Polyakov line models from lattice gauge theory, and the sign problem

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We are interested in the QCD phase diagram at finite temperature and baryon density. To get a finite baryon density, we introduce a quark chemical potential $\mu$ into the QCD Lagrangian.

The problem is that this addition makes $S_{\text{QCD}}$ complex, and $\exp[S_{\text{QCD}}]$ oscillatory. Standard Monte Carlo simulation via importance sampling breaks down! This is the "sign problem."

Motivation: The Sign Problem

Maybe the phase diagram looks like this. Nobody knows for sure.
Integrate out all the d.o.f. in a lattice gauge theory, subject to the constraint that Polyakov line holonomies are held fixed.

The resulting D=3 action is the **Effective Polyakov line model** (a.k.a “Effective spin model”).

Using the strong-coupling and hopping parameter expansions, this action at lowest order has the form

\[
S_{P} = \beta_{P} \sum_{x} \sum_{i=1}^{3} \left[ \text{Tr} U_{x}^{\dagger} \text{Tr} U_{x+\hat{i}} + \text{Tr} U_{x} \text{Tr} U_{x+\hat{i}}^{\dagger} \right] + \kappa \sum_{x} \left[ e^{\mu} \text{Tr} U_{x} + e^{-\mu} \text{Tr} U_{x}^{\dagger} \right]
\]

The model seems to have a relatively **mild** sign problem, for a large range of parameters $\beta_{P}, \kappa, \mu$. 

**Effective Polyakov line models**
The model, with finite $\mu$, can be solved in any one of several ways:

- Flux representation (Mercado & Gattringer)
- Reweighting (Philipsen, Langelage, et al.)
- Stochastic quantization (Aarts & James)
- even mean field is not too bad (Splittorff & JG)

If we knew the $S_p$ corresponding to $S_{QCD}$ at realistic gauge couplings and light quark masses, and if the sign problem remains mild, then we could find the phase diagram of $S_{QCD}$ by computing the phase diagram of $S_p$.

But – what is $S_p$ in the parameter range of interest?
Consider a lattice of $N_t=1/T$ lattice spacings in the time direction. Lattice coupling and quark masses are arbitrary, *but $\mu=0$ for now*. It is convenient to fix to temporal gauge, $U(x,t) = 1$ except on one timeslice, say $t=0$. Then by definition

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

Lets pick a set of “effective spin” configurations (anything we like):

$$
\left\{ \{U_x^{(i)}\}, \text{ all } x \in V_3, \; i = 1, 2, \ldots, M \right\}
$$

and imagine restricting the timelike links at $t=0$ to just this set.
Define the partition function of this system

\[
Z = \int D U_0(x,0) D U_k D \bar{\psi} D \psi \sum_{i=1}^{M} \left\{ \prod_{x} \delta[U^{(i)}_x - U_0(x,0)] \right\} e^{S_{QCD}}
\]

and consider the ratio

\[
\frac{\exp[S_P[U^{(j)}]]}{\exp[S_P[U^{(k)}]]} = \frac{\int D U_0(x,0) D U_k D \bar{\psi} D \psi \left\{ \prod_{x} \delta[U^{(j)}_x - U_0(x,0)] \right\} e^{S_{QCD}}}{\int D U_0(x,0) D U_k D \bar{\psi} D \psi \left\{ \prod_{x} \delta[U^{(k)}_x - U_0(x,0)] \right\} e^{S_{QCD}}}
\]

\[
= \frac{1}{Z} \frac{\int D U_0(x,0) D U_k D \bar{\psi} D \psi \left\{ \prod_{x} \delta[U^{(j)}_x - U_0(x,0)] \right\} e^{S_{QCD}}}{\int D U_0(x,0) D U_k D \bar{\psi} D \psi \left\{ \prod_{x} \delta[U^{(k)}_x - U_0(x,0)] \right\} e^{S_{QCD}}}
\]

both the numerator and denominator on the rhs have the interpretation of a probability

\[
\text{Prob}[U^{(j)}] = \frac{1}{Z} \int D U_0(x,0) D U_k D \bar{\psi} D \psi \left\{ \prod_{x} \delta[U^{(j)}_x - U_0(x,0)] \right\} e^{S_{QCD}}
\]
For numerical simulation of this system:

1. Update all d.o.f in the usual way, *except* for timelike links at $t=0$.

2. Update timelike links at $t=0$ simultaneously, choosing one of the $M$ effective spin configurations via the Metropolis algorithm.

