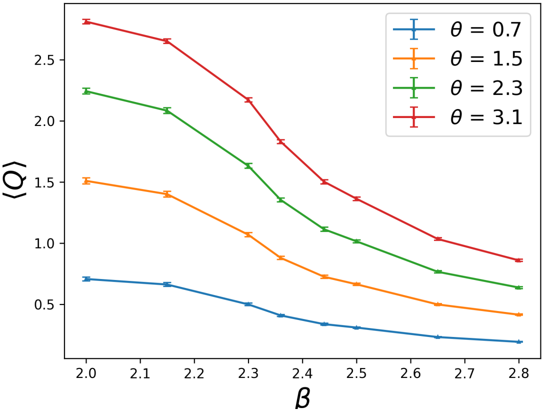


Very good agreement of conventional and DoS results for all temperatures considered.

Results for 4-d SU(2) gauge theory with a θ-term – III

$\langle Q \rangle$ as a function of θ and as a function of β:





First DoS results for topology at $\theta \neq 0$.

Summary

- We explore the possibility of using modern DoS techniques for treating lattice field theory with θ-terms.

- The key ingredients are a continuous and piecewise linear parameterization of $\ln\,\rho(x)$ combined with restricted VEVs for computing the parameters of $\ln\,\rho(x)$.

- To make theories with a θ-term accessible we need open boundary conditions to lift the integer quantization of the topological charge.

- Test results for 2-d U(1) lattice gauge theory with θ-term show that the approach works well. Analytical results provide a cross check and allow one to analyze finite volume effects and the general applicability of the DoS approach.

- Method is now applied to 4-d SU(2) lattice gauge theory with θ-term and cross checks with standard simulations at $\theta = 0$ indicate sufficient accuracy. First non-trivial results for $\theta \neq 0$ are obtained.

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