Density of states method for $SU(3)$-spin system

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Pascal Törek talk: Z_3 discrete variables $\Rightarrow$ exact DoS parametrization
SU(3)-spin system: continuous variables $\Rightarrow$ different DoS parametrization

Sign Problem: a brief review

- Monte-Carlo simulation of quantum field theories at finite density: Sign problem
- Different approaches to solve this problem:
  - Reweighting
  - Expansion methods
  - Stochastic differential equations
  - Mapping to dual variables
  - Et cetera...
- Density of states approach:
  - New development: Functional Fit Approach (FFA)
  - Tested in the SU(3)-spin system
  - SU(3)-spin system has a dual formulation [Gattringer Nuclear Physics B850 (2011) 242-252]

Density of states:

$Z = \int \mathcal{D}[C]\, e^{S_R[C]+iS_I[C]}$ where $S_I[C]$ is bounded: $S_I[C] \in [S_{I\,min}; S_{I\,max}]$

Use a Monte Carlo calculation to estimate the density:

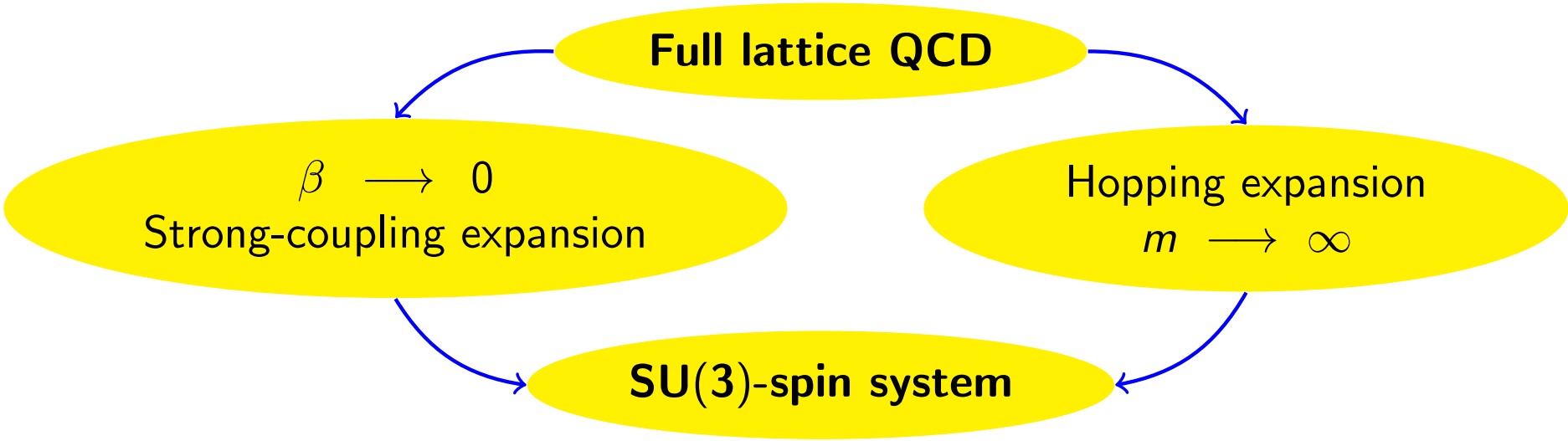
$$\rho(S_I) = \int \mathcal{D}[C]\, e^{S_R[C]}\, \delta(S_I - S_I[C])$$

$$Z = \int_{S_{I\,min}}^{S_{I\,max}} d[S_I]\, \rho(S_I)\, \{\cos(S_I) + i \sin(S_I)\}$$

$$\langle \mathcal{O} \rangle = \int_{S_{I\,min}}^{S_{I\,max}} d[S_I]\, \rho(S_I)\, \{\cos(S_I) + i \sin(S_I)\}\, \mathcal{O}(S_I)$$

Sine and cosine are oscillating functions so we need to know $\rho(S_I)$ with high precision

