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# Mean field theory of effective spin models as a baryon fugacity expansion

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The free energy of effective spin or ''Polyakov line'' models with a chemical potential, based on the U($N$) group, does not depend on the chemical potential. In a mean field-inspired expansion, we show how the condition of unit determinant, taking U($N$) to SU($N$), reintroduces the chemical potential, and allows us to express the free energy, as a function of mean field variational parameters, in terms of an expansion in the baryon (rather than the quark) fugacity at each lattice site. We solve the SU(3) mean field equations numerically to determine the phase diagram and compute observables. We also calculate the first corrections to the leading order mean field results, and find that these can significantly shift the endpoint of a line of first order transitions. The problem of deriving an effective spin model from full QCD is discussed.

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## I. INTRODUCTION

Polyakov line or ''effective spin'' models, with lattice actions of the form

$$S = \beta \sum_x \sum_{k=1}^{d} [\mathrm{Tr} U_x^\dagger \mathrm{Tr} U_{x+\hat{k}} + \mathrm{Tr} U_x \mathrm{Tr} U_{x+\hat{k}}^\dagger] + \kappa \sum_x [e^{\mu} \mathrm{Tr} U_x + e^{-\mu} \mathrm{Tr} U_x^\dagger], \quad (1)$$

are of interest as crude models of gauge theories in $D = d + 1$ dimensions at finite temperature and chemical potential [1]. Indeed, actions of this form can be extracted from QCD directly by integrating out most of the variables via a combined strong-coupling and hopping parameter expansion, while keeping the Polyakov line holonomies $U_x$ fixed, and therefore (1) is justified as an effective theory at least within the range of validity of these expansions.[1] At finite chemical potential $\mu$ the Polyakov line models have a sign problem, so that the usual Monte Carlo simulation is not directly applicable. There are, nonetheless, several different methods which can be used to solve this model. One of the earliest studies applied the complex Langevin equations to the SU(3) model [1–3]. A second method is the mean field approach, applied to the $\mu \neq 0$ case by Bilic *et al.* [2]. A third procedure, introduced in Ref. [4], is to convert the partition function to a ''flux'' representation, which, in the SU(3) case, has been simulated numerically by Mercado and Gattringer [5]. Finally, the model can also be solved, at least in some parameter range, by the reweighting technique [6].

In this article we will revisit the mean field strategy, because there are certain aspects of that approach which we find illuminating. It is generally believed that the free energy of effective spin models based on the U($N$) group do not depend on the chemical potential, and this is because one can shift the integration contour of a U(1) subgroup into the complex plane to absorb the factors of $e^{\pm\mu}$ (cf. Ref. [7]), providing no singularities are encountered. We first rederive this $\mu$-independence, in Sec. II, in the framework of a mean field-inspired expansion. We then go on to show, in Sec. III, how the restriction to a unit determinant, which converts U($N$) to SU($N$), not only reintroduces the chemical potential, but also converts the mean field formulation into an expansion in baryon fugacity. Numerical solutions of the mean field equations for the SU(3) case are presented in Sec. IV, and the phase diagram (projected to the $\beta$-$\mu$ plane) is obtained. We also display the effects of including the first correction to the mean field approximation. In Sec. V we present some comments on the problem of extracting the appropriate effective spin model from full QCD, in the range of gauge couplings and quark masses of interest. Our conclusions are in Sec. VI.

## II. U($N$) POLYAKOV LINE MODELS

We will begin with models in which the effective spin (or ''Polyakov line'') variable $U(x)$ is an element of the U($N$) group. As already noted, the chemical potential disappears from the free energy in this case, but the example will set the stage for the more interesting SU($N$) models.

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[1]Below we will refer to $\mu$ in Eq. (1) as the ''quark'' chemical potential, while keeping in mind the fact that, in the hopping parameter expansion, $\mu$ is actually related to the quark chemical potential of full QCD by a factor of inverse temperature.

Starting from the action (1), we mimic the mean field approach by first adding and subtracting constants $u$, $\nu$, which will eventually become variational parameters:

$$\begin{aligned} S &= \beta\sum_{x,k}[(\mathrm{Tr}U_x^\dagger - \nu + \nu)(\mathrm{Tr}U_{x+\hat{k}} - u + u) \\ &\quad + (\mathrm{Tr}U_x - u + u)(\mathrm{Tr}U_{x+\hat{k}}^\dagger - \nu + \nu)] \\ &\quad + \kappa\sum_x[e^{\mu}\mathrm{Tr}U_x + e^{-\mu}\mathrm{Tr}U_x^\dagger] \\ &= -2\beta dVu\nu + 2\beta d\nu\sum_x \mathrm{Tr}U_x + 2\beta du\sum_x \mathrm{Tr}U_x^\dagger \\ &\quad + \kappa\sum_x[e^{\mu}\mathrm{Tr}U_x + e^{-\mu}\mathrm{Tr}U_x^\dagger] + J. \end{aligned} \tag{2}$$

Here $V$ is the lattice volume, $d$ is its dimensionality, and

$$\begin{aligned} J = \beta\sum_{x,k}\{&(\mathrm{Tr}U_x^\dagger - \nu)(\mathrm{Tr}U_{x+\hat{k}} - u) \\ &+ (\mathrm{Tr}U_x - u)(\mathrm{Tr}U_{x+\hat{k}}^\dagger - \nu)\}. \end{aligned} \tag{3}$$

We then have

$$S = -2\beta dVu\nu + \sum_x[A_x\mathrm{Tr}U_x + B_x\mathrm{Tr}U_x^\dagger] + J, \tag{4}$$

where

$$\begin{aligned} A_x &= A \equiv 2\beta d\nu + \kappa e^{\mu} \quad \text{and} \\ B_x &= B \equiv 2\beta du + \kappa e^{-\mu}. \end{aligned} \tag{5}$$

Although $A_x$, $B_x$ are $x$-independent constants, it is useful below to regard them as variables. This allows us to differentiate with respect to each of them, with the understanding that all the $A_x$, $B_x$ are set to $A$ and $B$, respectively, after the differentiation.

Ordinary mean field theory amounts to dropping $J$ in the action and, in the absence of a chemical potential, setting, $u = \nu = m$, where $m$ is the mean field. One then varies $m$ to minimize the free energy. In our case, define

$$\begin{aligned} Z_{mf} &= e^{-F_{mf}} \\ &= e^{-2\beta dVu\nu}\prod_x\int dU_x \exp[A_x\mathrm{Tr}U_x + B_x\mathrm{Tr}U_x^\dagger], \end{aligned} \tag{6}$$

and

$$\frac{Z}{Z_{mf}} = e^{-\Delta F} = \frac{\int DU e^J \exp[\sum_x(A_x\mathrm{Tr}U_x + B_x\mathrm{Tr}U_x^\dagger)]}{\int DU\exp[\sum_x(A_x\mathrm{Tr}U_x + B_x\mathrm{Tr}U_x^\dagger)]}. \tag{7}$$

Also defining the operator

$$\begin{aligned} \tilde{J}\Big[u,\nu,\frac{\partial}{\partial A},\frac{\partial}{\partial B}\Big] \equiv \beta\sum_{x,k}\Big\{&\Big(\frac{\partial}{\partial B_x} - \nu\Big)\Big(\frac{\partial}{\partial A_{x+\hat{k}}} - u\Big) \\ &+ \Big(\frac{\partial}{\partial A_x} - u\Big)\Big(\frac{\partial}{\partial B_{x+\hat{k}}} - \nu\Big)\Big\}, \end{aligned} \tag{8}$$

we have

$$\begin{aligned} &\exp[-\Delta F] \\ &= \Big(\frac{e^{\tilde{J}[u,\nu,\frac{\partial}{\partial A},\frac{\partial}{\partial B}]}\int DU\exp[\sum_x(A_x\mathrm{Tr}U_x + B_x\mathrm{Tr}U_x^\dagger)]}{\int DU\exp[\sum_x(A_x\mathrm{Tr}U_x + B_x\mathrm{Tr}U_x^\dagger)]}\Big)_{|_{A_x=A,B_x=B}}. \end{aligned} \tag{9}$$

