Dynamical QCD thermodynamics with domain wall fermions

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We present results from numerical simulations of full, two flavor QCD thermodynamics at $N_t = 4$ with domain wall fermions. For the first time a numerical simulation of the full QCD phase transition displays a low temperature phase with spontaneous chiral symmetry breaking but intact flavor symmetry and a high temperature phase with the full $SU(2) \times SU(2)$ chiral flavor symmetry.

1. Introduction

QCD thermodynamics has been extensively studied using numerical simulations with staggered or Wilson fermions. However, both formulations break the chiral symmetry of the theory. The symmetry is recovered together with the Lorentz symmetry as the continuum limit is approached. In the past few years a novel fermion regulator was developed that provides a way of controlling the amount of chiral symmetry breaking at any lattice spacing. Domain wall fermions utilize an extra space–time dimension with free boundary conditions to separate the two chiral components of the Dirac spinor. The components are localized on the opposite boundaries (walls). If the extent of the fifth “dimension”, $L_s$, is infinite the two chiral components decouple and the theory has the full chiral symmetry, even at finite lattice spacing. For practical numerical simulations, $L_s$ must be finite and as a result there is a small mixing of the chiral components resulting in a residual mass. The important point is that the size of this residual chiral symmetry breaking can be controlled at any lattice spacing by increasing $L_s$. For the first time the approach to the chiral limit has been separated from the approach to the continuum limit.

In free field theory the localization is exponential and the effective quark mass is given by [1]:

$$m_{\text{eff}}^{(\text{free})} = m_0 (2 - m_0) \left[ m_f + (1 - m_0)^L \right]. \quad (1)$$

where $0 \leq m_0 < 2$ is the domain wall “height” and $m_f$ an explicit fermion mass. In the interacting theory there is numerical non-perturbative evidence that the general features of eq. 1 still hold with $m_0$ being renormalized [2], [3], [4].

Another unique property of domain wall fermions is that the $L_s = \infty$ limit can be studied using the overlap formalism [5]. In that limit it can be shown that for topological gauge field backgrounds there are exact fermionic zero modes. It has been demonstrated that for masses in the range of interest the effects of finite $L_s$ on the zero modes can be made arbitrarily small for classical [6], [7] and for quantum [8], [9] gauge field backgrounds. Domain wall fermions possess the key ingredient in reproducing anomalous effects.

For more details on domain wall fermions see the review [10] and references within.

2. Numerical Simulations

Dynamical domain wall simulations have been done in the past for the Schwinger model in the $L_s = \infty$ limit (overlap formalism) [11] and for finite $L_s$ using standard hybrid Monte Carlo (HMC) techniques. In this work we simulated QCD using standard HMC at finite $L_s$. The gauge fields are defined on the four-dimensional lattice while the fermion fields on the five-dimensional one. The five-dimensional Dirac operator is as in [12] with even-odd pre-
conditioning. The bulk effects of the $L_s$ heavy flavors were subtracted by introducing five-dimensional bosonic fields as in [3]. We used the $\Phi$ algorithm with trajectory length of 0.5 and step sizes $\sim 0.01 - 0.02$ resulting in acceptance rates $\sim 80\%$. The standard conjugate gradient inversion algorithm (CG) was used with a typical number of CG iterations ranging from 50 – 200. We used initial configurations in the opposite phase and 200 – 800 thermalization sweeps. The computational cost is linear in $L_s$.

3. The Phase Transition

In order to investigate the feasibility of studying QCD thermodynamics with domain wall fermions, to locate the critical coupling, and to investigate the parameter space of this new regulator $(m_0, m_f, L_s)$ we performed a large number of simulations at various couplings on $8^3 \times 4$ and $16^3 \times 4$ lattices using the QCDSP machine. This was possible due to the robustness of the machine and software that allowed us to split a 200 Gflops portion of it to 7 independent, 6 Gflops machines and 6 independent, 25 Gflops machines.

