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Sign Problem in Heavy-Dense QCD from a Density of States perspective

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Outline

- Introduction LLR
- Heavy-Dense QCD
- Moments method

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- Introduction LLR
- Heavy-Dense QCD
- Moments method

Other talks related to LLR

Parallels in Algorithms

R Pellegrini Tuesday @17:30

B Luicini @17:50

Plenary by Kurt Langfeld

Friday @ 10:15

Reminders

- Euclidean QCD partition function

$$Z = \int dU\, d\bar{\psi}\, d\psi\, \mathrm{e}^{-\bar{\psi} M \psi - S_{\mathrm{YM}}}$$

Integrate over the quark fields

$$Z = \int dU \; \det M\, \mathrm{e}^{-S_{\mathrm{YM}}}$$

Standard MC methods fail if the determinant has a non trivial phase

$$\det M[U] = |\det M[U]|\, \mathrm{e}^{i\phi[U]}$$

Reminders

- We follow the LLR method [Lucini, Langfeld, Rago, 1204.3243], modified for the phase

  We re-write the partition function as

$$
\begin{aligned}
Z &= \int DU\, \mathrm{e}^{-S_{\mathrm{YM}}[U]}\, |\det M[U]|\, \mathrm{e}^{i\phi[U]} \\
&= \int ds \int DU\, \mathrm{e}^{-S_{\mathrm{YM}}[U]}\, |\det M[U]|\, \delta(s-\phi[U])\, \mathrm{e}^{is} \\
&= \int ds\, \rho(s)\, \mathrm{e}^{is}
\end{aligned}
$$

  where we have defined the density

$$
\rho(s) = \int DU\, \mathrm{e}^{-S_{\mathrm{YM}}[U]}\, |\det M[U]|\, \delta(s-\phi[U])
$$

Density of state and the LLR method

We divide the support of the phase in n intervals

$$[s_0, s_1]\ , [s_1, s_2]\ , \ldots , [s_{n-1}, s_n]$$

On each interval $s \in [s_{i-1}, s_i]$, we assume that

$$\ln(\rho(s)) \sim a_i s\ , \quad \text{where } a_i = \text{unknown constant}$$

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On each interval $s \in [s_{i-1}, s_i]$, we assume that

$$\ln(\rho(s)) \sim a_i s \,, \quad \text{where } a_i = \text{unknown constant}$$

Therefore we approximate the density by

$$\rho(s) = \rho(s_{i-1}) \mathrm{e}^{a_i (s - s_{i-1})} \,, \quad \text{where } s_{i-1} \leq s \leq s_i$$

Reconstructing the Partition Function

- The density is given by

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Reconstructing the Partition Function

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Reconstructing the Partition Function

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- LLR provides a way to compute the coefficient a_i with good precision

- Once the a_i are known, we can reconstruct the density $\rho(s)$

  We still have to compute

$$Z = \int ds\, \rho(s)\mathrm{e}^{is}$$

  which can be numerically hard, but it's a 1D problem

LLR Brief History

- Belong to the class of Wang-Landau Techniques
- First paper, $U(1)$ [Lucini, Langfeld, Rago, 1204.3243]
- Z_3 spin model [Langfeld, Lucini, 2014]
- Exponential error suppression [Langfeld, Lucini, Rago, Pellegrini, Bongiovanni, 2015]
- Convergence, technical details, etc. [Langfeld, Lucini, Pellegrini, Rago, 2015]
- Bose Gas [Pellegrini, Bongiovanni, Langfeld, Lucini, Rago, 2016]

Heavy-dense QCD

Based on [NG & Langfeld, 1605.02709]

Heavy-Dense QCD

QCD with heavy quarks and large chemical potential μ, at low Temperature

[Bender, Hashimoto, Karsch, Linke, Nakamura, Plewnia, Stamatescu, Wetzel, '92] ,[Blum, Hetrick, Toussaint '96]

[Aarts, Attanasio, Jäger, Seiler, Sexty, Stamatescu '14]   [Rindlisbacher & de Forcrand '16]

$$Z(\mu) \;=\; \int dU \, \mathrm{e}^{-S_{\mathrm{YM}}[U]} \, \mathrm{Det} M(\mu)$$

and where the determinant takes the form

$$\mathrm{Det}\, M(\mu) = \prod_{\vec{x}} \det{}^2 \Big((1 + h\, \mathrm{e}^{\mu/T} P(\mathbf{x}))(1 + h\, \mathrm{e}^{-\mu/T} P^\dagger(\mathbf{x})) \Big) \,,$$

