Chiral dynamics and operator relations at non-zero chemical potential

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Abstract. We discuss Taylor expansions of operator expectation values in QCD with respect to chemical potentials of quarks. Maxwell’s relations between coefficients and Ward identities between series are used to relate the operators which give the Taylor coefficients of the series for the chiral condensate, the pseudoscalar susceptibility and the mass dependence of quark number susceptibilities. Through such relations the physics of chiral dynamics are explored. The renormalized expectation values of the chiral condensate and its Taylor coefficients are extracted from simulation.

1. Introduction

Direct lattice simulations at non-zero chemical potential are possible only along certain subspaces of the full parameter space, such as Re $\mu_f = 0$ or $\mu_u = -\mu_d$. However, Taylor expansions around $\mu_f = 0$ have proved to be useful in studying the physics for general $\mu_f$. Here we discuss the two flavour case $f \in \{u, d\}$ and with degenerate quark masses $m_u = m_d = m$. We shall freely go from the parameter space expressed in terms of $\mu_u$ and $\mu_d$ to the isoscalar $\mu_0 = (\mu_u + \mu_d)/2$ and the isovector $\mu_3 = (\mu_u - \mu_d)/2$ chemical potentials. These are simply related to the baryon and electric charge chemical potentials. Since we perform Taylor expansions around the point $\mu_f = 0$, all expectation values are computable by the standard methods of lattice gauge theory.

Various operators related to chiral dynamics in QCD are connected among themselves via chiral Ward identities and Maxwell relations, such that there are only few independent Taylor coefficients. For us the three independent parameters of interest in the chiral sector are the single linear response coefficient of the chiral condensate to $\mu$, and two quadratic response coefficients (QRCs). The linear coefficient vanishes by symmetry in an expansion around $\mu = 0$. Thus, the two chiral QRCs encapsulate the physics arising from the influence of baryon dynamics due to $\mu \neq 0$ on chiral fluctuations.

2. Taylor Expansion

2.1. Chiral condensate

Here we consider only the isoscalar condensate $C_S(m, T, \mu_u, \mu_d) = \frac{1}{2V_4} \left[ \langle uu \rangle + \langle dd \rangle \right]$, which can also be written as, $C_S(m, T, \mu_u, \mu_d) = \frac{1}{2V_4} \left( \frac{\partial \log Z}{\partial m_u} + \frac{\partial \log Z}{\partial m_d} \right) |_{m_u = m_d = m}$, where $V_4$ is the 4-volume.
of the lattice. In our present computations the volumes are taken large enough, but with non-zero quark masses. Since we work with staggered quarks, the mass renormalization is multiplicative, and so are the renormalization of the condensate and its Taylor coefficients. We are interested only on the variation of the condensate with $\mu$ at constant $T$, so we simply work with either of the ratios

$$\frac{C_S(m_R, T, \mu_u, \mu_d; a)}{C_S(m_R, 0, 0; a)} \quad \text{(Z scheme)} \quad \text{or} \quad \frac{C_S(m_R, T, \mu_u, \mu_d; a)}{C_S(m_R, T, 0, 0; a)} \quad \text{(T scheme).} \quad (1)$$

The computations have to be performed at fixed renormalized mass $m_R$. One expects the T scheme to be undefined for $T > T_c$ when $m_R = 0$, since the chiral condensate then vanishes. We perform a formal expansion here which will later be renormalized in either of these schemes.

$$C_S(m, T, \mu_0) = C^0_S + \left(C^{20}_S + C^{11}_S\right) \frac{\mu^2_0}{2} + \cdots$$

$$C_S(m, T, \mu_3) = C^0_S + \left(C^{20}_S - C^{11}_S\right) \frac{\mu^2_3}{2} + \cdots \quad (2)$$

where $C^{20}_S$ and $C^{11}_S$ are respectively the diagonal and off-diagonal coefficients.

2.2. Chiral Ward identities

Chiral Ward identities are consequences of certain operator equalities which follow from chiral symmetries. The prototypical chiral Ward identity is $C_S(T, \mu) = m\chi_\pi(T, \mu)$, where $\chi_\pi$ is the pseudo-scalar susceptibility. Taylor expansions of both sides of this identity can then be equated term by term. A second chiral Ward identity [1] relates the isovector scalar susceptibility to the mass derivative of the condensate: $\partial C_S / \partial m = -\chi_\epsilon$.

We show later that in the continuum limit of the high temperature phase the second derivatives of the condensate with respect to the chemical potential vanish. As a result, the pion susceptibilities are insensitive to chemical potential. Also, in this phase, symmetry arguments show that $\chi_\pi = \chi_\epsilon$ [2]. As a result, the scalar susceptibility is also independent of the isoscalar chemical potential, at least to quadratic order. Below $T_c$ this chain of logic does not hold. The scalar susceptibility is interesting because of speculation about the massless modes at the critical end point [3]. We will discuss it at greater length elsewhere.

