Relative Weights Approach to Dynamical Fermions at Finite Densities

Jeff Greensite
San Francisco State University

LATTICE 2016
University of Southampton
Southampton, UK $\notin$ EU

July 2016

with Roman Höllwieser, arXiv: 1603.09654

An Indirect Approach

There are several "direct" approaches to the sign problem in QCD, which are under development:

- **Reweighting + cumulant expansion**
- **Langevin equation**
- **Lefschetz thimble**
- **Density of States**
- **...**

The idea of the indirect approach is to first map the SU(3) gauge theory with dynamical fermions theory onto a much simpler theory − a **Polyakov line action** (or "SU(3) spin") model.

At finite density there is still a sign problem in the effective theory. This will be dealt with via mean field theory.

Previous application to SU(3) gauge-Higgs at finite μ: *Langfeld and JG, Phys.Rev. D90 (2014), 014507.*

Effective Polyakov Line Action

Start with SU(3) lattice gauge theory and integrate out all d.o.f. subject to the constraint that the Polyakov line holonomies are held fixed. In temporal gauge

$$e^{S_P[U_{\mathbf{x}}]} = \int DU_0(\mathbf{x},0) DU_k D\overline{\psi} D\psi \left\{ \prod_{\mathbf{x}} \delta[U_{\mathbf{x}} - U_0(\mathbf{x},0)] \right\} e^{S_L}$$

Given S_P at $\mu = 0$, the action at finite μ is simply

$$S_P^{\mu}[U_{\mathbf{x}}, U_{\mathbf{x}}^{\dagger}] = S_P^{\mu=0}[e^{N_t \mu} U_{\mathbf{x}}, e^{-N_t \mu} U_{\mathbf{x}}^{\dagger}]$$

For heavy quarks, the PLA can be derived via strong coupling/hopping parameter expansions (*Langelage, Philipsen et al., JHEP 1201 (2012) 042*).

We are interested in lighter quark masses, where those methods cannot be easily applied.

The Relative Weights Method

Let S'_L be the lattice action in temporal gauge with $U_0(\mathbf{x},0)$ fixed to $U'_{\mathbf{x}}$. It is not so easy to compute

$$\exp\Big[S_P[U'_{\mathbf{x}}]\Big] = \int DU_k D\overline{\psi} D\psi \; e^{S'_L}$$

directly. But the ratio (“relative weights”)

$$e^{\Delta S_P} = \frac{\exp[S_P[U'_{\mathbf{x}}]]}{\exp[S_P[U''_{\mathbf{x}}]]}$$

is easily computed as an expectation value

$$\begin{aligned}
\exp[\Delta S_P] &= \frac{\int DU_k D\overline{\psi} D\psi \; e^{S'_L}}{\int DU_k D\overline{\psi} D\psi \; e^{S''_L}} \\
&= \frac{\int DU_k D\overline{\psi} D\psi \; \exp[S'_L - S''_L] e^{S''_L}}{\int DU_k D\overline{\psi} D\psi \; e^{S''_L}} \\
&= \Big\langle \exp[S'_L - S''_L] \Big\rangle''
\end{aligned}$$

where $\langle ... \rangle''$ means the VEV in the Boltzman weight $\propto e^{S''_L}$.

Suppose $U_{\mathbf{x}}(\lambda)$ is some path through configuration space parametrized by λ, and suppose $U'_{\mathbf{x}}$ and $U''_{\mathbf{x}}$ differ by a small change in that parameter, i.e.

$$U'_{\mathbf{x}} = U_{\mathbf{x}}(\lambda_0 + \tfrac{1}{2}\Delta\lambda) \quad , \quad U''_{\mathbf{x}} = U_{\mathbf{x}}(\lambda_0 - \tfrac{1}{2}\Delta\lambda)$$

Then the relative weights method gives us the derivative of the true effective action S_P along the path:

$$\left(\frac{dS_P}{d\lambda}\right)_{\lambda=\lambda_0} \approx \frac{\Delta S}{\Delta\lambda}$$

The question is: which derivatives will help us to determine S_P itself?

Fourier components of P_x

$$P_{\mathbf{x}} \equiv \frac{1}{N_c} \mathrm{Tr}\, U_{\mathbf{x}} = \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}$$

We first set a particular momentum mode $a_{\mathbf{k}}$ to zero. Call the resulting configuration $\widetilde{P}_x$. Then define ($f \approx 1$)

$$\begin{aligned} P''_{\mathbf{x}} &= \left(\alpha - \frac{1}{2}\Delta\alpha\right) e^{i\mathbf{k}\cdot\mathbf{x}} + f\widetilde{P}_x \\ P'_{\mathbf{x}} &= \left(\alpha + \frac{1}{2}\Delta\alpha\right) e^{i\mathbf{k}\cdot\mathbf{x}} + f\widetilde{P}_x \end{aligned}$$

which uniquely determine (in SU(2) and SU(3)) the eigenvalues of the corresponding holonomies $U'_{\mathbf{x}}, U''_{\mathbf{x}}$. In this way we can compute

$$\frac{1}{L^3} \left(\frac{\partial S_P}{\partial a_{\mathbf{k}}}\right)_{a_{\mathbf{k}}=\alpha}$$

