Chiral dynamics in QCD at finite chemical potential

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We present the renormalized Taylor expansion of the chiral condensate with chemical potential. The relation with the Taylor coefficients of meson susceptibilities and the quark mass dependence of the quark number susceptibilities are obtained through chiral Ward identities and Maxwell relations. The continuum limit is obtained in quenched and two flavour QCD. In \( N_f = 2 \) QCD, the quadratic response coefficients (QRCs) of the chiral condensate to chemical potential indicate that pion fluctuations decrease at finite chemical potential toward the critical end point. We discuss how these observables can be used to test other features of the QCD phase diagram.

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I. INTRODUCTION

Studies of hot dense matter formed in heavy-ion colliders such as the RHIC \([1]\) need to be interpreted using theoretical predictions obtained from lattice computations. Most of these are performed at zero baryon density. However, it seems likely that the actual experimental conditions involve small but non-vanishing baryon chemical potential. In order to deal with this one has to consider the stability of various lattice predictions to the presence of a small chemical potential, \( \mu \).

This was once considered an insoluble problem in lattice QCD. The reason is that direct lattice Monte Carlo simulations at finite \( \mu \) are impossible since the weights in the partition function are not positive definite. However, developments in recent years \([2, 3, 4, 5]\) mean that QCD at finite \( \mu \) is no longer out of reach on the lattice. In this paper we investigate Taylor expansions in the chemical potential \([4, 6, 7]\), which have recently been used to compute the equation of state at finite \( \mu \) \([4, 5]\).

The first investigations of correlators at finite chemical potential was performed in \([7]\). Our approach differs from theirs in that we do a direct Taylor expansion of operators, rather than of parameters in fitting functions. There is a conceptual and practical gain. Putting chemical potentials on quarks can break the flavour x CP symmetry of QCD in many different ways, possibly affecting every observable in distinct fashion. However it turns out that there are enough relations between operators and their derivatives that, among all the observables related to chiral dynamics in QCD, there is only one set of independent Taylor coefficients. Taylor expansions of the operators utilize these relations with generality and economy.

There turn out to be three independent parameters of interest in the chiral sector— a 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. Since the phase diagram of QCD at small \( \mu \) is built up through the interplay of chiral and baryon dynamics \([8, 9, 10, 11]\), the QRCs provide direct information on this phase diagram.

Here we present the first systematic study of the renormalized Taylor expansion of the chiral condensate in QCD up to second order in the chemical potentials \([12]\). We define renormalization schemes which are simple to implement, and in which the Taylor expansion can be extrapolated to the continuum. We find the continuum limits at both high and low temperatures in quenched and dynamical \( N_f = 2 \) QCD.

In section 2 we write out generic Taylor expansions in the chemical potential, before specializing to pure glue operators, the chiral condensate and meson susceptibilities. The renormalization schemes for the condensate, Maxwell relations and chiral Ward identities are also dealt with in this section. The actual lattice simulations and results are in section 3, including the complete specification of the renormalization schemes and results above and below \( T_c \) in

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the quenched theory. This section also contains our results for QCD with dynamical quarks. Discussion of the results and the constraints that the QRCs can place on the QCD phase diagram can be found in the concluding section 4.

II. TAYLOR EXPANSIONS

The partition function of QCD at temperature $T$ and chemical potentials $\mu_f$ for each flavour $f$ of quarks is
\[
Z(\{m_f\}, T, \{\mu_f\}) = \int \mathcal{D}U e^{-S(T)} \prod_f \text{Det} M(m_f, T, \mu_f),
\]
where $m_f$ is the mass of quark flavour $f$. $S(T)$ denotes the gluon part of the action and $M$ is the lattice discretised Dirac operator. The expectation value of an operator $\mathcal{J}$ is defined as
\[
\langle \mathcal{J} \rangle \equiv J(\{m_f\}, T, \{\mu_f\}) = \frac{1}{Z} \int \mathcal{D}U \mathcal{J} e^{-S(T)} \prod_f \text{Det} M(m_f, T, \mu_f),
\]
where $\mathcal{J}$ may or may not contain explicit dependence on the parameters. Direct simulations are possible only along certain subspaces of the full parameter space, such as $\text{Re} \mu_f = 0$ or $\mu_u = - \mu_d$. However, Taylor expansions around $\mu_f = 0$ have proved to be a good method of studying the physics for general $\mu_f$. In the remainder of this paper we shall work mainly with 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 chemical potential $\mu_0 = (\mu_u + \mu_d)/2$ and the isovector $\mu_3 = (\mu_u - \mu_d)/2$. These are simply related to the baryon and electric charge chemical potentials.

