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MORE ON THE FIRST ORDER CHIRAL SYMMETRY TRANSITION IN QCD

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ABSTRACT

We present evidence from numerical simulations for a first order chiral symmetry restoration transition in QCD at finite temperature. Also, for quarks in the fundamental representation, there is a simultaneous deconfinement transition. These transitions are present only for small quark masses. We use an exact algorithm to incorporate the dynamical quarks.

In [1] we presented evidence for the chiral symmetry restoration and deconfinement transition at $6/g^2 = 4.9$ and $m_q = 0.025$. In this talk I shall present results at $6/g^2 = 4.95$. The work was done in collaboration with G. Guralnik, G. Kilcup, A. Patel and S. Sharpe at Los Alamos.

We are pursuing a program aimed at developing an algorithm efficient at small g and m_q . In particular we want to investigate how and when systematic biases become dominant in various approximate algorithms. To do this we have made extensive runs using the exact algorithm of Scalapino and Sugar [2] to act as a standard for comparison. The largest lattice on which this can be done with reasonable statistics is $4 \times 4 \times 4 \times 4$. In exploring the small quark mass limit we find evidence for the chiral transition. In this talk I will concentrate on this physics result. Due to the small lattice size, 4^4 , and the fact that $N_{spatial} = N_{time}$, we do not claim any quantitative results. Clearly, in a realistic finite temperature study, the transition temperature will be shifted. However, we think that the clarity of the signal of the transition in our data, together with our use of an exact algorithm, make our qualitative result interesting.

Simulations of pure gauge SU(3) show a strong first order transition at a temperature $T_c \approx \Lambda_{\overline{MS}}$ [3]. At this transition the global Z(3) symmetry of the theory is spontaneously broken. A non-zero expectation value of the Polyakov line $\langle L \rangle$ in the high temperature deconfined phase implies a finite free energy for the quarks. A second order parameter, the chiral condensate

$\bar{\chi}\chi$ measured in the quenched approximation, is also discontinuous at the transition. $\bar{\chi}\chi$, when extrapolated to $m_q = 0$, changes from a non-zero value at low T to zero in the high T phase.

Dynamical quarks act as external fields and explicitly break the $Z(3)$ symmetry. $\langle L \rangle$ is still a measure of the quark free energy but it is non-zero for all temperatures due to vacuum polarization. $\bar{\chi}\chi$ remains a good order parameter to study chiral symmetry. The only theoretical understanding of the realization of chiral symmetry comes from a renormalization group analysis of an effective spin model in $4 - \epsilon$ dimensions [4]. The conclusion is that QCD has a first order chiral symmetry transition for $N_f \geq 3$ and at $m_q = 0$. For $T < T_c$, one expects $\bar{\chi}\chi \neq 0$ when extrapolated to $m_q = 0$. For $T > T_c$ the chiral symmetry is restored, consequently $\bar{\chi}\chi \propto m_q$ for small m_q . This needs to be verified. Also, if, as in the pure gauge theory, there is a discontinuity in $\langle L \rangle$, then we expect to see interesting thermodynamical properties of the quark-gluon plasma [5] created in heavy ion collisions.

The expected phase diagram for QCD is as follows: The confinement transition at $m_q = \infty$ extends to some finite m_q in the $m_q - T$ phase plane, and similarly the chiral transition at $m_q = 0$ extends to some non-zero m_q . The questions to settle are whether these two transitions are connected and whether the chiral transition with the three physical light flavors is first order. The status of the chiral transition is not clear. We summarize the results for 4 flavors of staggered fermions obtained using approximate algorithms. The most detailed calculations are by Kogut *et al.* [6] who find a rapid crossover for $m_q = 0.1$ and 0.05 . They extrapolate the center of the cross-over to $m_q = 0$, and thereby estimate the transition coupling $6/g^2$ for $N_t = 6$ (4) to be 5.01 ± 0.025 (≈ 4.9). Further, assuming that asymptotic scaling is valid, they estimate the transition temperature to be $T_c = (2.14 \pm 0.1) \Lambda_{\overline{MS}}$. These results are obtained with both the micro-canonical and the hybrid algorithm. Similarly, Gavai, [7] does not find evidence for a first order transition using the pseudo-fermion algorithm. On the other hand, Fucito and Solomon [8] claim to see a first order transition at $m_q = 0.1$. They used perturbation theory to reduce the number of flavors to 3. Fukugita and Ukawa, [9] use the Langevin algorithm and also claim that at $m_q = 0.1$ the transition is already first order. The chief criticism against the last two calculations which found a hysteresis, i.e. two metastable states, has been that the runs were not long enough for complete thermalization. Also, the algorithm used to simulate fermions is different in each study so the reason for conflicting results may lie in the nature of the bias introduced due to the approximation.

In the exact algorithm the ratio of determinants $R \equiv \det(1 + M^{-1}\delta M)$ is calculated at each link update. Since we use staggered fermions (4 flavors), the algorithm requires a calculation of a 6×6 block of M^{-1} . Because M^{-1} is calculated with the conjugate gradient (CG) iterative algo-

Fig.1 Plot of a) 1×1 Wilson loop, b) $\langle L \rangle$ and c) $\bar{\chi} \chi$ with $\beta = 4.95$, $m_q = 0.05$ and $N_{cg} = 60$ versus Monte Carlo Sweeps.

rithm to some approximation, there can be a systematic bias. We discuss this later. In a Metropolis update, a link can be changed many times without having to recalculate M^{-1} . The multi-hit algorithm we use is that described in detail by Gavai and Gocksch [10]. We use antiperiodic boundary conditions in all directions. We update each link with 50 hits and the acceptance is adjusted to $\approx 30\%$. In solving $Ax_{even} = M^\dagger Mx_{even} = b$, we define the convergence by $C = \frac{\langle b - Ax | b - Ax \rangle}{\langle x | x \rangle}$, which depends on the number of CG iterations (N_{cg}).