3. Keep track of the number of times $N_n$ ($n=1,...,M$) that each member of the set is selected by Metropolis.
\textbf{Prob} [U^{(j)}] \text{ is just the probability for the j-th configuration to be found on the t=0 timeslice.}

Let \( N_j \) be the number of times the j-th configuration is selected in a Monte Carlo simulation,

Let \( N_{\text{tot}} \) be the total number of updates of the t=0 timeslice. Then

\[
\text{Prob}[U^{(j)}] = \lim_{N_{\text{tot}} \to \infty} \frac{N_j}{N_{\text{tot}}}
\]

and this gives us the \textbf{relative weights} of the effective Polyakov line action:

\[
\frac{\exp \left[ S_P[U^{(j)}] \right]}{\exp \left[ S_P[U^{(k)}] \right]} = \lim_{N_{\text{tot}} \to \infty} \frac{N_j}{N_k}
\]

From this information we can either test anyone’s proposal for \( S_p \), or, if we are lucky, deduce \( S_p \) from the data.

(For the potential part of the action, we don’t need luck.)
Let $\lambda$ parametrize a path $U_x(\lambda)$ through the configuration space of Polyakov lines. We can use the method of relative weights to compute derivatives $dS_p/d\lambda$.

Let $U^{(i)}$ correspond to $\lambda = \lambda_0 + \Delta \lambda$ and $U^{(k)}$ correspond to $\lambda = \lambda_0 - \Delta \lambda$. Then

$$
\left( \frac{dS_P[U_x(\lambda)]}{d\lambda} \right)_{\lambda=\lambda_0} \approx \frac{1}{2\Delta \lambda} \left\{ \log \frac{N_j}{N_{tot}} - \log \frac{N_k}{N_{tot}} \right\}
$$

More generally: Choose the set of configurations $\{U_x^{(n)} = U_x(\lambda_n), \ n=1,2,...,M\}$ and

$$
\lambda_n = \lambda_0 + \left( n - \frac{M + 1}{2} \right) \Delta \lambda , \quad n = 1, 2, ..., M
$$

for sufficiently small $\Delta \lambda$ we have

$$
\left( \frac{dS_P[U_x(\lambda)]}{d\lambda} \right)_{\lambda=\lambda_0} \approx \text{slope of log } \frac{N_n}{N_{tot}} \text{ vs. } \lambda_n
$$
The strategy is:

- First find $S_p$ at $\mu=0$ from $S_{QCD}$.
- Then obtain $S^\mu_p$ at finite $\mu$.
- From there, if the sign problem is mild, solve the theory by any means available (reweighting, flux representation, stochastic quantization, mean field…) to determine the phase diagram.

This is a tall order. First step (and the main topic of this talk): can we actually determine $S_p$ by the relative weights method, even at $\mu=0$?

For starters, make life easy. SU(2) gauge group (no sign problem, of course), and scalar matter.
First, can we determine $S_p$ by relative weights in a case where we already know the answer?

Choose: **SU(2)** gauge group, $\beta=1.2$ (strong coupling), $N_t = 4$, no matter fields. $S_p$ is readily computed via strong-coupling/character expansion methods:

$$S_P = \beta P \sum_{x} \sum_{i=1}^{3} P_x P_{x+i},$$

where

$$P_x \equiv \frac{1}{2} \text{Tr} U_x$$

$$\beta P = 4 \left[ 1 + 4N_t \left( \frac{I_2(\beta)}{I_1(\beta)} \right)^4 \right] \left( \frac{I_2(\beta)}{I_1(\beta)} \right)^{N_t}.$$
$S_p$ divides into kinetic + potential pieces $S_p = K_p + V_p$ where

$$K_P = \frac{1}{2} \beta_P \sum_x \sum_{i=1}^3 (P_x P_{x+i} - 2P_x^2 + P_x P_{x-i})$$

$$V_P = 3 \beta_P \sum_x P_x^2$$

First, we determine $V_p$ by relative weights. Choose a set of configurations (timelike links at $t=0$) consisting of link variables constant in space, but varying in amplitude

$$U_x^{(n)} = (P_0 + a_n) \mathbb{1} + i \sqrt{1 - (P_0 + a_n)^2} \sigma_3$$

$$a_n = \left(n - \frac{1}{2}(M + 1)\right) \Delta a , \quad n = 1, 2, ..., M$$

so in this case the path parameter is $\lambda = a$, and it is easy to see that

$$\frac{1}{L^3} \left(\frac{dS_P(U_x(a))}{da}\right)_{a=0} = \frac{1}{L^3} \frac{dV_P(P_0)}{dP_0}$$

where $L^3 = \text{spatial volume.}$
Here is the data, evaluated at \( L = 12 \) \((12^3 \times 4 \text{ lattice})\) and \( \beta = 1.2, \ P_0 = 0.5 \)

