Tricritical scaling at the $N_t = 6$ chiral phase transition for 2 flavour lattice QCD with staggered quarks.

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Abstract

We have simulated lattice QCD directly in the chiral limit of zero quark mass by adding an additional, irrelevant 4-fermion interaction to the standard action. Using lattices having temporal extent of six and spatial extents of twelve and eighteen, we find that the theory with 2 massless staggered quark flavors has a second order finite temperature phase transition. The critical exponents $\beta_{\text{mag}}, \delta$ and $\nu$ are measured and favour tricritical behaviour over that expected by universality arguments. The pion screening mass is consistent with zero below the transition, but is degenerate with the nonzero $\sigma(f_0)$ mass above the transition, indicating the restoration of chiral symmetry.

12.38.Mh, 12.38.Gc, 11.15.Ha
There are several bottlenecks in the simulation studies of lattice field theories by standard algorithms [1], [2]. One of the most harmful is that the chiral limit cannot be simulated directly because the standard algorithms fail to converge in the limit of vanishing bare fermion mass and become prohibitively expensive at small quark masses. Various chiral transitions, such as the finite temperature Quantum Chromodynamics (QCD) transition to be discussed here, have been difficult to study quantitatively because of this. In particular, studies of critical scaling and the extraction of critical exponents have been especially difficult. This has led people to extract the critical exponents associated with the mass dependence of the heights and positions of susceptibility peaks [3,4] and to compare the scaling behaviour of the chiral condensate as both the coupling constant and the quark mass are varied [5], rather than studying the scaling of order parameters in terms of the coupling constant and mass independently. The most extensive data has been obtained for $N_t = 4$ where it differs significantly from what universality arguments predict.

These problems are largely solved by adding a four-fermi interaction to standard lattice actions with staggered fermions [6]. The resulting lattice action can be simulated directly in the chiral limit because an auxiliary scalar field $\sigma$ (essentially the chiral condensate $\langle \bar{\psi}\psi \rangle$) acts as a dynamical (‘constituent’) quark mass term insuring that the inversion of the Dirac operator will be successful and very fast. This approach is far more efficient and physical than the traditional lattice algorithm in which the chiral limit is singular and a nonzero bare quark mass $m$ is a necessity.

Using this strategy we have simulated lattice Quantum Chromodynamics (QCD) with two flavors of staggered quarks on $12^3 \times 6$ and $18^3 \times 6$ lattices, at zero quark mass, in order to determine the position and nature of the finite temperature transition. In addition to measuring the standard order parameters, we have measured the pion and $\sigma(f_0)$ screening masses to probe the nature of chiral symmetry restoration at this transition. We find that the two flavor theory experiences a second order chiral symmetry restoring phase transition. We make independent determinations of the critical indices $\beta_{\text{mag}}, \nu,$ and $\delta$. $\beta_{\text{mag}}$ differs
significantly from that of the $O(4)$ (or $O(2)$) sigma model in 3 dimensions, expected in the standard scenario of dimensional reduction and universality for this transition [4], but is in excellent agreement with that of the 3-dimensional tricritical point. Since we have found that the $N_t = 4$ transition is first order at $\gamma = 10$ [6] and a tricritical point would be expected to separate a line of first order transitions from a line of second order transitions, this suggests that this theory would have a normal critical point with the critical exponents expected from universality for $N_t \geq 8$. If so, the anomalous behaviour of the $N_t = 4, 6$ transitions is due to irrelevant terms in the lattice action which are important only on coarse lattices.

In this letter we review the ‘standard’ expectations and alternative scenarios for the finite temperature transition in continuum and lattice QCD. We review the lattice formulation of QCD with chiral four-fermion interactions, and present our data and fits. We end with discussions and conclusions, and directions for future research.