- $h = (2\kappa)^{N_\tau}$,
- κ the Wilson hopping parameter (quark mass),
- $T = 1/aN_\tau$ the temperature,
- N_τ the number of sites in the time direction,
- $P_{\mathbf{x}}$ the Polyakov loop (not normalised) at the site $\mathbf{x}$

$$P(\mathbf{x}) \;=\; \prod_{t=1}^{N_t} U_4(\mathbf{x}, t) \,.$$

Heavy-Dense QCD

- Define a bare quark mass by $am = -\ln(2\kappa) \Rightarrow h = (2\kappa)^{N_\tau} = e^{-m/T}$

$$\mathrm{Det}\, M(\mu) = \prod_{\mathbf{x}} \det{}^2\Big((1 + \mathrm{e}^{(\mu-m)/T}\, P(\mathbf{x}))(1 + \mathrm{e}^{-(\mu+m)/T}\, P^\dagger(\mathbf{x}))\Big)$$

$\Rightarrow$ m is a mass gap for this theory

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$\Rightarrow m$ is a mass gap for this theory

- For $\mu \gg T$, we have $\mathrm{e}^{-(\mu+m)/T} \ll 1$, so

$$\mathrm{Det}\, M(\mu) \approx \prod_{\mathbf{x}} \det{}^2\Big(1 + \mathrm{e}^{(\mu-m)/T}\, P(\mathbf{x})\Big)$$

Heavy-Dense QCD

- For some specific values of μ the determinant is real

$\mu = 0$,

$$\mathrm{Det}\, M(0) = \prod_{\mathbf{x}} \det \left| 1 + \mathrm{e}^{-m/T} P_{\mathbf{x}} \right|^4$$

$\mu = m$, (to very good approximation)

$$\mathrm{Det}\, M(m) \approx \prod_{\mathbf{x}} 4(1 + \mathrm{Re}\, \mathrm{tr} \mathrm{P}_{\mathbf{x}})^2$$

$\mu = 2m$ (to very good approximation)

$$\mathrm{Det}\, M(2m) \approx \prod_{\mathbf{x}} e^{6m/T}$$

Heavy-Dense QCD

- In general the determinant is complex
- We can show that the partition function is real
- For certain values of μ the imaginary part of the determinant is very small

Heavy-Dense QCD

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  $\Rightarrow$ There are regions in which reweighing gives reliable results

Reweighting

- The Phase Quenched partition function is given by

$$Z_{PQ}(\mu) \;=\; \int dU\, \mathrm{e}^{-S_{\mathrm{YM}}[U]}\; |\mathrm{Det}\, M(\mu)|$$

Reweighting

- The Phase Quenched partition function is given by

$$Z_{PQ}(\mu) \;=\; \int dU \, \mathrm{e}^{-S_{\mathrm{YM}}[U]} \; |\mathrm{Det}\, M(\mu)|$$

- Connecting the Phase quenched theory to the full theory

$$\begin{aligned} Z &= \int dU \, \mathrm{e}^{-S_{\mathrm{YM}}[U]} \; |\mathrm{Det}\, M(\mu)| \times \frac{\int dU \, \mathrm{e}^{-S_{\mathrm{YM}}[U]} \; |\mathrm{Det}\, M(\mu)| \; \mathrm{e}^{i\phi[U]}}{\int dU \, \mathrm{e}^{-S_{\mathrm{YM}}[U]} \; |\mathrm{Det}\, M(\mu)|} \\ &= Z_{PQ} \times \langle \mathrm{e}^{i\phi} \rangle_{PQ} \end{aligned}$$

Heavy-Dense QCD

Fermionic density

$$\sigma(\mu) \;=\; \frac{T}{V}\,\frac{\partial\ \ln\ Z(\mu)}{\partial\mu} \;=$$

We can show that $Z(\mu) \approx \mathrm{e}^{6V(\mu-m)/T} Z(-\mu)$ and therefore we find

$$\sigma(\mu) \approx 6 - \sigma(-\mu)$$

Limiting cases

$$\begin{aligned} \mu \to 0, &\qquad \sigma(\mu) \to 0 \\ \mu \to \infty, &\qquad \sigma(\mu) \to 6\ (= 2N_c) \end{aligned}$$

