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Imaginary chemical potential and finite fermion density on the lattice

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Standard lattice fermion algorithms run into the well-known sign problem with a real chemical potential. In this paper we investigate the possibility of using an *imaginary* chemical potential and argue that it has advantages over other methods, particularly for probing the physics at finite temperature as well as density. As a feasibility study, we present numerical results for the partition function of the two-dimensional Hubbard model with an imaginary chemical potential. We also note that systems with a net imbalance of isospin may be simulated using a real chemical potential that couples to I_3 without suffering from the sign problem. [S0556-2821(99)05203-0]

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I. INTRODUCTION

The behavior of fermions in the presence of a chemical potential is relevant to condensed matter physics (Hubbard model away from half-filling) and particle physics (high quark density systems such as the early universe, neutron stars, and heavy-ion collisions). Furthermore, a remarkably rich phase structure has been conjectured for QCD at finite temperature and density [1,2].

The only reliable nonperturbative approach to QCD is numerical Monte Carlo evaluation of the functional integral using a lattice regulator. Unfortunately, standard Monte Carlo methods become inapplicable at finite quark density, since in the presence of a real chemical potential the measure is no longer positive. One approach to this problem is the ‘‘Glasgow method’’ [3], in which the partition function is expanded in powers of $e^{\beta\mu}$, and the coefficients are evaluated by the Monte Carlo method using an ensemble of configurations weighted by the $\mu=0$ action. Simulations using this method have so far given unphysical results; namely, the lattice starts to fill with baryons at a chemical potential well below the expected value of one-third the baryon mass. It seems plausible that this happens because the $\mu=0$ ensemble does not overlap sufficiently with the finite-density states of interest, and so the true effects of quark loops will only be seen at exponentially large statistics [3].

In this paper we look at an alternative: evaluating the partition function at an *imaginary* chemical potential, for which the measure remains positive and standard Monte Carlo methods apply. The canonical partition functions can then be obtained by a Fourier transform [4,5]. Since the dominant source of errors is now the Fourier transform rather than the poor overlap of the measure, it seems worthwhile to explore the imaginary chemical potential as an alternative to the Glasgow method.

An outline of the paper is as follows. We give criteria that a theory should satisfy in order for Monte Carlo simulations at finite density to be feasible. We describe a toy model where even-odd effects become visible. We find some interesting examples (e.g., QCD at finite isospin density) where lattice simulations are possible. As a feasibility study, we perform Monte Carlo simulations for the two-dimensional Hubbard model with imaginary chemical potential and find that it is indeed possible to obtain the canonical partition functions at low particle number. At the rather high temperature and low interaction strength that we study, we see no sign of electron pairing.

II. CHEMICAL POTENTIAL AND POSITIVITY OF THE MEASURE

Consider a generic system of fermions ψ and bosons ϕ, where the fermion Lagrange density is $\bar{\psi}M(\phi)\psi$. On integrating out the fermions, the partition function becomes

$$Z=\int \mathcal{D}\phi\, e^{-S_{\mathrm{bos}}(\phi)} \det M(\phi). \tag{2.1}$$

In order to perform Monte Carlo simulations, it is necessary that the measure be non-negative; so we have either to restrict ourselves to the cases where $\det M \geqslant 0$ or to treat $\det M$ as an observable. The latter option is usually not viable, as $\det M$ tends to be a rapidly varying function of ϕ. We will discuss it again at the end of this section.

To guarantee that the measure is positive, we must generally have an even number of flavors, for each of which $\det M$ is real (but not necessarily positive). One situation where $\det M$ is real is when there exists an invertible operator P such that

$$M^{\dagger}=PMP^{-1}. \tag{2.2}$$

For a Wilson lattice fermion at zero chemical potential, this relation holds, with $P=\gamma_5$, so any even number of flavors can be simulated by the Monte Carlo method. With a real chemical potential, Eq. (2.2) breaks down, but with an imaginary chemical potential it is valid, and again simulations are possible for an even number of flavors.