Ansatz for S_P

Motivated by the known fermion determinant for heavy-dense quarks:

$$e^{S_P} = \prod_{\mathbf{x}} \det[1 + he^{\mu/T}\text{Tr}U_{\mathbf{x}}] \det[1 + he^{-\mu/T}\text{Tr}U^{\dagger}_{\mathbf{x}}]$$
$$\times \exp\left[\sum_{\mathbf{x},\mathbf{y}} P_{\mathbf{x}} K(x-y) P^{\dagger}_{\mathbf{y}}\right]$$

where parameter h and kernel $K(\mathbf{x}-\mathbf{y})$ are to be determined from the data. (For heavy dense, $h = \kappa^{N_t}$ is fixed.)

Of course this ansatz is not exact. An important check: compute and compare, at $\mu = 0$, the Polyakov line correlator

$$G(R) = \langle P(\mathbf{x}) P^{\dagger}(\mathbf{y}) \rangle \quad , \quad R = |\mathbf{x} - \mathbf{y}|$$

in both the PLA, and the underlying lattice gauge theory.

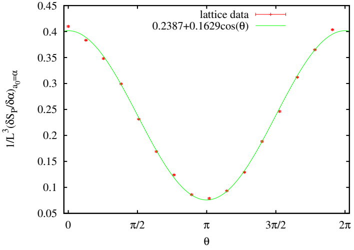
imaginary chemical potential

We gain precision by introducing an imaginary chemical potential $\mu/T = i\theta$. Construct $U'_{\mathbf{x}}, U''_{\mathbf{x}}$ as before, then set

$$U'(\mathbf{x},0) = e^{i\theta}U'_{\mathbf{x}} \quad , \quad U''(\mathbf{x},0) = e^{i\theta}U''_{\mathbf{x}}$$

To lowest order in h, we have

$$\frac{1}{L^3}\left(\frac{\partial S_P}{\partial a_0}\right)^{\mu/T=i\theta}_{a_0=\alpha} = 2\widetilde{K}(0)\alpha + 6h\cos\theta$$



Wilson action, staggered fermions, $\beta = 5.2$, $ma = 0.35$, $N_t = 4$ at $\alpha = 0.03$

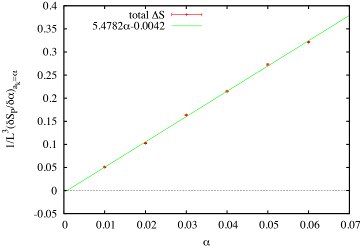
Data for the lhs, at various θ, determines $\widetilde{K}(0)$ and h on the rhs.

($\widetilde{K}(\mathbf{k})$ is the Fourier transform of $K(\mathbf{x}-\mathbf{y})$)

At $\mathbf{k} \neq 0$, lowest order in h:

$$\frac{1}{L^3}\left(\frac{\partial S_P}{\partial a^R_{\mathbf{k}}}\right)_{a_{\mathbf{k}}=\alpha} = 2\widetilde{K}(\mathbf{k})\alpha$$

Data for the lhs, at various α, determines $\widetilde{K}(\mathbf{k})$.



Derivative of S_P with respect to the Fourier component of the Polyakov line configuration at mode numbers (210). Wilson action, staggered fermions, $\beta = 5.2,\ ma = 0.35,\ N_t = 4$.

Fit to $K(\mathbf{x} - \mathbf{y})$

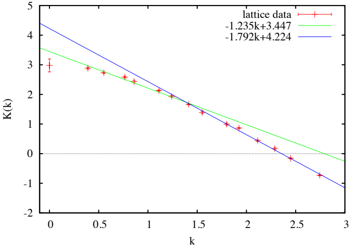
As in previous work with bosonic matter fields, we fit $\widetilde{K}(\mathbf{k})$ by two straight lines

$$\widetilde{K}^{fit}(\mathbf{k}) = \begin{cases} c_1 - c_2 k_L & k_L \le k_0 \\ d_1 - d_2 k_L & k_L \ge k_0 \end{cases}$$

where

$$k_L = 2\sqrt{\sum_{i=1}^{3} \sin^2(k_i/2)}$$

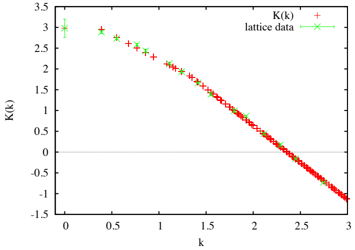
is the lattice momentum. The last few points are handled by a long distance cutoff