Next we need to evaluate the U($N$) integral

$$I = \int dU\exp[A\mathrm{Tr}U + B\mathrm{Tr}U^\dagger], \tag{10}$$

which, by standard methods (cf. Ref. [8]), becomes an angular integration[2]

$$\begin{aligned} I &= \int\prod_{n=1}^N\frac{d\phi_n}{2\pi}\frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}e^{i(j_1-i_1)\phi_1}\ldots e^{i(j_N-i_N)\phi_N} \\ &\quad\times\exp\Big[A\sum_{m=1}^N e^{i\phi_m} + B\sum_{m=1}^N e^{-i\phi_m}\Big] \\ &= \frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\prod_{n=1}^N\int\frac{d\phi_n}{2\pi}e^{i(j_n-i_n)\phi_n} \\ &\quad\times\exp[Ae^{i\phi_n} + Be^{-i\phi_n}] \\ &= \frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\prod_{n=1}^N\Big(\frac{\partial}{\partial A}\Big)^{j_n}\Big(\frac{\partial}{\partial B}\Big)^{i_n} \\ &\quad\times\int\frac{d\phi_n}{2\pi}\exp[Ae^{i\phi_n} + Be^{-i\phi_n}] \\ &= \frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\prod_{n=1}^N\Big(\frac{\partial}{\partial A}\Big)^{j_n}\Big(\frac{\partial}{\partial B}\Big)^{i_n}I_0[2\sqrt{AB}]. \end{aligned} \tag{11}$$

This gives us

$$\begin{aligned} Z_{mf} &= e^{-2\beta dVu\nu}\prod_x\frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\prod_{n=1}^N\Big(\frac{\partial}{\partial A_x}\Big)^{j_n} \\ &\quad\times\Big(\frac{\partial}{\partial B_x}\Big)^{i_n}I_0[2\sqrt{A_xB_x}]. \end{aligned} \tag{12}$$

[2]The solution for $I$ in the general case where $A$, $B$ are matrix-valued and located inside the trace is given in Ref. [9], and the answer involves Vandermonde determinants of the eigenvalues of $AB$. The SU($N$) case was presented in Ref. [10], but only for $B = A^\dagger$. For the later extension to SU($N$) with $A$ and $B$ arbitrary scalar constants, it is convenient for us to work out the scalar constant case explicitly here.

We now introduce rescaled variables

$$\begin{aligned} u &= e^{-\mu}u' \quad \text{and} \quad \nu = e^{\mu}\nu' \\ A_x &= (2\beta d\nu' + \kappa)e^{\mu} = A'_x e^{\mu} \\ B_x &= (2\beta d u' + \kappa)e^{-\mu} = B'_x e^{-\mu} \\ \frac{\partial}{\partial A_x} &= e^{-\mu}\frac{\partial}{\partial A'_x} \\ \frac{\partial}{\partial B_x} &= e^{\mu}\frac{\partial}{\partial B'_x}. \end{aligned} \tag{13}$$

Then $Z_{mf}$ becomes

$$\begin{aligned} Z_{mf} &= e^{-2\beta dVu'\nu'}\prod_x \frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\prod_{n=1}^{N} e^{(i_n-j_n)\mu}\left(\frac{\partial}{\partial A'_x}\right)^{j_n} \\ &\quad\times\left(\frac{\partial}{\partial B'_x}\right)^{i_n} I_0\left[2\sqrt{A'_x B'_x}\right] \\ &= e^{-2\beta dVu'\nu'}\prod_x \frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N} \\ &\quad\times\exp\left[\left(\sum_{m=1}^{N} i_m - \sum_{m=1}^{N} j_m\right)\mu\right] \\ &\quad\times\prod_{n=1}^{N}\left(\frac{\partial}{\partial A'_x}\right)^{j_n}\left(\frac{\partial}{\partial B'_x}\right)^{i_n} I_0\left[2\sqrt{A'_x B'_x}\right]. \end{aligned} \tag{14}$$

At this point we note that, because of the $\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\phi$ term,

$$\sum_{m=1}^{N} i_m = \sum_{m=1}^{N} j_m. \tag{15}$$

Therefore

$$\begin{aligned} Z_{mf} &= e^{-2\beta dVu'\nu'}\prod_x \frac{1}{N!}\varepsilon_{i_1\ldots i_N j_1\ldots j_N}\prod_{n=1}^{N}\left(\frac{\partial}{\partial A'_x}\right)^{j_n} \\ &\quad\times\left(\frac{\partial}{\partial B'_x}\right)^{i_n} I_0\left[2\sqrt{A'_x B'_x}\right] \\ &= e^{-2\beta dVu'\nu'}\prod_x \det\left[\left(\frac{\partial}{\partial B'_x}\right)^{i}\left(\frac{\partial}{\partial A'_x}\right)^{j} I_0\left[2\sqrt{A'_x B'_x}\right]\right]. \end{aligned} \tag{16}$$

As a function of the rescaled variational parameters $u'$, $\nu'$, $Z_{mf}$ is clearly $\mu$-independent, and of course it will remain $\mu$-independent when $F_{mf}$ is minimized with respect to $u'$, $\nu'$. Likewise, all $\mu$ dependence cancels in the $\tilde{J}$ operator

$$\begin{aligned} \tilde{J}\left[u,\nu,\frac{\partial}{\partial A},\frac{\partial}{\partial B}\right] &= \beta\sum_{x,k}\left\{\left(\frac{\partial}{\partial B_x}-\nu\right)\left(\frac{\partial}{\partial A_{x+\hat{k}}}-u\right)\right. \\ &\quad\left.+\left(\frac{\partial}{\partial A_x}-u\right)\left(\frac{\partial}{\partial B_{x+\hat{k}}}-\nu\right)\right\} \\ &= \beta\sum_{x,k}\left\{\left(\frac{\partial}{\partial B'_x}-\nu'\right)\left(\frac{\partial}{\partial A'_{x+\hat{k}}}-u'\right)\right. \\ &\quad\left.+\left(\frac{\partial}{\partial A'_x}-u'\right)\left(\frac{\partial}{\partial B'_{x+\hat{k}}}-\nu'\right)\right\}. \end{aligned} \tag{17}$$

From this we can conclude that both $F_{mf}$ and $\Delta F$, and therefore the free energy $F = F_{mf} + \Delta F$ itself, are independent of the chemical potential $\mu$ in Polyakov line models based on the group U($N$).[3]

Before proceeding to SU($N$), we note that the expression for $Z_{mf}$ can be simplified a little further, using the identity

$$\frac{\partial}{\partial A}\frac{\partial}{\partial B} I_0[2\sqrt{AB}] = I_0[2\sqrt{AB}], \tag{18}$$

which is evident from the fact that

$$I_0[2\sqrt{AB}] = \int\frac{d\phi}{2\pi} e^{Ae^{i\phi}+Be^{-i\phi}}. \tag{19}$$

Then, defining the derivative operator

$$D_{ij}(x) = \begin{cases} \left(\frac{\partial}{\partial B'_x}\right)^{i-j} & i \geq j \\ \left(\frac{\partial}{\partial A'_x}\right)^{j-i} & i < j \end{cases}, \tag{20}$$

we may write

$$Z_{mf} = e^{-2\beta dVu'\nu'}\prod_x \det\left[D_{ij}(x) I_0\left[2\sqrt{A'_x B'_x}\right]\right], \tag{21}$$

and

$$e^{-\Delta F} = \left(\frac{1}{Z_{mf}} e^{\tilde{J}[u',\nu',\frac{\partial}{\partial A'},\frac{\partial}{\partial B'}]} Z_{mf}\right)_{|_{A'_x=A',B'_x=B'}}. \tag{22}$$

Again, the $\mu$-independence of the free energy is manifest.[4]

## III. SU($N$) POLYAKOV LINE MODELS

We can convert the U($N$) models considered above to SU($N$) models by simply converting the U($N$) group integration in Eq. (11) to an SU($N$) integration. To accomplish this (cf. Ref. [10]) we have only to insert a periodic delta function into the angular integrations, which imposes the constraint that $\sum_n \phi_n = 0 \bmod 2\pi$. We use the identity

$$\delta_p\left(\sum_{n=1}^{N}\phi_n\right) = \frac{1}{2\pi}\sum_{s=-\infty}^{\infty}\exp\left[is\sum_{n=1}^{N}\phi_n\right]. \tag{23}$$

This introduces into each $\phi_n$ integration an additional factor of $\exp[is\phi_n]$. Tracing through the steps of the previous section, we arrive at

[3] A slight subtlety is that at $\kappa = 0$, the free energy depends not on $u'$, $\nu'$ separately, but only on the product $u'\nu' = u\nu$. Then one must appeal to the hermiticity of the action to set $u = \nu$. For any nonzero $\kappa$ and $\mu$, however, there is no such degeneracy.

