Hamiltonian lattice quantum chromodynamics at finite chemical potential

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At sufficiently high temperature and density, quantum chromodynamics (QCD) is expected to undergo a phase transition from the confined phase to the quark-gluon plasma phase. In the Lagrangian lattice formulation the Monte Carlo method works well for QCD at finite temperature; however, it breaks down at finite chemical potential. We develop a Hamiltonian approach to lattice QCD at finite chemical potential and solve it in the case of free quarks and in the strong coupling limit. At zero temperature, we calculate the vacuum energy, chiral condensate, quark number density and its susceptibility, as well as mass of the pseudoscalar, vector mesons and nucleon. We find that the chiral phase transition is of first order, and the critical chemical potential is $\mu_C = m_{\rm dyn}^{(0)}$ (dynamical quark mass at $\mu = 0$). This is consistent with $\mu_C \approx M_N^{(0)}/3$ (where $M_N^{(0)}$ is the nucleon mass at $\mu = 0$).

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I. INTRODUCTION

A. Motivation

According to the big bang model in cosmology, the early universe underwent a series of drastic changes. For some time it was a hot and dense quark-gluon plasma (QGP), where quarks and gluons were deconfined. Today it is in a low temperature and low density hadronic phase, where quarks are confined. The ultimate goal of machines such as the Relativistic Heavy Ion Collider (RHIC) at BNL and the Large Hadron Collider (LHC) at CERN is to create the QGP phase. The QGP may also exist in the core of very dense stars such as neutron stars. Quantum chromodynamics (QCD) is the fundamental theory of quarks and gluons. A precise determination of the QCD phase structure at finite temperature T and chemical potential μ will provide valuable information in the experimental search for the QGP. The lattice gauge theory (LGT) proposed by Wilson in 1974 is a very reliable technique for the investigation of phase transitions. There are no free parameters in LGT when the continuum limit is taken, in contrast with other nonperturbative techniques. Although the standard lattice Lagrangian Monte Carlo method works very well for QCD at finite temperature, it unfortunately breaks down at finite chemical potential (due to the so-called complex action problem). This is briefly summarized in Sec. I B. On the other hand, lattice QCD at finite chemical potential formulated in the Hamiltonian approach does not encounter a complex action problem. In Sec. II we develop a Hamiltonian approach to lattice QCD at finite chemical potential μ. We solve this in the case of free quarks and in the strong coupling limit.

B. Present status

LGT is an approach to QCD from first principles. However, it is not free of problems: (a) First, there are lattice artifacts: A finite volume and a finite lattice spacing introduce errors. (b) There is a no-go theorem for chiral fermions: There is species doubling of any local fermionic theory with continuous symmetries. For naive fermions, chiral symmetry is preserved, but the species are doubled and the chiral anomaly is wrong. Kogut-Susskind fermions preserve the continuous U(1) chiral symmetry, but break explicitly flavor symmetry. For Wilson fermions, the flavor symmetry exists, but chiral symmetry is explicitly broken. Kogut–Susskind fermions and Wilson fermions have been extensively used in numerical simulations. Recently, there has been evidence showing that those two approaches may give the topological charge or anomaly incorrectly [1] on a finite lattice. Therefore, it is far from clear whether correct results in the continuum can be obtained using those fermion formulations. Kaplan's domain wall fermions [2] and Neuberger's overlap fermion formulation [3] have attracted much attention, because they give the correct chiral modes, they also produce the correct anomaly and topological charge. For domain wall fermions there is an extra dimension and the lattice size in this dimension has to be very large. Thus algorithms suitable for those new fermion approaches need to be developed. In this paper, we do not address those problems.

Here we would like to investigate lattice QCD at finite chemical potential. In the continuum, the grand canonical partition function of QCD at finite temperature T and chemical potential μ is given by

$$Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)}, \quad \beta = (k_B T)^{-1}, \tag{1.1}$$

where k_B is the Boltzmann constant, H is the Hamiltonian, and N is particle number operator

$$N = \int d^3x\, \psi^\dagger(x)\psi(x). \tag{1.2}$$

The energy density of the system with free quarks is given by [4]

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$$\epsilon = \frac{1}{V}\frac{1}{Z}\mathrm{Tr}\, H e^{-\beta(H-\mu N)} = -\frac{1}{V}\frac{\partial \ln Z}{\partial \beta}\bigg|_{\mu\beta}. \quad (1.3)$$

Going over to $T\to 0$, the energy density (where the contribution of $\mu=0$ is subtracted) becomes

$$\epsilon_{\mathrm{sub}} = \frac{4\pi}{(2\pi)^4}\int_{-\infty}^{\infty} d^3p \times \Theta\left(\mu - \sqrt{\sum_{j=1}^{3} p_j^2 + m^2}\right)\sqrt{\sum_{j=1}^{3} p_j^2 + m^2}. \quad (1.4)$$

Here Θ is the step function. In the chiral limit $m\to 0$ one obtains

$$\epsilon_{\mathrm{sub}} = \frac{1}{4\pi^3}\int_{-\infty}^{\infty} d^3p\, \Theta(\mu - |\vec{p}|)|\vec{p}| = \frac{1}{\pi^2}\int_0^{\mu} |\vec{p}|^3 d|\vec{p}| = \frac{\mu^4}{4\pi^2}. \quad (1.5)$$