There are more exotic situations where Eq. (2.2) holds. For example, consider two-flavor QCD with a finite density of isospin. In this case M has a block-diagonal structure

$$M(\mu)=\begin{pmatrix} L(\mu) & 0 \\ 0 & L(-\mu) \end{pmatrix}, \tag{2.3}$$

where μ is the chemical potential for the isospin and $L(\mu)$ is a Dirac operator for one flavor with chemical potential μ. Here $L(\mu)$ satisfies $L(\mu)^{\dagger}=\gamma_5 L(-\mu)\gamma_5$; hence, Eq. (2.2) is satisfied by setting

$$P=\begin{pmatrix} 0 & \gamma_5 \\ \gamma_5 & 0 \end{pmatrix}. \tag{2.4}$$

Here $\det M(\mu)=|\det L(\mu)|^2 \geqslant 0$. More generally, consider QCD with N_f flavors. It has a global vectorlike symmetry $G=\mathrm{U}(1)_B\times \mathrm{SU}(N_f)$, where $\mathrm{U}(1)_B$ is the baryon number. One may consider a nonzero chemical potential coupled to any generator T of G. Then Eq. (2.2) is satisfied for some choice of P if and only if the nonzero eigenvalues of T come in pairs $\lambda,-\lambda$. Thus $\det M$ is real for QCD at nonzero isospin density but not for nonzero hypercharge density or baryon number density.

Another case where $\det M$ is real even in the presence of the chemical potential is when there exists an invertible operator Q such that

$$M^{*}=QMQ^{-1}. \tag{2.5}$$

Examples of this sort are afforded by models with four-fermion interactions, such as the Hubbard model and the Gross-Neveu model. There M is a real operator, and so $\det M$ is real too. Other examples are gauge theories with ‘‘quarks’’ in the real or pseudoreal representation of the gauge group. Thus $\det M$ is real for SU(2) with quarks in the fundamental representation or for SU(3) with quarks in the adjoint, even when the chemical potential is nonzero.

In some cases with $\det M$ real, but not positive, it appears that one can perform simulations by treating the sign of $\det M$ as an observable. The Hubbard model can be treated in this way far below half-filling [6]. This is also the case for the Gross-Neveu model with a nonzero chemical potential [7]. Reference [7] further argues that $\det M$ is non-negative for most of the configurations; so one can simply replace $\det M$ with $|\det M|$. In QCD the phase of the determinant contains important physical information, but calculations have been performed without it [8].

III. IMAGINARY CHEMICAL POTENTIAL

The fact that the fermion determinant for QCD is real in the presence of an imaginary chemical potential $\mu=i\nu$ makes this an attractive option for exploring finite quark density. Simulations with an imaginary chemical potential are more or less equivalent to simulating a canonical ensemble. Indeed, the partition function for the imaginary chemical potential,

$$Z(i\nu)=\mathrm{Tr}\, e^{-\beta\hat{H}}e^{i\beta\nu\hat{N}}, \tag{3.1}$$

which is a periodic function of ν with period $2\pi/\beta$, is the Fourier transform of the canonical partition function

$$Z(N)=\frac{\beta}{2\pi}\int_0^{2\pi/\beta} d\nu\, Z(i\nu)e^{-i\beta\nu N}. \tag{3.2}$$

In principle, one can compute $Z(i\nu)$ on a lattice as a function of ν and then use Eq. (3.2) to obtain the canonical partition function. In practice, this method can work only for low enough N, because for large N the integrand in Eq. (3.2) is a rapidly oscillating function, and the error of the numerical integration will grow exponentially with N. The method fails completely in the thermodynamic limit $N\to\infty$. This need not discourage us, however, because in lattice simulations one is always working in a finite and rather small volume. The real question is how high we can push N before the numerical integration in Eq. (3.2) becomes undoable. We will consider the two-dimensional Hubbard model as a testing ground for this approach. Related work has been performed in Ref. [4], but without using the freedom to simulate at any ν (see below).

Having a positive measure is not the end of the story. In practice, we want to be able to use importance sampling to calculate $Z(i\nu)$ with reasonable accuracy. To this end we rewrite $Z(i\nu)$ in the following form:

$$\frac{Z(i\nu)}{Z(i\nu_0)}=\int \mathcal{D}\phi\, e^{-S_{\mathrm{bos}}}\det M(i\nu_0)\frac{\det M(i\nu)}{\det M(i\nu_0)}. \tag{3.3}$$

Now we treat the ratio of determinants as an observable and the rest as the measure. In the case of a real chemical potential, one would have to take $\nu_0=0$, and in this ensemble the ratio of determinants would reach its correct value only at very high statistics, through important but rare fluctuations as the mismatched measure occasionally sampled the regions where the integrand is large. For an imaginary chemical potential, however, the fluctuations can be made arbitrarily small by choosing ν_0 close to ν.

We can therefore use Eq. (3.3) to calculate the partition function for a range of ν around a reference value ν_0 and cover the range $\nu=0\cdots 2\pi/\beta$ with a set of ‘‘patches’’ each centered on a different ν_0. We can use as many patches as are required; so the measure will always overlap arbitrarily well with the observables.

