Functional Fit Approach (FFA) for Density of States method: SU(3) spin system and SU(3) gauge theory with static quarks

Mario Giuliani

Christof Gattringer, Pascal Törek

Karl Franzens Universität Graz

FWF Der Wissenschaftsfonds.

NAWI Graz Natural Sciences

UNI GRAZ

Sign Problem: a brief review

- Different approaches to solve the sign problem:
  - Reweighting
  - Expansion methods
  - Stochastic differential equations
  - Mapping to dual variables
  - Et cetera...
- Density of states approach:
  - Method used **FFA** Functional Fit Approach (ARXIV: 1503.04947, 1607.07340)
  - See also **LLR** Linear Logarithmic Relaxation by K. Langfeld, B. Lucini and A. Rago (ARXIV:1204.3243, 1509.08391)

Density of States Method

- In QFT we want to compute for our theory:

$$Z = \int \mathcal{D}[\psi] e^{-S[\psi]} \qquad \langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\psi] \mathcal{O}[\psi] e^{-S[\psi]}$$

- In the density of states approach we divide the action into two parts:

$$S[\psi] = S_\rho[\psi] + \mathrm{c}\, X[\psi]$$

* $S_\rho[\psi]$ and $X[\psi]$ are real functionals of the fields ψ

* $S_\rho[\psi]$ is the part of the action that we include in the weighted density ρ

* Here c is purely imaginary: $\mathrm{c} = i\xi$

Density of States Method

- The weighted density is defined as:

$$\rho(x) = \int \mathcal{D}[\psi] e^{-S_\rho[\psi]} \delta(X[\psi] - x)$$

- Using $\rho(x)$ we can write Z and $\langle \mathcal{O} \rangle$s:

$$Z = \int_{x_{min}}^{x_{max}} dx\ \rho(x)\ e^{-i\xi x} \qquad \langle \mathcal{O} \rangle = \frac{1}{Z} \int_{x_{min}}^{x_{max}} dx\ \rho(x)\ e^{-i\xi x} \mathcal{O}[x]$$

- Usually there is a symmetry $\psi \longrightarrow \psi'$ such that we can write:

$$Z = 2 \int_0^{x_{max}} dx\ \rho(x) \cos(\xi x)$$

- ... and for the observables $\mathcal{O}$:

$$\langle \mathcal{O} \rangle = \frac{2}{Z} \int_0^{x_{max}} dx\, \rho(x) \left\{ \cos(\xi x) \mathcal{O}_{even}(x) - i \sin(\xi x) \mathcal{O}_{odd}(x) \right\}$$

Where $\mathcal{O}_{\text{even}} = \frac{\mathcal{O}(x)+\mathcal{O}(-x)}{2}$ and $\mathcal{O}_{\text{odd}} = \frac{\mathcal{O}(x)-\mathcal{O}(-x)}{2}$

First example: SU(3)-spin model Arxiv:1607.07340

- $SU(3)$ spin model is a 3D effective theory for heavy dense QCD
- Relevant d.o.f. is the Polyakov loop $\mathrm{P}(n) \in SU(3)$ (static quark source at n)
- The model has a real and positive dual representation $\Rightarrow$ reference data
- We have an action:

$$S[\mathrm{P}] = -\tau \sum_{n} \sum_{\nu=1}^{3} \left[\mathrm{Tr}\mathrm{P}(n)\, \mathrm{Tr}\mathrm{P}(n+\nu)^{\dagger} + c.c. \right] - \kappa \sum_{n} [e^{\mu}\, \mathrm{Tr}\mathrm{P}(n) + e^{-\mu}\, \mathrm{Tr}\mathrm{P}(n)^{\dagger}]$$

The action depends only on the trace $\Rightarrow$ simple parametrization

$$\mathrm{P}(n) = \begin{pmatrix} e^{i\theta_1(n)} & 0 & 0 \\ 0 & e^{i\theta_2(n)} & 0 \\ 0 & 0 & e^{-i(\theta_1(n)+\theta_2(n))} \end{pmatrix}$$