[4] This $\mu$-independence was also demonstrated in the $N = \infty$ limit in Ref. [11].

$$Z_{mf} = e^{-2\beta dVu\nu}\prod_x \frac{1}{2\pi}\sum_{s=-\infty}^{\infty}\frac{1}{N!}\varepsilon_{i_1\ldots i_N}\varepsilon_{j_1\ldots j_N}\prod_{n=1}^{N}\left(\frac{\partial}{\partial A_x}\right)^{j_n} \times\left(\frac{\partial}{\partial B_x}\right)^{i_n}\begin{cases}(s\geq 0) & \left(\frac{\partial}{\partial A_x}\right)^{s}\\ (s<0) & \left(\frac{\partial}{\partial B_x}\right)^{|s|}\end{cases} I_0[2\sqrt{A_xB_x}]. \tag{24}$$

Now expressing everything in terms of the rescaled variables of Eq. (13), this becomes

$$Z_{mf} = e^{-2\beta dVu'\nu'}\prod_x \frac{1}{N!}\epsilon_{i_1\ldots i_N}\epsilon_{j_1\ldots j_N}\frac{1}{2\pi} \times\left\{\sum_{s\geq 0}e^{-sN\mu}\prod_{n=1}^{N}\left(\frac{\partial}{\partial A'_x}\right)^{s+j_n}\left(\frac{\partial}{\partial B'_x}\right)^{i_n} + \sum_{s<0}e^{|s|N\mu}\prod_{n=1}^{N}\left(\frac{\partial}{\partial A'_x}\right)^{j_n}\left(\frac{\partial}{\partial B'_x}\right)^{i_n+|s|}\right\} I_0\left[2\sqrt{A'_xB'_x}\right]. \tag{25}$$

Defining

$$D^s_{ij}(x) \equiv \begin{cases} D_{i,j+s}(x) & s\geq 0\\ D_{i+|s|,j}(x) & s<0\end{cases}, \tag{26}$$

we can express $Z_{mf}$ compactly in the form

$$Z_{mf} = e^{-2\beta dVu'\nu'}(2\pi)^{-V}\prod_x\sum_{s=-\infty}^{\infty}e^{sN\mu}\det\left[D^{-s}_{ij}I_0\left[2\sqrt{A'_xB'_x}\right]\right], \tag{27}$$

where we have also changed variables $s\rightarrow -s$ in the sum. As before

$$e^{-\Delta F} = \left(\frac{1}{Z_{mf}}e^{\tilde{J}[u',\nu',\frac{\partial}{\partial A'},\frac{\partial}{\partial B'}]}Z_{mf}\right)_{|_{A'_x=A',B'_x=B'}}. \tag{28}$$

This gives a formal expression for the full free energy, $F(\mu) = F_{mf}(\mu) + \Delta F(\mu)$ in terms of the variational parameters $u'$, $\nu'$, which should be chosen to minimize $F(\mu)$.

The mean field expression for the free energy $F_{mf}$, as a function of the variational parameters $u'$, $\nu'$ (or equivalently $A'$, $B'$) has some features which are worth noting. In the first place, the mean field partition function $Z_{mf}$ has now been expressed in terms of a product, at each site, of a fugacity expansion of the form

$$\sum_{s=-\infty}^{\infty}e^{sN\mu}\det[D^{-s}_{ij}I_0[2\sqrt{A'B'}]]. \tag{29}$$

Here we see that the quark chemical potential $\mu$ only occurs in the combination $N\mu$, which is, in effect, the baryon chemical potential. So in fact we have an expansion in the baryon, rather than quark, fugacity. In Ref. [12] the determinant in an expansion of this sort is referred as the "canonical determinant." The second point is that parameter $s$, originally introduced in the representation (23) of the periodic delta function, has now emerged as the baryon number (which, if negative, is the number of antibaryons) per site.

Of course, one still has to minimize the free energy with respect to the variational parameters, and this will introduce some $N\mu$-dependence into the canonical determinants. Strictly speaking, it is the mean field expression of the partition function as a function of (freely varying) parameters $u'$, $\nu'$ which has the form of a fugacity expansion.

Successive improvements to the leading mean field result would be obtained by expanding the operator $\exp[\tilde{J}]$ in a Taylor series. In the case that $\kappa = 0$, and $\beta$ is so small that the minimum free energy is obtained at $u' = \nu' = 0$, then the Taylor series simply generates the strong-coupling expansion. At larger $\beta$ and $\kappa$, the series also generates corrections to the leading mean-field result. We will compute the effect of the leading correction in the next section.

At this point, we should draw attention to the similarities and differences between our approach and the much earlier work of Bilic *et al.* [2]. The starting point of the mean field treatment in Ref. [2] was the action (4) without the $J$-term. The SU(3) group integral was expanded as a power series in $A$, $B$, and for this reason it was not obvious that the partition function is an expansion in baryon fugacity, arising from the unit determinant condition. In the next section we determine the phase diagram (for both real and imaginary $\mu$), which was not displayed in Ref. [2], and work out leading corrections to the mean field result.

## IV. NUMERICAL RESULTS FOR THE SU(3) POLYAKOV LINE MODEL

We will now specialize to SU(3). From Eq. (27), we see that the mean field free energy per lattice site at $N = 3$ is

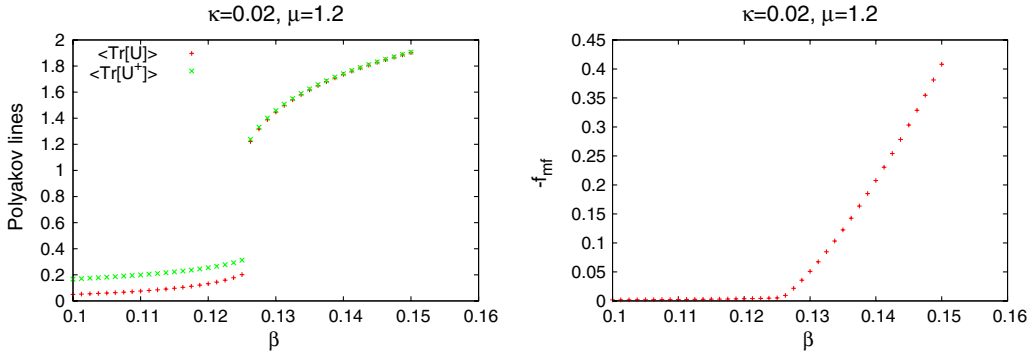
$$f_{mf} = 2\beta du'\nu' - \log\left[\sum_{s=-\infty}^{\infty}e^{3s\mu}\det[D^{-s}_{ij}I_0[2\sqrt{A'B'}]]\right], \tag{30}$$

where we have dropped an irrelevant constant. In numerical work we cannot sum $s$ over the full range $[-\infty,\infty]$, so it is necessary to cut off the sum at some maximum baryon/antibaryon number $s_{\max}$ per site

$$f_{mf} \approx 2\beta du'\nu' - \log[G(A',B')],$$
$$G(A',B') \equiv \sum_{s=-s_{\max}}^{s_{\max}}e^{3s\mu}\det[D^{-s}_{ij}I_0[2\sqrt{A'B'}]], \tag{31}$$

and of course it is important, when computing observables, to check sensitivity to the cutoff. We will return to this issue below.