The notation used above is $\langle O \rangle = 0$ have proved to be a good method of studying the physics for general $\mu_f$. In the remainder of this paper we shall work mainly with 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 chemical potential $\mu_0 = (\mu_u + \mu_d)/2$ and the isovector $\mu_3 = (\mu_u - \mu_d)/2$. These are simply related to the baryon and electric charge chemical potentials. Since we perform Taylor expansions around the point $\mu_f = 0$, all angular brackets in the rest of this paper shall mean expectation values at vanishing chemical potential. These are computable by the standard methods of lattice gauge theory.

We recall a few points about the expansion of the partition function \[1, 2\]. The $\mu_f$ appear only in the Fermion determinant. If a matrix $M(x)$ depends on a parameter $x$, then the identity $\text{Det} M(x) = \exp[\text{tr} \ln M(x)]$ yields, $[\text{Det} M(x)]' = \text{Det} M(x) \text{tr} M^{-1} M'$, where primes denote derivative with respect to the parameter $x$. Furthermore, the identity $M^{-1} M = 1$ yields $[M^{-1}]' = - M^{-1} M' M^{-1}$. This is enough to determine the Taylor coefficients of the partition function. The first order coefficients are proportional to the quark number densities—
\[
\frac{\partial Z}{\partial \mu_f} \bigg|_{\mu_f = 0} = ZZ_1, \quad \text{where} \quad Z_1 = \langle O_1 \rangle = \langle \text{tr} M_f^{-1} M_f' \rangle,
\]
which is flavour independent since $m_u = m_d$. When we need to keep track of the flavour we shall use the notation $\mathcal{O}_1^{(f)}$ and obvious generalizations for higher derivatives. The second order coefficients are
\[
\frac{\partial^2 Z}{\partial \mu_f \partial \mu_g} \bigg|_{\mu_f = 0} = ZZ_2^{(fg)} = Z \langle O_{11} + O_2 \delta_{fg} \rangle \quad \text{where} \quad \langle O_2 \rangle = - \langle \text{tr} M_f^{-1} M_f' M_f^{-1} M_f' \rangle.
\]
The notation used above is $O_{11} = O_1 O_1$. Flavour symmetry gives two independent components—$Z_2^{uu} = Z_2^{dd} = \langle O_2 + O_{11} \rangle$ and $Z_2^{ud} = \langle O_{11} \rangle$. Expansions for isoscalar ($\mu_u = \mu_d = \mu_0$) and isovector ($\mu_u = - \mu_d = \mu_3$) chemical potentials are—
\[
Z(m, T, \mu_u, \mu_d) = Z(m, T, 0, 0) \times \left\{ \begin{array}{ll} 1 & + \langle 2 O_{11} + O_2 \rangle \mu_0^2 + O(\mu_0^4) \, , \\ 1 & + \langle O_2 \rangle \mu_3^2 + O(\mu_3^4) \end{array} \right\}.
\]
The terms of odd order vanish by CP symmetry. Diagrammatic representations of these operators have been written down \[2\] and can be extended to other operators, as we outline later.

The double series expansion in terms of $\mu_u$ and $\mu_d$ of the pressure, $P = T(\log Z)/V$, has as coefficients the quark number densities, $n_f = (T/V) \langle O_1 \rangle = 0$, and the quark number susceptibilities. The two independent linear susceptibilities \[2\] are the diagonal ones $\chi_{uu} = \chi_{dd} = (T/V) \langle O_{11} + O_2 \rangle$ arising from taking two derivatives with respect to the same chemical potential, and the off-diagonal $\chi_{ud} = (T/V) \langle O_{11} \rangle$. In writing these expressions we have used the fact that the expansion is around $\mu_f = 0$. Higher order susceptibilities have also been used \[4\].

Similar Taylor expansions can be written for any operator $\mathcal{J}$. Here we write this out to second order. Using the notation $\mathcal{J}^{(f)}$ for the first derivative of $\mathcal{J}$ with respect to any explicit appearance of $\mu_f$ in it, and $\mathcal{J}^{(fg)}$ for the explicit
double derivative with respect to $\mu_f$ and $\mu_g$ we can write the first two Taylor coefficients in the expansion—

\[
J^{(f)}_1 = \left. \frac{\partial J}{\partial \mu_f} \right|_{\mu_f=0} = \langle O^{(f)}_1 J + J^{(f)} \rangle,
\]

\[
J^{(f)}_2 = \left. \frac{\partial^2 J}{\partial \mu_f \partial \mu_g} \right|_{\mu_f=0} = \left( \langle O_{11} + \delta_{fg} O_2 \rangle J + O_1 \left( J^{(f)} + J^{(g)} \right) + J^{(fg)} \right).
\]