In our data all the observables, $\bar{\chi}\chi$, $\langle L \rangle$, Wilson loops and R are correlated. In [1] we used $\bar{\chi}\chi$ to demonstrate that the transition for $m_q = 0.025$ exists at $6/g^2 = 4.9$. In Figs. 1 and 2 we show that with $N_{cg} = 60$ there is a transition for both $m_q = 0.05$ and $m_q = 0.025$ at $6/g^2 = 4.95$. The correlated flip-flops between the 2 states can be seen in $\bar{\chi}\chi$, $\langle L \rangle$ and in Wilson loops. So for $m_q = 0.05$, the transition appears between $6/g^2 = 4.9$ and 4.95 . Note that on increasing $6/g^2$, the physical temperature increases for fixed N_t and so does the quark mass when the bare lattice quark mass is held fixed. Thus, for any given constant m_q , and N_t we expect to go from the confined to the deconfined phase on increasing $6/g^2$. This is what we see with the transition remaining strongly first order. We also find that the nature of the transition is unchanged under changing the 3 spatial boundary conditions to periodic as shown in Fig 2c.

To further analyze the transition we study $\bar{\chi}\chi$ as a function of m_q . The estimates for $\bar{\chi}\chi$ in the two phases are shown in Fig. 3. In the confined phase we estimate $(\bar{\chi}\chi - 0.3) \propto m_q$ from the data at $6/g^2 = 4.9$. To study $\bar{\chi}\chi$ in the high temperature phase, we made runs with $N_{cg} = 60$ at $6/g^2 = 4.95$ and $m_q = 0.05, 0.025, 0.02$ and 0.015 . We find a flip-flop at the two heavier m_q , while the system is predominately in the deconfined phase at the two smaller m_q . The agreement with the expected behavior $\bar{\chi}\chi \propto m_q$ in the deconfined phase is good. Unfortunately, this behavior though significant is not sufficient proof of the order of the transition. Thus a corroboration on lattices with larger N_t and with $N_s \gg N_t$ is necessary. Further shortcomings of using Staggered fermions are that the flavor symmetry at finite lattice spacing is not $SU(n_f)$ and second the phenomenologically interesting case of 3 flavors is hard to achieve.

In [1] we presented an analysis of the systematic biases in our simulation. Our implementation of the CG algorithm tends to underestimate the effects of the fermions, i.e. it tends to give too small a value for $S \equiv |\ln(R)|$. We have studied this by changing a single link and comparing the exact R with that calculated with a variety of CG sweeps. The exact R is obtained by calculating the determinants, before and after changing the link, using gaussian elimination. To study if there is an accumulation of the bias, we compare the product of the accepted determinant ratios ($A \equiv \ln R_{acc}$) with

Fig.2 Plot of a) $\langle L \rangle$, b) $\bar{\chi} \chi$ with anti-periodic b.c. in all directions and c) $\bar{\chi} \chi$ with periodic b.c. in space --- at $\beta = 4.95$, $m_q = 0.025$ and $N_{eq} = 60$ versus Monte Carlo Sweeps.

the exact answer (T).

The bias at $6/g^2 = 4.95$ is similar to that at 4.9. The disagreement between A and T gets progressively worse with decreasing N_{CG} , but C is consistently a factor of ≈ 20 smaller in the high temperature phase. Conversely, the bias decreases as m_q increases. We again find that $C \leq 10^{-7}$ is necessary to avoid a bias at $m_q=0.025$ in both phases.

In Fig. 4 we show a distribution of the generated values of R and those accepted in the Metropolis algorithm. We expect this distribution of R to be a gaussian for a single link change in a fixed environment. That this is still approximately true when averaged over all links, as shown by the data, suggests that in a local update algorithm, the environment of any link is well described by a mean field approximation. Some properties of the distribution of the generated values of R are; 1) the mean which is always less than one becomes smaller and 2) the width increases with decreasing quark mass and increasing $6/g^2$. However, the change is small on going from $m_q = 0.05$ to $m_q = 0.015$. The relevance of this data is that for a method that gives an unbiased estimator for R to be efficient, the spread of the estimate must be smaller than the narrow width shown.

Fig.3 Plot of $\bar{\chi}\chi$ versus the bare quark mass in lattice units. The expected chiral behavior is seen in both phases.

Fig.4 Distribution of the value of R generated at each hit per link update. Also shown is the distribution of R for the hits accepted in the Metropolis algorithm. The data is at $\beta = 4.95$, $m_q = 0.025$ and $N_{cg} = 60$.

To conclude, we present evidence that there does exist a first order chiral/thermal transition at small m_q . Since hadronic matter at high temperature and density is expected to undergo a transition to quark-gluon plasma, which can be checked by the planned heavy ion experiments, it is therefore very important to understand the nature of the transition and determine the transition temperature. Further, a first order transition in standard cosmology (thermal history) would dump entropy and affect the cosmological constant unless it occurs without appreciable supercooling. Thus one needs to know the transition rate. I hope these questions can be addressed by future lattice calculations.

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