Minimizing the free energy with respect to the variational parameters $u'$, $\nu'$, or, equivalently, with respect to $A' = 2\beta d\nu' + \kappa$, $B' = 2\beta du' + \kappa$, leads to two equations




(a) Polyakov lines vs. $\beta$. (b) - free energy/site vs. $\beta$.

FIG. 1 (color online). Observables vs $\beta$ at fixed $\kappa = 0.02$ and $\mu = 1.2$, evaluated at mean field level for SU(3).

$$\frac{B' - \kappa}{2\beta d} - \frac{1}{G(A', B')}\frac{\partial G}{\partial A'} = 0$$
$$\frac{A' - \kappa}{2\beta d} - \frac{1}{G(A', B')}\frac{\partial G}{\partial B'} = 0, \tag{32}$$

whose roots may be determined numerically.[5] At the minimum, we can regard $A' = A'(\beta, \kappa, \mu)$ and $B' = B'(\beta, \kappa, \mu)$ as functions of the parameters of the theory.

Apart from the free energy itself, the observables of interest are $\mathrm{Tr}[U]$, $\mathrm{Tr}[U^\dagger]$, and the baryon number density $n$ (baryon number per lattice site). The latter is given by

$$\langle n\rangle = -\frac{\partial f_{mf}}{\partial(3\mu)}$$
$$= \frac{1}{G(A', B')}\sum_{s=-s_{\max}}^{s_{\max}} s e^{3s\mu}\det[D_{ij}^{-s} I_0[2\sqrt{A'B'}]]$$
$$-\frac{1}{3}\left(\frac{\partial A'(\beta,\kappa,\mu)}{\partial\mu}\frac{\partial}{\partial A'} + \frac{\partial B'(\beta,\kappa,\mu)}{\partial\mu}\frac{\partial}{\partial B'}\right) f_{mf}(A', B'), \tag{33}$$

where it is understood that the derivative is taken at the point where $f_{mf}(A', B')$ is minimized. But at this point, the first derivatives of $f_{mf}$ with respect to $A'$ and $B'$ vanish. Therefore

$$\langle n\rangle = \frac{1}{G(A', B')}\sum_{s=-s_{\max}}^{s_{\max}} s e^{3s\mu}\det[D_{ij}^{-s} I_0[2\sqrt{A'B'}]]. \tag{34}$$

[5]Note that these are real-valued equations with real-valued roots, despite the complex character of the action (1). Ultimately this is due to the fact, which one can easily show using the reality of the Haar measure and the property $DU = DU^\dagger$, that $\langle \mathrm{Tr}U\rangle$, $\langle \mathrm{Tr}U^\dagger\rangle$ and $F$ are all real-valued quantities.

From (6) we see that

$$\langle \mathrm{Tr}U\rangle = \frac{1}{V}\sum_x \frac{\partial}{\partial A_x}\log Z_{mf} = \frac{\partial}{\partial A}\log G(A', B')$$
$$= e^{-\mu}\frac{\partial}{\partial A'}\log G(A', B'). \tag{35}$$

At the minimum of the free energy, determined by the roots of (32), this simply becomes

$$\langle \mathrm{Tr}U\rangle \equiv \frac{1}{V}\sum_x \langle \mathrm{Tr}U_x\rangle = e^{-\mu}u' = u, \tag{36}$$

and likewise

$$\langle \mathrm{Tr}U^\dagger\rangle \equiv \frac{1}{V}\sum_x \langle \mathrm{Tr}U_x^\dagger\rangle = e^{\mu}v' = v. \tag{37}$$

This is, of course, reminiscent of the standard mean field approach to a spin system, in which the variational parameter becomes the average spin. It must be understood, however, that due to the complex weight there is no constraint that the "average" values of $\mathrm{Tr}U$ and $\mathrm{Tr}U^\dagger$ are necessarily bounded by $\mathrm{Tr}\mathbb{1}$.

We now have all the tools needed to evaluate observables and map out the phase diagram. Figure 1 shows a typical result for $\langle \mathrm{Tr}U\rangle$, $\langle \mathrm{Tr}U^\dagger\rangle$ and the mean field free energy per site $f_{mf}$, as a function of $\beta$, at fixed $\kappa = 0.02$ and chemical potential $\mu = 1.2$. There is a clear first order phase transition at $\beta = 0.1257$. As the chemical potential is increased at fixed $\kappa = 0.2$, the discontinuity at the transition decreases, until it disappears altogether at $\mu = 1.67$. At larger $\mu$, there is only a crossover.

Repeating this procedure, we can map out the region of first order transitions in the $\beta$, $\mu$, $\kappa$ parameter space. In Fig. 2 we show sample first-order phase transition lines in the $\beta$-$\mu$ plane at $\kappa = 0, 0.02, 0.03, 0.04, 0.05, 0.059$. At $\kappa = 0$ the transition, at $\beta = 0.1339$, is of course independent of $\mu$. At fixed, finite $\kappa$ the transition line terminates at some value of $\mu$, and this termination point happens at smaller and smaller values of $\mu$ as $\kappa$ increases. The transition line

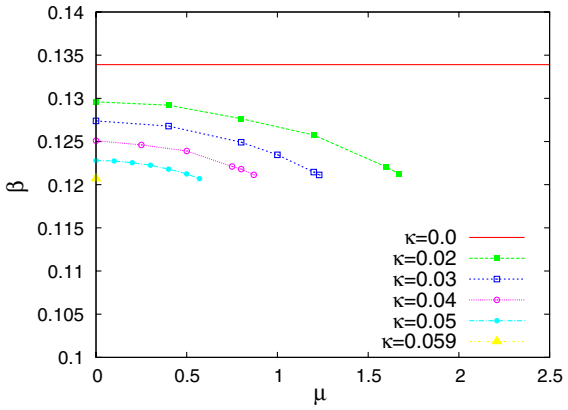



FIG. 2 (color online). Phase diagram of the Polyakov line model (1) for the SU(3) group, obtained via mean field methods, in the $\beta$-$\mu$ plane at several values of $\kappa$. The lines indicate first order transitions. Beyond $\kappa = 0.059$, there are no transitions at any value of $\mu$.

shrinks to a point at $\mu = 0$ for $\kappa = 0.059$, and beyond this value of $\kappa$ there are no further transitions.

We can also solve the mean field equations for imaginary $\mu$. The results for several values of $\kappa$ are shown in Fig. 3. The continuity of first order transition lines, as $\mu$ varies from real to imaginary values, as well as the weakening of the transition at larger values of $\kappa$, ties in with the considerations of Ref. [13].