SU(3)-spin model

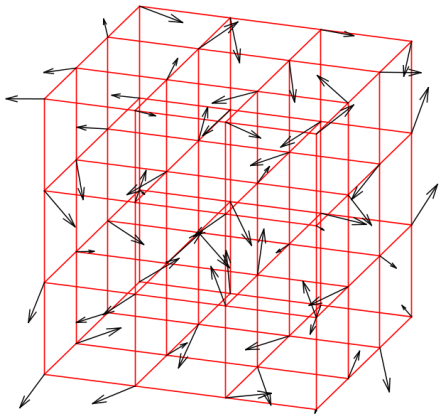


- We have a system with action:

$$S[\mathrm{P}] = \tau \sum_x \sum_{\nu=1}^{3} \Big[\mathrm{TrP}(x)\, \mathrm{TrP}(x+\nu)^\dagger + c.c. \Big] + k \sum_x [e^{\mu}\, \mathrm{TrP}(x) + e^{-\mu}\, \mathrm{TrP}(x)^\dagger]$$

The action depends only on the trace

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



DoS for the SU(3) spin model

- Term with chemical potential can be decomposed into real and imaginary parts:

$$k \sum_x \left[e^{\mu} \, \mathrm{Tr}\mathrm{P}(x) + e^{-\mu} \, \mathrm{Tr}\mathrm{P}(x) \right] =$$

$$2k \cosh(\mu) \sum_x \mathrm{Re}\left[\mathrm{Tr}\mathrm{P}(x) \right] + i2k \sinh(\mu) \sum_x \mathrm{Im}\left[\mathrm{Tr}\mathrm{P}(x) \right]$$

- Definition:

– $\sum_x \mathrm{Im}\left[\mathrm{Tr}\mathrm{P}(x) \right] = F[P] = \sum_x \left[\sin(\theta_1(x)) + \sin(\theta_2(x)) - \sin(\theta_1(x) + \theta_2(x)) \right]$

– $F[P] \in [-\frac{3\sqrt{3}}{2} V_3; \frac{3\sqrt{3}}{2} V_3] \equiv [-I_{max}, I_{max}]$

Definition of density of states

- We define the weighted density of states:

$$\rho(I) = \int \mathcal{D}[\mathrm{P}]\, e^{S_R[\mathrm{P}]}\, \delta(I - F[\mathrm{P}]) \qquad I \in [-I_{max}, I_{max}]$$

- The density of states is an even function of I:

$$\rho(-I) = \rho(I)$$

  because of symmetry properties under $\mathrm{P}(x) \to \mathrm{P}(x)^*$

- This simplifies the partition function:

$$Z = \int_{-I_{max}}^{I_{max}} dI\, \rho(I) \cos(2k \sinh(\mu) I) = 2 \int_{0}^{I_{max}} dI\, \rho(I) \cos(2k \sinh(\mu) I)$$

DoS Observables

- We can also use $\rho(I) = \rho(-I)$ for the expectation value of the observables
- As observables we consider functions of $F[\mathrm{P}]$, and define even and odd parts:

$$\mathcal{O}[F] = \mathcal{O}_E[F] + \mathcal{O}_O[F]$$

$$\mathcal{O}_E[F] = \frac{1}{2}(\mathcal{O}[F] + \mathcal{O}[-F]) \quad ; \quad \mathcal{O}_O[F] = \frac{1}{2}(\mathcal{O}[F] - \mathcal{O}[-F])$$