Dimensional reduction and universality predict that 2-flavour QCD has the critical behaviour of the 3-dimensional $O(4)$ sigma model [4]. This theory has a second order phase transition with critical indices [4], $\nu = .73(2), \beta_{mag} = .38(1), \delta = 4.82(5)$, etc. The lack of full flavour symmetry of the staggered fermion method is expected to reduce this to an $O(2)$ sigma model with critical indices $\nu = .71(2), \beta_{mag} = .35(1)\) and $\delta = 4.81(1)$ [4]. A breakdown of such arguments or the presence of lattice artifacts can produce a first order transition. If both a first and simple second order transitions are possible, so is a tricritical point for which $\nu = \frac{1}{2}, \beta_{mag} = \frac{1}{4}$ and $\delta = 5$ or 3, the second value being for a second independent symmetry breaking operator this more complex transition admits [10]. Finally, if dimensional reduction fails to occur, one would expect a mean field transition with $\nu = \frac{1}{2}, \beta_{mag} = \frac{1}{2}$ and $\delta = 3$.

This suggests that a direct measurement of $\beta_{mag}$, requiring simulations at $m = 0$ will be crucial in determining the nature of the finite temperature chiral transition in 2-flavour (lattice) QCD.

The lattice QCD action used in this study contains an additional chirally invariant
4-fermion interaction. Because the extra interaction is irrelevant, such an action should lie in the same universality class as the standard action. Ideally, such an interaction should be chosen to have the $SU(N_f) \times SU(N_f)$ flavour symmetry of the original QCD action. However, when one introduces auxiliary scalar and pseudoscalar fields to render this action quadratic in the fermion fields — which is necessary for lattice simulations —, the fermion determinant is no longer real, even in the continuum limit. Thus for 2-flavour QCD ($N_f = 2$), we make a simpler choice and choose a 4-fermion term with the symmetry $U(1) \times U(1) \subset SU(2) \times SU(2)$, where $U(1) \times U(1)$ is generated by $(\tau_3, \gamma_5 \tau_3)$, which preserves the symmetries of the lattice action. The euclidean Lagrangian density for this theory is

$$L = \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} (\not{D} + \sigma + i \pi \gamma_5 \tau_3 + m) \psi + \frac{\gamma N_f}{2} (\sigma^2 + \pi^2)$$

when we have introduced auxiliary fields $\sigma$ and $\pi$ to render it quadratic in the fermion fields. $\gamma \equiv 3/\lambda^2$, where the quartic term in the original Lagrangian had coefficient $\lambda^2/6N_f$. The molecular dynamics Lagrangian for a particular staggered fermion lattice transcription of this theory has been given in reference [6]. There we reported simulation results on lattices with $N_t = 4$ and discussed the choice of parameters as well as systematic errors. Here we shall discuss higher precision simulations on larger lattices, $18^3 \times 6$ and $12^3 \times 6$.

By doing simulations on two lattice sizes we were able to isolate finite volume effects in several observables and check that they had the behaviour expected of finite size scaling theory. We ran simulations at $\gamma = 10$ and 20 on a $12^3 \times 6$ and $\gamma = 20$ on an $18^3 \times 6$ lattice. We carefully checked that our results do not depend on $\gamma$ or on the lattice size. These technically important results will be discussed at greater length elsewhere [8].

Since our $m = 0$ lattice action does not single out a preferred chiral direction, we accumulate the magnitude of the order parameter, $\sqrt{\langle \bar{\psi} \psi \rangle^2 + \langle \bar{\psi} \gamma_5 \tau_3 \psi \rangle^2}$, rather than the order parameter itself, which averages to zero. This is not a true order parameter since it does not vanish identically in the symmetric phase. However, for a large system of volume $V$, its values in the high temperature phase are of order $1/\sqrt{V}$. In the low temperature phase
the order parameter can be fit to a standard critical form, $A(\beta_c - \beta)^{\beta_{mag}}$, if $\beta$ is chosen within the model’s scaling window near $\beta_c$. Of course, we cannot simulate the model with $\beta$ chosen too close to $\beta_c$ where the order parameter is very small, and finite size rounding in this effective order parameter is considerable. This forces us to work slightly away from the critical point and would produce indecisive results if the scaling window were particularly small. These potential problems bear close scrutiny.

