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ON THE FINITE TEMPERATURE TRANSITION OF QCD

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ABSTRACT

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What happens to Quantum Chromodynamics (QCD) as the temperature is increased? Is there a phase transition to a quark-gluon plasma, and if so what is its order? Despite much work, the answers to these questions remain controversial for the realistic case of very light u and d quarks and an intermediate mass s quark. In this letter we present evidence from numerical simulations suggesting the presence of a strong first order phase transition at finite temperature for such quark masses.

The significance of this result is twofold. First, planned heavy ion experiments will be able to investigate hadronic matter at temperatures up to a few hundred MeV. The signature of a transition to a plasma phase depends upon the order of the transition and upon its properties [1]. Second, as the early universe cools down it passes through the transition. If the transition is first order, entropy production reduces the baryon to photon ratio. Furthermore, a first order transition changes the vacuum energy density and thus the cosmological constant. More exotic scenarios, such as neutron-proton separation [2], also depend crucially on the order and strength of the transition.

Our results have been obtained using an exact algorithm to incorporate the dynamical fermions. The advantage of this algorithm is that one need make no extrapolations in a step parameter, reducing the possibility of systematic errors. The disadvantage is that the algorithm is very slow, and can only be applied on the smallest non-trivial lattice— 4×4^3 for staggered fermions. Although this lattice is small, previous results suggest that it provides a reliable guide to the bulk thermodynamic behavior of the theory. Indeed, our earlier results with four light flavors of quarks on this size lattice [3] [4], which found evidence for a first order transition, have been confirmed by results on larger asymmetric lattices [5] [6]. Because of this success, we have extended our calculations so as to address the questions raised above. Of course, since we use a symmetric lattice, we cannot measure the latent heat or other thermodynamical quantities. Thus we concentrate on studying the order of the transition.

Let us first review the expectations for the phase diagram of a theory simpler than QCD: $SU(3)$ gauge theory with n_f degenerate flavors of quarks. The parameters are the quark mass m_q and the temperature T . For $m_q = \infty$ the theory reduces to pure gauge $SU(3)$. There is considerable numerical evidence [7] that this theory has a first order deconfinement transition. The Polyakov line $\langle L \rangle$ is the order parameter for this transition, vanishing below the transition temperature T_c , but having a non-zero value above. The global $Z(3)$ symmetry of the pure gauge theory is spontaneously broken above T_c . Quarks with finite mass act as external fields coupled to $\langle L \rangle$, and their inclusion weakens the transition. The $Z(3)$ symmetry is explicitly broken, so $\langle L \rangle$ is never zero, but it is still discontinuous at the transition, and thus remains an indicator that the transition is associated with deconfinement. As m_q decreases it is possible that the transition vanishes, allowing an analytic connection between confined and deconfined phases. Also possible is

that the transition joins continuously onto the chiral transition, which we now discuss.

For $m_q = 0$ the theory possesses an exact $SU(n_f) \times SU(n_f)$ chiral symmetry. For high T there is an additional approximate axial $U(1)$ symmetry. It is believed that these symmetries are spontaneously broken at low temperatures, but are restored above a critical temperature. The order parameter for this chiral transition is $\langle \bar{\chi}\chi \rangle$, which is non-zero only below T_c . An ϵ -expansion suggests that the transition is first order for $n_f \geq 3$, but may be first or second order for $n_f = 2$ [8]. For $n_f = 3$ this conclusion is supported by a calculation using an approximate renormalization group equation [9]. Quark masses explicitly break the chiral symmetry, and weaken the transition. At strong gauge coupling, in a Hamiltonian treatment of the $n_f = 2$ theory [10], and in both Hamiltonian and Lagrangian treatments of the $n_f = 4$ theory [11], the chiral transition is of second order. Turning on m_q removes the transition, and the high and low temperature phases are analytically connected at finite quark mass. As the gauge coupling decreases, however, it is possible that the transition extends out to finite m_q . For finite m_q , $\langle \bar{\chi}\chi \rangle$ is always non-zero, but may be discontinuous across a transition. If so, this would signify that the transition is associated with chiral symmetry breaking. In fact, if chiral symmetry breaking is driven by confinement, as is suggested by all present evidence, then it may be that, for weak enough gauge coupling, the chiral phase transition line matches onto the deconfinement transition line, cutting the phase plane in two.