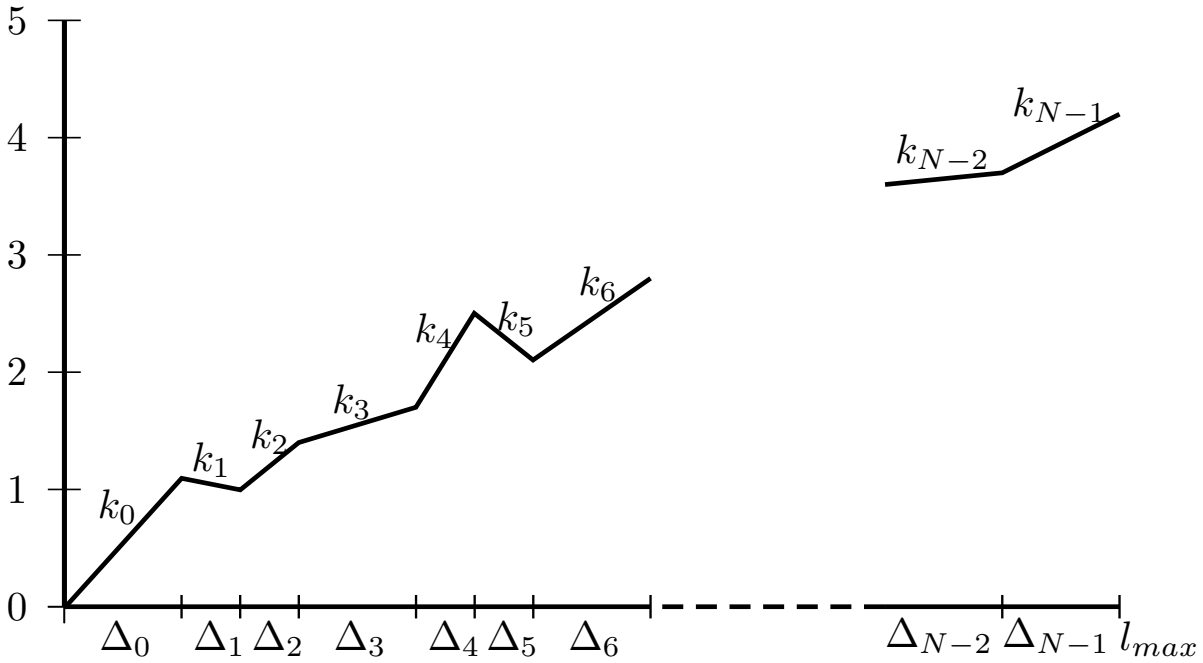
- We have for the expectation value of the observable:

$$\langle \mathcal{O}[F] \rangle = \frac{2}{Z} \int_0^{I_{max}} dI\, \rho(I) \left[\mathcal{O}_E[I] \cos(2k \sinh(\mu) I) + i\, \mathcal{O}_O[I] \sin(2k \sinh(\mu) I) \right]$$

- We need $\rho(I)$ only for $I \geq 0$
- For large k and μ the sine and cosine are strongly oscillating functions

Parametrization of the density $\rho(l)$

- Ansatz for the density: $\rho(l) = e^{-L(l)}$, normalization $\rho(0) = 1 \Rightarrow L(0) = 0$
- We divide the interval $[0, l_{max}]$ into N intervals $n = 0, 1, \ldots, N-1$.
- $L(l)$ 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 $\lambda \in \mathbb{R}$:

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

$$Z_n(\lambda) = \int \mathcal{D}[\mathrm{P}]\, e^{S_R[\mathrm{P}]+\lambda F[\mathrm{P}]}\, \theta_n\big[F[\mathrm{P}]\big]$$

$$\theta_n\big[I\big] = \begin{cases} 1 \text{ for } I \in [I_n, I_n + 1] \\ 0 \text{ otherwise} \end{cases}$$

- Expressed in terms of the density of states ($I = F[\mathrm{P}]$):

$$\langle\langle \mathcal{O} \rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \int_{-I_{max}}^{I_{max}} dI\, \rho(I)\, e^{\lambda I}\, \mathcal{O}\big[I\big]\theta_n\big[I\big] = \frac{1}{Z_n(\lambda)} \int_{I_n}^{I_{n+1}} dI\, \rho(I)\, e^{\lambda I}\, \mathcal{O}\big[I\big]$$

$$Z_n(\lambda) = \int_{-I_{max}}^{I_{max}} dI\, \rho(I)\, e^{\lambda I}\, \theta_n\big[I\big] = \int_{I_n}^{I_{n+1}} dI\, \rho(I)\, e^{\lambda I}$$