The corresponding Taylor expansion is

\[
J(m, T, \mu_u, \mu_d) = J_0 + J^{(u)}_1 \mu_u + J^{(d)}_1 \mu_d + \frac{1}{2} \left[ \left( J_{2}^{(uu)} - J_0 Z_{2}^{(uu)} \right) \mu_u^2 + \left( J_{2}^{(dd)} - J_0 Z_{2}^{(dd)} \right) \mu_d^2 + 2 \left( J_{2}^{(ud)} - J_0 Z_{2}^{(ud)} \right) \mu_u \mu_d \right] + \cdots
\]

where $J_0 = J(m, T, 0, 0)$. CP symmetry cannot be used to simplify the expansion in general, since the operator may not transform nicely under CP. Special simplifications occur for purely gluon operators, as we discuss later.

A. Pure gauge operators

Since pure gauge operators have no explicit dependence on the chemical potentials,

\[
J_1 = \langle O_1 J \rangle,
\]

and

\[
J^{(fg)}_2 = \left( \left( O_{11} + \delta_{fg} O_2 \right) J + O_1 \left( J^{(f)} + J^{(g)} \right) + J^{(fg)} \right).
\]

The corresponding Taylor expansion is

\[
J(m, T, \mu_u, \mu_d) = J_0 + J_1 (\mu_u + \mu_d) + \frac{1}{2} \left[ \left( J_{2}^{(uu)} - J_0 Z_{2}^{(uu)} \right) (\mu_u^2 + \mu_d^2) + 2 \left( J_{2}^{(ud)} - J_0 Z_{2}^{(ud)} \right) \mu_u \mu_d \right] + \cdots
\]

In general the linear term vanishes exactly only when $\mu_0 = 0$. However, for CP even operators, such as real parts of traces of products of links, the odd order terms can be shown to vanish by summing over CP orbits before performing the remaining part of the path integral.

B. Chirality Condensate

From the flavoured condensates $\langle \bar{u}u \rangle$ and $\langle \bar{d}d \rangle$, one can build the isoscalar and isovector condensates which are, respectively,

\[
C_S(m, T, \mu_u, \mu_d) = \frac{1}{2} \left[ \langle \bar{u}u \rangle + \langle \bar{d}d \rangle \right] \quad \text{and} \quad C_V(m, T, \mu_u, \mu_d) = \frac{1}{2} \left[ \langle \bar{u}u \rangle - \langle \bar{d}d \rangle \right].
\]

For equal mass quarks, $C_V$ vanishes at vanishing chemical potential. This vector flavour symmetry is not broken by $\mu_0$ since a sign flip in $\mu_0$ carries the quark of each flavour to its own antiquark. As a result, $C_V$ vanishes at all $\mu_0$, and the series expansion for $C_S(\mu_0)$ is even. A sign flip in $\mu_3$ carries a quark of a given flavour to the antiquark of the opposite flavour, thus mixing the vector flavour symmetry with CP. The same arguments can still be followed through to show that $C_V$ vanishes to all orders in the expansion around $\mu_3 = 0$ and $C_S(\mu_3)$ is even. In the remainder of this paper we consider only $C_S$.

Recall that the quark condensate can also be written as

\[
C_S(m, T, \mu_u, \mu_f) = \frac{1}{2V_4} \left( \frac{\partial \log Z}{\partial m_u} + \frac{\partial \log Z}{\partial m_d} \right) \bigg|_{m_u=m_d=m}
\]

where $V_4$ is the 4-volume of the lattice. Spontaneous breaking of chirality symmetry is signaled by a non-zero value of the condensate in the limit $m \to 0$. We shall not be concerned with this limit in this paper, and can consequently neglect the known subtleties of taking the limits $m \to 0$ and $V_4 \to \infty$. We shall however, check that in actual numerical work the volumes are large enough to obtain correct physical results.