The crucial issue for QCD is whether, for quarks with the actual masses observed in nature, the transition is first order, second order or not present at all. We address this first by ignoring the strange quark, and the differences in mass between up and down quarks, and asking whether for $n_f = 2$ with small m_q there is a transition. Even if our quarks are somewhat heavier than the physical quarks, if we find a transition, as we do, it seems very likely that the transition will strengthen for smaller m_q , and thus apply to the physical masses.

It is most likely that the addition of the strange quark to the dynamics will not change this conclusion. The success of PCAC for processes involving Kaons implies that the strange quark is light enough to have a significant remnant of the chiral symmetry. Nevertheless, it is possible that the strange quark could smooth out the transition. We have addressed this issue indirectly by studying the $n_f = 4$ theory with masses close to the strange quark mass. We find that the first order transition found for $m_q \ll m_s$ remains for $m_q \sim m_s$. In fact we have preliminary evidence that the transition joins the deconfinement transition line. These results show that 4 flavors of strange quarks do not destroy the chiral transition, and thus strongly suggest that the addition of a single strange quark will not significantly effect the first order transition found for the up and down quarks.

In recent months there have been many results addressing similar issues. However

these results, all of which are obtained using approximate algorithms, are in conflict over the points addressed here. We restrict ourselves in this discussion to staggered fermion data with $N_t = 4$, which is the bulk of the data. For $n_f = 2$, Gottlieb *et al.* [6] see no clear evidence of a transition for $m_q a = 0.0125 - 0.2$. In contrast, Kogut and Sinclair [12] find a first order transition for $m_q a = 0.0125$, but no transition for $m_q a = 0.025$. However, Gavai *et al.* [13] do find a transition for $m_q a = 0.025$, while Fukugita *et al.* [14] see one for $m_q a = 0.1$. We should also mention that Gavai *et al.* [15] have found that the transition is first order along an interpolation between $n_f = 2$ and $n_f = 3$ where two quarks are held at $m_q a = 0.025$, while the mass of the third is varied between 0.025 and ∞ . For $n_f = 4$, there is a transition for masses lighter than $m_q a = 0.05$, but for $m_q a = 0.05 - 0.1$ the evidence is ambiguous [6][16]. For still heavier masses, $m_q a = 0.2 - 0.5$, [6][16] appear to see no transition. They interpret this as the appearance of the gap between chiral and deconfinement transition lines.

Given these disagreements between the results from approximate algorithms, we think that it is particularly important to study the question using an exact algorithm [17]¹. We use the algorithm of Scalapino and Sugar [18], in which the ratio of determinants, $R \equiv \det(1 + M^{-1}\delta M)$, is calculated at each link update. Here M is the staggered fermion Dirac operator. Due to species doubling, this operator automatically describes four degenerate flavors of fermions in the continuum limit. Thus one can change the number of flavors by using $R^{n_f/4}$ in the Boltzmann factor of the Metropolis update. We comment on this naive prescription below.

The particular implementation of the algorithm we use is that described in detail by Gavai and Gocksch [19]. 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 $Ax_{\text{even}} = M^\dagger Mx_{\text{even}} = b$, we define the convergence by $C = \frac{\langle b - Ax | b - Ax \rangle}{\langle x | x \rangle}$. C depends on the number of conjugate gradient CG iterations (N_{cg}). By using $N_{cg} = 30, 60$ and 90 and observing flip-flops in all cases, we rule out the possibility that the order of the transition is affected by the systematic bias due to incomplete convergence of M^{-1} [3]. Also, we have found that periodic boundary conditions in the spatial directions give similar results [4].