In the Hamiltonian formulation of LGT, Eq. (1.1) in well defined. For Wilson fermions or Kogut–Susskind fermions, the relation Eq. (1.5) is satisfied (see below). However, if one constructs the fermionic lattice Lagrangian via Legendre transformation of the Hamiltonian, one cannot reproduce the continuum relation Eq. (1.5). Let us take the naive fermions as an example. The action obtained via Legendre transformation of H reads

$$S_f = a^4\sum_x m\bar{\psi}(x)\psi(x) + \frac{a^3}{2}\sum_x\sum_{k=\pm 1}^{\pm 4}\bar{\psi}(x)\gamma_k\psi(x+\hat{k}) + a^4\mu\sum_x \psi^{\dagger}(x)\psi(x), \quad (1.6)$$

where $\gamma_{-k} = -\gamma_k$. This action gives the following result for the subtracted energy density:

$$\epsilon_{\mathrm{sub}} = \frac{-a^{-4}}{4\pi^4}\int_{-\pi}^{\pi} d^4p\, \frac{\sum_{j=1}^{3}\sin^2 p_j + (ma)^2}{(\sin p_4 - i\mu a)^2 + \sum_{j=1}^{3}\sin^2 p_j + (ma)^2} - [\mu = 0]. \quad (1.7)$$

Taking the limit $m\to 0$ and the continuum limit $a\to 0$, $\epsilon_{\mathrm{sub}} \propto (\mu/a)^2$, i.e., becoming quadratically divergent, and therefore it is inconsistent with the continuum result of Eq. (1.5). This problem is not due to the species doubling of naive fermions, because the case of Kogut–Susskind fermions or Wilson fermions is similar.

Hasenfratz and Karsch [5] proposed the following solution: If $(\sin p_4 - i\mu)^2$ is replaced by $\sin^2(p_4 - i\mu)$ the continuum result Eq. (1.5) is reproduced, except for a factor of 16. Correspondingly in the action, the chemical potential is introduced in the following way:

$$S_f = a^4\sum_x m\bar{\psi}(x)\psi(x) + \frac{a^3}{2}\sum_x\sum_{j=1}^{3}[\bar{\psi}(x)\gamma_j\psi(x+\hat{j}) - \bar{\psi}(x+\hat{j})\gamma_j\psi(x)] + \frac{a^3}{2}\sum_x [e^{\mu a}\bar{\psi}(x)\gamma_4\psi(x+\hat{4}) - e^{-\mu a}\bar{\psi}(x+\hat{4})\gamma_4\psi(x)]. \quad (1.8)$$

The chemical potential can be introduced analogously for KS as well as for Wilson fermions. Such treatment of the chemical potential is numerically feasible in the quenched approximation (where the fermionic determinant $\det\Delta$ is constraint to be 1, and quark loops are suppressed). However, there is evidence [6] that the quenched approximation produces an unphysical onset of the critical chemical potential at the value $\mu_C = M_\pi(m\neq 0)/2$, being in conflict with other theoretical predictions $\mu_C \approx M_N^{(0)}/3$ [$M_N^{(0)}$ is the nucleon mass at $\mu=0$ and $M_\pi(m\neq 0)$ is the pion mass at finite bare quark mass m. A finite bare quark mass must be introduced in most of the numerical simulations]. The unphysical onset of μ_C is considered as a defect of the quenched approximation.

For full QCD, the fermionic degrees of freedom have to be integrated out. In the measure occurs the fermionic determinant $\det\Delta$. For finite chemical potential $\det\Delta$ becomes complex (complex action problem), which renders numerical simulations extremely difficult. Much effort has been made to solve the notorious complex action problem. (1) The Glasgow group has suggested to treat $\det\Delta$ as observable [7]. This method requires a very large number of configurations, in particular for $\mu\approx\mu_C$. Even on a very small lattice $V=4^4$, the computational costs exceed the current computer capacity [8]. (2) In the imaginary chemical potential method [9] $\det\Delta$ becomes real, which works well for numerical simulations at high temperature and low density. But it might not work at low temperature and high density. (3) It has been proposed to utilize a special symmetry [10]. This is the only successful method in Lagrangian lattice QCD, but it works only for the SU(2) gauge group. (4) Recently, a new approach has been proposed in [11], using quantum spin variables. It remains to be seen whether this can be applied to QCD.

II. HAMILTONIAN APPROACH

A. Free fermions at zero chemical potential

The lattice Hamiltonian describing noninteracting Wilson fermions in $d+1$ dimensions at $\mu=0$ reads

$$H = \sum_x m\bar{\psi}(x)\psi(x) + \frac{1}{2a}\sum_{x,k=\pm j}\bar{\psi}(x)\gamma_k\psi(x+\hat{k}) + \frac{r}{2a}\sum_{x,k=\pm j}[\bar{\psi}(x)\psi(x) - \bar{\psi}(x)\psi(x+\hat{k})]. \quad (2.1)$$