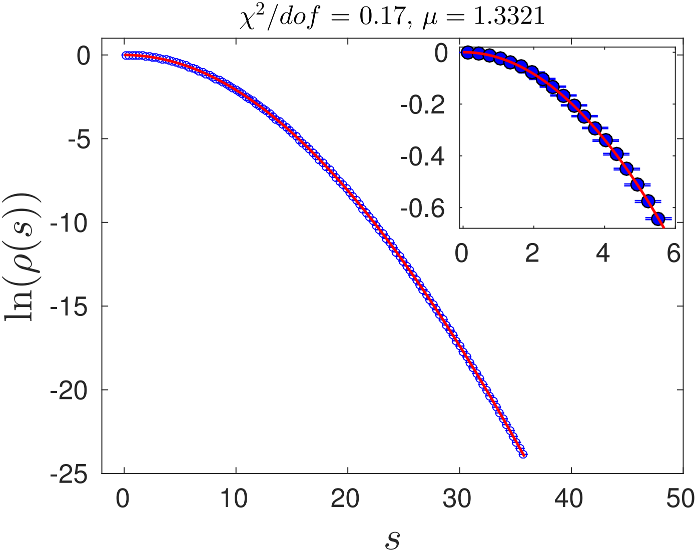
Numerical details

We choose the Wilson action :

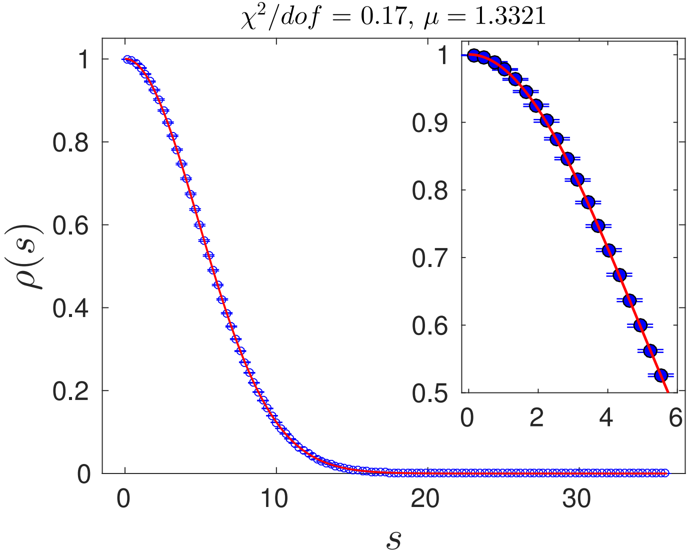
$$S_{\mathrm{YM}}[U] = \frac{\beta}{3} \sum_{x,\mu>\nu} \mathrm{Re}\,\mathrm{tr}\Big[U_\mu(x)\, U_\nu(x+\mu)\, U^\dagger_\mu(x+\nu)\, U^\dagger_\nu(x) \Big]$$