Effect of the long-range cutoff: Define

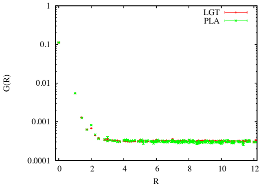
$$K(\mathbf{x}-\mathbf{y}) = \begin{cases} \frac{1}{L^3}\sum_{\mathbf{k}} \widetilde{K}^{fit}(k_L) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} & |\mathbf{x}-\mathbf{y}| \le r_{max} \\ 0 & |\mathbf{x}-\mathbf{y}| > r_{max} \end{cases}$$

and Fourier transform again to $\widetilde{K}(k)$. Compare the result with the relative weights data:

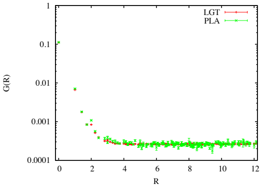


Wilson action, $N_t = 4$

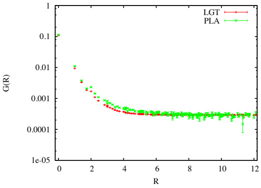
We determine the effective action and compare Polyakov line correlators at $\mu = 0$ in the PLA and the underlying gauge theory.



$\beta = 5.04, \; ma = 0.2, \; N_t = 4.$



$\beta = 5.2, \; ma = 0.35, \; N_t = 4.$



$\beta = 5.4, \; ma = 0.6, \; N_t = 4.$

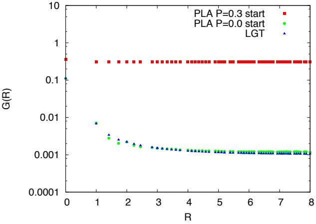
So far so good, but...

Metastable States in the PLA

We also tried the Lüscher-Wiesz gauge action at $\beta = 7.0$, $ma = 0.3$, $N_t = 6$. Unlike previous cases, the couplings in the effective action are completely non-local: all spins coupled to all other spins, at least on a 16^3 lattice.

In this instance, we found that the simulation of the PLA depends on the starting point; i.e. there are long-lived metastable states persisting for many thousands of sweeps.
An unfortunate ambiguity in this case!

A start with $P_{\mathbf{x}} = 0$ seems to choose the phase which agrees with underlying lattice gauge theory.



Lüscher-Weisz gauge action, $\beta = 7.0$, $ma = 0.3$, $N_t = 6$.

Apart from this ambiguity: *How do we solve a given PLA at $\mu \neq 0$?* There is still a sign problem!

Mean Field Theory

- Mean field theory *likes* systems with couplings of each spin to many spins. The PLA is a system of that type.
- The method has been applied to such models, at $\mu \neq 0$, with results compared to solution by Langevin equation (J.G., arXiv:1406.4558).
- Result: Mean field and Langevin agree perfectly, except where Langevin fails due to the Mollgaard-Splittorff ("singular drift") problem. (Mollgaard and Splittorff, arXiv:1309.4335)

So this is the method we apply to solve the PLA at $\mu \neq 0$.

Mean Field Theory for the effective actions

We follow the approach of *Splittorff and JG (2012)*.
The idea is to localize the part of the action S_P^0 containing products of terms at different sites:

$$\begin{aligned} S_P^0 &= \frac{1}{9}\sum_{\mathbf{xy}} \mathrm{Tr}[U_{\mathbf{x}}]\mathrm{Tr}[U_{\mathbf{y}}^\dagger]K(\mathbf{x}-\mathbf{y}) \\ &= \frac{1}{9}\sum_{(\mathbf{xy})} \mathrm{Tr}[U_{\mathbf{x}}]\mathrm{Tr}[U_{\mathbf{y}}^\dagger]K(\mathbf{x}-\mathbf{y}) + a_0 \sum_{\mathbf{x}} \mathrm{Tr}[U_{\mathbf{x}}]\mathrm{Tr}[U_{\mathbf{x}}^\dagger] \end{aligned}$$

where we have introduced the notation for the double sum, excluding $\mathbf{x} = \mathbf{y}$,

$$\sum_{(\mathbf{xy})} \equiv \sum_{\mathbf{x}} \sum_{\mathbf{y}\neq\mathbf{x}} \quad \text{and} \quad a_0 \equiv \frac{1}{9}K(0)$$

Next, introduce parameters u, v

$$\mathrm{Tr}U_{\mathbf{x}} = (\mathrm{Tr}U_{\mathbf{x}} - u) + u \quad , \quad \mathrm{Tr}U_{\mathbf{x}}^\dagger = (\mathrm{Tr}U_{\mathbf{x}}^\dagger - v) + v$$