We want to diagonalize H so that the fermionic field ψ can be expressed in terms of up and down 2-spinors ξ and $\eta^{\dagger}$,

$$\psi=\begin{pmatrix}\xi\\ \eta^{\dagger}\end{pmatrix}. \tag{2.2}$$

We define the bare vacuum state $|0\rangle$ as

$$\xi|0\rangle=\eta|0\rangle=0. \tag{2.3}$$

Since the up and down components are coupled via the γ_k matrices, the bare vacuum is not an eigenstate of H. Let $|\Omega>$ denote the physical vacuum state, and E_Ω the vacuum energy. One can use a unitary transformation to decouple the up and down components [12],

$$H'=\exp(-iS)H\exp(iS). \tag{2.4}$$

Such a transformation is similar to the Foldy-Wouthuysen transformation [13]. Then the physical vacuum state of H can be expressed as

$$|\Omega\rangle=\exp(iS)|0\rangle. \tag{2.5}$$

The operator S can be computed explicitly. For Wilson ($r\neq 0$) or naive ($r=0$) fermions it reads [12]

$$\begin{aligned}S&=\sum_p \theta_p S_p,\\ S_p&=-\frac{1}{A_p}\sum_{j=1}^{d}\psi_p^{\dagger}\gamma_j\psi_p\frac{\sin p_j a}{a},\\ A_p&=\left[\sum_{j=1}^{d}\left(\frac{\sin p_j a}{a}\right)^2\right]^{1/2},\end{aligned} \tag{2.6}$$

and p is the momentum. The transformed Hamiltonian becomes

$$\begin{aligned}H'=\sum_p\Bigg[&\left[m+\frac{2r}{a}\sum_{j=1}^{d}\sin^2(p_j a/2)\right]\cos 2\theta_p\\ &+A_p\sin 2\theta_p\Bigg]\overline{\psi}_p\psi_p+\Bigg[\cos 2\theta_p-\left[m+\frac{2r}{a}\right.\\ &\left.\times\sum_{j=1}^{d}\sin^2(p_j a/2)\right]\frac{\sin 2\theta_p}{A_p}\Bigg]\sum_{j=1}^{d}\overline{\psi}_p i\gamma_j\frac{\sin p_j a}{a}\psi_p.\end{aligned} \tag{2.7}$$

The vacuum energy is given by

$$\begin{aligned}E_\Omega&=\langle\Omega|H|\Omega\rangle=\langle 0|H'|0\rangle\\ &=-2N_c N_f\sum_p\Bigg[\left[m+\frac{2r}{a}\sum_{j=1}^{d}\sin^2(p_j a/2)\right]\cos 2\theta_p\\ &\quad+A_p\sin 2\theta_p\Bigg],\end{aligned} \tag{2.8}$$

where N_c and N_f, respectively, are the number of colors and number of flavors. The vacuum energy E_Ω is minimized under variation of the parameters θ_p if

$$\tan 2\theta_p=\frac{A_p}{m+\frac{2r}{a}\sum_{j=1}^{d}\sin^2(p_j a/2)}. \tag{2.9}$$

This condition also leads to the cancellation of the second term in Eq. (2.7) coupling the up and down components such that

$$H'|0\rangle=\sum_p A_p'\overline{\psi}_p\psi_p|0\rangle=E_\Omega|0\rangle, \tag{2.10}$$

where we denote

$$A_p'=\left[\left[m+\frac{2r}{a}\sum_{j=1}^{d}\sin^2(p_j a/2)\right]^2+A_p^2\right]^{1/2}. \tag{2.11}$$

The vacuum energy becomes

$$E_\Omega=-2N_c N_f\sum_p A_p'. \tag{2.12}$$

It can be easily seen that $|\Omega\rangle$ is the eigenstate of H and E_Ω is its eigenvalue. For Wilson fermions, in the continuum limit $a\to 0$, for any finite momentum p, we have

$$A_p'\to\sqrt{m^2+p^2}, \tag{2.13}$$

giving the correct dispersion relation.

B. Free fermions at nonzero chemical potential

We follow the same steps as in the case $\mu=0$. According to Eq. (1.1), the role of the Hamiltonian is now played by

$$H_\mu=H-\mu N, \tag{2.14}$$

where H is given by Eq. (2.1) and N is given by Eq. (1.2). Let us define the state $|n_p,\overline{n_p}\rangle$ by

$$\begin{aligned}&\xi_p|0_p,\overline{n_p}\rangle=0,\quad \xi_p^{\dagger}|0_p,\overline{n_p}\rangle=|1_p,\overline{n_p}\rangle,\\ &\xi_p|1_p,\overline{n_p}\rangle=|0_p,\overline{n_p}\rangle,\quad \xi_p^{\dagger}|1_p,\overline{n_p}\rangle=0,\\ &\eta_p|n_p,0_p\rangle=0,\quad \eta_p^{\dagger}|n_p,0_p\rangle=|n_p,1_p\rangle,\\ &\eta_p|n_p,1_p\rangle=|n_p,0_p\rangle,\quad \eta_p^{\dagger}|n_p,1_p\rangle=0.\end{aligned} \tag{2.15}$$

The numbers n_p and $\overline{n_p}$ take the values 0 or 1 due to the Pauli principle. By definition, the up and down components of the fermion field are decoupled. Obviously, this is not an eigenstate of H_μ due to the nondiagonal form of H. However, they are eigenstates of H_μ', which are related to H_μ by a unitary transformation

$$H_\mu'=\exp(-iS)H_\mu\exp(iS)=H'-\mu N. \tag{2.16}$$

For the vacuum eigenstate of H_μ we make an ansatz of the following form:

$$|\Omega\rangle = \exp(iS)\sum_p f_{n_p,\bar{n}_p}|n_p,\bar{n}_p\rangle. \tag{2.17}$$