Parameters: $\beta = 5.8, \kappa = 0.12, N_\tau = L/a = 8,$

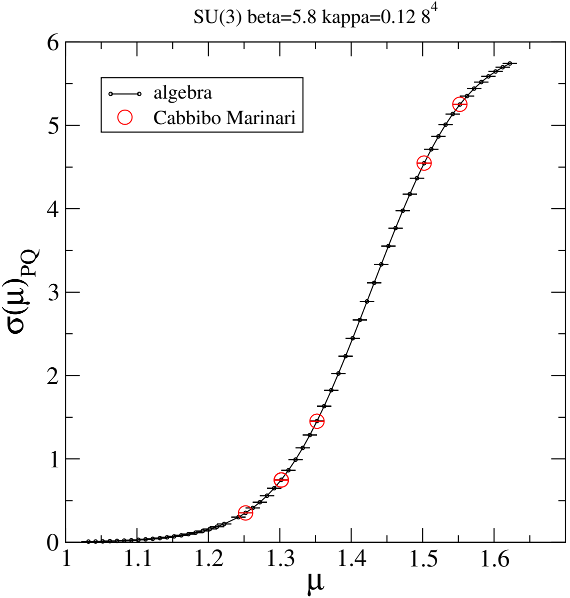
LLR results: the density



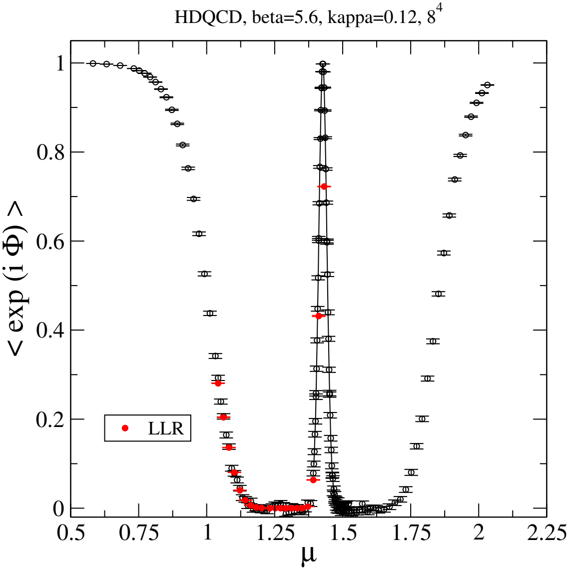
LLR results: the density



LLR results: the Fermionic density



Results: Phase Quenched vs LLR



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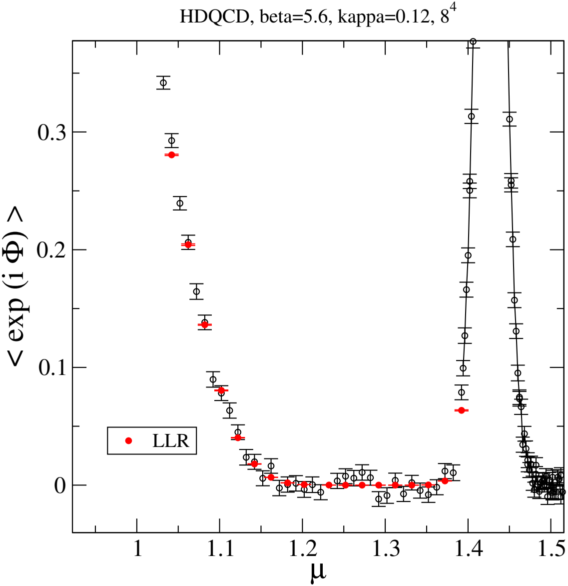
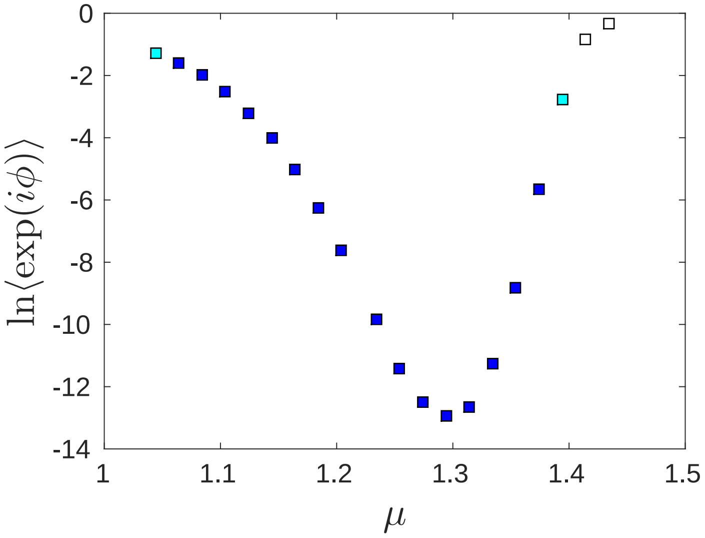


LLR Results: Phase Factor Expectation value



Work in Progress

Folding the density

$$
\begin{aligned}
Z &= \int_{-\infty}^{+\infty} ds\, \rho(s) \cos(s) \\
&= \sum_{k \in \mathbb{Z}} \int_{-\pi+2k\pi}^{\pi+2k\pi} ds\, \rho(s) \cos(s)
\end{aligned}
$$

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\end{aligned}
$$

The substitution $x = s - 2k\pi$ gives

$$
\begin{aligned}
Z &= \sum_{k \in \mathbb{Z}} \int_{-\pi}^{\pi} dx\, \rho(x + 2k\pi) \cos(x) \\
&= \int_{-\pi}^{\pi} dx \left(\sum_{k \in \mathbb{Z}} \rho(x + 2k\pi) \right) \cos(x) \\
&\equiv \int_{-\pi}^{\pi} dx\, \rho_F(x)\, \cos(x)
\end{aligned}
$$

we have defined the folded density

$$
\rho_F(x) \equiv \sum_{k \in \mathbb{Z}} \rho(x + 2k\pi)
$$

Folding the density

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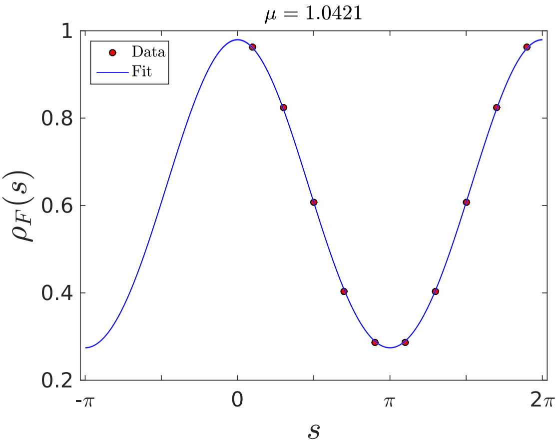
$$\rho_F(x) \equiv \sum_{k\in\mathbb{Z}} \rho(x+2k\pi)\ , \quad x = s - 2k\pi$$

