Chemical potential on the lattice

R. V. Gavai
Physics Department, Brookhaven National Laboratory, Upton, New York 11973
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Imposing a physically desirable constraint, we obtain a class of lattice actions for nonzero chemical potential. Unfortunately, none of them lead to a real fermion determinant in general.

I. INTRODUCTION

Investigations of quantum chromodynamics (QCD) under unusual conditions, such as at finite temperature or finite densities, are of a great interest by themselves. Furthermore, one expects these studies to lead to important consequences for ultrarelativistic heavy-ion collisions[1] and the early universe.[2] Introduction of the lattice regularization[3] of QCD and the Monte Carlo methods[4] to simulate it have yielded a wealth of information at finite temperature,[5] including the prediction of a phase transition at a temperature $T_c \simeq 200$–250 MeV. Most of these calculations were performed in a world with zero net baryon number, i.e., with chemical potential $\mu = 0$, and it appears natural that one extends this only known method of obtaining nonperturbative results in QCD to $\mu \neq 0$ as well.

One encounters problems,[6,7] however, in introducing the chemical potential on the lattice; even for an ideal gas of quarks, which should be the $\mu \to \infty$ limit of QCD, physical quantities such as the energy density diverge quadratically in the continuum limit. The divergence is not a lattice artifact. Indeed, it is present in the continuum theory itself. There one uses some prescription to get rid of it, e.g., in the contour method[8] one throws away the contributions of the contour integrals at infinity. On the lattice one has the freedom of choosing the action, which can be exploited as an appropriate prescription. The remedies proposed in the literature to get rid of the above-mentioned divergence[6,7,9] have done precisely that. The modified actions still have a drawback from the point of view of numerical simulations: They lead to a complex fermion determinant in general, whereas all the methods[5] known so far to perform a full calculation need a real determinant. One, therefore, needs either a better form of action or a cleverer method of numerical simulation. Starting from a general form I obtain a class of actions by requiring that it yield well-behaved physical quantities. The proposals made earlier[6,7,9] fall in this general class, enabling us to understand why they work despite their differences. On the other hand, all these actions still give rise to a complex determinant. A better strategy of numerical simulation which will be able to deal with a complex determinant therefore appears necessary for realistic numerical calculations with $\mu \neq 0$.

II. A CLASS OF ACTIONS FOR $\mu \neq 0$

Let us start with a general fermionic action for an ideal quark gas with $\mu \neq 0$:

$$S_F = \tfrac{1}{2}\bar{\psi}(x)\Bigg\{\sum_{\mu=1}^{3}[(r+\gamma_\mu)\delta_{x,x'-\hat{\mu}} + (r-\gamma_\mu)\delta_{x,x'+\hat{\mu}}] + \frac{a_\sigma}{a_\beta}[(r+\gamma_0)\delta_{x,x'-\hat{0}} f(\mu a_\beta) + (r-\gamma_0)\delta_{x,x'+\hat{0}} g(\mu a_\beta)] + 2ma_\sigma\delta_{x,x'}\Bigg\}\psi(x') \quad . \tag{1}$$

Our notation is a fairly standard one. a_σ and a_β are the lattice spacings in the space and time directions, respectively. If $r = 0$, S_F describes naive (or, after appropriate transformations,[10] staggered) fermions, whereas $r = 1$ defines Wilson fermions. We will choose below $r = 0$ for the sake of clarity and come back to other cases at the end. Choosing

$$f(\mu a_\beta) = e^{\mu a_\beta}, \quad g(\mu a_\beta) = e^{-\mu a_\beta} \quad , \tag{2}$$

one obtains the action proposed in Refs. 6 and 9, while

$$f(\mu a_\beta) = (1+\mu a_\beta)/(1-\mu^2 a_\beta^2)^{1/2} \quad ,$$
$$g(\mu a_\beta) = (1-\mu a_\beta)/(1-\mu^2 a_\beta^2)^{1/2} \tag{3}$$

yields the action of Ref. 7, where it is also shown that

$$f(\mu a_\beta) = 1+\mu a_\beta \quad ,$$
$$g(\mu a_\beta) = 1-\mu a_\beta \tag{4}$$

is the straightforward, naive choice to introduce the chemical potential. As mentioned earlier, the last choice leads to quadratic divergences, however. Note also that $f(0) = g(0) = 1$ in all the cases. I will retain this obvious condition for f and g below.