S is given by Eq. (2.6) and the parameter θ_p is given by Eq. (2.9). Both S and θ_p do not depend on μ because the quark number operator N commutes with S. H' is given by Eq. (2.7). The vacuum energy thus obeys

$$\begin{aligned} E_\Omega &= \langle\Omega|H_\mu|\Omega\rangle = \sum_{p',p} f_{n_{p'},\bar{n}_{p'}} f_{n_p\bar{n}_p}\langle n_{p'}\bar{n}_{p'}|H'_\mu|n_p,\bar{n}_p\rangle \\ &= \sum_p C_{n_p,\bar{n}_p}\langle n_p,\bar{n}_p|H'-\mu N|n_p,\bar{n}_p\rangle, \end{aligned} \tag{2.18}$$

where we have introduced the notation $C_{n_p,\bar{n}_p} = f^2_{n_p,\bar{n}_p}$. From Eq. (2.15) follows

$$\begin{aligned} E_\Omega &= \sum_p C_{n_p,\bar{n}_p}(A'_p\langle n_p,\bar{n}_p|\bar{\psi}_p\psi_p|n_p,\bar{n}_p\rangle \\ &\quad -\mu\langle n_p,\bar{n}_p|\psi_p^\dagger\psi_p|n_p,\bar{n}_p\rangle) \\ &= 2N_cN_f\sum_p C_{n_p,\bar{n}_p}[(A'_p-\mu)n_p+(A'_p+\mu)\bar{n}_p-A'_p-\mu]. \end{aligned} \tag{2.19}$$

We have not yet specified the function $C_{n_p,\bar{n}_p}$. For this purpose we use the condition of stability of the vacuum. Because $\mu>0$, the vacuum energy increases with n_p. This means the vacuum is unstable unless $\bar{n}_p=0$. This simplifies Eq. (2.19) to

$$E_\Omega = 2N_cN_f\sum_p C_{n_p}[(A'_p-\mu)n_p-A'_p-\mu], \tag{2.20}$$

where we use the abbreviation $C_{n_p}=C_{n_p,0}$. From the normalization condition $C_{0_p}+C_{1_p}=1$, we obtain

$$E_\Omega = 2N_cN_f\sum_p [C_{1_p}(A'_p-\mu)-A'_p-\mu]. \tag{2.21}$$

C_{1_p} depends on the value of μ and its dependence can be seen by inspection of the derivative

$$\frac{\partial E_\Omega}{\partial C_{1_p}} = 2N_cN_f(A'_p-\mu). \tag{2.22}$$

For $\mu>A'_p$, the right-hand side is negative. Maximizing C_{1_p} means minimizing the vacuum energy. Therefore, $C_{1_p}=1$. On the other hand, for $\mu<A'_p$, the right-hand side is positive and for any C_{1_p} the vacuum is unstable. Therefore, $C_{1_p}=0$. We can summarize these properties by writing

$$C_{1_p} = \Theta(\mu-A'_p). \tag{2.23}$$

Thus the vacuum energy becomes

$$E_\Omega = 2N_cN_f\sum_p (C_{1_p}A'_p-A'_p). \tag{2.24}$$

The subtracted energy density reads

$$\begin{aligned} \epsilon_{\rm sub} &= \frac{E_\Omega - E_\Omega|_{\mu=0}}{N_cN_fN_s} = \frac{2}{N_s}\sum_p C_{1_p}A'_p \\ &= \frac{2}{(2\pi)^3}\int_{-\infty}^{\infty} d^3p\, A'_p\Theta(\mu-A'_p). \end{aligned} \tag{2.25}$$

Here N_s is the number of spatial lattice sites. In case of Wilson fermions, for $m=0$ and in the continuum $a=0$, for any finite momentum p, one has $A'_p=|p|$. In 3+1 dimensions, at the corners of the Brillouin zone $p_ja=(\pi,0,0)$, $(0,\pi,0)$, $(0,0,\pi)$, $(\pi,\pi,0)$, $(0,\pi,\pi)$, $(\pi,0,\pi)$, (π,π,π), one has $\Theta(\mu-A'_p)=0$. Therefore, in the continuum we find

$$\epsilon_{\rm sub} = \frac{8\pi}{(2\pi)^3}\int_0^\mu p\, d^3p = \frac{\mu^4}{4\pi^2}. \tag{2.26}$$

Thus we have proven that we can reproduce in the Hamiltonian formulation the continuum result of the vacuum energy density, Eq. (1.5). For naive fermions, in the continuum limit $a=0$, there will be an extra factor of 2^d.

C. Strong coupling QCD at nonzero chemical potential

1. Structure of the Hamiltonian

As is well known, lattice QCD at $\mu=0$ confines quarks and spontaneously breaks chiral symmetry. For a sufficiently large chemical potential, this picture may change. At lattice spacing $a\neq0$, as discussed in Sec. I B, none of the standard approaches to lattice fermions is satisfactory. Here we set out to investigate finite density QCD in the strong coupling regime $1/g^2\ll1$, using the Hamiltonian formulation. One of the goals is to get a better understanding of the mechanism of chiral phase transition. According to Ref. [12], H' in Eq. (2.16) now is replaced by

$$\begin{aligned} H' &= \left[m[1-(2\theta_0)^2d]+\frac{(2\theta_0)d}{a}\right]\sum_x \bar{\psi}(x)\psi(x) \\ &\quad + \frac{g^2C_N(2\theta_0)^2}{8aN_c}\sum_x\sum_{k=\pm j}\psi^\dagger_{c_1,f_1}(x)\gamma_k\psi_{c_2,f_1}(x+\hat{k}) \\ &\quad \times\psi^\dagger_{c_2,f_2}(x+\hat{k})\gamma_k\psi_{c_1,f_2}(x), \end{aligned} \tag{2.27}$$

where $d=3$ denotes the spatial dimension, c_1, c_2 are color indices and f_1, f_2 are flavor indices (summation over repeated indices is understood), $\theta_0=1/(4ma+g^2C_N)$, and $C_N=(N_c^2-1)/(2N_c)$. The four-fermion interaction is induced by gauge interactions with fermions. A very similar Hamiltonian has been derived in Ref. [14] using strong coupling and large N_c expansion. After a Fierz transformation, H' becomes [12]

TABLE I. Γ matrices and coefficients.