The slope of the line gives us \( (dS/da)/\text{vol} = (dV_P/dP_0)/\text{vol} \) at \( P_0 = 0.5 \).
Repeating the calculation for various values of $P_0$, we find that $\frac{dV_p}{dP_0}$ is linear in $P_0$:

Integrating, and dropping an irrelevant constant of integration, we find

\[
V(P_x) = \begin{cases} 
0.1721(8) \sum_x \frac{1}{2} P_x^2 & \text{relative weights method} \\
0.1710 \sum_x \frac{1}{2} P_x^2 & \text{strong-coupling expansion}
\end{cases}
\]
Now for the kinetic term, which by definition $= 0$ for spatially constant configurations. We choose a set of plane wave deformations around a constant background

$$U^{(n)}_x = P^{(n)}_x \mathbb{1} + i \sqrt{1 - (P^{(n)}_x)^2} \sigma_3$$

$$P^{(n)}_x = P_0 + a_n \cos(k \cdot x)$$

$$k_i = \frac{2\pi}{L} m_i$$

it is convenient to let $\lambda = a^2$ be the path parameter. We compute $dS_P/d(a^2)$ as before, from the slope of $\log(N_n/N_{tot})$ vs. $a^2$, at fixed $k$ and $P_0$, and define lattice momentum as usual:

$$P_0 = 0.5$$

$$k_L^2 \equiv 4 \sum_{i=1}^{3} \sin^2\left(\frac{1}{2} k_i\right)$$
Then \[ \frac{1}{L^3 \frac{dS_P}{d(a^2)}} = -A k_L^2 + B \], and from runs at other values of \( P_0 \) we find that the constants \( A \) and \( B \) are independent of \( P_0 \). Then we have

\[
S_P[U_x(a)] = L^3 \{ -A a^2 k_L^2 + B a^2 + f(P_0) \}
\]

and from the data on the potential, the constant of integration \( f(P_0) = C P_0^2 \) is determined. Expressing \( a^2 k_L^2 \) in terms of Polyakov lines \( P_x \), we find

\[
S_P = 4A \sum_x \sum_{i=1}^{3} P_x P_{x+i} + \left[(B - 6A)a^2 + (C - 12A)P_0^2 \right] L^3
\]

with

\[
A = 7.3(2) \times 10^{-3} \quad B = 4.30(3) \times 10^{-2} \quad C = 8.61(4) \times 10^{-2}
\]

With these numbers, we find that \( B-6A \) and \( C-12A \) are consistent with zero, so finally

\[
S_P = \left\{ \begin{array}{ll}
0.0292(8) \sum_x \sum_{i=1}^{3} P_x P_{x+i} & \text{(relative weights method)} \\
0.0285 \sum_x \sum_{i=1}^{3} P_x P_{x+i} & \text{(strong-coupling expansion)}
\end{array} \right.
\]
Conventions: The potential term is **local**. The kinetic term **vanishes** for spatially constant configurations. Then

\[ V_P = \sum_{x} \mathcal{V}(U_x) \quad \text{and} \quad \mathcal{V}(U) = \frac{1}{L^3} S_P(U) \]

(By definition, \( K_P \equiv S_P[U_x] - V_P[U_x] \))

The point is that to compute the potential, we only have to compute the action for \( x \)-independent configurations \( U \). So as at strong coupling, we again choose the set

\[ U_x^{(n)} = (P_0 + a_n) \mathbb{I} + i \sqrt{1 - (P_0 + a_n)^2} \sigma_3 \]

\[ a_n = \left( n - \frac{1}{2} (M + 1) \right) \Delta a \quad , \quad n = 1, 2, \ldots, M \]

and compute \( dS_p/da \), but this time at \( \beta = 2.2 \), \( N_t = 4 \).
so we compute, as before

$$\frac{1}{L^3} \frac{dV_P}{dP_0} = \frac{1}{L^3} \frac{dS_P}{d\alpha}$$

and fit to a polynomial. A cubic polynomial $c_1 P_0 + c_2 P_0^2 + c_3 P_0^3$ works nicely...
But wait! **This violates center symmetry!** In SU(2), we must have $V(P) = V(-P)$, and therefore the derivative must be an odd function. This *seems* to be violated by the $c_2 P_0^2$ term. So let’s try only odd polynomial fits ($= \text{expansion of } V(P) \text{ in } j=\text{integer } \text{SU}(2) \text{ characters})$...