Since the mass is subject to renormalization as the cutoff changes, one must bother about cutoff dependence of the condensate as well as its Taylor coefficients. Since we work with staggered quarks, the mass renormalization is
multplicative, \( m_R(a) = \sqrt{Z_m(a)} m \), where the renormalization constant depends on the ultraviolet cutoff, the lattice spacing \( a \), but not on \( T \) and \( \mu \). Throughout this paper we write the bare quark mass as \( m \). The quark condensate is also renormalized by \( Z_m \). If we are not interested in the absolute value of the condensate, but only on its variation with \( \mu \) at constant \( T \), then one can simply work with either of the ratios

\[
\frac{C_S(m_R, T, \mu_u, \mu_d; a)}{C_S(m_R, 0, 0; a)} \quad \text{(Z scheme)} \quad \text{or} \quad \frac{C_S(m_R, T, \mu_u, \mu_d; a)}{C_S(m_R, T, 0, 0; a)} \quad \text{(T scheme)}. \tag{12}
\]

One expects the T scheme to be undefined for \( T > T_c \) when \( m_R = 0 \), since the chiral condensate then vanishes. Elsewhere there is a finite multiplicative relation between the schemes which has the interpretation of the \( T \)-dependence of \( C_S \) at \( \mu = 0 \). The computations have to be performed at fixed renormalized mass. We perform a formal expansion here which will later be renormalized in either of these schemes.

For the \( u \) quark condensate \( \langle C_u \rangle = \langle \bar{u} u \rangle = \langle \text{Re} \, \text{tr} \, M_u^{-1} \rangle \), clearly \( C_u^{(d)} = C_u^{(ud)} = C_u^{(dd)} = 0 \). The non-vanishing derivatives are \( C_u^{(a)} = -\text{Re} \, \text{tr} \, M_u^{-1} M_u^{a-1} = C' \), and \( C_u^{(ud)} = \text{Re} \, \text{tr} \, (2 M_u^{-1} M_u^{a-1} M_u^{d-1} - M_u^{-1} M_u^{d-1} M_u^{a-1}) = C'' \). For the \( d \) quark condensate, the corresponding relations can be found by flipping \( u \) and \( d \) indices. Since the Taylor series expansion is carried out at \( \mu = 0 \), in the limit of degenerate masses the quantities \( C' \) and \( C'' \) are flavour independent. In this limit the Taylor expansion coefficients of the flavoured condensates are flavour independent, and we need to evaluate the four quantities—

\[
\begin{align*}
C^0_S &= \langle C \rangle, \\
C^1_S &= \langle 2 \mathcal{O}_1 C + C' \rangle, \\
C^{20}_S &= \langle 2(\mathcal{O}_{11} + \mathcal{O}_2) C + 2 \mathcal{O}_1 C' + C'' \rangle - 2 \langle \mathcal{O}_{11} + \mathcal{O}_2 \rangle \langle C \rangle, \\
C^{11}_S &= \langle 2 \mathcal{O}_{11} C + \mathcal{O}_1 (C') - 2 \langle \mathcal{O}_{11} \rangle \langle C \rangle, \\
\end{align*}
\tag{13}
\]

A direct check shows that \( C^1_S \) vanishes, as does every odd term in the expansion. \( C^{20}_S \) is the diagonal, and \( C^{11}_S \) is the off-diagonal QRC.

A diagrammatic representation of the expansion of the chiral condensate is shown in Fig. 1. This builds on a previous diagrammatic representation of the expansion of the partition function \( \langle \varphi_0 \rangle \). Every line denotes a fermion propagator, a dot denotes a derivative with respect to \( \mu_f \) (an insertion of \( \varphi_0 \) in the continuum), every cross is a derivative with respect to \( m_f \) (a mass insertion), and every closed line is a trace over Fermion coordinates. The fermions have to be dressed in all possible ways by gluon insertions. Power counting arguments \( \langle \varphi_0 \rangle \) can be easily extended to estimate the power of the gauge coupling \( g \) associated with the connected parts which appear in eqs. \( \langle \varphi_0 \rangle \) when they are evaluated at high temperatures. The largest quark-loop-disconnected quantity is \( \langle \mathcal{O}_2 C \rangle_c \) which is of order \( g^4 \). Both \( \langle \mathcal{O}_{11} \rangle \) and \( \langle \mathcal{O}_1 C' \rangle_c \) are of order \( g^6 \), and \( \langle \mathcal{O}_{11} \rangle \) is of order \( g^8 \). These powers may be modified by log \( g \) terms due to infrared singularities. \( \langle C'' \rangle \) is of order \( g^0 \), and, because it is non-vanishing, generically gives the largest contribution in the high temperature phase.
The Taylor expansions of $C_S$ are

\[
C_S(m, T, \mu_0) = C_S^0 + \left(C_S^{20} + C_S^{11}\right) \frac{\mu_0^2}{2} + \cdots
\]

\[
C_S(m, T, \mu_3) = C_S^0 + \left(C_S^{20} - C_S^{11}\right) \frac{\mu_3^2}{2} + \cdots
\]