Definition of density of states

- We define the weighted density of states with $S_\rho[\mathrm{P}] = \mathrm{Re}[S[\mathrm{P}]]$ and $\mathrm{Im}[S[\mathrm{P}]] = 2\kappa \sinh(\mu) X[\mathrm{P}]$:

$$\rho(x) = \int \mathcal{D}[\mathrm{P}]\, e^{-S_\rho[\mathrm{P}]}\, \delta(x - X[\mathrm{P}]) \qquad x \in [-x_{max}, x_{max}]$$

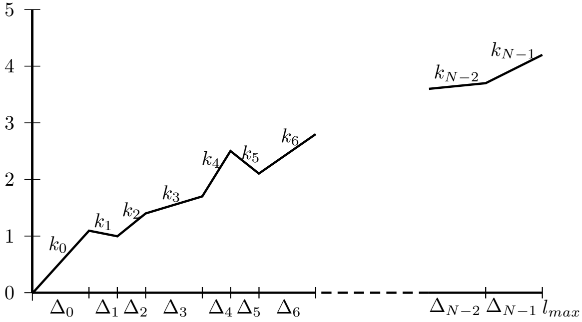
- Symmetry $\mathrm{P}(n) \to \mathrm{P}(n)^*$ implies $\rho(-x) = \rho(x)$
- This simplifies the partition function:

$$Z = \int_{-x_{max}}^{x_{max}} dx\, \rho(x) \cos(2\kappa \sinh(\mu) x) = 2 \int_0^{x_{max}} dx\, \rho(x) \cos(2\kappa \sinh(\mu) x)$$

$$\langle \mathcal{O}[X] \rangle = \frac{2}{Z} \int_0^{x_{max}} dx\, \rho(x) \left[\mathcal{O}_E(x) \cos(2\kappa \sinh(\mu) x) + i\, \mathcal{O}_O(x) \sin(2\kappa \sinh(\mu) x) \right]$$

Parametrization of the density $\rho(x)$

- Ansatz for the density: $\rho(x) = e^{-L(x)}$, normalization $\rho(0) = 1 \Rightarrow L(0) = 0$
- We divide the interval $[0, x_{max}]$ into N intervals $n = 0, 1, \ldots, N-1$.
- $L(x)$ is continuous and linear on each of the intervals, with a slope k_n:



Determination of the slopes k_n

- How do we find the slopes k_n?
  Restricted expectation values which depend on a parameter $\lambda \in \mathbb{R}$:

$$\langle\langle\mathcal{O}\rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \int \mathcal{D}[\mathrm{P}]\, e^{-S_\rho[\mathrm{P}]+\lambda X[\mathrm{P}]}\, \mathcal{O}\big[X[\mathrm{P}]\big]\, \theta_n\big[X[\mathrm{P}]\big]$$

$$Z_n(\lambda) = \int \mathcal{D}[\mathrm{P}]\, e^{-S_\rho[\mathrm{P}]+\lambda X[\mathrm{P}]}\, \theta_n\big[X[\mathrm{P}]\big]$$

$$\theta_n\big[x\big] = \begin{cases} 1 \text{ for } x \in [x_n, x_{n+1}] \\ 0 \text{ otherwise} \end{cases}$$

- Update with a restricted Monte Carlo
- Vary the parameter λ to fully explore the density

Functional Fit Approach FFA

- Expressed in terms of the density:

$$Z_n(\lambda) = \int_{-x_{max}}^{x_{max}} dx\, \rho(x)\, e^{\lambda x}\, \theta_n\left[x\right] = \int_{x_n}^{x_{n+1}} dx\, \rho(x)\, e^{\lambda x} = c \int_{x_n}^{x_{n+1}} dx\, e^{(-k_n+\lambda)x}$$

$$= c\, \frac{e^{(\lambda x - k_n) x_{n+1}} - e^{(\lambda x - k_n) x_n}}{\lambda - k_n}$$

- For computing the slopes we use as observable $X[\mathrm{P}]$:

$$\langle\langle X[\mathrm{P}]\rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \int_{x_n}^{x_{n+1}} dx\, \rho(x)\, e^{\lambda x}\, x = \frac{\partial}{\partial\lambda} \ln\left[Z_n(\lambda)\right]$$