![Graph showing data points and fits]

Rather poor fits. A little like fitting a step function with a truncated Fourier series.
Could it be that \( V_p(P) \) is a non-analytic function? In other words

\[
\frac{1}{L^3} \frac{dV_P}{dP_0} = c_1 P_0 + c_2 \text{sign}(P_0) P_0^2 + c_3 P_0^3
\]

so that \( dV_p/dP \) is still an odd function. Look at the full range \(-1 \leq P_0 \leq 1\):

Here we plot the derivative at \( P_0 > 0 \), and also at \( P_0 < 0 \) multiplied by \(-1\). Since the data points for \( \pm P_0 \) fall on top of each other, \( dV_p/dP \) is an odd function, as it must be.
Integrating w.r.t. $P_0$, we find for the potential term of the effective Polyakov line action

$$V_P = \sum_x \left( \frac{1}{2} c_1 P_x^2 + \frac{1}{3} c_2 |P_x|^3 + \frac{1}{4} c_3 P_x^4 \right)$$

$c_1 = 4.61(2)$, $c_2 = -4.5(1)$, $c_3 = 1.77(8)$

which is center-symmetric but non-analytic. It is not the form expected from strong-coupling expansions.

One might have thought instead that an analytic expression such as

$$V_P = \sum_x \sum_{j=1}^{j_{max}} c_j \chi_j(U_x)$$

would be a good approximation, for relatively small $j_{max}$. That seems wrong.
Towards the kinetic term

To help determine the kinetic term we consider two different sets of configurations.

A. Plane Wave deformations around a constant background

\[ U^{(n)}_x = P^{(n)}_x \mathbb{1} + i \sqrt{1 - (P^{(n)}_x)^2 \sigma_3} \]
\[ P^{(n)}_x = P_0 + a_n \cos(k \cdot x) \]
\[ k_i = \frac{2\pi}{L} m_i \]

The \( a \)-dependence of \( S_P \) begins at \( O(a^2) \), so again we take \( \lambda = a^2 \), and compute

\[ \frac{1}{L^3} \left. \frac{dS_P}{d(a^2)} \right|_{a=0} \]

But unlike the case at strong couplings, this path derivative depends on \( P_0 \).
B. Pure plane waves \((P_0 = 0)\)

\[ U^{(n)}_x = P^{(n)}_x \mathbb{1} + i \sqrt{1 - (P^{(n)}_x)^2} \sigma_3 \]

\[ P^{(n)}_x = A_n \cos(\mathbf{k} \cdot \mathbf{x}) \]

\[ A_n = A_0 + \left( n - \frac{1}{2} (M + 1) \right) \Delta A , \quad n = 1, 2, ..., M \]

and this time we compute

\[ \frac{dS_P}{dA} \]

by the relative weights method.
It turns out that the action which fits the data, for configurations of Types A and B, is

\[
S_P = 2c \left\{ \sum_{xy} P_x \left( \sqrt{-\nabla^2_L + gP_{av}^2 + g'\Delta P^2} \right) P_y - \sum_x \sqrt{gP_{av}^2 + g'\Delta P^2 P_x^2} \right\} \\
+ \sum_x \left( \frac{1}{2} c_1 P_x^2 + \frac{1}{3} c_2 |P_x|^3 + \frac{1}{4} c_3 P_x^4 \right)
\]

where

\[
P_{av} = \frac{1}{L^3} \sum_x P_x \quad \text{and} \quad \Delta P^2 = \frac{1}{L^3} \sum_x (P_x - P_{av})^2
\]