Functional Fit Approach FFA

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

$$\langle\langle F[\mathrm{P}]\rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \int_{I_n}^{I_{n+1}} dI\, \rho(I)\, e^{\lambda I}\, I = \frac{\partial}{\partial\lambda} \ln\big[Z_n(\lambda)\big]$$

- Explicit evaluation:

$$Z_n(\lambda) = e^{(\lambda - k_n) n\Delta}\, \frac{1 - e^{-\Delta(k_n - \lambda)}}{k_n - \lambda}$$

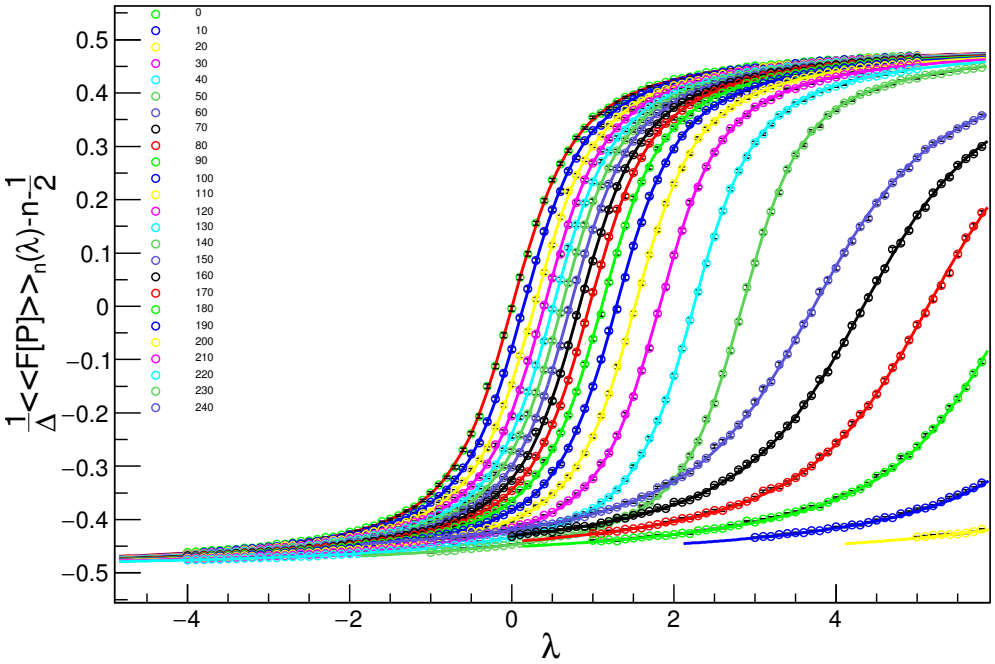
$$\langle\langle F[\mathrm{P}]\rangle\rangle_n(\lambda) = n\Delta + \frac{\Delta}{1 - e^{\Delta(k_n - \lambda)}} + \frac{1}{k_n - \lambda}$$