The partition function Z for the ideal quark gas is given by

$$Z = \int \prod_x d\psi(x)\, d\bar{\psi}(x) e^{-S_F} \quad , \tag{5}$$

and the energy density can be obtained from it by using

$$\epsilon = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln Z\Big|_{\substack{V=\text{const}\\ \beta\mu=\text{const}}} \quad , \tag{6}$$

where V is the volume of the system and $\beta^{-1} = T$ is its temperature. If the lattice has N_σ sites in each space direction and N_β sites in the time direction, then $V = N_\sigma^3 a_\sigma^3$ and

$\beta = N_\beta a_\beta$ and Eq. (6) becomes

$$\epsilon = -\frac{1}{N_\beta N_\sigma^3 a_\sigma^3}\frac{\partial}{\partial a_\beta}\ln Z\Big|_{\substack{a_\sigma=\text{const}\\ \mu a_\beta=\text{const}}} . \tag{7}$$

Carrying out the integration in Eq. (5) exactly, one obtains the following expression for $\ln Z$ in momentum space (see Ref. 7 for more details):

$$\ln Z = \sum_p \ln \det \Delta_p , \tag{8}$$

where

$$\Delta_p = i\sum_{\mu=1}^{3}\gamma_\mu \sin p_\mu a_\sigma + \frac{a_\sigma}{a_\beta}\left[\frac{f(\mu a_\beta)-g(\mu a_\beta)}{2}\right]\gamma_0 \cos p_0 a_\beta + i\frac{a_\sigma}{a_\beta}\left[\frac{f(\mu a_\beta)+g(\mu a_\beta)}{2}\right]\gamma_0 \sin p_0 a_\beta + m a_\sigma \tag{9}$$

and

$$p_i a_\sigma = \frac{2\pi j_i}{N}, \quad p_0 a_\beta = \frac{2\pi(j_0+\frac{1}{2})}{N_\beta} ,$$

with

$$j_i = 0, \pm 1, \pm 2, \ldots, \pm\frac{N_\sigma}{2}$$

and

$$j_0 = 0, \pm 1, \ldots, \pm\frac{N_\beta}{2} .$$

Let

$$\frac{f+g}{2} = R\cosh\theta$$

and

$$\frac{f-g}{2} = R\sinh\theta . \tag{10}$$

Then $R = \sqrt{f\cdot g}$ and

$$\tanh\theta = (f-g)/(f+g) \tag{11}$$

and

$$\Delta_p = i\sum_{\mu=1}^{3}\gamma_\mu \sin p_\mu a_\sigma + \frac{a_\sigma}{a_\beta} i\gamma_0 R\sin(p_0 a_\beta + i\theta) + m a_\sigma .$$

Using Eqs. (7) and (8) one obtains, for $a_\sigma = a_\beta = a$,

$$\epsilon = \frac{4}{N_\sigma^3 N_\beta a^4}\sum_p\left[\frac{R^2\sin^2(p_0 a + i\theta)}{R^2\sin^2(p_0 a + i\theta) + \sum_{\mu=1}^{3}\sin^2 p_\mu a}\right] . \tag{12}$$

Letting $N_\beta \to \infty$ at fixed a to achieve $T=0$ in the expression above and subtracting the vacuum contribution ($\mu = 0$) from it, one obtains the energy density for $\mu \neq 0$, $T=0$:

$$\epsilon = \frac{4}{a^4 N_\sigma^3}\sum_{\mathbf{p}}\frac{1}{2\pi}\int_{-\pi}^{\pi} d(p_0 a_\beta)\left[\frac{R^2\sin^2(p_0 a + i\theta)}{R^2\sin^2(p_0 a + i\theta) + \sum_{\mu=1}^{3}\sin^2 p_\mu a} - \frac{\sin^2 p_0 a}{\sin^2 p_0 a + \sum_{\mu=1}^{3}\sin^2 p_\mu a}\right] . \tag{13}$$