The simulations of the lattice version of Equation 1 were performed using the hybrid molecular-dynamics algorithm with “noisy” fermions allowing us to tune $N_f$ to 2 flavours \cite{6}. The simulations on an $18^3 \times 6$ lattice were performed at 14 $\beta$ values from 5.39 to 5.45, the observed chiral transition occurring close to $\beta = 5.423$. This enabled us to fit order parameters in the scaling window on both sides of the transition. Runs at single $\beta$’s varied in length from 5,000 to 50,000 molecular-dynamics time units close to the critical point (this computer “time” is the same as that used in related works by other groups, such as \cite{11}). We were forced to make such lengthy runs because of critical slowing down. Order parameters measured included the local chiral condensates $\langle \bar{\psi} \psi \rangle$ and $\langle \bar{\psi} \gamma_5 \tau_3 \psi \rangle$, their counterparts in terms of the auxiliary fields viz $\langle \sigma \rangle$ and $\langle \pi \rangle$, the thermal Wilson line, the plaquette, and operators contributing to the partial entropies of each field. These were measured every 2 time units and binned to minimize the effect of correlations on error estimates. The molecular dynamics “time” increment for updating was $dt = 0.05$ \cite{8}. This was large enough that the order parameters $\langle \sigma \rangle$ and $\langle \pi \rangle$ have sizable $O(dt^2)$ errors. However, since these errors can be absorbed in a redefinition of the couplings in the action, they should not affect universality.

The data for the magnitude of the order parameter $\sqrt{\langle \bar{\psi} \psi \rangle^2 + \langle \bar{\psi} \gamma_5 \tau_3 \psi \rangle^2}$ is plotted against $\beta$ in Figure 1. The points between $\beta$ values of 5.41 and 5.4225 were fitted to a simple powerlaw $A(\beta_c - \beta)^{\beta_{mag}}$. The fit has a confidence level of 94 percent and determined the parameters $\beta_c = 5.4230(2)$, $a = 1.19(12)$ and, most importantly, the critical index $\beta_{mag} = 0.27(2)$, in good agreement with the 0.25 of the tricritical point, but inconsistent with the $O(4)$, $O(2)$, and mean field values.
We see in the figure that points at stronger coupling than $\beta = 5.41$ are outside the scaling window. For example, if the points at $\beta = 5.4$ and $\beta = 5.405$ were included in the fit, the confidence level would fall to 28 percent while the predicted best value for $\beta_{mag}$ does not change significantly. Our simulations on $12^3 \times 6$ lattices produced values for the order parameter which were essentially identical to those shown in the figure for $\beta \leq 5.4225$, but were considerably larger for $\beta > 5.4225$. Using the 2 lattice sizes to remove the finite volume
effects gave $\beta_{\text{mag}} = 0.24(2)$ consistent with the above. The data on the weak coupling side of the transition is, in fact, compatible with the finite size scaling prediction that the magnitude of the order parameter should fall to zero as $1/\sqrt{V_s}$, where $V_s$ is the volume of the spatial box. For the $12^3 \times 6$ lattice and $\gamma = 10$, our fits predicted $\beta_{\text{mag}} = 0.27(3)$, in good agreement with the $18^3 \times 6$, $\gamma = 20$ results, while $\beta_c = 5.4650(1)$.

A second independent critical index is $\delta$ which controls the size of the order parameter at the critical temperature as the quark mass is turned on with $\beta$ fixed at $\beta_c$. The order parameter should scale as $\langle \bar{\psi}\psi \rangle = am^{1/\delta}$. We accumulated data at quark masses ranging from 0.004 to 0.030, as shown in Figure 2 on a $12^3 \times 6$ lattice with the strength of the four fermi coupling set to $\gamma = 10$. (We repeated this for $\gamma = 20$.) Since the quark mass is different from zero in these simulations, the real order parameters $\langle \sigma \rangle$, $\langle \bar{\psi}\psi \rangle$ can be measured rather than their absolute values. Our best fit gives $a = 1.66(2)$ and critical index $\delta = 3.89(3)$. The fact that this fit has only a 4% confidence is due to the point at $m = 0.01$ which lies 2.5 standard deviations above the curve and is a problem for any smooth fit to the “data”. Its removal increases the confidence to 33% with negligible change in the parameters of the fit. This lies between 3 and 5, the $\delta$ values for the 2 leading symmetry breaking operators at the tricritical point. Since $\langle \bar{\psi}\psi \rangle$ could be expected to be a linear combination of these operators (and a third operator with $\delta = 1$ which is normally ignored), the more general scaling relation at $\beta = \beta_c$ is given by