Γ_A	1	γ_j	γ_4	γ_5	$i\gamma_4\gamma_5$	$i\gamma_4\gamma_j$	$i\epsilon_{jj_1j_2}\gamma_{j_1}\gamma_{j_2}$	$i\epsilon_{jj_1j_2}\gamma_4\gamma_{j_1}\gamma_{j_2}$
L_A	1	$-1+2\delta_{k,j}$	-1	-1	1	$1-2\delta_{k,j}$	$-1+2\delta_{k,j}$	$1-2\delta_{k,j}$

$$H'=\left[m[1-(2\theta_0)^2d]+\frac{(2\theta_0)d}{a}\right]\sum_x \bar{\psi}(x)\psi(x)$$
$$+\frac{g^2C_Nd(2\theta_0)^2}{4a}\sum_x \psi^\dagger(x)\psi(x)$$
$$-\frac{g^2C_N(2\theta_0)^2}{32aN_c}\sum_x\sum_{k=\pm j} L_A\psi^\dagger_{f_1}(x)\Gamma_A\psi_{f_2}(x)\psi^\dagger_{f_2}(x+k)$$
$$\times\Gamma_A\psi_{f_1}(x+k). \tag{2.28}$$

The matrices Γ_A and L_A are given in Table I.

Let us define the following operators [12,15]:

$$\Pi(x)_{f_1f_2}=\frac{1}{2\sqrt{-\bar{v}}}\psi^\dagger_{f_1}(x)(1-\gamma_4)\gamma_5\psi_{f_2}(x),$$
$$V_j(x)_{f_1f_2}=\frac{1}{2\sqrt{-\bar{v}}}\psi^\dagger_{f_1}(x)(1-\gamma_4)\gamma_j\psi_{f_2}(x), \tag{2.29}$$

where

$$\bar{v}=\frac{1}{N_fN_s}\sum_p C_{n_p,\bar{n}_p}\langle n_p,\bar{n}_p|\bar{\psi}_p\psi_p|n_p,\bar{n}_p\rangle$$
$$=\frac{2N_c}{N_s}\sum_p C_{n_p,\bar{n}_p}(n_p+\bar{n}_p-1). \tag{2.30}$$

Using mean field approximation, one can show that [15]

$$[\Pi(x),\Pi^\dagger(x')]=\delta_{x,x'},$$
$$[V_j(x),V_j^\dagger(x')]=\delta_{x,x'}. \tag{2.31}$$

Thus the operators Π and V_j, defined in Eq. (2.29), behave like pseudoscalar and vector operators. In Ref. [15] it has been shown that the operator $\bar{\psi}\psi$ satisfies the same commutation relations as $\bar{v}+2\Pi^\dagger\Pi+2\Sigma_jV_j^\dagger V_j$. Therefore, H' in Eq. (2.28) can be written in terms of pseudoscalar and vector particle operators in the following way:

$$H'=E_\Omega^{(0)}+G_1\sum_x\left(\Pi^\dagger(x)\Pi(x)+\sum_j V_j^\dagger(x)V_j(x)\right)$$
$$+\frac{G_2}{2}\sum_{x,k}\left(\Pi^\dagger(x)\Pi^\dagger(x+k)+\sum_j V_j^\dagger(x)V_j^\dagger(x+k)\right.$$
$$\left.\times(1-2\delta_{jk})+\text{H.c.}\right), \tag{2.32}$$

where

$$E_\Omega^{(0)}=N_fN_s\left[m[1-(2\theta_0)^2d]+\frac{(2\theta_0)d}{a}\right]\bar{v}$$
$$+N_fN_s\frac{g^2C_Nd(2\theta_0)^2}{4a}v^\dagger-N_fN_s\frac{g^2C_N(2\theta_0)^2d}{16aN_c}$$
$$\times(v_2^\dagger-\bar{v_2}),$$
$$G_1=2\left[m[1-(2\theta_0)^2d]+\frac{(2\theta_0)d}{a}\right]+\frac{g^2C_Nd(2\theta_0)^2}{4aN_c}\bar{v},$$
$$G_2=-\frac{g^2C_N(2\theta_0)^2}{8aN_c}\bar{v},$$
$$v^\dagger=\frac{1}{N_fN_s}\sum_p C_{n_p,\bar{n}_p}\langle n_p,\bar{n}_p|\psi_p^\dagger\psi_p|n_p,\bar{n}_p\rangle$$
$$=\frac{2N_c}{N_s}\sum_p C_{n_p,\bar{n}_p}(n_p-\bar{n}_p+1),$$
$$v_2^\dagger=\frac{1}{N_fN_s}\sum_p C_{n_p,\bar{n}_p}$$
$$\times\langle n_p,\bar{n}_p|\psi^\dagger_{f_1,p}\psi_{f_2,p}\psi^\dagger_{f_2,p}\psi_{f_1,p}|n_p,\bar{n}_p\rangle$$
$$=\frac{(2N_c)^2}{N_s}\sum_p C_{n_p,\bar{n}_p}(n_p-\bar{n}_p+1)^2,$$
$$\bar{v}_2=\frac{1}{N_fN_s}\sum_p C_{n_p,\bar{n}_p}$$
$$\times\langle n_p,\bar{n}_p|\bar{\psi}_{f_1,p}\psi_{f_2,p}\bar{\psi}_{f_2,p}\psi_{f_1,p}|n_p,\bar{n}_p\rangle$$
$$=\frac{(2N_c)^2}{N_s}\sum_p C_{n_p,\bar{n}_p}(n_p+\bar{n}_p-1)^2. \tag{2.33}$$