$\rho_F(s)$ is computed in two different ways

- From the fitted $\rho(s)$
- We re-compute the $a(s)$ with $\delta_s = 2/(n\pi)$

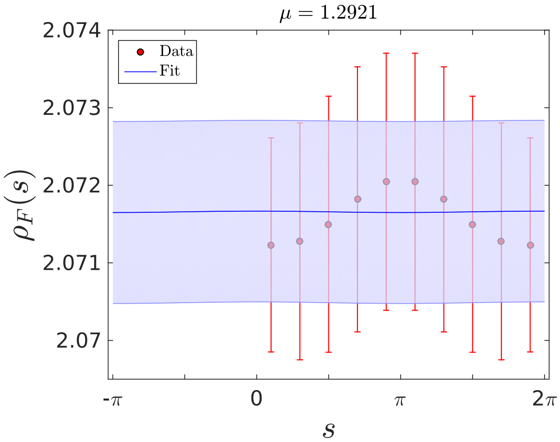
  $\Rightarrow$ direct determination of $\rho_F(s)$ (no fit dependence)

Folding the density



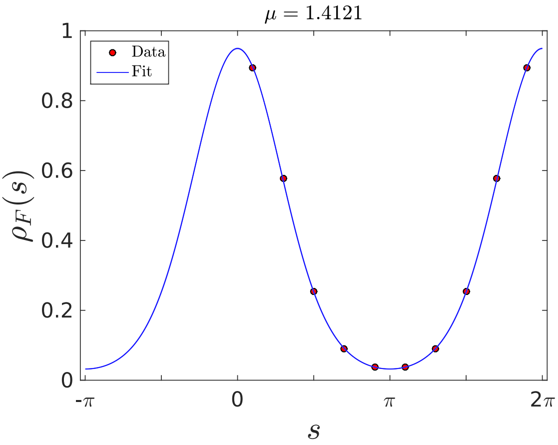
Low μ region

Folding the density



Middle μ region (Strong Sign Problem !)

Folding the density



High μ region

Moment expansion

Expanding the folded density

See eg [Ejiri '08; WHOT-QCD '10, '14; Greensite, Myers, Splittorf '14]

The elementary moments are given by

$$\langle s^{2n} \rangle = \int_{-\pi}^{\pi} s^{2n} \rho_F(s)\, ds$$

In the strong sign-problem region $\rho_F(s)$ is almost constant, therefore we expand

$$\rho_F(s) = \left(1 + \epsilon d_1 s^2 + \epsilon^2 d_2 s^4 + \epsilon^3 d_3 s^6 + \dots\right)/N$$

Expanding the folded density

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$$\rho_F(s) = \left(1 + \epsilon d_1 s^2 + \epsilon^2 d_2 s^4 + \epsilon^3 d_3 s^6 + \dots\right) / N$$

Plugging this expansion in the partition function gives

$$\begin{aligned} Z &= \int_{-\pi}^{\pi} dx \, \rho_F(x) \, \cos(x) \\ &= \left[-4\pi\epsilon d_1 + (48\pi - 8\pi^3)\epsilon^2 d_2 + (240\pi^3 - 12\pi^5 - 1440\pi)\epsilon^3 d_3 + \dots \right] / N \end{aligned}$$

Moment expansion

- We can use the expanded ρ_F to compute the moments, for example

$$\langle s^2 \rangle = \Big[\frac{2\pi^3}{3} + \frac{2\pi^5}{5}\epsilon d_1 + \frac{2\pi^7}{7}\epsilon^2 d_2 + \frac{2\pi^9}{9}\epsilon^3 d_3 + \ldots \Big] / N$$

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- At leading order, ie up to $\mathcal{O}(\epsilon^2)$, we impose

$$Z = k_1 \langle s^2 \rangle + k_2 \langle s^4 \rangle \ , \qquad \forall \ d_1$$