Figure 2 can be compared directly to the phase diagram recently obtained by Mercado and Gattringer [5] via a Monte Carlo simulation in the flux representation. The two diagrams are qualitatively, and even quantitatively, very similar. The main difference is that we only show first order transition points, and most of these are found in Ref. [5] to be crossover points, rather than first order transitions. According to Mercado and Gattringer [5], the

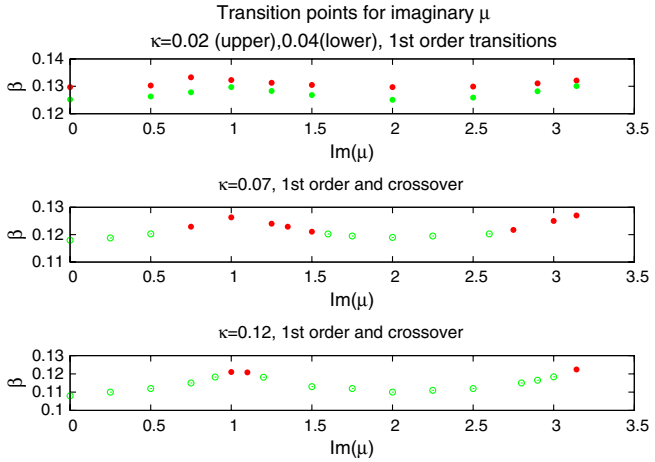



FIG. 3 (color online). Some transition points for Polyakov line models in the $\beta - \mathrm{Im}(\mu)$ plane, for imaginary values of the chemical potential, at several values of $\kappa$. Filled circles indicate first order transition points, open circles indicate a crossover.

endpoint of a line of first order transitions, at a given $\kappa$, occurs at a much smaller value of $\mu$ than we find in our mean field calculations. So an interesting question is whether inclusion of higher order corrections, beyond the leading order mean field result, would bring our endpoints to smaller values of $\mu$, in closer agreement with Ref. [5]. We will turn to this question in subsection IV B below.

### A. Effect of the baryon number cutoff

The data displayed above was obtained using a cutoff $s_{\max} = 4$ in the sum over baryon number, but the results shown are quite insensitive to increasing the cutoff to $s_{\max} = 6$, and even to decreasing the limit to $s_{\max} = 2$. The reason for this insensitivity is that the phase transitions occur at values of the baryon number density which are very small compared to the cutoff. Only when the chemical potential is raised to values such that the number density becomes comparable to $s_{\max}$ does the cutoff dependence become apparent. To illustrate this dependence, we fix $\beta = 0.1257$ and $\kappa = 0.02$ (where we have found a transition at $\mu = 1.2$), and compute the Polyakov lines and number density over a wider range of $\mu$.

The results, for $\mu \leq 10$ and $s_{\max} = 2, 4$, are shown in Fig. 4. We see that $\langle \mathrm{Tr}U \rangle$ and $\langle \mathrm{Tr}U^\dagger \rangle$ are comparable to one another and of $O(1)$ until $\langle n \rangle$ approaches the cutoff in $s$. Beyond that point, $\langle \mathrm{Tr}U \rangle$ falls exponentially as $e^{-\mu}$, and $\langle \mathrm{Tr}U^\dagger \rangle$ diverges as $e^{\mu}$, exactly as in the U($N$) theory, and the results are no longer valid for the SU($N$) case. When $\langle n \rangle$ saturates the cutoff then, in order to probe a larger range of $\mu$, it is necessary to increase $s_{\max}$. For the purpose of determining the phase diagram, however, $s_{\max} = 4$, which can be interpreted as a limit of no more than four baryons per lattice site, appears to be more than sufficient.[6]

### B. The leading correction to the mean field free energy

Going back to Eq. (7), we have

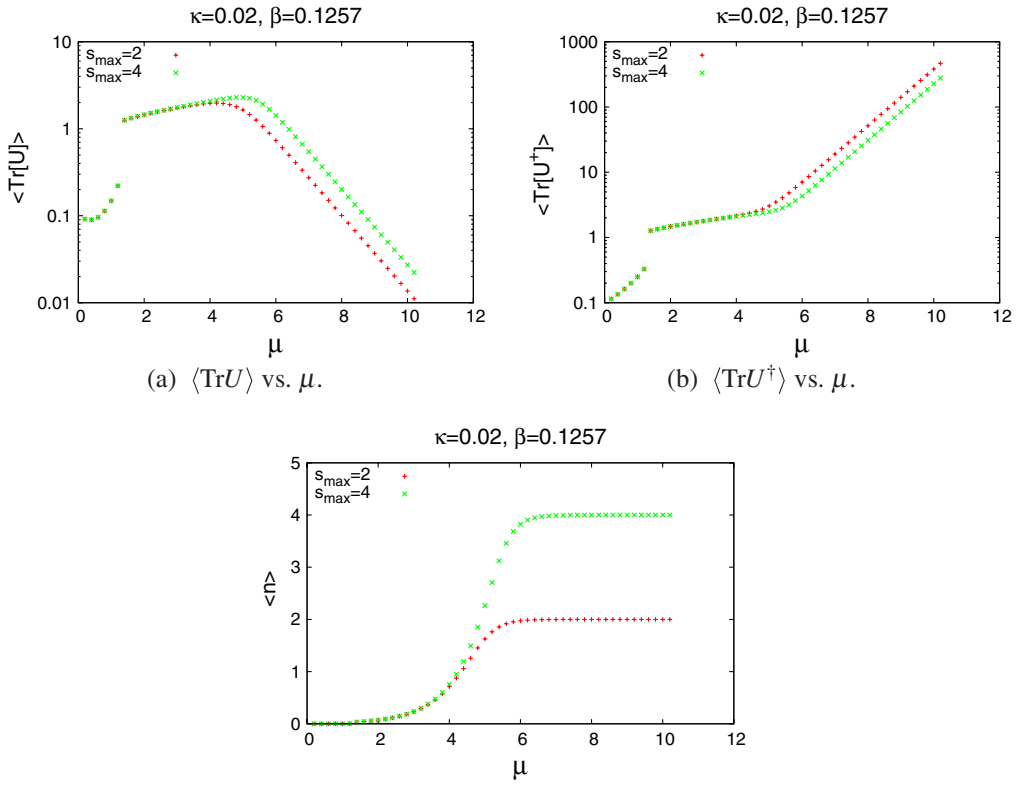
$$e^{-\Delta F} = \langle e^J \rangle_{mf} = \left\langle \prod_{x,k} e^{J_{x,k}} \right\rangle_{mf}. \tag{38}$$

The product is over all links, where

$$J_{x,k} = \beta\{(\mathrm{Tr}U_x^\dagger - \nu)(\mathrm{Tr}U_{x+\hat{k}} - u) + (\mathrm{Tr}U_x - u)(\mathrm{Tr}U_{x+\hat{k}}^\dagger - \nu)\}, \tag{39}$$

and the $\langle\rangle_{mf}$ notation denotes the expectation value with respect to the mean field action, as in (7). The expansion of $\exp[J]$ generates products of terms such as $J_{l_1} J_{l_2} \ldots J_{l_n}$, where the $l_i$ denote links, some of which may be the same.

[6]It should be emphasized that saturation of the $s_{\max}$ cutoff has nothing to do with the Pauli principle, and corresponding limit on baryons per site. That limit is not really seen in the simple effective spin model discussed here.




(a) $\langle \mathrm{Tr}U \rangle$ vs. $\mu$. (b) $\langle \mathrm{Tr}U^\dagger \rangle$ vs. $\mu$.

(c) number density vs. $\mu$.

FIG. 4 (color online). Observables $\langle \mathrm{Tr}U \rangle$, $\langle \mathrm{Tr}U^\dagger \rangle$ and $\langle n \rangle$ vs $\mu$ at fixed $\kappa = 0.02$ and $\beta = 0.1257$, for two values of the cutoff $s_{\max}$. Note that these observables are independent of the baryon/site cutoff $s_{\max}$, until a little beyond $\mu = 4$, which is well past the value of $\mu$ at the first order transition.