We have made extensive runs with two flavors at $m_q a = 0.02$. We observe flip-flops and metastability for $\beta = 5.21, 5.23$ and 5.25 . The discontinuities are visible in $\langle \bar{\chi}\chi \rangle$ and $\langle L \rangle$, as well as in Wilson loops. They are also clear in R , and in the convergence C for fixed N_{cg} . The transitions are between a high temperature state with large $\langle L \rangle$, small $\langle \bar{\chi}\chi \rangle$ and larger Wilson loops, and a low temperature phase with small $\langle L \rangle$, large $\langle \bar{\chi}\chi \rangle$ and smaller Wilson loops. In all these variables the jumps are correlated, but the cleanest signal is in

¹ The value of $\langle \bar{\chi}\chi \rangle$ quoted in [3] and [4] and in this reference was inadvertently that per color. Thus it should be multiplied by 3 to compare with the results of [5], and by 1.5 to compare with [6]. In this paper we use the standard normalization of [5]

$\langle \bar{\chi}\chi \rangle$. This we show in Fig. 1 for $\beta = 5.21, 5.23$ and 5.25 . Our estimate of the critical coupling is ≈ 5.23 . We consider the fact that the system performs a flip-flop, i.e. jumps from one phase to the other, and then back again, as strong evidence for two states and a first order transition. The discontinuities in observables are large, in fact comparable to the those seen for $n_f = 4$. This suggests that the transition will remain for considerably larger quark masses, as we find below for $n_f = 4$. This is consistent with the transition seen at $m_q a = 0.1$ by Ref. [14].

We now turn to our $n_f = 4$ data. Here we display $\langle \bar{\chi}\chi \rangle$, and the 1×1 Wilson loop for $m_q a = 0.025$ (Fig. 2), $m_q a = 0.05$ (Fig. 3), $m_q a = 0.1$ (Fig. 4) and $m_q a = 0.2$ (Fig. 5). For each mass, β_c is chosen to maximize the discontinuity in observables. In fact, the discontinuity in $\langle L \rangle$ is roughly constant over the width of the transition region, so β_c is determined by $\langle \bar{\chi}\chi \rangle$. It turns out that this criterion puts β_c very close to the low β end of the transition region.

At all four masses the system shows sharp transitions between two states, with all but $m_q a = 0.2$ data displaying flip-flops. We take these results to indicate that there is a first order transition characterized by deconfinement and chiral symmetry breaking at all these masses. As further evidence of this, we show in Fig. 6 the behavior of $\langle \bar{\chi}\chi \rangle$ as a function of $m_q a$. In the confined phase we estimate $(\langle \bar{\chi}\chi \rangle - 0.9) \propto m_q$. The intercept is clearly non-zero, consistent with chiral symmetry being broken. In the high temperature phase, on the other hand, the data is consistent with $\langle \bar{\chi}\chi \rangle \propto m_q a$ for small $m_q a$.

An important feature of the data is that the discontinuity in $\langle L \rangle$ is nearly the same for all values of m_q . The discontinuity in the Wilson Loop does decrease as m_q increases, but if one extrapolates it seems likely that the transition remains first order until at least $m_q a = .3$, and may extend to $m_q a = \infty$. Evidence for the latter option comes from runs with $m_q = \infty$, i.e. pure gauge $SU(3)$, on a 4^4 lattice. We find that $\beta_c \approx 5.6$, and that the discontinuity in $\langle L \rangle$ remains at about 0.15, i.e. very close to the value seen for finite quark masses. The Wilson loop jumps from $\sim .53$ to $\sim .55$ at the transition, a discontinuity smaller than that of about 0.05 seen in the figures.

We have checked these results using an alternative exact algorithm suggested in Ref. [20]. Our particular implementation uses Hybrid evolution to propose changes [21]. We have extended these runs to $N_s = 6, N_s = 4$ lattices. Preliminary results confirm the above scenario in the heavier mass region [22]. For $m_q a = 0.3$ we find $\beta_c \approx 5.3$, while for $m_q a = 0.5$ we have $\beta_c \approx 5.4$. If one plots these values on the $1/m_q - \beta$ plane, then they interpolate between the $m_q = \infty$ and small m_q results. This is consistent with there being a single phase line dividing the plane. We are continuing the calculation on larger N_t and N_s lattices using this algorithm.

To convert the values for m_q into physical units we use the preliminary result $T_c \approx 140$

MeV [23]. The region of interest for the strange quark is $m_q/T_c \approx 1$ ². Thus $m_q a = 0.2$, which gives $m_q/T_c = 0.8$, is close to m_s . If the transition remains out to $m_q = 0.3$ ($m_q/T_c = 1.2$), as our results strongly suggest, then we have encompassed the region of the strange quark mass.