The integrals in Eq. (13) can be evaluated by introducing the contour in Fig. 1 and one obtains

$$\epsilon a^4 = \frac{4}{N_\sigma^3}\sum_{\mathbf{p}}\left[\frac{1}{2\pi}\oint_c \frac{R^2\sin^2 p_0 a}{R^2\sin^2 p_0 a + \sum_{\mu=1}^{3}\sin^2 p_\mu a} d(p_0 a) - \frac{1}{2\pi}\int_{\pi+i\theta}^{\pi}\frac{R^2\sin^2 p_0 a}{R^2\sin^2 p_0 a + \sum_{\mu=1}^{3}\sin^2 p_\mu a} d(p_0 a)\right.$$
$$\left. - \frac{1}{2\pi}\int_{-\pi}^{-\pi+i\theta}\frac{R^2\sin^2 p_0 a}{R^2\sin^2 p_0 a + \sum_{\mu=1}^{3}\sin^2 p_\mu a} d(p_0 a)\right]$$

$$= \frac{4}{N_\sigma^3}\sum_{\mathbf{p}}\left\{\left[\frac{\sum_{\mu=1}^{3}\sin^2 p_\mu a}{R^2 + \sum_{\mu=1}^{3}\sin^2 p_\mu a}\right]^{1/2}\Theta\left[\frac{f(\mu a)-g(\mu a)}{2} - \left(\sum_{\mu=1}^{3}\sin^2 p_\mu a\right)^{1/2}\right] + \left[\frac{\sum_{\mu=1}^{3}\sin^2 p_\mu a}{1+\sum_{\mu=1}^{3}\sin^2 p_\mu a}\right]^{1/2} - \left[\frac{\sum_{\mu=1}^{3}\sin^2 p_\mu a}{R^2 + \sum_{\mu=1}^{3}\sin^2 p_\mu a}\right]^{1/2}\right\} . \tag{14}$$

In the limit $a \to 0, N_\sigma \to \infty$ ($V = \text{const}$) the first term contributes only if

$$f(\mu a) - g(\mu a) \propto \mu a \quad \text{for small } \mu a .$$

In all other cases it does not contribute at all. On the other hand, the other two terms contribute always in this limit and, as can be easily verified, lead to divergences, unless $R = 1$. The conditions for obtaining $\epsilon = 16\mu^4/4\pi^2$ from Eq. (14) in the $a \to 0$ limit thus are

$$f(\mu a)g(\mu a) = 1 \tag{15}$$

and

$$f(\mu a) - g(\mu a) = 2\mu a + O(\mu^2 a^2)$$

or, equivalently [using Eq. (15)],

$$df(\mu a)/d(\mu a)|_{\mu a = 0} \neq 0 . \tag{16}$$

It may be noted that both the earlier proposals[6,7,9] to modify the action for $\mu \neq 0$ given by Eqs. (2) and (3) satisfy the conditions (15) and (16). Furthermore, we also see from Eq. (15) that if forward quark propogation is enhanced by a factor $f(\mu a)$, the forward propagation of antiquarks is dampened by a factor $1/f(\mu a)$, and that quarks winding around the temperature axis (for $T \neq 0$) an even number of times do not contribute to any μ dependence. This has been already pointed out by the authors of Refs. 6 and 9 for the choice of f and g given by Eq. (2). I just note here that it is more general.

I used naive (or staggered) fermions in deriving the conditions given by Eqs. (15) and (16). It is, however, easily checked that a similar analysis as above results in the same conditions for $r=1$ fermions (Wilson fermions) as well, although it may be more convenient there to use the method of Ref. 7 to obtain the energy density. Also, in both the $r=0$ and $r=1$ cases, these same conditions yield the correct number density in the limit $a \to 0$.