In Eq. (2.32), we have ignored the nonmeson terms which give no contribution to the energy. Making a Fourier transformation, one obtains

$$H'=E_\Omega^{(0)}+G_1\sum_p\left(\Pi^\dagger(p)\Pi(p)+\sum_j V_j^\dagger(p)V_j(p)\right)$$
$$+G_2\sum_p(\Pi^\dagger(p)\Pi^\dagger(-p)+\text{H.c.})\sum_j\cos p_ja$$
$$+G_2\sum_{p,j}(V_j^\dagger(p)V_j^\dagger(-p)+\text{H.c.})$$
$$\times\left(\sum_{j'}\cos p_{j'}a-2\cos p_ja\right). \tag{2.34}$$

This can be diagonalized by a Bogoliubov transformation [12]

$$P(p)=\cosh u(p)a(p)+\sinh u(p)a^{\dagger}(-p),$$
$$V_j(p)=\cosh v_j(p)b(p)+\sinh v_j(p)b^{\dagger}(-p), \tag{2.35}$$

where

$$\tanh 2u(p)=\frac{-2G_2}{G_1}\sum_j \cos p_j a,$$
$$\tanh 2v_j(p)=\frac{-2G_2}{G_1}\left(\sum_{j'} \cos p_{j'} a-2\cos p_j a\right). \tag{2.36}$$

This condition also minimizes the vacuum energy. The Bogoliubov transformed Hamiltonian eventually becomes

$$\begin{aligned}H''=E_{\Omega}^{(0)}&+\frac{N_f^2}{2}G_1\sum_p [\sqrt{1-\tanh^2 2u(p)}-1]\\&+\frac{N_f^2}{2}G_1\sum_{p,j} [\sqrt{1-\tanh^2 2v_j(p)}-1]\\&+G_1\sum_p \sqrt{1-\tanh^2 2u(p)}a^{\dagger}(p)a(p)\\&+G_1\sum_{p,j} \sqrt{1-\tanh^2 2v_j(p)}b_j^{\dagger}(p)b_j(p).\end{aligned} \tag{2.37}$$

2. Vacuum energy

The vacuum energy is given by

$$\begin{aligned}E_{\Omega}=\langle\Omega|H_{\mu}|\Omega\rangle=E_{\Omega}^{(0)}&-N_fN_s\mu v^{\dagger}\\&+\frac{N_f^2}{2}G_1\sum_p [\sqrt{1-\tanh^2 2u(p)}-1]\\&+\frac{N_f^2}{2}G_1\sum_{p,j} [\sqrt{1-\tanh^2 2v_j(p)}-1].\end{aligned} \tag{2.38}$$

From Eqs. (2.33)–(2.37), we get for $m=0$

$$\begin{aligned}\frac{E_{\Omega}}{2N_fN_c}=&\sum_{n_p,\bar{n}_p} C_{n_p,\bar{n}_p}[(m_{\rm dyn}^{(0)}-\mu)n_p+(m_{\rm dyn}^{(0)}+\mu\\&+2m_{\rm dyn}^{(0)}n_p)\bar{n}_p]-(\mu+m_{\rm dyn}^{(0)})\sum_{n_p,\bar{n}_p} C_{n_p,\bar{n}_p}\\&+\frac{N_f}{2}G_1\sum_p [\sqrt{1-\tanh^2 2u(p)}-1]\\&+\frac{N_f}{2}G_1\sum_{p,j} [\sqrt{1-\tanh^2 2v_j(p)}-1].\end{aligned} \tag{2.39}$$

Here $m_{\rm dyn}^{(0)}=d/(ag^2C_N)$ is the dynamical quark mass at $\mu=0$. It is obvious that $\bar{n}_p=0$, otherwise, the vacuum is unstable. Using the notation and normalization condition for the coefficient as in Sec. II B, we obtain

$$\begin{aligned}\frac{E_{\Omega}}{2N_cN_f}=&\sum_p C_{1_p}(m_{\rm dyn}^{(0)}-\mu)-\sum_p (m_{\rm dyn}^{(0)}+\mu)\\&+\frac{N_f}{2}G_1\sum_p [\sqrt{1-\tanh^2 2u(p)}-1]\\&+\frac{N_f}{2}G_1\sum_{p,j} [\sqrt{1-\tanh^2 2v_j(p)}-1].\end{aligned} \tag{2.40}$$