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- Sovling for k_1 and k_2 gives

$$k_1 = \frac{105}{2\pi^4}\ , \qquad k_2 = -\frac{175}{2\pi^6}$$

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$$k_1 = \frac{105}{2\pi^4} \,, \qquad k_2 = -\frac{175}{2\pi^6}$$

- Can easily be generalised to higher orders

Moment expansion

Numerical analysis, for $\mu = 1.2921$ (strong sign problem)

$$\begin{aligned} \langle s^2 \rangle &= 3.289859(2) \\ \langle s^4 \rangle &= 19.48175(1) \\ \langle s^6 \rangle &= 137.3408(1) \end{aligned}$$

$\Rightarrow$ The moments are computed with high precision

Moment expansion

Application: phase factor expectation value

$$\langle e^{i\phi} \rangle = \frac{175}{2\pi^6} \left[\frac{3\pi^2}{5} \langle s^2 \rangle - \langle s^4 \rangle \right] + \mathcal{O}(\epsilon^2)$$

Moment expansion

Application: phase factor expectation value

$$\langle \mathrm{e}^{i\phi} \rangle = \frac{175}{2\pi^6}\left[\frac{3\pi^2}{5}\langle s^2\rangle - \langle s^4\rangle\right] + \frac{4851\,(27-2\pi^2)}{8\pi^{10}}\left[\frac{5\pi^4}{21}\langle s^2\rangle - \frac{10\pi^2}{9}\langle s^4\rangle + \langle s^6\rangle\right] + \mathcal{O}(\epsilon^3)$$

Moment expansion

Application: phase factor expectation value

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\begin{aligned}
\langle \mathrm{e}^{i\phi} \rangle &= \frac{175}{2\pi^6}\left[\frac{3\pi^2}{5}\langle s^2\rangle - \langle s^4\rangle\right] \\
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&+ \frac{57915\,(3\pi^4-242\pi^2+2145)}{16\pi^{14}}\left[\frac{35\pi^6}{429}\langle s^2\rangle - \frac{105\pi^4}{143}\langle s^4\rangle + \frac{21\pi^2}{13}\langle s^6\rangle - \langle s^8\rangle\right] + \mathcal{O}(\epsilon^4)
\end{aligned}
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\end{aligned}
$$

Numerically, for $\mu = 1.2921$ (strong sign problem)

$$\langle \mathrm{e}^{i\phi} \rangle = 10^{-6}\ (\ 1.45(28)\ +\ 0.67(13) + 0.068(13)\ +\ \ldots)$$

Looks like it's converging

Moment expansion: Numerical cancellations

$$\mathcal{O}(\epsilon) \quad = \quad \frac{175}{2\pi^6}\left[\frac{3\pi^2}{5}\langle s^2\rangle - \langle s^4\rangle\right]$$

$$\begin{aligned} \frac{3\pi^2}{5}\langle s^2\rangle &= 19.4817\,661\,(99) \\ -\langle s^4\rangle &= -19.481\,7501\,(129) \\ \hline [\quad\quad] &= 0.000\,0160\,(30) \end{aligned}$$

Moment expansion: Numerical cancellations

$$\mathcal{O}(\epsilon^2) \quad = \quad \frac{4851\,(27-2\pi^2)}{8\pi^{10}} \left[\frac{5\pi^4}{21} \langle s^2 \rangle - \frac{10\pi^2}{9} \langle s^4 \rangle + \langle s^6 \rangle \right]$$

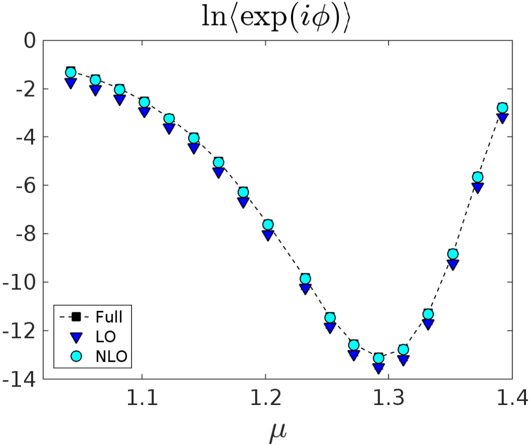
$$\begin{array}{rcr} \frac{5\pi^4}{21} \langle s^2 \rangle & = & 76.300\,526\,(39) \\ -\frac{10\pi^2}{9} \langle s^4 \rangle & = & -213.641\,297\,(141) \\ \langle s^6 \rangle & = & 137.340\,785\,(100) \\ \hline [\qquad] & = & 0.000\,014\,(3) \end{array}$$