Some qualitative features of the system can be inferred from the knowledge of $Z(i\nu)$ alone, without performing the Fourier transform. For example, consider a model of interacting fermions on a lattice (the example of the Hubbard model will be discussed further below). At some filling fraction the system may undergo a phase transition to a BCS superconducting phase. In that phase, the system will be populated with Cooper pair; so the partition function will be dominated by sectors in which the charge is a multiple of 2. This will be clearly visible in $Z(i\nu)$, which will not only be periodic with period $2\pi/\beta$, but acquire a significant subharmonic at period $2\pi/(2\beta)$. This would be a signal that for some range of densities the energy of the system has a minimum when the number of electrons is a multiple of 2.

This can be illustrated by a simple toy model containing a fermion with mass M_f and charge 1, and a boson with mass M_b and charge 2. If we make M_b less than M_f, then, assuming some very weak charge-conserving interactions that establish equilibrium, states of even charge will be favored.

The free energy is the sum of the fermion and boson contributions,

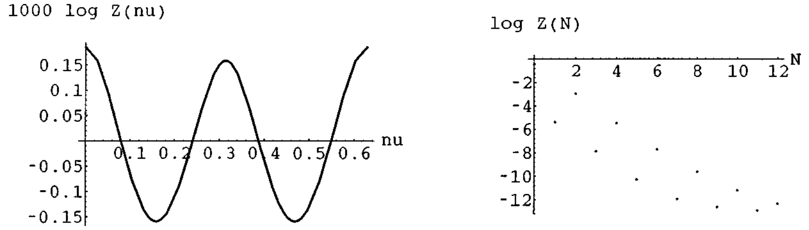

FIG. 1. Free energy as a function of imaginary chemical potential ν (left) and logarithm of the canonical partition function as a function of particle number (right) for our illustrative toy model (3.4), with $\beta = 10$, $\beta M_b = 1$, and $\beta M_f = 5$.

$$F(\mu,T) = F_{\text{fermion}}(M_f,\mu,T) + F_{\text{boson}}(M_b,2\mu,T), \quad (3.4)$$

where F_{fermion} and F_{boson} are the free energies of free fermions and bosons, respectively,

$$F_{\substack{\text{fermion}\\ \text{boson}}}(M,\mu,T) = \int \frac{d^3p}{(2\pi)^3} \pm \ln[1 \pm 2\cosh(\beta\mu) e^{-\beta E(p)} + e^{-i\beta E(p)}],$$

$$E(p)^2 = p^2 + M^2. \quad (3.5)$$

The pairing of fermions into bosons is clearly visible in $Z(N)$ (Fig. 1, for which $\beta = 10$) and also directly in $Z(i\nu)$, which is not only periodic with period $2\pi/\beta$, but also approximately periodic with a smaller period $2\pi/(2\beta)$. This is a signal that the energy of a system has a minimum when the number of particles is a multiple of 2. However, to infer the existence of an ''unpairing'' transition at high chemical potential, a visual inspection of the plot of $Z(i\nu)$ would not suffice: this information is encoded in the high-frequency behavior of the Fourier transform of $Z(i\nu)$.

IV. HUBBARD MODEL WITH IMAGINARY CHEMICAL POTENTIAL

At densities away from half-filling, the single-flavor Hubbard model has a real but not necessarily positive fermionic determinant [9]. Like QCD, the measure becomes positive at imaginary chemical potential. Since this model is of physical interest and also much less computationally demanding than QCD, it is interesting to use it to study the feasibility of performing simulations with an imaginary chemical potential. In fact, the model is so simple that for this initial investigation we were able to dispense with the usual hybrid Monte Carlo algorithm [9] for evaluating the fermion determinant and perform the whole calculation with the computer mathematics tool ''MATHEMATICA,'' using its ''Det'' function to calculate the fermionic determinants.

Using the formulation described above [see Eq. (3.3)], we calculated the partition function as a function of imaginary chemical potential ν. We used a $4^2 \times 10$ lattice with inverse temperature $\beta = 1.5$. (Lower statistics were also gathered on $4^2 \times 20$, to check that temporal discretization errors were under control.) The results are given in Fig. 2. By particle-hole symmetry, $Z(i\nu) = Z(-i\nu)$, and Z has period $2\pi/\beta$; so we only plot $\nu = 0$ to π/β.