Because $\langle \mathrm{Tr}[U] \rangle_{mf} = u$ and $\langle \mathrm{Tr}[U^\dagger] \rangle_{mf} = \nu$, it is clear that the expectation values of such products are only nonzero if each endpoint of a link $l_i$ appearing in the product is also an endpoint of at least one other link appearing in the product. The simplest product whose expectation value is nonvanishing, containing the minimum number of $J$ factors, is simply the product of $J_l J_l$ on the same link. Therefore, to leading order, we approximate

$$e^{-\Delta F} = \left\langle \prod_{x,k} e^{J_{x,k}} \right\rangle_{mf} \approx \prod_{x,k} \langle e^{J_{x,k}} \rangle_{mf} \approx \prod_{x,k} \left( 1 + \frac{1}{2} \langle J_{x,k}^2 \rangle_{mf} \right). \tag{40}$$

Now

$$\begin{aligned} \langle J_{x,k}^2 \rangle_{mf} &= \beta^2 \langle (\mathrm{Tr}U_x^\dagger - \nu)^2 (\mathrm{Tr}U_{x+\hat{k}} - u)^2 + (\mathrm{Tr}U_x^\dagger - \nu)(\mathrm{Tr}U_x - u)(\mathrm{Tr}U_{x+\hat{k}} - u)(\mathrm{Tr}U_{x+\hat{k}}^\dagger - \nu) + \mathrm{H.c.} \rangle_{mf} \\ &= 2\beta^2 [(\langle \mathrm{Tr}U \mathrm{Tr}U \rangle_{mf} - u^2)(\langle \mathrm{Tr}U^\dagger \mathrm{Tr}U^\dagger \rangle_{mf} - \nu^2) + (\langle \mathrm{Tr}U \mathrm{Tr}U^\dagger \rangle_{mf} - u\nu)^2] \\ &= 2\beta^2 [(\langle (e^\mu \mathrm{Tr}U)^2 \rangle_{mf} - u'^2)(\langle (e^{-\mu} \mathrm{Tr}U^\dagger)^2 \rangle_{mf} - \nu'^2) + (\langle (e^\mu \mathrm{Tr}U)(e^{-\mu} \mathrm{Tr}U^\dagger) \rangle_{mf} - u'\nu')^2], \end{aligned} \tag{41}$$

and we use

$$\langle (e^\mu \mathrm{Tr}U)^m (e^{-\mu} \mathrm{Tr}U^\dagger)^n \rangle_{mf} = \frac{1}{G(A', B')} \left( \frac{\partial}{\partial A'} \right)^m \left( \frac{\partial}{\partial B'} \right)^n G(A', B'). \tag{42}$$

Putting all the pieces together, the free energy per unit volume is

$$f(A', B') = 2\beta du\nu - \tilde{f}(A', B'), \tag{43}$$

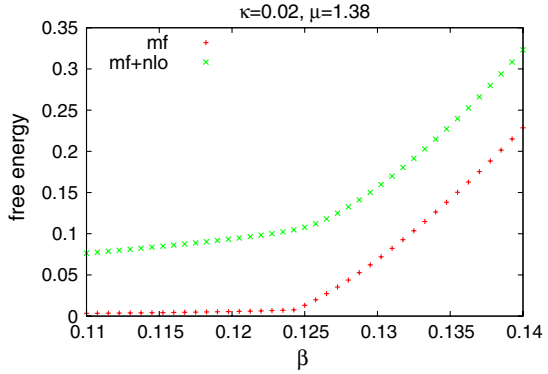



FIG. 5 (color online). $-F$ in lowest order mean field theory, and in mean field + next leading order. Inclusion of the next leading order can change a first-order transition to a crossover, as seen clearly in Fig. 6.

where

$$\tilde{f} = \log G(A', B') + d\log\Big[1 + \beta^2\Big\{\Big(\frac{1}{G}\frac{\partial^2 G}{\partial A'^2} - u'^2\Big)\Big(\frac{1}{G}\frac{\partial^2 G}{\partial B'^2} - \nu'^2\Big) + \Big(\frac{1}{G}\frac{\partial^2 G}{\partial A'\partial B'} - u'\nu'\Big)^2\Big\}\Big], \tag{44}$$

and $G(A', B')$ is as defined in (31). Note that the terms inside the logarithm, which correct the leading mean field expression, depend on fluctuations around the mean field values.

The variational parameters $A'$, $B'$ are again derived by minimizing $f(A', B')$, which implies

$$\frac{B' - \kappa}{2\beta d} - \frac{\partial}{\partial A'}\tilde{f} = 0, \qquad \frac{A' - \kappa}{2\beta d} - \frac{\partial}{\partial B'}\tilde{f} = 0, \tag{45}$$

whose roots may again be determined numerically. It is also still true that $u = \langle \mathrm{Tr} U\rangle$, $\nu = \langle \mathrm{Tr} U^\dagger\rangle$, which can be seen as follows: Define

$$\tilde{Z} \equiv e^{V\tilde{f}} = \int DU e^J \exp[\sum_x (A\mathrm{Tr}U_x + B\mathrm{Tr}U_x^\dagger)]. \tag{46}$$

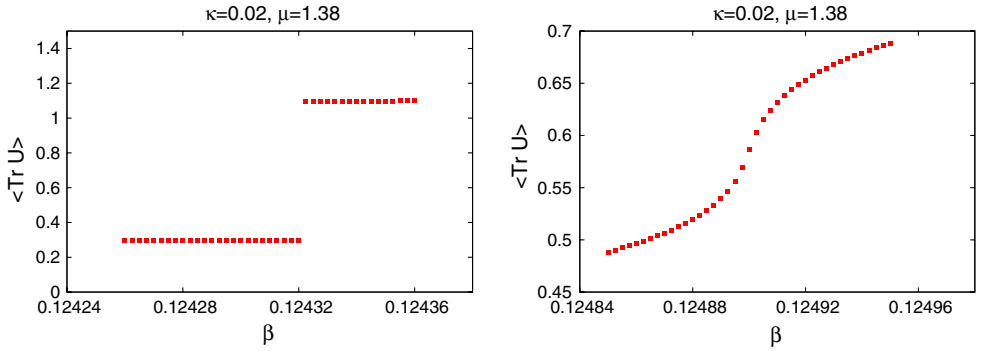
Then it is clear that

$$\langle \mathrm{Tr} U\rangle = \frac{1}{V}\frac{\partial}{\partial A}\log\tilde{Z} = \frac{\partial}{\partial A}\tilde{f}. \tag{47}$$

Applying the first of Eqs. (45), and the definitions (13), we arrive at $u = \langle \mathrm{Tr} U\rangle$. In the same way, we can show that $\nu = \langle \mathrm{Tr} U^\dagger\rangle$. Thus the correspondence between the variational parameters $u$, $\nu$ and the observables $\langle \mathrm{Tr} U\rangle$, $\langle \mathrm{Tr} U^\dagger\rangle$ is maintained exactly, in fact to all orders beyond the leading mean field expressions.

We can now study how inclusion of the leading correction will modify the phase diagram shown in Fig. 2. It turns out that the location of the phase transition points changes very little. Generally, at fixed $\kappa$, $\mu$, the value of $\beta$ at the transition changes by less than one percent. What does change significantly are the endpoints of the first-order transition lines. For example, at $\kappa = 0.02$, the endpoint of the transition line was at $\mu = 1.67$, $\beta = 0.1213$. Inclusion of the first correction brings the endpoint down to $\mu = 1.38$, $\beta = 0.1249$. The free energy at lowest order (mf), and the free energy after inclusion of the first correction (mf + nlo) is shown in Fig. 5. The free energy changes substantially, but the transition point hardly at all (from $\beta = 0.1243$ to $\beta = 0.1249$). However, at $\mu = 1.38$, the order of the transition changes, from first order in the leading mean-field approximation, to a sharp crossover when the first correction is included. In Fig. 6 we show a closeup of the $\langle \mathrm{Tr} U\rangle$ in the near neighborhood of the transition in both cases.

We also find that at $\kappa = 0.04$, the endpoint of the line of first order transitions moves from $\mu = 0.87$, $\beta = 0.1211$ to $\mu = 0.46$, $\beta = 0.1246$. At $\kappa = 0.045$ the line of transitions shrinks to a point, at $\mu = 0$, $\beta = 0.1245$. Beyond $\kappa = 0.045$, there are no transitions. The corresponding phase diagram, including the leading correction, is shown in Fig. 7.




(a) mean field (b) mean field + NLO

FIG. 6 (color online). Closeup of $\langle \mathrm{Tr} U\rangle$ in the transition region, at $\kappa = 0.02$ and $\mu = 1.38$, showing the effect of inclusion of the leading correction to the mean field free energy. With the inclusion of the leading correction, this is the endpoint of the $\kappa = 0.02$ line of transitions, down from the value $\mu = 1.67$, which is the endpoint without the first correction.