Moment expansion: Numerical cancellations

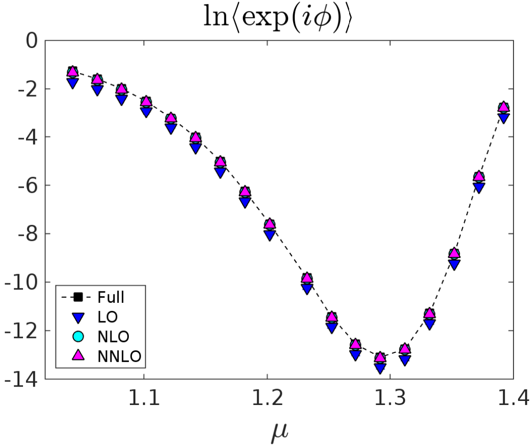
$$\mathcal{O}(\epsilon^3) = \frac{57915\,(3\pi^4 - 242\pi^2 + 2145)}{16\pi^{14}} \left[\frac{35\pi^6}{429}\langle s^2\rangle - \frac{105\pi^4}{143}\langle s^4\rangle + \frac{21\pi^2}{13}\langle s^6\rangle - \langle s^8\rangle \right]$$

$$\begin{aligned}
\frac{35\pi^6}{429}\langle s^2\rangle &= 258.040\,170\,(131)\\
-\frac{105\pi^4}{143}\langle s^4\rangle &= -1393.415\,773\,(921)\\
\frac{21\pi^2}{13}\langle s^6\rangle &= 2189.652\,588\,(1594)\\
-\langle s^8\rangle &= -1054.276\,980\,(804)\\
\hline
[\quad\quad] &= 0.000\,004\,(1)
\end{aligned}$$

Moment expansion, Results



Moment expansion, Results



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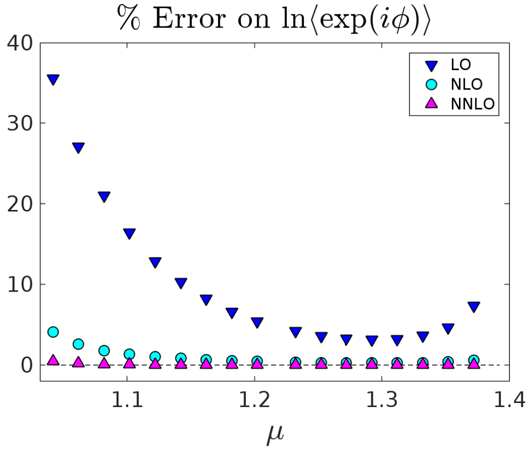
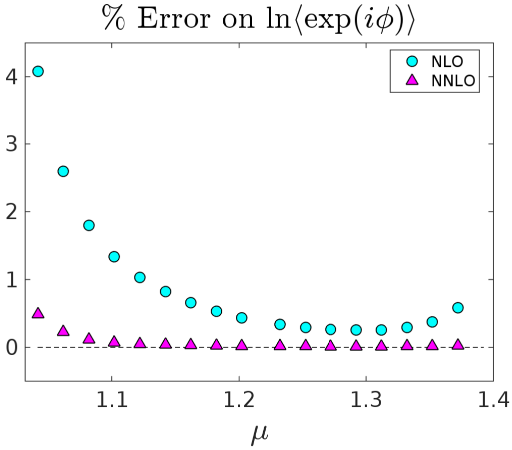


Moment expansion, Results



Conclusions and outlook

- We study a theory of QCD in the cold heavy-dense limit
- Combine LLR and re-weighting techniques
- Obtain robust results for the phase expectation value for a large range of μ
- Determine the moments with very good precision
- Moment expansion seems to work very well (converges quickly)

Conclusions and outlook

Future investigations

- How does the method scale with the volume ?
- Or toward the continuum limit ?
- Applications to different physical systems, eg Hubbard model, ϕ^4
- What about QCD ? LLR for HMC ?