Three ''patches'' were used (see Sec. III), centered at $\beta\nu_0 = 0$, $\pi/2$, and π. At the temperature we study, the error in $Z(i\nu)/Z(i\nu_0)$ rises rapidly with $|\nu - \nu_0|$; so it is crucial to use multiple patches to keep the statistical errors in $Z(i\nu)$ under control. In turn, via the Fourier transform, this controls the errors in $Z(N)$ for $N > 0$. In contrast, Ref. [4] only used $\nu_0 = 0$, which is adequate only for the small volume, low temperature, and low particle number ($N \leqslant 2$) they studied.

We then fitted $Z(i\nu)$ to various *Ansätze* and Fourier transformed them to obtain the canonical partition function Z_N (Fig. 3). Even using our very inefficient updating algorithm, we are easily able to get accurate results up to $N = 6$. The error bars reflect the statistical errors in the $Z(i\nu)$ data. We used fit functions of the form $Z(i\nu) = \exp(-a\nu^2) \times$spline.

It has been suggested that at some filling fraction the 2D Hubbard model may exhibit superconductivity, through pairing of the electrons, to form Cooper pairs, which then con-

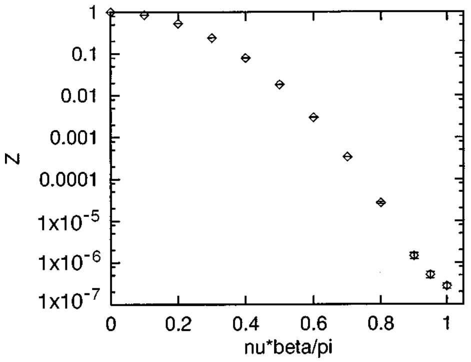

FIG. 2. Partition function for the 2D Hubbard model as a function of imaginary chemical potential ν, in units of π/β. This is on a $4^2 \times 10$ lattice, with $\beta = 1.5$, hopping term $K = 1$, and interaction strength $U = 0.1$, following the conventions of Creutz [9].

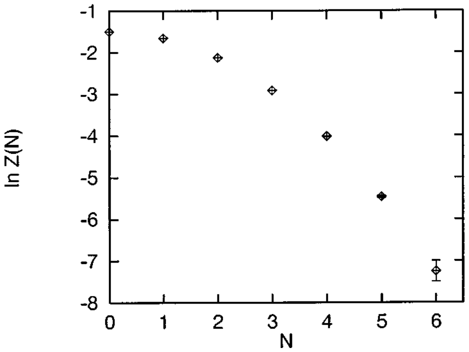

FIG. 3. Logarithm of the canonical partition function Z_N for the 2D Hubbard model, obtained by Fourier transform of $Z(i\nu)$ (Fig. 2).

dense. Along the lines described in Sec. III, we would expect such pairing to manifest itself as an even-odd periodicity of Z_N, leading to a characteristic extra bump in $Z(i\nu)$. At the temperature and coupling that we studied, we see no such evidence of pairing. Obviously, it would be very interesting to explore a wider range of parameters. This method might also be suitable for exploring the metal-insulator transition near half-filling, where the sign problem becomes particularly virulent [6]. As noted in Ref. [4], however, it will become much harder to extract the Z_N at low temperatures, where the $N=0$ contribution dominates $Z(i\nu)$. We should note that the Glasgow method has also been applied to the Hubbard model [10] to explore the scaling of Yang-Lee zeros. It would be interesting to make a systematic comparison of the relative merits of the two methods, for the Hubbard model as well as for QCD.

V. CONCLUSIONS

Let us conclude with a few remarks concerning the possible utility of imaginary chemical potential in QCD. An imaginary chemical potential does not systematically bias the ensemble to large density, so that to pick out the effect of states of nonzero baryon number density one must rely on fluctuations (which, when they occur, are appropriately weighted by the action). These fluctuations will occur most readily when the temperature is high and the gap in the baryon number channel is small. And even then one can only realistically hope, on the small lattices likely to be practical, to fluctuate to a few baryons. So a reasonable procedure would seem to be to start with a high temperature and work down, looking for qualitative changes as a function of temperature. In this way, one could realistically hope to use the methods described in this paper to study how properties of the quark-gluon plasma are affected by a net quark density. One could also study the deconfinement crossover, near which the baryons become light, and in particular locate the critical point in the T-μ plane predicted for two-flavor QCD [2,11]. All these phenomena are of immediate interest, since they will be explored in the next generation of heavy-ion collision experiments.

Another possibility is to work with large numbers of quark species, close to 16, so that the theory is perturbative. Then there is no mass gap to baryons, and so fluctuations are cheap, and also the contribution of interest, due to the quarks, is not swamped by gluons. In this case the cancellations may not be so bad even with a real chemical potential, and the imaginary chemical potential approach should also work better, since the fluctuations of interest will occur frequently.

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