We can think of at least three reasons why some of the previous calculations might have failed to see the transition at masses where we show flip-flops. First, in simulations using molecular dynamics or Langevin algorithms, a noisy estimate of $\langle \bar{\chi}\chi \rangle$ is made using pseudofermions. This should be compared to the exact algorithm, where during each sweep $\langle \bar{\chi}\chi \rangle$ is calculated 8 times on each site. In tests on our 4^4 lattices we find that the noisy estimator gives a distribution centered about the exact $\langle \bar{\chi}\chi \rangle$, but with a variance which increases with decreasing m_q . For $m_q a = 0.1$ the standard deviation is ≈ 0.25 , which is comparable to the discontinuity seen in Fig. 4. Thus for this and larger masses, large statistics would be required to resolve a first order transition using the noisy estimator. Second, the changes introduced by the finite step size approximation are not understood beyond lowest non-trivial order. It is possible that the shift in the parameters due to finite step size are different for the two states. Third, it is not clear how fast different algorithms move through configuration phase. Thus one does not know how long one has to run to see tunneling. Very long runs may be necessary, as found by Kovacs *et al.* [24] in their study of the $n_f = 4$ theory for $m_q a = 0.025$ on lattices with $N_t = 6$. Finally, there is the problem of the need to make subjective judgments; for example Gavai *et al.* [13] call the transition at $n_f = 2, m_q a = 0.025$ first order with a flip-flop, while Gottlieb *et al.* [6] are not sure if the transitions in their $n_f = 2$ data are genuine tunnelling events.

We close with a note of caution concerning the use of staggered fermions at such strong couplings. Away from $g = 0$, the staggered fermion symmetry group is $U(1) \times U(1)$ (plus some discrete parts), rather than $U(1) \times SU(4) \times SU(4)$. Thus it is possible that one is studying the chiral dynamics of the smaller group when one uses small N_t . Furthermore, it is no longer true that one can dial the number of fermions by dialing the power of the determinant, since the determinant does not factorize. Finally, for all n_f , $\langle \bar{\chi}\chi \rangle$ is calculated with a single species of staggered fermions, so that there are always four flavors of valence quarks, even though the numbers of dynamical quarks has been varied.

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² The current quark mass for the strange quark is ≈ 125 MeV at a scale of 1 GeV. We are evaluating m_s at a scale of about $4T_c \approx 400$ MeV, so m_s will be somewhat larger than this

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Figure Captions

- 1) Time history of $\frac{n_f}{4} \langle \bar{\chi} \chi \rangle$ at (a) $\beta = 5.21$ (b) $\beta = 5.23$ and (c) $\beta = 5.25$ versus Monte Carlo Sweeps for $m_q = 0.02$, $n_f = 2$ and $N_{cg} = 60$. The solid lines ($\times$ marks) are for cold (hot) starts. The tunneling is correlated in all observables.
- 2) Time history of (a) $\langle \bar{\chi} \chi \rangle$ (b) $\langle L \rangle$ and (c) 1×1 plaquette versus Monte Carlo Sweeps at $\beta = 4.95$, $m_q = 0.025$, $n_f = 4$ and $N_{cg} = 90$. The tunneling is correlated in all observables.
- 3) Same as Fig. 2 except at $\beta = 4.95$, $m_q = 0.05$, $n_f = 4$ and $N_{cg} = 60$.
- 4) Same as Fig. 2 except at $\beta = 5.04$, $m_q = 0.1$, $n_f = 4$ and $N_{cg} = 30$.
- 5) Same as Fig. 2 except at $\beta = 5.18$, $m_q = 0.2$, $n_f = 4$ and $N_{cg} = 30$.
- 6) $\langle \bar{\chi} \chi \rangle$ versus m_q for $n_f = 4$. The upper line is for the low T phase, the lower for the high T phase.

Fig.1: $m_q=0.02$ $n_f=2$ $N_{CG}=60$

Fig.2: $m_q=0.025$ $\beta=4.90$ $N_{CG}=90$

Fig.3: $m_q=0.050$ $\beta=4.95$ $N_{CG}=60$

Fig.4: $m_q=0.10$ $\beta=5.04$ $N_{CG}=30$

Fig.5: $m_q=0.20$ $\beta=5.18$ $N_{CG}=30$

Fig. 6