2.3. Maxwell relations

A Maxwell relation is the equality of two distinct physical interpretations of a mixed derivative obtained by interchanging the order of the derivatives. From the Taylor expansion of the chiral condensate in eq. (2) we can find Maxwell relations with the change of quark number susceptibilities (QNS) with the quark mass. The leading order relation $\frac{\partial C_S}{\partial \mu} = \frac{\partial n}{\partial m}$ was first noted in [4]. It is trivially true at $\mu = 0$ since the first derivative on the left vanishes, as does $n$ for all quark masses. The second derivatives give two non-trivial Maxwell relations and consequent relations using the chiral Ward identities discussed earlier,

$$C^{20}_S = \frac{\partial^2 C_S}{\partial \mu_u^2} = m \frac{\partial^2 \chi_\pi}{\partial \mu_u^2} = \frac{\partial \chi_{uu}}{\partial m},$$

$$C^{11}_S = \frac{\partial^2 C_S}{\partial \mu_u \partial \mu_d} = m \frac{\partial^2 \chi_\pi}{\partial \mu_u \partial \mu_d} = \frac{\partial \chi_{ud}}{\partial m}. \quad (3)$$

Here, as a byproduct of our computation of the renormalized chiral condensate, we shall give the continuum limit of the derivative of the susceptibility. Also, the relative rates of strange and light quark production in heavy-ion collisions i.e. the Wroblewski parameter on the lattice [5] is

$$\lambda_s = \frac{\chi_{ss}}{\chi_{uu}}. \quad (4)$$
with obvious extensions to the production rates of heavier quarks. Since it is hard to perform
lattice computations at realistic values of light quark masses due to constraints of computer time,
one can lighten the computational burden by using a Taylor series for the mass dependence of
the susceptibilities utilizing the above Maxwell relation. Then one can compute $\lambda_s$ at some
reasonably light quark mass, corresponding to, say, the pion mass being two to three times
heavier than in the real world, and extrapolate to the physical quark mass values using the
Maxwell relation. Extrapolating the results of our measurements at heavier quark masses to the
realistic values we find the change in $\lambda_s < 1\%$.

3. Results

3.1. Continuum limit in quenched QCD

3.1.1. $T > T_c$ We used stored gauge configurations from the study in [6] for our measurements.
These were obtained on $N_t = 4, 8, 10, 12$ and 14 lattices for temperatures $T = 1.5T_c, 2T_c$ and $3T_c$
respectively.

The diagonal QRC in the T scheme is shown in Figure 1. It is clear that there is significant $\mu$-
dependence on coarser lattices. However, this Taylor coefficient vanishes at the 99% confidence
limit on extrapolation to the continuum. The identities in eq. (3) then imply that $\chi_{uu}$ is
insensitive to changes in the quark mass and $\chi_\pi$ is insensitive to $\mu$ in this range of temperatures.
Since $\chi_{uu}$ agrees with a perturbative evaluation for $T \geq 1.5T_c$, its insensitivity to $m$ can be
understood from the fact that the effective infrared cutoff is given by the Matsubara frequency
$\pi T$ and not by $m$ when $m/T_c < \pi T/T_c$.

3.1.2. $T < T_c$ We also made a series of simulations at fixed $T/T_c = 0.75$ for $N_t = 6, 8, 10$
and 12 in quenched QCD with the Wilson action. We found that the continuum limit of both
$\langle O_2 \rangle$ and $\langle O_{11} \rangle$ were consistent with zero within reasonably small errors. However, note that
at coarser lattices the values were increasing with increasing temperature, but below $T_c$ the
behaviour is reversed. We then do a dynamical simulation near $T_c$ to investigate this further.

3.2. Dynamical staggered quarks

We give the results of a series of computations with two flavours of dynamical quarks as the
temperature varies between $0.75T_c$ and $2T_c$. The simulations were performed using the R-
algorithm with two flavours of quarks with bare mass of $0.1T_c$. Three lattice sizes were used in
most of the simulations, namely $4 \times 8^3$, $4 \times 12^3$ and $4 \times 16^3$. Lattice computations with dynamical
quarks are still too costly for the continuum limit to be taken easily. However, in order to have
some idea of the continuum limit we have also performed two further simulations with $6 \times 12^3$
and $8 \times 16^3$ lattices at $T = 0.9T_c$. In addition, we have results at $T_c$ on $6 \times 12^3$ lattices.
Consistent with our previous observations, $C^1_S$ was seen to vanish with small errors across the full range of temperatures considered. The diagonal QRC was negative and differed significantly from zero, as shown in Figure 2. Eq. (3) then implies the suppression of pion fluctuations and increase in pion mass as one approaches the critical end point. Note a small shift of the peak from $T_c$. This may be an indicator of a crossover transition. For comparison, results from the quenched theory at the same bare quark mass are also shown. The $T$-dependence is seen to be a little different; this could reflect either the difference in the value of $m_\pi/m_\rho$ or be a quenching artifact. The off-diagonal QRC was consistent with zero within small errors above $T_c$. Near and below $T_c$ larger fluctuations are seen. Although still consistent with zero at the 3-$\sigma$ level, the averages increase by several orders of magnitude compared to $T > T_c$, and seem to be comparable in magnitude to the diagonal QRC. Reduction of the noise in measurement is required to get a clearer signal. Any non-zero value of $C^{20}_S$ would imply an asymmetry of the phase diagram in the $\mu_0$ and $\mu_3$ directions (see eq. 2)

The results of our preliminary investigation of the continuum limit with dynamical quarks are shown in Figure 3. At $0.9T_c$ the 3-$\sigma$ error band on the extrapolation of the diagonal QRC is consistent with zero. At $T_c$ the continuum extrapolation perforce had to be performed with data from only two lattice spacings. With this caveat, our data currently points to a non-zero continuum extrapolation of renormalized $C^{20}_S$ at $T_c$.

Acknowledgments
For more details of this work please refer to [7]

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