It can be shown that the \( g' \Delta P^2 \) term doesn’t contribute to the \( dS_p/d(a^2) \) path derivative (from Type A), and of course \( g P_{av}^2 = 0 \) for type B configurations. So we use Type A to determine constants \( c \) and \( g' \), and then Type B to determine \( g' \).
Here is the data (red) and best fit (green) to
$$\frac{1}{L^3} \frac{dS_P}{d(a^2)} \bigg|_{a=0}$$
from the Type A configurations
here is the data (red) and best fit (green) to \[ \frac{dS_P}{dA} \]

from type B configurations, which determines \( g' = 3.45(4) \).
The relative weights method has been used to investigate the effective Polyakov line action corresponding to pure SU(2) gauge theory at $\beta = 2.2$ and $N_t = 4$. Denoting the action as a sum $S_p = K_p + V_p$ of a kinetic and a potential term:

- The potential term is found to be center symmetric, but non-analytic:

$$V_P = \sum_x \left( \frac{1}{2} c_1 P_x^2 + \frac{1}{3} c_2 |P_x|^3 + \frac{1}{4} c_3 P_x^4 \right)$$

- Based on plane wave data, the kinetic term is conjectured to be

$$K_P = 2c \left\{ \sum_{xy} P_x \left( \sqrt{-\nabla_L^2 + gP_{av}^2 + g'\Delta P^2} \right)_{xy} P_y \right. - \left. \sum_x \sqrt{gP_{av}^2 + g'\Delta P^2} P_x \right\}$$
Next Steps...

- Study the $\beta$-$T$ dependence of the various coefficients in $S_p$, in particular the evolution from strong to weaker couplings.
- See if the conjectured $K_p$ is valid for more complicated configurations.
- Move on to SU(3), matter fields, and, of course, the sign problem.
Extra Slides
We want to compare $V_p$ on a $12^3 \times 4$ lattice at $\beta = 2.2$ (confined phase) and at $\beta = 2.4$ (deconfined phase).

For this purpose it is useful to plot

$$\frac{1}{L^3} \frac{dV_P}{d(P_0^2)} = \frac{1}{L^3} \frac{1}{2P_0} \frac{dV_P}{dP_0} \quad \text{vs.} \quad P_0^2$$

When the data is plotted this way, a curious feature does show up...
Note the “dip” near $P_0=0$ in the deconfined phase. I have no idea about its significance.
$S^\mu_{QCD}$ is obtained from $S_{QCD}$ at $\mu=0$ by the replacement at timeslice $t=0$

$$S^\mu_{QCD} = S_{QCD} \left[ U_0(x,0) \rightarrow e^{N_t\mu} U_0(x,0), U_0^\dagger(x,0) \rightarrow e^{-N_t\mu} U_0^\dagger(x,0) \right]$$

According to the strong coupling/hopping parameter expansion, we obtain $S^\mu_P$ from $S_P$ by the same replacement:

$$U_x \rightarrow e^{N_t\mu} U_x \quad , \quad U_x^\dagger \rightarrow e^{-N_t\mu} U_x^\dagger$$

Another option: expand the domain of $U_0(x,0)$ from SU(N) to U(N), allowing these links to take on values

$$U_0(x,0) = \exp[i\theta] \times \text{SU}(N) \text{ matrices}.$$ 

If we can determine $S_P$ for these configurations, then we analytically continue

$$\theta \rightarrow -i N_t \mu$$

to get $S^\mu_P$. 

finite chemical potential
Now we add a matter field in the fundamental representation of the gauge group.

Keep it simple: a fixed-modulus scalar field, which can be mapped onto an SU(2)-valued field $\Phi$. The action is

$$S = \beta \sum_{plaq} \frac{1}{2} \text{Tr}[UUU^\dagger U^\dagger] + \gamma \sum_{x,\mu} \frac{1}{2} \text{Tr}[\phi^\dagger(x) U_\mu(x) \phi(x + \vec{\mu})]$$

Center symmetry is broken explicitly, and the model has only one phase in an infinite volume. There is, however, a line of 1st order transitions going into a line of sharp crossovers. At $\beta=2.2$, the crossover is around $\gamma = 0.84$. 

![Plaquette Energy](image)
Here is the data for $dV_P/dP_0$ at $\beta=2.2$, $\gamma=0.75$, $N_t=4$. ($<P_x> = 0.03$)

Best fit to the data yields (after integration wrt $P_0$)

$$V_P = \sum_{x} \left( c'_0 P_x + \frac{1}{2} c'_1 P_x^2 + \frac{1}{3} c'_2 |P_x|^3 + \frac{1}{4} c'_3 P_x^4 \right)$$

$c'_{0}=.025(1)$, $c'_{1} = 4.70(2)$, $c'_{2}=-4.70(8)$, $c'_{3}=1.91(7)$