$$\langle \bar{\psi}\psi \rangle = a\phi + \frac{1}{3}b\phi^3 + \frac{1}{5}c\phi^5$$

with $\phi$ the solution of

$$\phi^5 - m(a + b\phi^2 + c\phi^3) = 0$$

A fit to this form over the whole mass range yields $a = 1.05(2)$, $b = 2.5(4)$ and $c = -3.0(1.4)$. Although the confidence level of this fit is only 2%, removing the $m = 0.01$ point improves this to an acceptable 34%.
FIG. 2. The order parameter plotted against $m$ at criticality on a $12^3 \times 6$ lattice. The solid line is the fit $\langle \bar{\psi} \psi \rangle = am^{1/\delta}$.

The hadronic screening lengths determine the manner in which chiral symmetry is restored as we pass through the transition from hadronic matter to a quark-gluon plasma. Here we concentrate on the $\pi$ and $\sigma(f_0)$ propagators which can be calculated from the $\pi$ and $\sigma$ auxiliary fields. For these we stored the $\pi$ and $\sigma$ fields averaged over each $z$-slice of the lattice, every 2 time units. Because the orientation of the condensate changes continuously throughout the runs, we relabeled the component of these fields in the direction of the
condensate as $\sigma$ and the orthogonal component as $\pi$ for each configuration. These fields were then correlated to calculate the average $\sigma$ and $\pi$ screening propagators. The sum of these propagators is easily seen to give the joint $\sigma/\pi$ propagator in the plasma phase. The screening mass obtained from this unsubtracted propagator is plotted in Figure 3 as a function of $\beta$. It flattens out in the hadronic matter phase when the fields develop a vacuum expectation value heralding a truly massless pion. While good fits of the pion propagator to a massless boson propagator are obtained in this region, fits in which the mass is allowed to float typically give masses $\sim 0.2$. To get clearer evidence for a massless pion would require a lattice of larger spatial extent (and/or better statistics). Until then we appeal to Goldstone’s theorem for the knowledge that the pion is exactly massless in the chirally broken phase [6]. The fit for the screening mass in the plasma phase is also shown. The fit used the data points at $\beta = 5.4225$ through $\beta = 5.45$ and used the form $a(\beta - \beta_c)^\nu$. It predicted a correlation length exponent of $\nu = 0.59(7)$, an amplitude $a = 2.66(71)$ and a critical coupling $\beta_c = 5.4196(7)$. As is clear from the figure, the data here suffers from errors, both statistical and systematic, that are larger than in our other analyses. The prediction $\nu = 0.59(7)$ is compatible with the 0.5 of the tricritical point.

In summary, our measurements of $\beta_{mag}$ at $N_t = 6$, made possible by our new action which permits zero mass simulations, strongly favour tricritical scaling at the chiral phase transition over the $O(4)/O(2)$ transition expected from universality arguments. Combined with the first order transition we have observed at $N_t = 4$ it gives hope that $O(4)/O(2)$ scaling will be observed for $N_t \geq 8$. This ‘anomalous’ behaviour for $N_t = 4,6$ offers a potential explanation as to why simulations with the standard staggered fermion action produce unexpected results [3,4].

The extra symmetry breaking operator at the tricritical point provides a possible explanation of the scaling of the chiral condensate with mass at $\beta_c$ and the measured value of $\delta$. $\nu$ is consistent with its tricritical value.

Simulations on $N_t = 8$ lattices should be performed to determine whether the contin-
FIG. 3. The pion screening mass plotted against $\beta$ on a $18^3 \times 6$ lattice. The solid line is the fit discussed in the text.

uum limit shows universal critical behaviour. Lattices with larger spatial extent are needed to obtain better predictions of $\nu$.

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