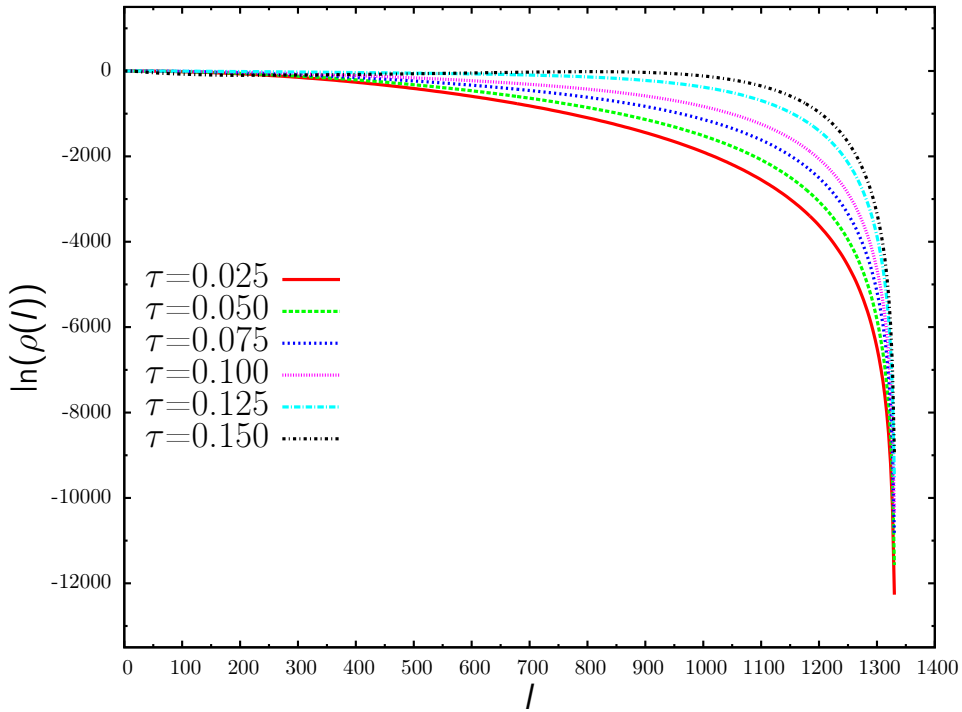
- Evaluate $\langle\langle F[\mathrm{P}]\rangle\rangle_n(\lambda)$ for different values of $\lambda \Rightarrow$ Fit these values to obtain k_n

Fit of slopes $\Rightarrow$ density $\rho(l)$

Example $\Rightarrow$ **Lattice:** 8^3, $k = 0.005$, $\mu = 0.0$

$\tau = 0.075$ $\qquad$ $\tau = 0.025, 0.050, .., 0.150$





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

Observables

- We use the density of states to compute observables:
- Particle number density n:

$$n = \frac{1}{iV_3} F[\mathrm{P}] = \frac{1}{V_3}\left(-\frac{1}{2k}\right)\frac{\partial}{\partial \sinh(\mu)} \ln Z$$

- ... and the corresponding susceptibility χ_n:

$$\chi_n = \frac{1}{2k}\frac{\partial}{\partial \sinh(\mu)} n = \frac{1}{V_3}\left(-\frac{1}{(2k)^2}\right)\frac{\partial^2}{(\partial \sinh(\mu))^2} \ln Z$$
$$= \frac{1}{V_3}\left(-\frac{1}{(2k)^2}\right)\left[\frac{1}{Z}\frac{\partial^2 Z}{(\partial \sinh(\mu))^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial \sinh(\mu)}\right)^2\right]$$

Density of States Method

- In terms of the density of states $\rho(l)$ we have:

$$Z = 2 \int_0^{l_{max}} dl\, \rho(l)\, \cos(2k \sinh(\mu) l)$$

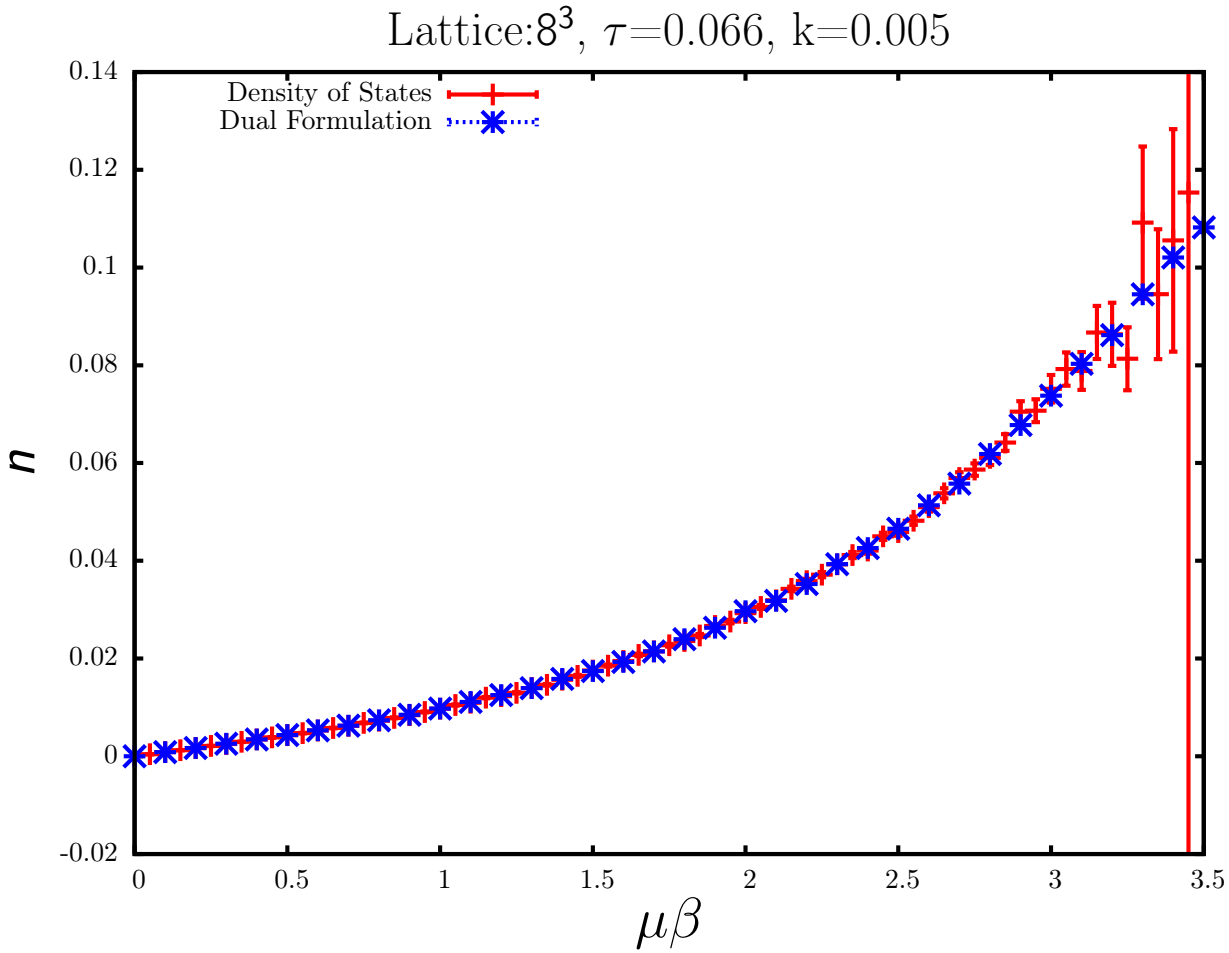
$$n = \frac{1}{V_3} \frac{2}{Z} \int_0^{l_{max}} dl\, \rho(l)\, \sin(2k \sinh(\mu) l)\, l$$

$$\chi_n = \frac{1}{V_3} \left\{ \frac{2}{Z} \int_0^{l_{max}} dl\, \rho(l)\, \cos(2k \sinh(\mu) l)\, l^2 + \left(\frac{2}{Z} \int_0^{l_{max}} dl\, \rho(l)\, \sin(2k \sinh(\mu) l) \right)^2 \right\}$$

- For reliable results we need intervals of order $\Delta_n \approx \frac{1}{2k \sinh \mu}$