(14)

where the temperature dependence of the coefficients has not been shown explicitly. Note that in the T scheme the Taylor series begin with a constant term of exactly unity. In this scheme one can rewrite the series as an expansion in $\mu/T$ and render all the coefficients dimensionless. Then the remaining Taylor coefficients have the significance of fractional changes due to non-zero values of $\mu$. The power counting argument shows that for $T \gg T_c$ the coefficient of the quadratic term is dominated by the operators $\langle C^\prime \rangle_\epsilon$, and the two expansions differ only by terms subleading in $g$. In the low-temperature phase these arguments fail, and the two series could have significantly different behaviour. Near and below $T_c$ other arguments, outlined in Section IV also lead us to expect different behaviour for the two series.

C. Chiral Ward identities for meson susceptibilities

A meson operator is $M(x) = \bar{\psi}(x)\Gamma\psi(x)$, where $\psi$ is a quark field operator and $\Gamma$ is a Hermitian spin-flavour matrix. The conjugate operator is $M^\dagger(x) = \bar{\psi}^\dagger\Gamma^\dagger\psi = \pm \bar{\psi}\Gamma\psi$, where the plus sign is obtained for the Dirac matrices $\Gamma^0$ and $\gamma_5 \gamma_0$ and the negative sign for $\gamma_5 \gamma_i$ and $\gamma_5 \gamma_i$. The meson correlators are

\[
C(x, y) = \langle M(x)M^\dagger(y) \rangle = \langle \text{tr} \Gamma M^{-1} \Pi(y) \bar{\Gamma}(M^\dagger)^{-1} \Pi(x) \rangle,
\]

(15)

where $M$ is the Dirac operator, and $\Pi(x)$ is the projector to one site $x$. The final expression on the right was obtained using the relation $\Pi^2 = \Pi$ and the fact that $\Pi$ and $\Gamma$ commute since they act on different spaces. In [17] the correlator was parametrized in the form $A \cosh m(L/2 - x)$ and the derivatives with respect to $\mu$ of the parameters $A$ and $m$ were related to operator expectation values obtained by taking derivatives of the right hand side of eq. (15). However, since CP symmetry is explicitly broken on introduction of chemical potentials, one need no longer have $C(x, y) = C(|x - y|)$. This is explicitly visible in the computations reported in [16, 17].

A little tinkering does not help, since it is the transfer matrix formalism that needs to be re-examined at finite $\mu$, because a non-zero value of this parameter introduces an explicit breaking of time reversal symmetry. It is much more straightforward to deal with the meson susceptibilities [18].

\[
\chi_T = \frac{1}{V} \sum_{x,y} C(x, y) = \frac{1}{V} \langle \text{tr} \Gamma M^{-1} \bar{\Gamma}(M^\dagger)^{-1} \rangle.
\]

(16)

If a single pole dominates this propagator then the corresponding mass, $m_T \propto 1/\sqrt{\Lambda_T}$. However, this quantity more generally measures mesonic fluctuations [15].

Chiral Ward identities are consequences of certain operator equalities which follow from chiral symmetries. Each formulation of lattice fermions can preserve a different subset of these identities; a basic set for staggered fermions can be found in [18]. The remaining continuum identities are violated at finite lattice spacing, and hence can be used to check the approach to the continuum. The prototypical chiral Ward identity is $C_S(T, \mu) = m\chi_S(T, \mu)$, where $\chi_S$ is the pseudo-scalar susceptibility. Furthermore, this chiral Ward identity allows us to define a renormalized $\chi_S$ using the simultaneous renormalization of the quark mass and the condensate. Taylor expansions of both sides of this identity can then be equated term by term. Another conclusion is that the Taylor expansion of $\chi_S$ must be even in $\mu$. Explicit construction of the first Taylor coefficient shows that it vanishes, in conformity with this proof.

A second chiral Ward identity [20] relates the isovector scalar susceptibility to the mass derivative of the condensate:

\[
\partial C_S/\partial m = -\chi_S.
\]

Again this can be used to renormalize $\chi_S$ and relate two Taylor series. We emphasize that this involves the isovector scalar, i.e., the scalar meson susceptibility implicated here is obtained out of a connected quark loop.