Again, using the same argument as in Sec. II B, the coefficient C_{1_p} must be

$$C_{1_p}=\Theta(\mu-m_{\rm dyn}^{(0)}). \tag{2.41}$$

Substituting into Eq. (2.40) yields

$$\begin{aligned}\frac{E_{\Omega}}{2N_cN_fN_s}=&(m_{\rm dyn}^{(0)}-\mu)\Theta(\mu-m_{\rm dyn}^{(0)})-m_{\rm dyn}^{(0)}-\mu\\&+\frac{N_f}{2N_s}G_1\sum_p [\sqrt{1-\tanh^2 2u(p)}-1]\\&+\frac{N_f}{2N_s}G_1\sum_{p,j} [\sqrt{1-\tanh^2 2v_j(p)}-1].\end{aligned} \tag{2.42}$$

3. Chiral condensate and critical μ

According to the Feynman–Hellmann theorem, the chiral condensate is related to the ground state energy by

$$\langle\bar{\psi}\psi\rangle=\frac{1}{N_fN_s}\lim_{m\to 0}\frac{\partial E_{\Omega}(m\neq 0)}{\partial m}=\langle\bar{\psi}\psi\rangle^{(0)}[1-\Theta(\mu-m_{\rm dyn}^{(0)})], \tag{2.43}$$

where $\langle\bar{\psi}\psi\rangle^{(0)}$ is the chiral condensate at $\mu=0$

$$\langle\bar{\psi}\psi\rangle^{(0)}=-2N_C\left(1-\frac{4d}{g^4C_N^2}\right)\left(1-\frac{N_f}{N_c}I_1-\frac{N_f}{N_c}I_2\right) \tag{2.44}$$

and for $d=3$

$$I_1=\frac{1}{2(2\pi)^3}\int_{-\pi}^{\pi}d^3p'\left(\frac{1}{\sqrt{1-\left(\frac{1}{3}\sum_j \cos p_j'\right)^2}}-1\right)$$
$$=0.078\,354\pm 2\times 10^{-6},$$

$$I_2=\frac{1}{2(2\pi)^3}\sum_j\int_{-\pi}^{\pi}d^3p'\times\left(\frac{1}{\sqrt{1-\left(\frac{1}{3}\left(\sum_{j'}\cos p'_{j'}-2\cos p'_j\right)\right)^2}}-1\right)=0.235\,075\pm4\times10^{-6}. \quad (2.45)$$

According to Eq. (2.43), for $\mu<m_{\rm dyn}^{(0)}$, $\langle\bar\psi\psi\rangle=\langle\bar\psi\psi\rangle^{(0)}\neq0$, i.e., chiral symmetry is spontaneously broken. For $\mu>m_{\rm dyn}^{(0)}$, $\langle\bar\psi\psi\rangle=0$, i.e., chiral symmetry is restored. Therefore, there is a first order chiral phase transition and the critical value of μ is given by

$$\mu_C=m_{\rm dyn}^{(0)}=\frac{d}{g^2C_Na}. \quad (2.46)$$

The critical chemical potential μ_C is equal to the dynamical quark mass at $\mu=0$, which agrees with the result from an entirely different method [16]. (The authors argued this was a second order phase transition, in contrast we clearly observe a first order transition.) Our result is consistent with other theoretical predictions $\mu_C\approx M_N^{(0)}/3$, because (see below) at $\mu=0$ holds $M_N^{(0)}\approx3m_{\rm dyn}^{(0)}$.

4. Quark number density and susceptibility

We can compute now the quark number density in the chiral limit $m=0$, which yields

$$n_q=\frac{-1}{2N_cN_fN_s}\frac{\partial E_\Omega}{\partial\mu}-1=\frac{\langle\Omega|\sum_x\psi^\dagger(x)\psi(x)|\Omega\rangle}{2N_cN_fN_s}-1=\Theta(\mu-\mu_C), \quad (2.47)$$

which is consistent with the $\beta=0$ simulation results described in [17], and however, is different from the large μ behavior in the continuum (i.e., the Stefann–Boltzmann law $n_q\propto\mu^3$). It remains to be seen whether higher order $1/g^2$ calculations will improve this behavior.

The quark number susceptibility, standing for the response of the quark number density to infinitesimal changes in μ, is

$$\chi_q=\frac{\partial n_q}{\partial\mu}=\delta(\mu-\mu_C). \quad (2.48)$$

5. Mass spectrum

Finally, let us look at some implications on the thermal mass spectrum of the pseudoscalar meson, vector meson and nucleon. The thermal mass is defined by $M_h^\star=\langle h|H-\mu N|h\rangle-E_\Omega$. For the pseudoscalar meson, in the chiral limit $m=0$,

$$M_\pi^\star=G_1\sqrt{1-\tanh^2\,2u(p=0)}=\begin{cases}0 & \text{for } \mu<\mu_C,\\ 4m_{\rm dyn}^{(0)} & \text{for } \mu>\mu_C.\end{cases} \quad (2.49)$$

Therefore, in the broken phase, the pseudoscalar is a Goldstone boson ($M_\pi^\star\propto\sqrt{m}\to0$), and in the symmetric phase, it is no longer a Goldstone boson. For the vector meson,

$$M_V^\star=G_1\sqrt{1-\tanh^2\,2v_j(p=0)}=\begin{cases}M_V^{(0)} & \text{for } \mu<\mu_C,\\ 4m_{\rm dyn}^{(0)} & \text{for } \mu>\mu_C,\end{cases} \quad (2.50)$$

where $M_V^{(0)}=4\sqrt{d-1}/(ag^2C_N)$ is the vector mass at $\mu=0$. Therefore, $\partial M/\partial\mu\propto\delta(\mu-\mu_C)$ for the pseudoscalar and vector mesons. It is worth mentioning in Ref. [18], the authors found $\partial M/\partial\mu=0$ outside the critical region. To see the critical behavior at zero temperature, one should be very close to μ_C. This behavior is consistent with that of the quark number density discussed in Sec. II C 4. To see whether the meson thermal masses depend on μ, higher order $1/g^2$ corrections must be included.