Functional Fit Approach FFA

- Explicit expression for restricted expectation values:

$$\frac{1}{\Delta_n}\left[\langle\langle X[\mathrm{P}]\rangle\rangle_n(\lambda) - \sum_{j=0}^{n-1}\Delta_j\right] - \frac{1}{2} = \mathrm{h}\big((\lambda - k_n)\Delta_n\big)$$

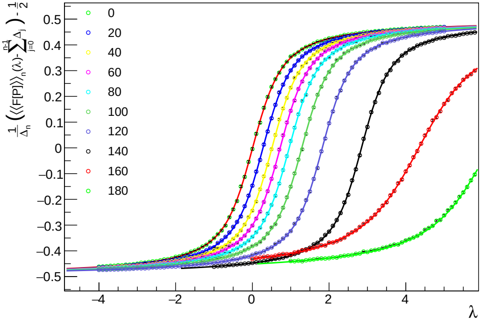
$$\mathrm{h}(r) = \frac{1}{1-e^{-r}} - \frac{1}{r} - \frac{1}{2}$$

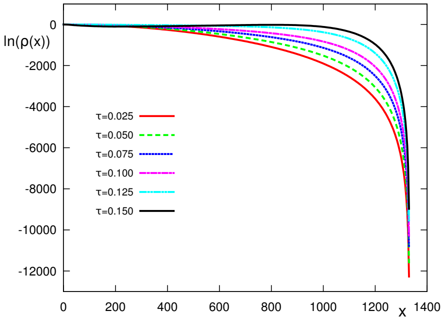
- Strategy to find k_n:
  1. Evaluate $\langle\langle X[\mathrm{P}]\rangle\rangle_n(\lambda)$ for different values of λ
  2. Fit these Monte Carlo data $h((\lambda - k_n)\Delta_n)$
  3. k_n are obtained from simple one parameter fits

- The quality of the fit provide a self-consistent check of our simulation

Example: 8^3, $\kappa = 0.005$, $\mu = 0.0$

$\tau = 0.075$





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

Observables

1. Particle number density n:

$$n = \frac{1}{V}\,\frac{1}{2\kappa}\,\frac{\partial}{\partial\,\mathrm{sinh}(\mu)}\ln Z = \frac{1}{V}\,\frac{2}{Z}\int_0^{x_{max}} dx\,\rho(x)\;\mathrm{sin}(2\kappa\,\mathrm{sinh}(\mu)x)\,x$$

2. ... and the corresponding susceptibility χ_n:

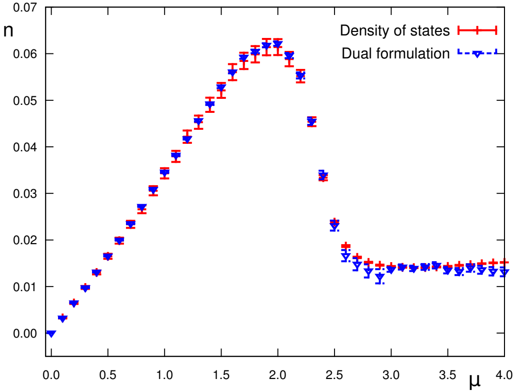
$$\chi_n = \frac{1}{2\kappa}\,\frac{\partial}{\partial\,\mathrm{sinh}(\mu)}\,n$$
$$= \frac{1}{V}\left\{\frac{2}{Z}\int_0^{x_{max}} dx\,\rho(x)\;\mathrm{cos}(2\kappa\,\mathrm{sinh}(\mu)x)\,x^2 + \left(\frac{2}{Z}\int_0^{x_{max}} dx\,\rho(x)\;\mathrm{sin}(2\kappa\,\mathrm{sinh}(\mu)x\right)^2\right\}$$

Comparison with dual approach

- With large statistic and small intervals we are able to explore results up to $\mu = 4$:

Particle number density n

Lattice 8^3, $\tau = 0.130$ and $\kappa = 0.005$:

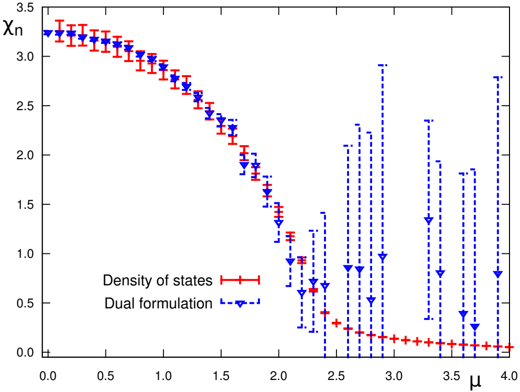


- We find a good agreement for chemical potential up to $\mu \approx 4.0$

Comparison with dual approach

Susceptibility χ_n

Lattice 8^3, $\tau = 0.130$ and $\kappa = 0.005$:



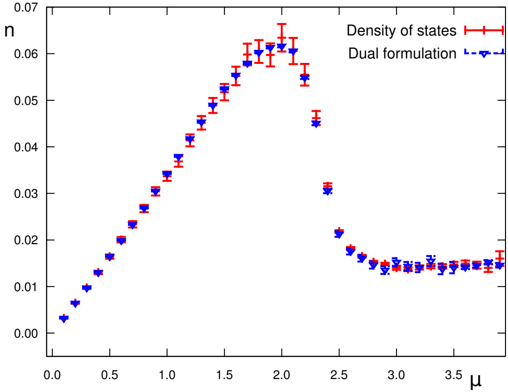
- The density performs fine up to $\mu \approx 4$

Comparison with dual approach

- We can also go to bigger lattice size with the same parameters:

Particle number density n

Lattice 12^3, $\tau = 0.130$ and $\kappa = 0.005$:

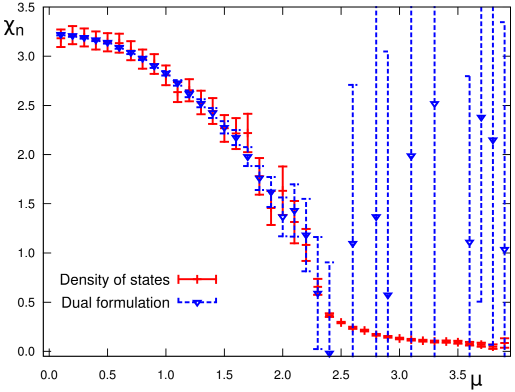


- We find a good agreement for chemical potential up to $\mu \approx 4.0$

Comparison with dual approach

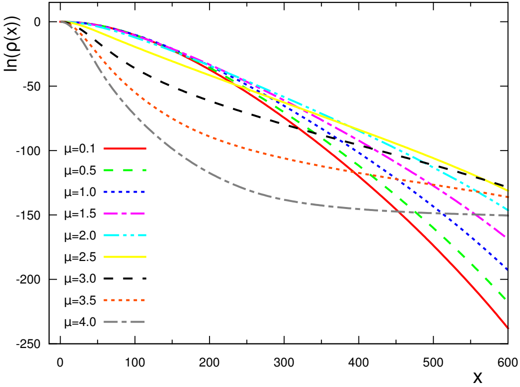
Susceptibility χ_n

Lattice 12^3, $\tau = 0.130$ and $\kappa = 0.005$:



- The density performs fine up to $\mu = 4$

- We find smaller error bars for larger μ
- The oscillating factor is bigger, but we still have: $\Delta_n \ll \frac{2\pi}{2\kappa \sinh \mu}$
- This can be explained looking at the different densities:



- The changed shape of the density above $\mu \approx 2.25$ weakens the piling up of the errors on the singles k_n

Second example: SU(3) static quarks

- Further step towards a real QCD system
- $SU(3)$ static quarks is a 4D effective theory for heavy dense QCD
- A $SU(3)$ gauge theory plus the static quarks represented by Polyakov loops
- We have the following action:

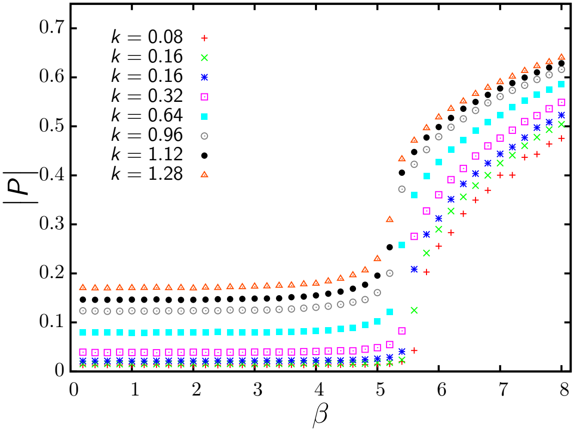
$$S[\mathrm{U}] = -\frac{\beta}{3}\sum_{n}\sum_{\mu<\nu}\mathrm{Re}\Big[\mathrm{Tr}\mathrm{U}_{\mu\nu}(n)\Big] - \kappa\Big[e^{\mu N_T}\sum_{\vec{n}}\mathrm{P}(\vec{n}) + e^{-\mu N_t}\sum_{\vec{n}}\mathrm{P}(\vec{n})^{\dagger}\Big]$$

Where the Polyakov loops are:

$$\mathrm{P}(\vec{n}) = \frac{1}{3}\mathrm{Tr}\prod_{n_4=0}^{N_T-1}\mathrm{U}_4(\vec{n}, n_4)$$

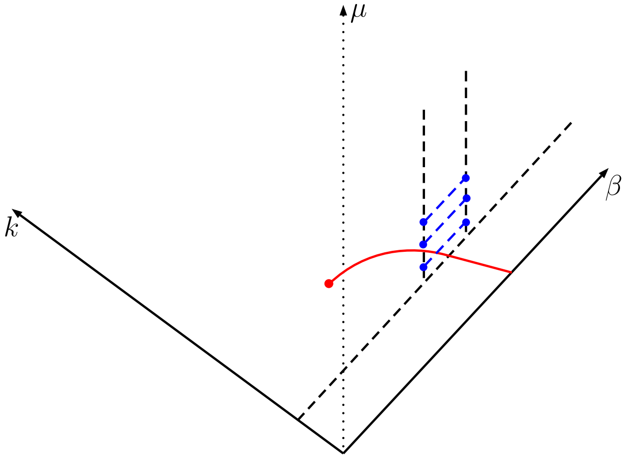
What is the idea of our simulation?

- We can do a simulation for $\mu = 0$, where we don't have the sign problem
- We can find a transition looking at the norm of the Polyakov loop
- We see that for larger κ we have a shift towards smaller β



Phase diagram

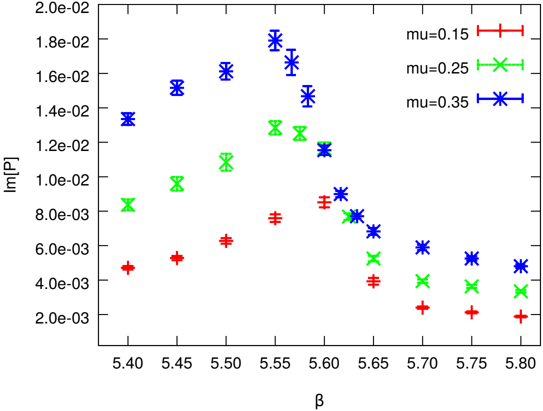
- The phase diagram would be something like:



- Simulating the blue lines we hope to find the bending of the phase transition

Preliminary results

- For now we find something in agreement with that idea:



- They are preliminary results so we need to improve them
- We should find a different method to check our results

Conclusions

- DoS is a general approach but its crucial point is the accuracy of ρ
- At very large μ the rapidly oscillating factor limits the accuracy of DoS
- FFA uses restricted Monte Carlo and probes the density with an additional Boltzmann weight
- Tested in $SU(3)$ Spin model: good agreement and now we have a good understanding how to scale the intervals size and the statistics
- Testing towards theory more similar to QCD: SU3 static quarks. First results are encouraging
- For the future it would be interesting to introduce dynamical fermions in our system