QCD Thermodynamics with Domain-Wall Fermions

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Abstract. The study of the QCD chiral phase transition on the lattice has been hampered in the past by the lack of a chiral-invariant fermion formulation. Only recently has it become possible to perform fully dynamical simulations with chiral formulations such as domain-wall and overlap fermions. Here we present results for various chiral observables at finite temperature that were obtained using domain-wall fermions. We also present results showing that the axial anomaly is still present even above the chiral phase transition. Lastly, we show our results for the Dirac spectrum at finite temperature and speculate on the mechanism of $U(1)_A$ breaking beyond the chiral phase transition.

1. Chiral Symmetry and the QCD Phase Diagram
The restoration of a spontaneously broken continuous global symmetry is the prototype of a phase transition in several quantum field theories. In QCD for e.g. while the Lagrangian for $N_f \geq 2$ massless quarks is formally invariant under separate $SU(N_f)$ rotations of the right- and left-handed quarks, interactions break this group down to its vector subgroup i.e. the familiar isospin symmetry. According to the conventional picture of Pisarski and Wilczek [1], the restoration of this chiral symmetry at high temperatures is expected to be second-order for two massless flavors. For massive quarks the transition is widely believed to be a crossover.

On the other hand, the singlet part of the axial group viz. $U(1)_A$, is broken by the famous axial anomaly [2, 3] at the perturbative level itself so that there is no question of its complete restoration at any finite temperature [4, 5, 6, 7]. However the configurations that contribute to the axial anomaly are Boltzmann-suppressed at high temperatures due to the screening of the coupling constant [8]. It is conceivable that this suppression is nearly complete by some temperature that is not too high. We may then speak of an effective restoration of the axial symmetry. If this temperature is close to the chiral phase transition temperature $T_c$, then the chiral phase transition can even be of first order [1].

1.1. Chiral Symmetry on the Lattice
Since chiral symmetry breaking is a non-perturbative effect, the only way of studying it from first principles is through lattice QCD. Unfortunately the study of chiral symmetry on the lattice is not straightforward owing to the well-known fermion doubling problem: Any discretization $D$ of the Dirac operator which preserves exact chiral symmetry i.e. $\{\gamma_5, D\} = 0$, will necessarily describe more than one fermion species in the continuum[9, 10]. Traditionally, this problem has been circumvented through the use of either staggered or Wilson fermions. Wilson fermions break chiral symmetry explicitly by adding an irrelevant second derivative term, the Wilson term, which does not commute with $\gamma_5$. Although chiral symmetry is regained in the continuum, its
loss at finite lattice spacing leads to problems such as unwanted additive renormalizations and operator mixing as well as exceptional configurations. Staggered fermions on the other hand preserve a $U(1)$ subgroup of the full chiral symmetry group. Unfortunately one does not get rid of all the doublers; four of these remain even in the continuum limit and introduce additional complications at finite lattice spacing [11, 12, 13]. From the point of view of the phase transition, the biggest problem in this case is that the chiral and continuum limits do not commute: The continuum limit must be taken separately for each pion mass before a chiral extrapolation can be performed.

Lastly, neither action satisfies an index theorem and therefore the famous relation between topology and the zero modes of the Dirac operator is regained only in the continuum.

All these problems may be avoided by the use of chiral fermions such as the overlap [14, 15], domain-wall [16, 17] or fixed-point [18]. For example, chiral fermions satisfy an exact, if altered, definition of chiral symmetry at finite lattice spacing $a$, namely [19]

$$\psi_x \rightarrow \left[1 + i\theta \gamma_5 \left(1 - \frac{a}{2} D_{xx'}\right)\right] \psi_{x'}, \quad \bar{\psi}_x \rightarrow \bar{\psi}_{x'} \left[1 + i\theta \left(1 - \frac{a}{2} D_{xx'}\right)\right] \gamma_5. \quad (1)$$

This works provided the Dirac matrix $D$ satisfies the famous Ginsparg-Wilson relation [20]

$$\{\gamma_5, D\} = aD\gamma_5 D. \quad (2)$$

Chiral fermions avoid the doubling problem since $\{\gamma_5, D\} \neq 0$. They also satisfy the index theorem even at finite $a$. The downside is that all three actions are much more expensive to simulate than either staggered or Wilson fermions. Of the three, the overlap and fixed-point operators satisfy the Ginsparg-Wilson relation, Eq (2) exactly. By contrast, domain-wall fermions live in five dimensions and satisfy the Ginsparg-Wilson relation only when the fifth dimension becomes infinite, $L_s = \infty$ [21]. For $L_s < \infty$ the quark mass receives an additive correction $m_{\text{res}}$ even when its input value is set to zero.

Both domain-wall and overlap fermions encounter difficulties during evolution due to dislocations. Dislocations occur whenever the system tunnels from one topological sector to another. In the case of overlap fermions, they significantly increase the cost of the HMC algorithm. As a result, overlap simulations are generally performed at fixed topology. In the case of domain-wall fermions, dislocations result in a large value of $m_{\text{res}}$ [22, 23]. In this work we used the Dislocation Suppressing Determinant Ratio (DSDR) action which suppresses dislocations, while still allowing for topology change, by augmenting the gauge action with a ratio of Wilson determinants [24, 25, 26]. Our lattice sizes were $16^3 \times 8$, with $L_s = 32$ or 48. Our pion mass was held fixed at approximately 200 MeV.