Other talks related to LLR

Parallels in Algorithms

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B Luicini @17:50

Plenary by Kurt Langfeld

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BACKUP SLIDES

Enter at your own risks

Determination of the a_i

Define the double bracket expectation value $\langle\langle s \rangle\rangle_{[i]}$ on the interval $[s_{i-1}, s_i]$

$$\langle\langle s \rangle\rangle_{[i]}(a) = \frac{1}{N_{[i]}(a)} \int_{s_{i-1}}^{s_i} ds\ s\rho(s)\mathrm{e}^{-as}$$

where N is the usual normalisation

$$N_{[i]}(a) = \int_{s_{i-1}}^{s_i} ds\rho(s)\mathrm{e}^{-as}$$

Determination of the a_i

Using the Ansatz $\rho(s) = \rho(s_{i-1})\mathrm{e}^{a_i(s-s_{i-1})}$ gives

$$\langle\langle s \rangle\rangle_{[i]}(a) = \frac{\displaystyle\int_{s_{i-1}}^{s_i} ds\, s\, \mathrm{e}^{s(a_i-a)}}{\displaystyle\int_{s_{i-1}}^{s_i} ds\, \mathrm{e}^{s(a_i-a)}}$$

For $a = a_i$, we find

$$\langle\langle s \rangle\rangle_{[i]}(a_i) = \frac{\displaystyle\int_{s_{i-1}}^{s_i} ds\, s}{\displaystyle\int_{s_{i-1}}^{s_i} ds} = \frac{\frac{1}{2}(s_i^2 - s_{i-1}^2)}{s_i - s_{i-1}} = \frac{1}{2}(s_{i-1} + s_i)$$

$$= s_{i-1} + \frac{1}{2}(s_{i-1} - s_i) \equiv s_{i-1} + \frac{1}{2}\delta s$$

Computing $\langle\langle s \rangle\rangle_{[i]}$

Recall that on the interval $[s_{i-1}, s_i]$

$$\langle\langle s \rangle\rangle_{[i]}(a) = \frac{1}{N_{[i]}(a)} \int_{s_{i-1}}^{s_i} ds\; s\rho(s)\mathrm{e}^{-as}$$

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Reconstructing the density

1. Using the numerical esitmates a_k, we build the function

$$
\begin{aligned}
P(s) &= -\sum_{k=1}^{n-1} a_i \, \delta s - a_n \, \delta s/2 \\
s &= s_n + \delta s/2
\end{aligned}
$$

2. We fit the result to a even-powers polynomial

$$P(s) = \sum_i c_{2i} \, s^{2i}$$

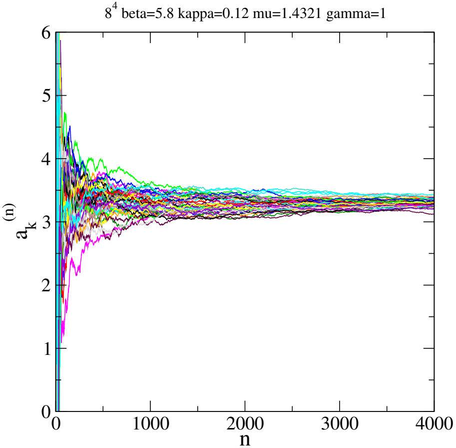
3. From the fit result, we reconstruct the density

$$\rho(s) = \exp(P(s))$$

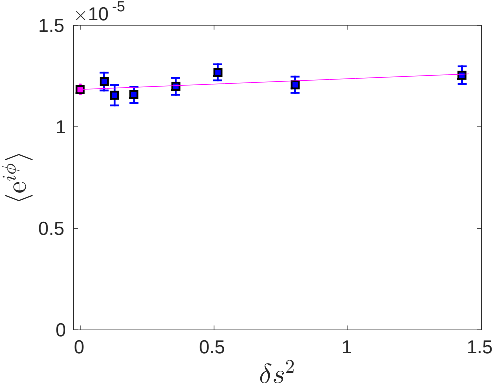
4. Finally, we compute the LLR integral semi-analytically

$$\langle \mathrm{e}^{i\phi} \rangle = \frac{\displaystyle\int_0^{\phi_{\max}} \rho(s) \cos(s) \; ds}{\displaystyle\int_0^{\phi_{\max}} \rho(s) \; ds}$$

Thermalisation of the a_i



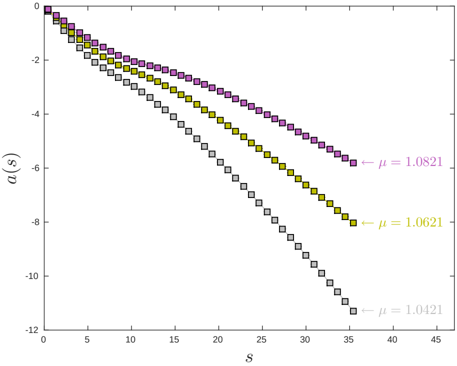
40 independent random starts



$\langle e^{i\phi} \rangle$ for $\mu = 1.3321$ as a function of δs^2

statistical error only

The a_i vs the phase for low μ



The a_i vs the phase for high μ