Simulating Lattice QCD at Finite Density *

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Abstract

A new method of simulating systems with a complex action is applied to lattice QCD at finite density. At infinite gauge coupling we obtain a phase diagram which, in nice agreement with mean field theory, gives a critical value of the chemical potential unrelated to the baryon mass. At the same time we demonstrate explicitly the failure of the quenched approximation.

In this talk I would like to discuss an algorithm for the simulation of lattice QCD at finite density. In it's present form it grew out of earlier work by Bhanot et. al. [1]. I have tested the algorithm in the highly nontrivial case of infinite gauge coupling. The results are in agreement with mean field theory and beautifully demonstrate why the quenched approximation fails so miserably when applied to this problem.

The most elegant way of introducing a chemical potential on the lattice is to make the substitution [2] $U_0(x) \rightarrow e^{\mu} U_0(x)$ and $U_0{}^{\dagger}(x) \rightarrow e^{-\mu} U_0{}^{\dagger}(x)$ in the fermion matrix (I use Kogut-Susskind fermions)

$$M(x,y) = m\delta_{x,y} + \frac{1}{2}\sum_{\mu} \eta_{\mu}(x)(U_{\mu}(x)\delta_{y,x+\mu} - U_{\mu}{}^{\dagger}(y)\delta_{y,x-\mu}). \qquad (1)$$

Unfortunatly, this substitution leeds to a complex fermionic determinant. Since Monte Carlo methods require a positive definite measure they cannot be applied here.

The quenched approximation represents the most radical attempt at dealing with a complex determinant by setting it equal to one. This bold approach which works so well for most aspects of QCD unfortunately fails here. It was found [3], that contrary to our expectations chiral symmetry is restored for all values of μ greater than a critical value of $\mu_c = \frac{m_\pi}{2}$. This means in particular that as the quark mass $m \rightarrow 0$ chiral symmetry is restored for ***arbitrarily small*** μ. The expected result was $\mu_c = \frac{m_B}{3}$, m_B being the baryon mass.

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The algorithm that I use is a straight forward application of a general method for simulating systems with a complex action [5]. It is a descendant of the "spectral density method" to compute partition functions which was introduced in ref. [6]. A detailed study of the phase structure of lattice QCD using this method can be found in ref. [7]. The quantity of interest is the expectation value of an operator O

$$< O[U] >= \frac{1}{Z} \int [DU] |detM[U]| O[U] e^{\beta S_G + i\theta[U]}. \tag{2}$$

In (2), Z is the partition function, S_G is the pure gauge part of the action (I use the standard Wilson action), $\beta = \frac{1}{g^2}$ is the inverse of the gauge coupling and $e^{i\theta[U]}$ is the phase of the determinant. The integration is over the $SU(3)$ Haar measure. Introducing

$$\rho(E) = \int [DU] |detM[U]| \delta_P(\theta[U] - E) e^{\beta S_G}, \tag{3}$$

the expectation value (2) can be expressed as

$$< O >= \frac{\int_{-\pi}^{+\pi} dE < O >_M \rho(E) e^{iE}}{\int_{-\pi}^{+\pi} dE \rho(E) e^{iE}}. \tag{4}$$

In (3) $\delta_P(x)$ is a *periodic* delta function and $< O >_M$ stands for the "microcanonical" average

$$< O >_M (E) = \frac{1}{\rho(E)} \int [DU] |detM[U]| O[U] \delta_P(\theta[U] - E) e^{\beta S_G} \tag{5}.$$

In the following I will refer to $\rho(E)$ as the density of states. Note that it is by definition a *periodic* function of E with period 2π. To calculate (4) we need both (3) and (5). The interval $[-E_{min}, E_{max}]$ is split up into n_S overlapping sets of b bins each. The simulation is started by bringing the system into one of the edge sets. Configurations $\{U\}$, distributed according to $P(U)[DU] \sim |detM[U]| e^{S_G}[DU]$ are then generated. If the "energy" E of a configuration thus proposed falls into one of the bins in the edge set the configuration is accepted and the event recorded. If it does not, the configuration is rejected but the event is still recorded. After a specified number of hits one moves to the next set and the procedure is repeated. It is clear that one is basically performing a Monte Carlo simulation in each set. Hence the evaluation of the expectation value (4) is straight forward. After one has accumulated enough statistics in each set one still has to normalize the density of states. The relative normalization of two adjacent sets can be obtained from the counts in the overlap bin(s) and hence $\rho(E)$ can be determined up to an overall constant which cancels out in (4). At the end (4) is of course approximated by a Riemann sum or an appropriate higher order integration scheme is used. Because the algorithm basically

represents Riemann integration of a stochastically generated integrand I call the method the "Riemann Walk".

I still have to specify how I move between configurations. Note that both real and imaginary part of the determinant are needed after each link update. Hence an exact algorithm that recomputes the determinant after each accepted change is *absolutely essential.* I use the exact algorithm studied in ref. [8], which computes the change in the fermion determinant to a specified accuracy. So the way I move around in configuration space is the following: I start with an ordered configuration which has $E = 0$. Then I generate configurations using the exact update. The current value of the energy is computed by adding up the changes. The change in E is given by $\delta E = Im[clog(\delta(detM))]$ where *clog* is the FORTRAN complex logarithm. δE defined this way lives in the interval $[-\pi, \pi]$. Obviously this way the "energy" of the system can attain any desired value. But because we measure the energy mod 2π, the density of states will be periodic with period 2π, in agreement with its definition (3).

I have applied the above procedure to the case of infinite gauge coupling, i.e. $\beta = 0$. I employed 2^4 lattices with antiperiodic boundary conditions in the time direction and periodic in space. The lattice size may appear very small but remember that at infinite coupling all hadrons are pointlike and correlations are small. In the exact fermion update the conjugate gradient algorithm was used to compute the elements of the inverse of $M(x,y)$ which are needed in the computation of the change in the determinant. After each accepted change I recompute $\bar{\psi}\psi$. This quantity is estimated from the 6 diagonal elements of the inverse of $M(x,y)$ which are needed in the computation of the change in the determinant.

I ran the algorithm at three different values of the quark mass m, $m = 0.1$, $m = 0.2$ and $m = 0.4$. I did not use multiple Metropolis hits in the Metropolis part of the exact update. The links to be updated were chosen at random.

My simulations lead to the following picture. Away from the critical region the density of states is a highly peaked function whose width decreases with the volume. In this case quenched and unquenched averages agree within errors. By "quenched" averages I mean averages computed by dropping the phase in eq. (2,4). As we tune μ into the critical region the density of states begins to flatten out and quenched and unquenched averages no longer agree. This is because all points in the integration interval are equally important and the phase can no longer be neglected.

The phase diagram of strong coupling QCD that emerges from the numerical simulation is in good agreement with the predictions of mean field theory. This was also observed to be the case in SU(4) strong coupling lattice gauge theory [4]. Hence also in the case of color SU(3) with a fermionic baryon we do not see a threshold tied to the baryon mass as one might have guessed. Rather before this value is reached chiral symmetry is restored. If

mean field theory is correct in detail, this happens in a first order fashion. As observed in [4] this might be a strong coupling artifact. To check this we have to go to a finite g^2. This requires one to go to larger lattices. The growth with volume of the present algorithm is V^2 due to the use of the exact update. I should stress that there is nothing that prevents us from going to finite β except for the need of using larger lattices.

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