Then

$$S_P^0 = J_0 \sum_{\mathbf{x}} (v \text{Tr} U_{\mathbf{x}} + u \text{Tr} U_{\mathbf{x}}^\dagger) - uvJ_0 V + a_0 \sum_{\mathbf{x}} \text{Tr}[U_{\mathbf{x}}]\text{Tr}[U_{\mathbf{x}}^\dagger] + E^0$$

where $V = L^3$ is the lattice volume, and we have defined

$$E^0 = \sum_{(\mathbf{xy})} (\text{Tr} U_x - u)(\text{Tr} U_{\mathbf{y}}^\dagger - v) \frac{1}{9} K(\mathbf{x} - \mathbf{y}) ,$$

$$J_0 = \frac{1}{9} \sum_{\mathbf{x} \neq 0} K(\mathbf{x})$$

If we drop E_0, the total action (including $\mu \neq 0$) is local and and the group integrations can be carried out analytically.

The trick is to choose u and v such that E_0 can be treated as a perturbation, to be ignored as a first approximation. In particular, $\langle E_0 \rangle = 0$ when

$$u = \langle \text{Tr} U_x \rangle \quad , \quad v = \langle \text{Tr} U_x^\dagger \rangle$$

This is *equivalent to stationarity* of the mean field free energy, with respect to variations in u, v, and is solved numerically.

check mean field at $\mu = 0$

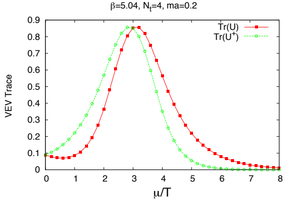
At $\mu = 0$ we can compute the Polyakov line expectation value by numerical simulation of the underlying lattice gauge theory, and by mean field solution of the PLA.

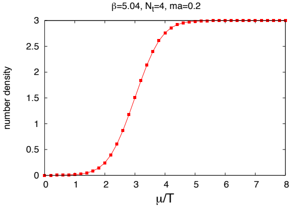
action	N_t	β	ma	$\frac{1}{3}\langle \mathrm{Tr}U \rangle$	$\frac{1}{3}\langle \mathrm{Tr}U \rangle_{mf}$
Wilson	4	5.04	0.2	0.01778(3)	0.01765
Wilson	4	5.2	0.35	0.01612(4)	0.01603
Wilson	4	5.4	0.6	0.01709(5)	0.01842
Lüscher-Weisz I	6	7.0	0.3	0.03580(4)	0.03212
Lüscher-Weisz II	6	7.0	0.3	0.554(1)	0.5580

For Lüscher-Weisz II, the value in column 5 is obtained by numerical simulation of the PLA with a cold start.

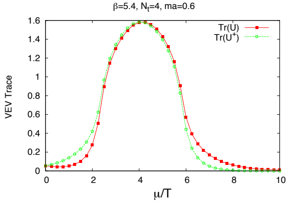
Results I - Wilson action

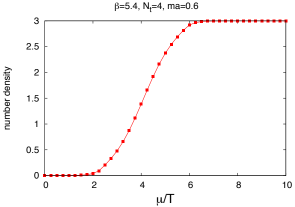
$\beta = 5.04, \ ma = 0.2, \ N_t = 4.$





$\beta = 5.4, \ ma = 0.6, \ N_t = 4.$

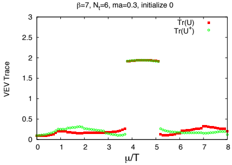




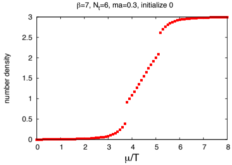
Similar to results seen in the heavy-dense quark case.

Results II - Lüscher-Weisz action

In the metastable situation, the solutions of the mean-field equations are not unique.
small *u*, *v* mean-field solutions:

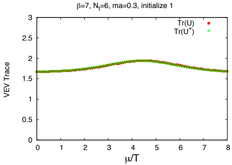


(a)

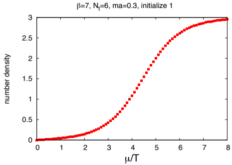


(b)

large *u*, *v* mean-field solutions:



(c)



(d)

The large *u*, *v* solutions have smallest free energy...but this is the phase which does *not* correspond to the underlying lattice gauge theory at $\mu = 0$!

Conclusions

- We have extended the relative weights methods to dynamical fermions in SU(3) lattice gauge theory.
- Relative weights data is fit to a simple ansatz for the Polyakov line action, motivated by the heavy quark form.
- At $\mu = 0$ we find good agreement between Polyakov line correlators in the effective action, and underlying lattice gauge theory. The effective theory can be solved at $\mu \neq 0$ by a mean field technique. *Would be interesting to compare to other methods!*
- Metastability problem for highly non-local S_P. Not a finite density issue!
- We either need a criterion for selecting the right metastable phase, or else must restrict the method to a region of parameter space where metastable states are not an issue.