Comparison with dual approach

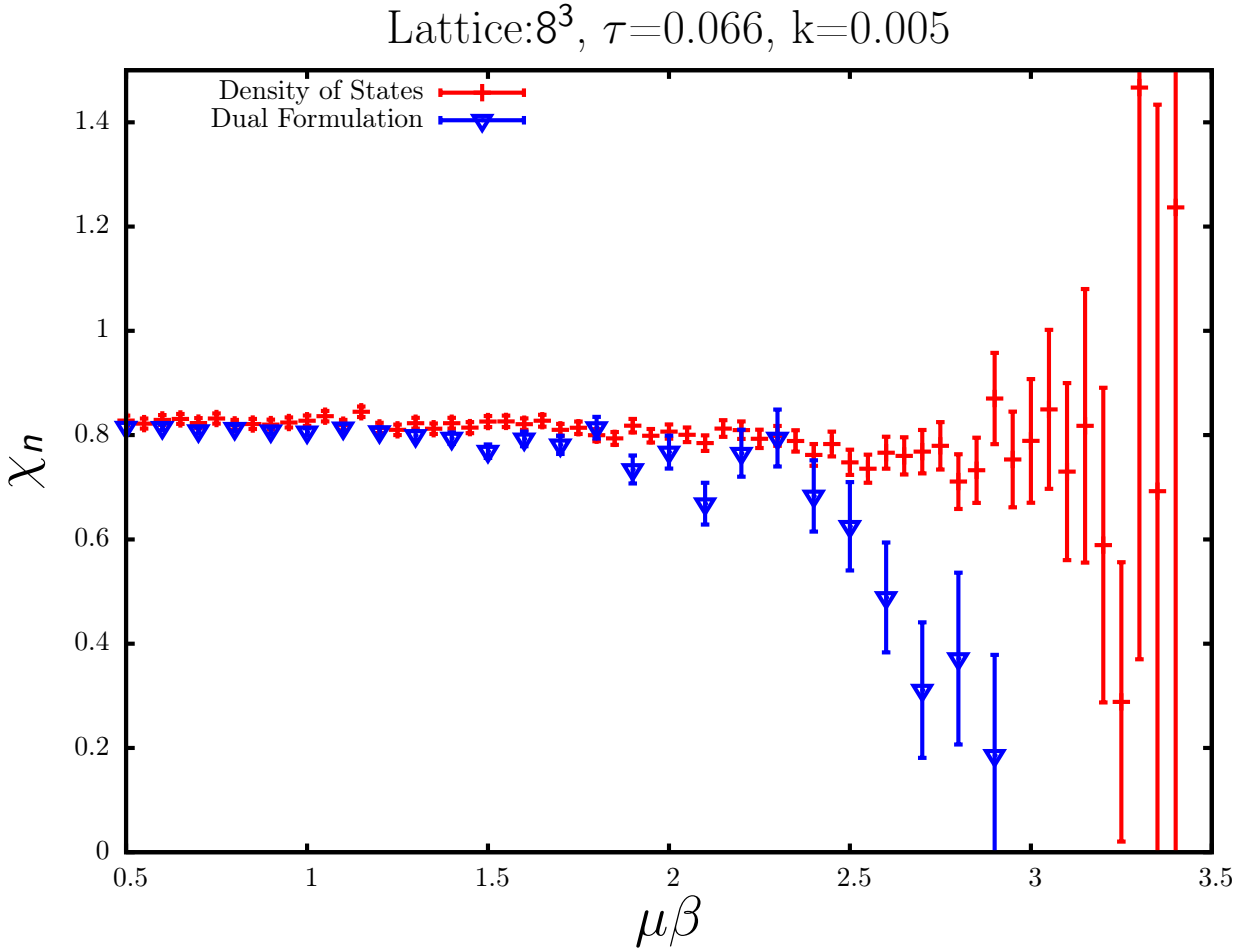
Particle number density n



- For dual results see Y.D.Mercado, C. Gattringer Nuclear Physics B862 (2012) 737-750
- We find a good agreement for chemical potential up to $\mu\beta \approx 3$

Comparison with dual approach

Susceptibility χ_n



- We find a good agreement for chemical potential up to $\mu\beta \approx 2$
- We need to reduce the size of the intervals Δ to explore larger $\mu\beta$

Conclusions

- We have developed further the density of states using the SU(3)-spin system
- The density of states has been calculated with restricted Monte Carlo updates and the functional fit approach (FFA)
- Good agreement with results from the dual approach
- At very large μ the rapidly oscillating factor $\cos(2k \sinh(\mu)l)$ limits the accuracy of DoS