Relative Weights Approach to Dynamical Fermions at Finite Densities

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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 $\mu$: *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

\[ e^{S_P[U_x]} = \int DU_0(x, 0) DU_k D\bar{\psi} D\psi \left\{ \prod_x \delta[U_x - U_0(x, 0)] \right\} e^{S_L} \]

Given \( S_P \) at \( \mu = 0 \), the action at finite \( \mu \) is simply

\[ S_P^{\mu}[U_x, U_x^\dagger] = S_P^{\mu=0}[e^{N_t \mu} U_x, e^{-N_t \mu} U_x^\dagger] \]

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

$$\exp[S_P[U'_x]] = \int DU_k D\bar{\psi} D\psi e^{S'_L}$$

directly. But the ratio ("relative weights")

$$e^{\Delta S_P} = \frac{\exp[S_P[U'_x]]}{\exp[S_P[U'_x']]}$$

is easily computed as an expectation value

$$\exp[\Delta S_P] = \frac{\int DU_k D\bar{\psi} D\psi e^{S'_L}}{\int DU_k D\bar{\psi} D\psi e^{S''_L}}$$

$$\quad = \frac{\int DU_k D\bar{\psi} D\psi \exp[S'_L - S''_L] e^{S''_L}}{\int DU_k D\bar{\psi} D\psi e^{S''_L}}$$

$$\quad = \langle \exp[S'_L - S''_L] \rangle''$$

where $\langle \ldots \rangle''$ means the VEV in the Boltzman weight $\propto e^{S''_L}$. 
Suppose $U_x(\lambda)$ is some path through configuration space parametrized by $\lambda$, and suppose $U'_x$ and $U''_x$ differ by a small change in that parameter, i.e.

\[
U'_x = U_x(\lambda_0 + \frac{1}{2} \Delta \lambda) \, , \, \, U''_x = U_x(\lambda_0 - \frac{1}{2} \Delta \lambda)
\]

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 $P_x$

\[ P_x \equiv \frac{1}{N_c} \text{Tr} U_x = \sum_k a_k e^{i k \cdot x} \]

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

\[ P''_x = \left( \alpha - \frac{1}{2} \Delta \alpha \right) e^{i k \cdot x} + f \tilde{P}_x \]
\[ P'_x = \left( \alpha + \frac{1}{2} \Delta \alpha \right) e^{i k \cdot x} + f \tilde{P}_x \]

which uniquely determine (in SU(2) and SU(3)) the eigenvalues of the corresponding holonomies $U'_x, U''_x$. In this way we can compute

\[ \frac{1}{L^3} \left( \frac{\partial S_P}{\partial a_k} \right)_{a_k=\alpha} \]
Motivated by the known fermion determinant for heavy-dense quarks:

\[
e^{S_P} = \prod_x \det[1 + he^{\mu/T} \text{Tr} U_x] \det[1 + he^{-\mu/T} \text{Tr} U_x^\dagger] \times \exp \left[ \sum_{x,y} P_x K(x - y) P_y^\dagger \right]
\]

where parameter $h$ and kernel $K(x - y)$ 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

\[
G(R) = \langle P(x) P^\dagger(y) \rangle , \quad R = |x - y|
\]

in both the PLA, and the underlying lattice gauge theory.
We gain precision by introducing an imaginary chemical potential $\mu/T = i\theta$. Construct $U'_x$, $U''_x$ as before, then set

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

To lowest order in $h$, we have

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

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

$(\tilde{K}(k)$ is the Fourier transform of $K(x - y))$
At $k \neq 0$, lowest order in $h$:

$$\frac{1}{L^3} \left( \frac{\partial S_P}{\partial a^R_k} \right)_{a_k = \alpha} = 2\tilde{K}(k)\alpha$$

Data for the lhs, at various $\alpha$, determines $\tilde{K}(k)$.

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

\[ 5.4782\alpha - 0.0042 \]
Fit to $K(x - y)$

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

\[
\tilde{K}^{\text{fit}}(k) = \begin{cases} 
  c_1 - c_2 k_L & k_L \leq k_0 \\
  d_1 - d_2 k_L & k_L \geq k_0 
\end{cases}
\]

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

\[ K(x - y) = \begin{cases} \frac{1}{L^3} \sum_k \tilde{K}^{fit}(k_L) e^{i k \cdot (x - y)} & |x - y| \leq r_{max} \\ 0 & |x - y| > r_{max} \end{cases} \]

and Fourier transform again to \( \tilde{K}(k) \). 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...
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 $P_x = 0$ seems to choose the phase which agrees with underlying lattice gauge theory.

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 $S^0_P$ containing products of terms at different sites:

$$S^0_P = \frac{1}{9} \sum_{xy} \text{Tr}[U_x] \text{Tr}[U_y^\dagger] K(x - y)$$

where we have introduced the notation for the double sum, excluding $x = y$,

$$\sum_{(xy)} \equiv \sum_x \sum_{y \neq x}$$

and

$$a_0 \equiv \frac{1}{9} K(0)$$

Next, introduce parameters $u, v$

$$\text{Tr} U_x = (\text{Tr} U_x - u) + u, \quad \text{Tr} U_x^\dagger = (\text{Tr} U_x^\dagger - v) + v$$
Then

\[ S_P^0 = J_0 \sum_x (v \text{Tr} U_x + u \text{Tr} U_x^\dagger) - uv J_0 V + a_0 \sum_x \text{Tr}[U_x] \text{Tr}[U_x^\dagger] + E^0 \]

where \( V = L^3 \) is the lattice volume, and we have defined

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

\[ J_0 = \frac{1}{9} \sum_{x \neq 0} K(x) \]

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

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

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

<table>
<thead>
<tr>
<th>action</th>
<th>$N_t$</th>
<th>$\beta$</th>
<th>$ma$</th>
<th>$\frac{1}{3}\langle\text{Tr}U\rangle$</th>
<th>$\frac{1}{3}\langle\text{Tr}U\rangle_{mf}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wilson</td>
<td>4</td>
<td>5.04</td>
<td>0.2</td>
<td>0.01778(3)</td>
<td>0.01765</td>
</tr>
<tr>
<td>Wilson</td>
<td>4</td>
<td>5.2</td>
<td>0.35</td>
<td>0.01612(4)</td>
<td>0.01603</td>
</tr>
<tr>
<td>Wilson</td>
<td>4</td>
<td>5.4</td>
<td>0.6</td>
<td>0.01709(5)</td>
<td>0.01842</td>
</tr>
<tr>
<td>Lüscher-Weisz I</td>
<td>6</td>
<td>7.0</td>
<td>0.3</td>
<td>0.03580(4)</td>
<td>0.03212</td>
</tr>
<tr>
<td>Lüscher-Weisz II</td>
<td>6</td>
<td>7.0</td>
<td>0.3</td>
<td>0.554(1)</td>
<td>0.5580</td>
</tr>
</tbody>
</table>

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

![Graphs showing VEV Trace and number density for small $u, v$ mean-field solutions.](image)

Large $u, v$ mean-field solutions:

![Graphs showing VEV Trace and number density for large $u, v$ mean-field solutions.](image)

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.