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 QNS are insensitive to variations of the quark mass, and the pion susceptibilities are insensitive to chemical potential. Also, in this phase, symmetry arguments show that $\chi_\pi = \chi_T$ [21], implying that $C_S$ vanishes linearly with $m$. As a result, we can deduce that 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 [22]. We will discuss it at greater length elsewhere.
D. Maxwell relations

A Maxwell relation is the equality of two distinct physical interpretations of a mixed derivative obtained by inter-changing the order of the derivatives. From the Taylor expansion of the chiral condensate in eq. (14) we can find Maxwell relations with the change of quark number susceptibilities with the quark mass. The leading order relation

\[ \frac{\partial \langle \bar{\psi} \psi \rangle_S}{\partial \mu} = \frac{\partial n}{\partial m} \]  

(17)

was first noted in [23]. 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,

\[ C_{S}^{20} = \frac{\partial^2 \langle \bar{\psi} \psi \rangle_S}{\partial \mu_d^2} = m \frac{\partial^2 \chi_\pi}{\partial \mu_d^2} = \frac{\partial \chi_{uu}}{\partial m}, \]

\[ C_{S}^{11} = \frac{\partial^2 \langle \bar{\psi} \psi \rangle_S}{\partial \mu_u \partial \mu_d} = m \frac{\partial^2 \chi_\pi}{\partial \mu_u \partial \mu_d} = \frac{\partial \chi_{ud}}{\partial m}. \]  

(18)

There are higher order relations between the mass derivative of the non-linear susceptibilities and the higher Taylor coefficients of the condensate. This class of Maxwell relations can be checked by explicit differentiation. Preliminary results have been reported in [24] and a mixed version of this has been used later to correct for the mass dependence of a Taylor expansion of the pressure [25]. Here, as a byproduct of our computation of the renormalized chiral condensate, we shall give the continuum limit of the derivative of the susceptibility.

The relative rates of strange and light quark production in heavy-ion collisions [26] is

\[ \lambda_s = \frac{\chi_{ss}}{\chi_{uu}} \]  

(19)

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. One can also investigate the stability against small variations in the heavy quark mass by similar means.

III. RESULTS

A. Implementing the renormalization scheme

In eq. (12) we have defined a renormalization scheme in which the multiplicative renormalization of the chiral condensate at temperature \( T \) and chemical potential \( \mu \) is absorbed by the bare condensate at \( T = 0 \) or \( \mu = 0 \) evaluated at the same lattice spacing \( a \). In order to implement this scheme this compensation must be performed at a constant renormalized quark mass. We complete the renormalization prescription by choosing to trade the pion mass for the renormalized quark mass. The practical question is then the choice of the bare quark mass which corresponds to a fixed pion mass.

The lattice spacing has been connected to the temperature scale using the QCD \( \beta \)-function at full two-loop order [27]. This scale determination was used to tune the bare couplings in the Wilson action required to simulate the quenched theory at a fixed physical temperature while changing the lattice spacing [28]. Here we used the same bare couplings to extract the pion mass using \( T = 0 \) simulations.

The series of bare couplings used correspond to fixed \( T = 1.5T_c \) on lattices with \( N_t = 4, 8, 10 \) and 12 and to fixed \( T = 0.75T_c \) for \( N_t = 8, 10 \) and 12. The lattice sizes, \( L \), were selected so that \( Lm_\pi \geq 6 \) in order to keep finite volume effects under control. At the two coarsest lattice spacings a previous determination of meson masses [29] could be used to estimate \( m_\pi \) and select an appropriate value of \( L \). Then one could successively use the already determined masses to estimate the size which would be required at finer lattice spacing. Quenched configurations were generated using the Wilson action. At each lattice spacing the first 500–1000 sweeps were discarded for thermalisation and a configuration was kept after every subsequent 50 sweeps.
TABLE I: Meson masses in quenched QCD with Wilson action and staggered quarks. The $\chi^2$ for pions is obtained by fitting local masses to a constant. The rho meson mass is obtained with a four parameter fit to the vector correlator. Details are discussed in the text.