Introducing SU(N) gauge interactions in Eq. (1) and using Eq. (15), one has

$$S_F = \bar{\psi}_x Q_{xx'} \psi_{x'} \tag{17}$$

with

$$Q_{xx'} = \sum_{\mu=1}^{3} [(r+\gamma_\mu) U_x^\mu \delta_{x,x'-\hat{\mu}} + (r-\gamma_\mu) U_{x'}^{\mu\dagger} \delta_{x,x'+\hat{\mu}}] + \frac{a_\sigma}{a_\beta} \left[f(\mu a_\beta)(r+\gamma_0) U_x^0 \delta_{x,x'-\hat{0}} + \frac{1}{f(\mu a_\beta)} (r-\gamma_0) U_{x'}^{0\dagger} \delta_{x,x'+\hat{0}} \right] + 2m a_\sigma \delta_{xx'}$$
$$\equiv D_{xx'} + 2m a_\sigma \delta_{xx'} \ . \tag{18}$$

One notes that in general $\det Q$ is complex except for SU(2) theory, which has real determinant due to its following property:[11]

$$\sigma_1 U_1 \sigma_1 = U^\dagger \quad \forall U \in \mathrm{SU}(2) \ . \tag{19}$$

Since all the methods known so far[5] to include the determinant in Monte Carlo simulations require a real, positive-definite $\det Q$, none of the actions belonging to the class defined by Eqs. (15) and (16) will be suitable for obtaining numerical results with the full theory. $\det Q$ can be made real and positive definite (at least for $r=0$) by allowing $f(\mu a)$ to be complex and then by requiring

$$|f(\mu a)| = 1 \quad \forall \mu a \ . \tag{20}$$

However, this leads to an imaginary chemical potential.

III. CONCLUSION

The property of asymptotic freedom of QCD tells us that for large chemical potential μ, QCD matter will behave as an ideal gas of quarks. Physical quantities, such as energy density, evaluated for an ideal quark gas on the lattice diverge as the lattice spacing is made to vanish. This divergence, like its analog in the continuum theory, can be removed by a suitable prescription. Demanding that the continuum limit of these physical quantities be well behaved I obtained a general class of lattice action for $\mu \neq 0$. The existing specific proposals belong to this class, enabling one to understand why they achieve a similar effect despite their differences.

In the presence of SU(N) interactions, $N \geq 3$, none of these actions lead to a real, positive-definite fermion determinant, suggesting that new, more general methods are needed to simulate the full theory for $\mu \neq 0$.

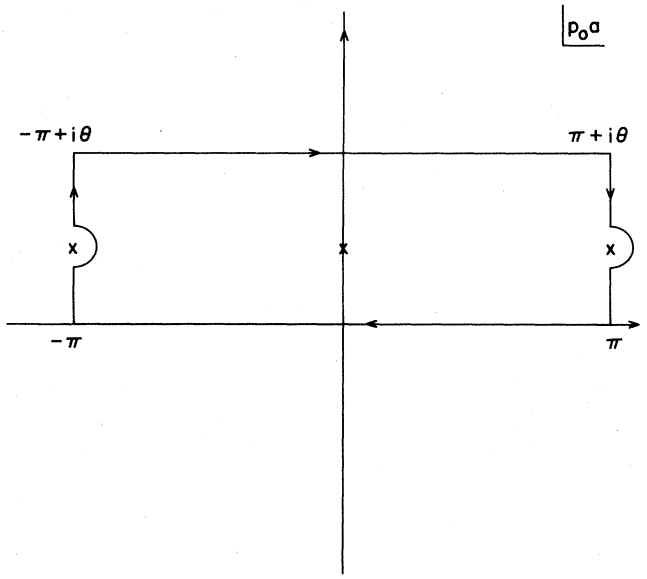

FIG. 1. The contour C used in Eq. (14). Poles of the integrand are denoted by ×.

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