For the nucleon, we obtain the expected behavior

$$M_N^\star=M_N^{(0)}-3\mu \quad (2.51)$$

for $\mu<\mu_C$, where $M_N^{(0)}\approx3m_{\rm dyn}^{(0)}$. This leads to $M_N^\star=0$ at $\mu=\mu_C$.

III. OUTLOOK

In this paper, we have developed a Hamiltonian approach to lattice QCD at finite density. It avoids the usual problem of either an incorrect naive continuum limit or a premature onset of the transition to nonzero quark density as μ is raised. The main result in the free case is given by Eq. (2.26), and those in the strong coupling regime are given by Eqs. (2.42)–(2.51). We have seen that the approach works well in the free case and also in the strong coupling regime. We predict that at strong coupling, the chiral transition is of first order, and the critical chemical potential $\mu_C\approx M_N^{(0)}/3$.

Here we have only considered zero temperature. In the case of finite temperature, contributions from thermal excitations will make the calculations quite complicated. We plan to address this issue in a future paper.

We are also aware that the strong coupling limit is not compatible with the continuum limit where $a\to0$ and $1/g^2\to\infty$. For pure gauge theory, within a Hamiltonian approach, we can extend to the intermediate coupling and obtain meaningful results for the glueballs [19]. For fermions, the calculation is far from trivial. Recently we proposed a Monte Carlo technique in the Hamiltonian formulation [20] for the purpose to do nonperturbative numerical simulations, by combining the virtues of the Monte Carlo algorithm with importance sampling and the Hamiltonian approach. We hope to apply it to QCD and with the aim to obtain useful information for RHIC physics.

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[1] M. Teper, hep-lat/9909124; T. W. Chiu, hep-lat/9911010.
[2] D. Kaplan, Phys. Lett. B **288**, 342 (1992).
[3] H. Neuberger, Phys. Lett. B **417**, 141 (1998).
[4] J. R. Li, *Introduction to Quark Matter Theory* (Hunan Education Press, 1989); J. Kapusta, *Finite Temperature Field Theory* (Cambridge University Press, Cambridge, England, 1989); B. Freedman and L. Mclerran, Phys. Rev. D **16**, 1130 (1977); **16**, 1147 (1977); **16**, 1169 (1977).
[5] P. Hasenfratz and F. Karsch, Phys. Lett. **125B**, 308 (1983).
[6] J. Kogut, M. P. Lombardo, and D. Sinclair, Phys. Rev. D **51**, 1282 (1995); I. Barbour, S. Morrison, E. Klepfish, J. Kogut, and M. Lombardo, *ibid.* **56**, 7063 (1997); M. A. Stephanov, Phys. Rev. Lett. **76**, 4472 (1996).
[7] I. Barbour, C. Davies, and Z. Sabeur, Phys. Lett. B **215**, 567 (1988).
[8] R. Aloisio, V. Azcoiti, G. DiCarlo, A. Galante, and A. Grillo, Phys. Lett. B **453**, 275 (1999).
[9] M. Alford, A. Kapustin, and F. Wilczek, Phys. Rev. D **59**, 054502 (1999); M. P. Lombardo, hep-lat/9908006.
[10] S. Hands, J. Kogut, M. P. Lombardo, and S. Morrison, Nucl. Phys. **B558**, 327 (1999).
[11] S. Chandrasekharan and U. Wiese, Phys. Rev. Lett. **83**, 3116 (1999).
[12] X. Q. Luo and Q. Chen, Phys. Rev. D **46**, 814 (1992); Q. Chen and X. Luo, *ibid.* **42**, 1293 (1990).
[13] J. Bjorken and S. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York); P. Roman, *Advanced Quantum Theory* (Addison-Wesley, New York).
[14] J. Smit, Nucl. Phys. **B175**, 307 (1980); J. Greensite and J. Primack, *ibid.* **B180**, 170 (1981).
[15] S. Guo, J. Liu, and Q. Chen, Commun. Theor. Phys. **3**, 575 (1984).
[16] A. Le Yaouanc, L. Oliver, O. Pene, J. Raynal, M. Jarfi, and O. Lazrak, Phys. Rev. D **37**, 3691 (1988); **37**, 3702 (1988).
[17] R. Aloisio, V. Azcoiti, G. DiCarlo, A. Galante, and A. Grillo, Nucl. Phys. **B564**, 489 (2000).
[18] F. Klingl, N. Kaiser, and W. Weise, Nucl. Phys. **A624**, 527 (1997); QCD-TARO Collaboration, Nucl. Phys. B (Proc. Suppl.) **73**, 477 (1999).
[19] X. Q. Luo and Q. Chen, Mod. Phys. Lett. A **11**, 2435 (1996); X. Q. Luo, Q. Chen, S. Guo, X. Fang, and J. Liu, Nucl. Phys. B (Proc. Suppl.) **53**, 243 (1997).
[20] H. Jirari, H. Kröger, X. Q. Luo, and K. Moriarty, Phys. Lett. A **258**, 6 (1999).