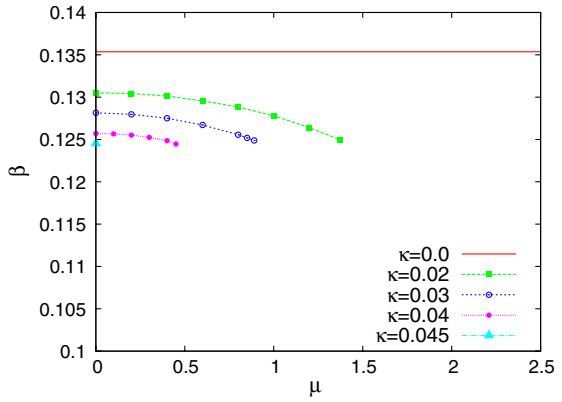



FIG. 7 (color online). Phase diagram of the Polyakov line model (1) for the SU(3) group, obtained via mean field methods, now including contributions at next-to-leading order (NLO). The main effect of the NLO corrections is that the endpoints of the first-order transition lines at fixed $\kappa$ occur at lesser values of $\beta$, as compared to the leading order result.

So the first correction to mean field is taking us in the right direction, in the sense of bringing the endpoint of the first order transition line to smaller values of $\mu$. Mercado and Gattringer [5] find that the endpoints of the first-order transition lines are located at yet smaller values of $\mu$. It would be interesting to see if the next higher-order corrections generated by $\exp[J]$ would bring the endpoints still closer to the endpoints found in Ref. [5]. We leave this exercise for a future study.

## V. EFFECTIVE SPIN MODELS AND FULL QCD

It seems to be easier to solve effective spin models at finite chemical potential, by a variety of methods, than to solve full QCD at finite chemical potential. This means that if we knew the effective spin models corresponding to full QCD at relevant points in the plane of temperature and quark chemical potential, then by solving the effective models we could determine the QCD phase diagram. We know how to derive the effective spin model in the strong coupling and hopping parameter expansions; for $\mu = 0$ this has been done in Refs. [14,15], and for $\mu \neq 0$ in Ref. [6]. Reference [6] uses high-order strong-coupling/hopping parameter expansions to derive an effective spin model, which is then used to determine critical couplings. We still think it desirable, however, to be able to extract the effective spin model without reliance on either the hopping parameter or the strong-coupling expansions.[7]

In principle the effective Polyakov line model is derived from full QCD by integrating out the quark and gauge field variables, under the constraint that the Polyakov lines are fixed. It is convenient to impose a temporal gauge on the periodic lattice, in which all timelike links are set to the unit matrix except on a single time slice, $t = 0$ say. Then the effective theory, at chemical potential $\mu = 0$, is defined by integrating over all quark fields and link variables with the exception of the timelike links at $t = 0$, i.e.,

$$Z(\beta, T, m_f) = \int DU_0(\mathbf{x}, 0) \int DU_k D\bar{\psi} D\psi e^{S_{\rm QCD}} = \int DU_0(\mathbf{x}, 0) e^{S_{\rm eff}[U_0, U_0^\dagger]}, \tag{48}$$

where $\beta$ is the gauge coupling, $T = 1/N_t$ is the temperature in lattice units with $N_t$ the lattice extension in the time direction, and $m_f$ represents the set of quark masses. Because temporal gauge has a residual symmetry under time-independent gauge transformations, it follow that $S_{\rm eff}$ is invariant under $U_0(\mathbf{x}, 0) \to g(\mathbf{x}) U_0(\mathbf{x}, 0) g^\dagger(\mathbf{x})$, and therefore can depend on the timelike links only through their eigenvalues. This just means that $S_{\rm eff}$ is a Polyakov line action of some kind.

Let $S^\mu_{\rm QCD}$ denote the QCD action with a chemical potential, which can be obtained from $S_{\rm QCD}$ by the following replacement of timelike links at $t = 0$:

$$S^\mu_{\rm QCD} = S_{\rm QCD}[U_0(\mathbf{x}, 0) \to e^{N_t \mu} U_0(\mathbf{x}, 0), U_0^\dagger(\mathbf{x}, 0) \to e^{-N_t \mu} U_0^\dagger(\mathbf{x}, 0)]. \tag{49}$$

The effective Polyakov line action, at finite chemical potential is defined via

$$Z(\mu, \beta, T, m_f) = \int DU_0(\mathbf{x}, 0) \int DU_k D\bar{\psi} D\psi e^{S^\mu_{\rm QCD}} = \int DU_0(\mathbf{x}, 0) e^{S^\mu_{\rm eff}[U_0, U_0^\dagger]}. \tag{50}$$

As already mentioned, the integration over $U_k$, $\bar{\psi}$, $\psi$ can be carried out in a strong gauge-coupling and hopping parameter expansion, to obtain $S_{\rm eff}$ and $S^\mu_{\rm eff}$. It is not hard to see that each contribution to $S_{\rm eff}$ in the strong coupling + hopping parameter expansion of (48) maps into a corresponding contribution to $S^\mu_{\rm eff}$, in the expansion of (50), by the replacement

$$U_x \to e^{N_t \mu} U_x, \qquad U_x^\dagger \to e^{-N_t \mu} U_x^\dagger, \tag{51}$$

where we have identified $U_x \equiv U_0(\mathbf{x}, 0)$. Since this mapping holds to all orders in the strong coupling + hopping expansion, it is reasonable to assume that it holds in general, i.e.,

$$S^\mu_{\rm eff}[U_x, U_x^\dagger] = S_{\rm eff}[U_x \to e^{N_t \mu} U_x, U_x^\dagger \to e^{-N_t \mu} U_x^\dagger]. \tag{52}$$

Equation (52) is a rather trivial, but potentially powerful identity. It suggests that if, by some means, one could obtain $S_{\rm eff}$ at fixed $\{\beta, m_f, T\}$ and chemical potential $\mu = 0$, then one would immediately also have the effective action $S^\mu_{\rm eff}$ at the same set of parameters $\{\beta, m_f, T\}$, but any chemical potential $\mu$, by the replacement shown.

[7]For efforts at deriving the effective Polyakov line model in pure gauge theories, cf. Ref. [16] and references therein.

Unfortunately, there is some degree of ambiguity in $S_{\rm eff}$ at $\mu = 0$. Suppose we have some ansatz for $S_{\rm eff}[U_x, U_x^\dagger]$, depending on some small set of parameters, which we would like to fix by comparing to the full theory at $\mu = 0$. The problem is that whatever ansatz we make for $S_{\rm eff}$, there is another form which is identical to that ansatz at $\mu = 0$, but differs under (51). In the case of SU(3), the identity

$$\mathrm{Tr}\, U_x^\dagger = \frac{1}{2}[(\mathrm{Tr} U_x)^2 - \mathrm{Tr} U_x^2], \tag{53}$$

allows us to replace $\mathrm{Tr} U_x^\dagger$ everywhere in $S_{\rm eff}$ by the right hand side of (53), but this again produces quite a different theory at $\mu \neq 0$ under the rule (52). Of course a similar identity holds for $\mathrm{Tr} U_x$, so we can convert the original $S_{\rm eff}$ to another theory which may be symmetric in $U_x$, $U_x^\dagger$, but which has quite a different extension to finite chemical potential.