A sharp change on the value of the chiral condensate $\langle \psi \bar{\psi} \rangle$ and the magnitude of the Wilson line $|W|$ was observed as $\beta = 6/g_0^2$ (with $g_0$ being the gauge coupling constant) was varied. This can be seen in figure 1 for an $8^3 \times 4$ lattice with $m_0 = 1.9$, $m_f = 0.1$ and $L_s = 12$. The fits are to $c_0 + c_1 e^{-c_2 L_s}$ that go through the three points. The horizontal lines are the $\langle \psi \bar{\psi} \rangle = c_0$ lines. As can be seen in the broken phase ($\beta = 5.2$ lines) where the coupling is larger, the decay rate $c_2$ is larger than the one in the symmetric phase ($\beta = 5.45$) as expected from the Schwinger model [4]. At $L_s = 16$ and $\beta = 5.2$ $\langle \psi \bar{\psi} \rangle$ is within 7% of the extrapolated value while at $\beta = 5.45$ it agrees within the error bars.

![Figure 1](image1.png)

**Figure 1.** $8^3 \times 4$, $L_s = 12$, $m_f = 0.1$, and $m_0 = 1.9$. $|W|$ (crosses) and $\langle \psi \bar{\psi} \rangle$ (diamonds).

![Figure 2](image2.png)

**Figure 2.** $8^3 \times 4$, $\beta = 5.20$ (squares), $8^3 \times 4$, $\beta = 5.45$ (diamonds), $16^3 \times 4$, $\beta = 5.45$ (crosses), with $L_s = 16$ and $m_0 = 1.9$. The stars are the $m_f = 0$ linearly extrapolated values.

The dependence on $m_0$ is more subtle. In free field theory $m_0 < 0$ corresponds to no light flavors, $0 \leq m_0 < 2$ to one and $2 \leq m_0 < 4$ to four light flavors. Also, for positive but small $m_0$ the number of low momentum states becomes small (for more details and numerical results see [3]). In order to study these effects we located $\beta_c$ using $\langle \psi \bar{\psi} \rangle$ and $|W|$, for various values of $m_0$ on $8^3 \times 4$ lattices. The results are in figure 4. The depen-
The evidence of $\beta_c$ on $m_0$ can be viewed as an expected renormalization effect.

Figure 3. $8^4 \times 4$, $m_f = 0.1$ and $m_0 = 1.9$. $\beta = 5.20$ (crosses), $\beta = 5.45$ (diamonds).

Figure 4. $8^4 \times 4$, $L_s = 12$ and $m_f = 0.1$. $\beta_c$ from $|W|$ (crosses) and from $\langle \psi \psi \rangle$ (diamonds).

4. The $U(1)$ Axial Symmetry

Due to the exceptional zero mode properties of domain wall fermions the possibly anomalous breaking of the $U_A(1)$ symmetry just above the transition can be investigated with clarity and without subtleties such as zero mode shift effects (staggered fermions) or proximity to the Aoki phase (Wilson fermions). We measured the difference of the screening masses of the $\delta$ and $\pi$ as a function of $m_f$ on a $16 \times 4$ lattice at $\beta = 5.45$ with $m_0 = 1.9$ and $L_s = 16$. The data fits to $c_0 + c_2 m_f^2$ with $\chi^2/dof \approx 0.5$ and $c_0 = 3.1(9) \times 10^{-2}$. The small $\chi^2/dof$ and the near-zero, small-mass limit of $\langle \psi \psi \rangle$ indicate that the chiral symmetry breaking effects due to the fermion regulator ($L_s < \infty$) are negligible so that this preliminary, non-zero $c_0$ value suggests that $U_A(1)$ remains broken just above the transition.

Figure 5. $16^4 \times 4$, $L_s = 16$, $\beta = 5.45$, and $m_0 = 1.9$. The fit is to $c_0 + c_2 m_f^2$ and the star is the $m_f = 0$ extrapolated value.

5. Conclusions

We presented results from numerical simulations of full, two flavor QCD thermodynamics at $N_t = 4$ with domain wall fermions. They indicate the presence of a low temperature phase with spontaneous chiral symmetry breaking but intact flavor symmetry and a high temperature phase with the full $SU(2) \times SU(2)$ chiral flavor symmetry. Given this, we interpret the difference seen in the $\pi$ and $\delta$ screening lengths just above the transition as preliminary evidence for the anomalous breaking of the $U_A(1)$ symmetry.

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