| $aT_c$ | $\beta$ | size | $a m_\rho$ | $a^2 m_\pi^2$ | $\chi^2$ | Range | $a m_\rho$ | $\chi^2$ | Range $m_\pi/m_\rho$ |
|--------|---------|------|------------|---------------|----------|-------|------------|----------|---------------------|
| 0.1667 | 5.8941  | $16^3 \times 32$ | 0.01667 | 0.119(1) | 1.99 | 7-10 | 0.66(2) | 1.43 | 5-17 | 0.52(2) |
|        |         | $30^4$ | 0.02    | 0.141(2) | 2.82 | 7-10 | 0.68(2) | 1.72 | 5-17 | 0.55(2) |
|        |         |       | 0.03    | 0.205(2) | 1.39 | 8-10 | 0.74(2) | 2.54 | 5-17 | 0.61(2) |
|        |         |       | 0.01667 | 0.123(3) | 4.41 | 6-11 | 0.71(4) | 10.73 | 3-16 | 0.49(3) |
|        |         |       | 0.02    | 0.142(2) | 5.59 | 6-10 | 0.72(3) | 11.08 | 3-16 | 0.52(2) |
|        |         |       | 0.03    | 0.214(4) | 4.10 | 6-11 | 0.77(3) | 11.78 | 3-16 | 0.60(2) |
| 0.1333 | 6.0150  | $20^3 \times 40$ | 0.01333 | 0.080(1) | 1.66 | 7-13 | 0.56(2) | 4.95 | 5-21 | 0.50(2) |
| 0.1111 | 6.14    | $24^3 \times 48$ | 0.01111 | 0.0515(9) | 1.64 | 9-13 | 0.42(1) | 2.62 | 7-25 | 0.54(1) |
| 0.0833 | 6.3384  | $40^4$ | 0.0083  | 0.035(1) | 6.58 | 9-17 | 0.333(9) | 2.55 | 7-21 | 0.56(2) |
|        |         |       | 0.01    | 0.040(1) | 5.06 | 10-17 | 0.341(8) | 2.64 | 7-21 | 0.59(2) |
| 0.0667 | 6.525   | $42^4$ | 0.0067  | 0.022(1) | 2.45 | 13-19 | 0.25(1) | 7.35 | 8-22 | 0.60(3) |
|        |         |       | 0.005   | 0.018(1) | 2.85 | 13-19 | 0.25(1) | 6.67 | 8-22 | 0.54(3) |
| 0.0556 | 6.65    | $50^4$ | 0.0056  | 0.0161(3) | 8.13 | 13-23 | 0.21(1) | 15.0 | 10-25 | 0.60(3) |

FIG. 2: The dimensionless ratio $m_\pi^2(T = 0)/mT$ for fixed bare quark mass $m/T_c = 0.1$ at a succession of lattice spacings corresponding to fixed $T = 1.5T_c$ at varying $N_t$ shown as a function of $1/N_t^2 = a^2 T^2$. The constancy of the ratio shows that this procedure correctly holds the renormalized quark mass constant and thereby implements the renormalization scheme of eq. (12).

The stored configurations were used to determine the chiral condensate, through a noisy evaluation of the trace of the inverse of the fermion matrix, and meson correlators. The stopping criterion on the staggered fermion matrix inversion was decreased by factors of 10 until the extracted value of $m_\pi$ was seen to stabilize. It was observed that while decreasing lattice spacing keeping $m_\pi$ fixed the stopping criterion had to be decreased significantly. We attribute this to the fact that as the lattice spacing decreases at zero temperature the eigenvalues near a rapidly decreasing renormalized quark mass take more conjugate gradient steps to resolve.

Our extraction of pion masses was based on effective (local) mass extraction, $m(t)$, and cross checked by fits. As has been known for a long time, this is contaminated at small distances by higher lying states and at large distances
FIG. 3: The diagonal QRC in the T scheme, at fixed $T/T_c = 1.5$ holding the renormalized quark mass fixed by fixing the bare mass to be $m/T_c = 0.1$. The full lines show the 1-$\sigma$ band on the continuum extrapolation and the dashed lines show the 3-$\sigma$ confidence band.

FIG. 4: The diagonal QRC in the T scheme, at fixed $T/T_c = 0.75$ holding the renormalized quark mass fixed by fixing the bare mass to be $m/T_c = 0.1$. The lines show the 1-$\sigma$ band on the continuum extrapolation.

by periodic lattice artifacts. When a plateau can be seen, that value is taken as an estimate of the ground state mass. We converted this into an automatic task by varying $t_{\min}$ and $t_{\max}$ and for each fixed value of this parameter checking
whether the data on \(m(t)\) could be fitted to a constant. We accepted the largest interval over which this could be done and took the corresponding constant as an estimate of the mass (see Table \(I\)). For the vector meson the local mass is harder to stabilize, and we used four parameter fits to extract the mass, varying the fit interval to look for stability.

In simulations at the coarser lattice spacings we performed a series of computations at larger bare quark mass. These are useful in order to check that the lattice volumes are under control. The near constancy of the ratio \(a^2m_\pi^2/(am_q)\) at fixed \(a\) on the coarser lattices indicates that the lattice volumes are sufficiently large that one can extrapolate to the correct continuum physics.