2. Symmetry Restoration: $SU(2)_L \times SU(2)_R$ Versus $U(1)_A$

A convenient way of studying symmetry restoration on the lattice is by looking at the appropriate correlators of Dirac bilinears. For example, the vector ($\rho$) and axial vector ($a_1$) correlators become equal when chiral symmetry is restored. Similarly, the scalar ($\delta$) and pseudoscalar ($\pi$) correlators are expected to become degenerate once $U(1)_A$ is restored. Fig. 1 presents our results for these correlators: We see that while the $\rho$ and $a_1$ become degenerate around $T_c \approx 160$ MeV, the scalar ($\delta$) and pseudoscalar ($\pi$) correlators remain distinct even at $T = 195$ MeV. This suggests that $U(1)_A$ stays broken at the chiral phase transition, although it must be remembered that we are still quite far from the chiral limit.

This difference may be quantified in terms of susceptibilities, obtained by integrating the appropriate correlators. Fig. 2 shows how the correlators in the scalar-pseudoscalar sector are related by chiral and axial symmetries. Chiral symmetry relates the flavored mesons $\pi$ and $\delta$ to the flavor-singlets $\sigma$ and $\eta'$. While the flavor-singlet correlators are hard to measure, their susceptibilities are somewhat easier since they are related to the fluctuations of $(\bar{\psi}\psi)$ and
Figure 1. (Left) The vector (\(\rho\)) and axial vector (\(a_1\)) correlators for \(T = 159\) MeV. (Right) The scalar (\(\delta\)) and pseudoscalar (\(\pi\)) correlators for \(T = 195\) MeV.

Figure 2. (Left) The expected relations between the different correlators whenever chiral/axial symmetry is restored. (Right) Our results for these susceptibilities as a function the temperatures. The relation to the topological susceptibility is expected on the basis of the Ward identity.

\[ \langle \overline{\psi} \gamma_5 \psi \rangle \]. From Fig. 2, one can derive relations among the susceptibilities that must hold once either symmetry is restored; the extent to which these are satisfied by our data is shown in the plot on the right. Although strictly speaking these relations are valid only in the chiral limit, they hold to a good degree for our current simulations.

3. Eigenvalue Distribution
In the domain-wall formalism, the chiral, four-dimensional fermion operator arises in the low-energy limit of the five-dimensional operator. As a result, the low-lying spectrum of both operators should be the same. Unfortunately lattice artifacts complicate this picture at finite lattice spacing. Furthermore although we may set the bare quark mass to zero, we cannot similarly eliminate the residual mass \(m_{\text{res}}\) from the four-dimensional theory. We could subtract \(m_{\text{res}}\) from each eigenvalue for each configuration, but it must be remembered that \(m_{\text{res}}\) is defined only as an ensemble average rather than on a configuration-by-configuration basis. However the spectral density \(\rho(\lambda)\) is also an ensemble-averaged quantity and subtracting \(m_{\text{res}}\) from each eigenvalue is equivalent to simply shifting the origin of \(\rho(\lambda)\).

We display our results for \(\rho(\lambda)\) in Fig. 3. In each of these figures, \(\lambda = \sqrt{\Lambda^2 - (m_l + m_{\text{res}})^2}\), where \(\Lambda\) are the eigenvalues obtained directly from our lattice calculations. Lattice artifacts appear as eigenvalues \(\Lambda < m_l + m_{\text{res}}\); we have binned these eigenvalues in the unphysical region.
\( \lambda < 0; \) we refer the reader to our paper [27] for details.

We see that the eigenvalue density at the origin shrinks rapidly as the temperature is increased, as one would expect on the basis of the Banks-Casher relation [28]. Nevertheless, a small peak at the origin persists even at \( T = 195 \) MeV i.e. well above the chiral phase transition temperature [29]. This could be consistent with a spectral density of the type \( \rho(\lambda) = m^2 \delta(\lambda). \) Such a form is expected within the Dilute Instanton Gas framework, but it is not the only possibility. There are atleast two other possibilities, namely \( \rho(\lambda) \propto \lambda \) and \( \rho(\lambda) \propto m. \) These yield qualitatively different predictions for thermodynamic observables (Table 1). Studies on larger volumes and at smaller quark masses should thus be useful in distinguishing between these possibilities. In this way, it is hoped that one may be eventually able to shed light on the mechanism of \( U(1)_A \) breaking at high temperatures.

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\begin{array}{|c|cccccc|}
\hline
\text{Term} & \langle \psi \psi \rangle & \chi_\pi & \chi_\delta & \chi_\pi - \chi_\delta & \chi^{\text{disc}} \\
\hline
\lambda & -2m \ln(m) & -2 \ln(m) & -2 \ln(m) & 0 & 0 \\
m & \pi m & \pi & 0 & \pi & \pi \\
m^2 \delta(\lambda) & m & 1 & -1 & 2 & 2 \\
\hline
\end{array}
\]

**Table 1.** Scaling forms for the chiral condensate and the various susceptibilities depending on the possible form of \( \rho(\lambda, m) \) near the origin i.e. for \( \lambda \to 0, m \to 0 \). The leading \( m \)-dependence comes from dimensional analysis, however the additional logarithmic dependence can result in divergences in the chiral limit, such as in \( \chi_\pi \) for \( \rho(\lambda) \propto \lambda \).

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