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

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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:

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

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

\[
S[\psi] = S_\rho[\psi] + c X[\psi]
\]

* \(S_\rho[\psi]\) and \(X[\psi]\) are real functionals of the fields \(\psi\)
* \(S_\rho[\psi]\) is the part of the action that we include in the weighted density \(\rho\)
* Here \(c\) is purely imaginary: \(c = i\xi\)
Density of States Method

- The weighted density is defined as:

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

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

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

- Usually there is a symmetry \( \psi \rightarrow \psi' \) such that we can write:

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

- ... and for the observables \( O \):

\[ \langle O \rangle = \frac{2}{Z} \int_0^{x_{\text{max}}} dx \rho(x) \left\{ \cos(\xi x) O_{\text{even}}(x) - i \sin(\xi x) O_{\text{odd}}(x) \right\} \]

Where \( O_{\text{even}} = \frac{O(x) + O(-x)}{2} \) and \( O_{\text{odd}} = \frac{O(x) - O(-x)}{2} \)
First example: SU(3)-spin model

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

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

The action depends only on the trace ⇒ simple parametrization

\[
P(n) = \begin{pmatrix}
e^{i\theta_1(n)} & 0 & 0 \\
0 & e^{i\theta_2(n)} & 0 \\
0 & 0 & e^{-i(\theta_1(n)+\theta_2(n))}
\end{pmatrix}
\]
We define the weighted density of states with $S_\rho[P] = \text{Re}[S[P]]$ and $\text{Im}[S[P]] = 2\kappa \sinh(\mu)X[P]$: \[
\rho(x) = \int D[P] e^{-S_\rho[P]} \delta(x - X[P]) \quad x \in [-x_{\text{max}}, x_{\text{max}}]
\]

Symmetry $P(n) \rightarrow P(n)^*$ implies $\rho(-x) = \rho(x)$

This simplifies the partition function:
\[
Z = \int_{-x_{\text{max}}}^{x_{\text{max}}} dx \rho(x) \cos(2\kappa \sinh(\mu)x) = 2 \int_0^{x_{\text{max}}} dx \rho(x) \cos(2\kappa \sinh(\mu)x)
\]
\[
\langle O[X] \rangle = \frac{2}{Z} \int_0^{x_{\text{max}}} dx \rho(x) \left[ O_E(x) \cos(2\kappa \sinh(\mu)x) + iO_O(x) \sin(2\kappa \sinh(\mu)x) \right]
\]
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 $\lambda \in \mathbb{R}$:

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

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

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

- Update with a restricted Monte Carlo

- Vary the parameter $\lambda$ to fully explore the density
Functional Fit Approach FFA

- Expressed in terms of the density:

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

- For computing the slopes we use as observable \(X[P]\):

\[
\langle\langle X[P] \rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \int_{x_n}^{x_{n+1}} dx \, \rho(x) \, e^{\lambda x} \, x = \frac{\partial}{\partial \lambda} \ln[Z_n(\lambda)]
\]
Functional Fit Approach FFA

- Explicit expression for restricted expectation values:

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

\[ h(r) = \frac{1}{1 - e^{-r}} - \frac{1}{r} - \frac{1}{2} \]

- Strategy to find \( k_n \):
  1. Evaluate \( \langle\langle X[P]\rangle\rangle_n(\lambda) \) for different values of \( \lambda \)
  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
Fit of slopes ⇒ density $\rho(l)$

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

$\tau = 0.075$

\[ k_n \rightarrow L(x) \rightarrow \rho(x) = e^{-L(x)} \]
1. Particle number density $n$:

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

2. ... and the corresponding susceptibility $\chi_n$:

$$\chi_n = \frac{1}{2\kappa} \frac{\partial}{\partial \sinh(\mu)} n$$

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

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 $\chi_n$

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 $\mu$

• 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:

$$S[U] = -\frac{\beta}{3} \sum_n \sum_{\mu<\nu} \text{Re} \left[ \text{Tr} U_{\mu\nu}(n) \right] - \kappa \left[ e^{\mu N_T} \sum P(\vec{n}) + e^{-\mu N_t} \sum P(\vec{n})^\dagger \right]$$

Where the Polyakov loops are:

$$P(\vec{n}) = \frac{1}{3} \text{Tr} \prod_{n_4=0}^{N_T-1} U_4(\vec{n}, n_4)$$
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 $\kappa$ we have a shift towards smaller $\beta$. 

![Graph showing transition points with different $k$ values]

$k = 0.08 \quad +$
$k = 0.16 \quad x$
$k = 0.16 \quad *$
$k = 0.32 \quad o$
$k = 0.64 \quad t$
$k = 0.96 \quad c$
$k = 1.12 \quad .$
$k = 1.28 \quad v$

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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 $\rho$

- At very large $\mu$ 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