It may be possible to overcome this ambiguity, however. Suppose we take the timelike link variables at $t = 0$ to be U(3), rather than SU(3) matrices. Then the ambiguity due to (53) is no longer present, but the effective spin theory still only depends on the eigenvalues of the U(3) matrices. Then let us suppose that we have some reasonable ansatz for $S_{\rm eff}$ in a physically interesting range of parameters $\beta$, $m_f$, $T$, e.g.,

$$\begin{aligned} S_{\rm eff} = & \sum_{x,y} J(\mathbf{x} - \mathbf{y}) \mathrm{Tr}[U_x] \mathrm{Tr}[U_y^\dagger] \\ & + \sum_{x,y} J'(\mathbf{x} - \mathbf{y}) (\mathrm{Tr}[U_x] \mathrm{Tr}[U_y] + \mathrm{Tr}[U_x^\dagger] \mathrm{Tr}[U_y^\dagger]) \\ & + \sum_x V(U_x, U_x^\dagger), \end{aligned} \tag{54}$$

where $J(x)$, $J'(x)$ are parametrized by a few constants (such as nearest and next-nearest neighbor couplings), and $V(U_x, U_x^\dagger)$ can be limited to a few terms involving the characters of U(3). In that case, the effective spin model is specified by a handful of constants $\{c_j\}$, which of course depend on $\{\beta, m_f, T\}$.

Since there is no sign problem at $\mu = 0$ and $U_x = U_0(\mathbf{x}, t = 0) \in U(3)$, it should be possible to numerically simulate both the effective theory and the full theory. Then one can imagine a number of strategies for obtaining the constants $\{c_j\}$. One possibility is to simply calculate an appropriate set of observables in both theories (Polyakov lines in various representations and Polyakov line correlators), and fix the set of constants $\{c_j\}$ in $S_{\rm eff}$ so that the two theories yield the same results. Or perhaps some variant of the inverse Monte Carlo method could be applied [16]. A third procedure is inspired by a recent study of the Yang-Mills vacuum wave functional [17]. The idea is to select a finite set of $M$ timelike link configurations

$$\{U_x^{(i)} = U_0^{(i)}(\mathbf{x}, t = 0) \in U(3), i = 1, 2, \ldots, M\}, \tag{55}$$

where each member $U_0^{(i)}$ of the set specifies the timelike link variables at every spatial site $\mathbf{x}$ and $t = 0$. Then the Monte Carlo simulation of the full theory proceeds in the usual way, except that on the $t = 0$ timeslice, one member of the given set of timelike link configurations is selected by the Metropolis algorithm, and all timelike links on that timeslice are updated simultaneously. Let $N_i$ be the number of times that the $i$th configuration is selected by the algorithm, and $N_{\rm tot} = \sum_i N_i$. Then it is not hard to show that

$$\frac{\exp[S_{\rm eff}[U^{(i)}]]}{\exp[S_{\rm eff}[U^{(j)}]]} = \lim_{N_{\rm tot} \to \infty} \frac{N_i}{N_j}. \tag{56}$$

Information derived from a number of such simulations, each using a different set of configurations at $t = 0$, can in principle completely determine the $\{c_j\}$. However, since the $\{N_i\}$ vary exponentially with $S_{\rm eff}$, the variation of $S_{\rm eff}$ within a given set must be kept relatively small, i.e., $\delta S_{\rm eff} \approx 5$–$7$, in order to ensure a reasonable acceptance rate for all members of the set. For details of the algorithm, and its application to the vacuum wave functional of pure Yang-Mills theory, cf. Ref. [17].

Once the set of constants $\{c_j\}$ is found, by whatever method, the effective theory at finite chemical potential, $S_{\rm eff}^\mu$, for any $\mu$ but the same set $\{\beta, m_f, T\}$, is given by the identity (52). The final step is simply to note that SU(3) $\subset$ U(3), so that the theory we want, $S_{\rm eff}^\mu$, is obtained by restricting the $U_x$ matrices to the SU(3) subset. Equivalently, since we can always express the U(3) matrices as[8]

$$U_x = \exp[i\theta_x] U_x^{SU(3)}, \qquad U_x^\dagger = \exp[-i\theta_x] (U_x^{SU(3)})^\dagger, \tag{57}$$

the conversion from $S_{\rm eff}$ to $S_{\rm eff}^\mu$ is obtained by setting $\theta_x = -iN_t\mu$.

With the effective Polyakov line model $S_{\rm eff}^\mu$ in hand, the theory can be solved by the mean field approach discussed above, or by other methods such as complex Langevin [1–3], the flux representation [5], or reweighting [6]. To check that the method is working at $\mu \neq 0$, one would compare full QCD with the effective spin model at, e.g., small or imaginary $\mu$, where the $\mu$-dependence of the full theory can be obtained by other means.

This approach can be expected to break down at sufficiently large $\mu$. At some point, terms in the potential involving high powers of $U_x$ and $U_x^\dagger$, which might be negligible for computing observables at $\mu = 0$ because they are multiplied by very small coefficients, could become important under the replacement (52). To what extent this effect will inhibit the study of the phase diagram remains to be seen.

[8] Allowing for the $Z_3$ subgroup of SU(3), the angle $\theta_x$ can be restricted to the range $[0, 2\pi/3)$.

There is no doubt that determining the set of constants $\{c_j\}$ in full QCD would be computationally demanding. As a first step, it may be worth trying to extract the effective spin theory from gauge theories with scalar, rather than fermionic, matter fields.

## VI. CONCLUSIONS

The mean field expansion for effective spin models with a chemical potential turns out to have an interesting structure. The constraint taking U($N$) to SU($N$) is responsible for the $\mu$-dependence of the free energy, and this constraint introduces an infinite sum whose index, as it turns out, can be interpreted as the baryon number at each site. The partition function can then be formally expressed in terms of a baryon fugacity expansion.

If we ignore the distinction between first-order and crossover points, then even the lowest order mean field equations do a reasonably good job of accounting for phase structure. The main error lies in the location of the endpoints of first-order transition lines, which occur, for fixed $\kappa$, at higher values of $\mu$ than those determined by other methods. The first correction to the mean field result moves those endpoints in the right direction, i.e., to lower values of $\mu$. It remains to be seen whether realistic results for the endpoints would be obtained from still higher orders in the mean field expansion.

We have also commented on the problem of deriving effective spin models from full QCD, and on certain subtleties associated with continuing those models from zero to finite chemical potential. We have suggested that a method which was previously applied to study the Yang-Mills vacuum wave functional may be useful in this context, and hope to discuss this further at a later time.

## ACKNOWLEDGMENTS

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[1] F. Karsch and H. Wyld, Phys. Rev. Lett. **55**, 2242 (1985).
[2] N. Bilic, H. Gausterer, and S. Sanielevici, Phys. Rev. D **37**, 3684 (1988).
[3] G. Aarts and F. A. James, J. High Energy Phys. 01 (2012) 118.
[4] C. Gattringer, Nucl. Phys. **B850**, 242 (2011).
[5] Y. D. Mercado and C. Gattringer, Nucl. Phys. **B862**, 737 (2012).
[6] M. Fromm, J. Langelage, S. Lottini, and O. Philipsen, J. High Energy Phys. 01 (2012) 042.
[7] A. Dumitru, R. D. Pisarski, and D. Zschiesche, Phys. Rev. D **72**, 065008 (2005).
[8] J. B. Kogut, M. Snow, and M. Stone, Nucl. Phys. **B200**, 211 (1982).
[9] B. Schlittgen and T. Wettig, J. Phys. A **36**, 3195 (2003).
[10] R. Brower, P. Rossi, and C.-I. Tan, Nucl. Phys. **B190**, 699 (1981).
[11] C. H. Christensen, Phys. Lett. B **714**, 306 (2012).
[12] J. Danzer and C. Gattringer, arXiv:1204.1020.
[13] P. de Forcrand and O. Philipsen, Phys. Rev. Lett. **105**, 152001 (2010).
[14] F. Green and F. Karsch, Nucl. Phys. **B238**, 297 (1984).
[15] M. Ogilvie, Phys. Rev. Lett. **52**, 1369 (1984).
[16] C. Wozar, T. Kaestner, A. Wipf, and T. Heinzl, Phys. Rev. D **76**, 085004 (2007).
[17] J. Greensite, H. Matevosyan, Š. Olejník, M. Quandt, H. Reinhardt, and A. P. Szczepaniak, Phys. Rev. D **83**, 114509 (2011).