In simulations at a sequence of lattice spacings, \(a\), corresponding to a fixed temperature and varying \(N_t\) \((a = 1/TN_t)\), with a sequence of bare quark masses \(m/Tc = 0.1\), we found that the dimensionless ratio \(m_\pi^2/mT\) is fixed. This is shown in Figure 2. The constancy of this ratio shows that this sequence of bare quark masses corresponds to a fixed renormalized quark mass, and gives an easy method to tune the bare quark mass in order to fix the renormalized quark mass. At this quark mass, we found that \(m_\pi/m_\rho \approx 0.6\), indicating that \(m_\rho\) could also have been chosen to fix the renormalized quark mass. For the parameters chosen here, the fact that the renormalized quark mass is rather heavy is seen both in the fact that the ratio \(m_\pi/m_\rho\) is larger than the physical value and also in that \(m_\pi/Tc \approx 2.3\). We recall that with two flavours of dynamical staggered quarks choosing \(m/Tc = 0.1\) corresponds to \(m_\pi/m_\rho = 0.36 \pm 0.01\), and that on reducing the bare quark mass to \(m/Tc = 0.03\) the ratio \(m_\pi/Tc\) became physical 30.

## B. Continuum limit in quenched QCD

### 1. \(T > T_c\)

We used stored gauge configurations from the study in 28 for our measurements. These were obtained on \(N_t = 4, 8, 10, 12\) and 14 lattices for temperatures \(T = 1.5Tc, 2Tc\) and 3\(Tc\) respectively. The main concern in choosing the spatial size \(N_s\) is to avoid gross distortions of the infinite volume result. For this it is sufficient to have \(N_s/N_t > \max(2, T/Tc)\). For \(N_t = 4\) we have used \(N_s = 12\). For all the other \(N_t\) the spatial size was chosen to be \(N_s = 2N_t + 2\) for \(T/Tc = 1.5\) and 2, and \(N_s = 3N_t + 2\) for \(T/Tc = 3\). For details of the generation of the configurations and their statistical properties, we refer the reader to 28. In this work we recomputed, as a check, the operators \(O_1\), \(O_{11}\) and \(O_2\) which were studied in 28 and supplemented these by computations of \(C, C'\) and \(C''\) needed for the computation of the Taylor expansion of the chiral condensate. The traces were evaluated by the noisy method (see 28 for details). For the conjugate gradient algorithm to obtain the matrix inverses, we used a stopping criterion that the norm of the residual should be less than \(10^{-3}\sqrt{N_tN_s}\).

The vanishing of the expectation values \(\langle O_1 \rangle\) and \(\langle C' \rangle\) are checks of the accuracy of the computation. On each lattice and at every temperature, we found that the expectation values were zero to within a part in \(10^6\) with the above stopping criterion. In the high temperature phase of QCD, where we work, \(\chi_{ud}\) is small, and therefore one expects a noisy and almost vanishing signal for its derivative with respect to the quark mass. In agreement with this expectation, we find that \(C_{S}^{11}\) is too small and noisy to be measured. We return to this in Section 1V.

The diagonal QRC in the T scheme is shown in Figure 3. It is clear that there is significant \(\mu\)-dependence on coarser lattices; in fact for \(N_t = 4\) we found that \(T^2C_{S}^{11}(T)/C_{S}(T) \approx -0.096\) at \(T/Tc = 1.5\). However, this Taylor coefficient vanishes at the 99% confidence limit on extrapolation to the continuum. The conversion from T scheme to Z scheme involves a finite multiplicative factor \(C_{S}(m_R, T)/C_{S}(m_R, 0)\) which also has an interpretation as the temperature dependence of the condensate. At \(T = 1.5Tc\) we find on extrapolation to the continuum that this factor is \(0.26 \pm 0.01\) for \(m_R\) such that \(m_\pi/m_\rho \approx 0.6\). With decreasing quark mass this factor is expected to decrease.

A vanishing continuum limit of the QRC is also found for \(m/Tc = 0.1\) at the two other temperatures that we have studied. The identities in eq. (18) 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 \(T \geq 1.5Tc\), 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 \(m/Tc < \pi T/Tc\).

### 2. \(T < T_c\)

We also made a series of simulations at fixed \(T/Tc = 0.75\) for \(N_t = 6, 8, 10\) and 12 in quenched QCD with the Wilson action. Three hits of pseudo-heat-bath followed by one Metropolis step made up one composite sweep. The first 500 sweeps were discarded for thermalization and subsequently one configuration was saved once every 500 sweeps. Between 35 and 45 such stored configurations were used on each lattice for this work. Measurements were made with the bare quark mass \(m/Tc = 0.1\) and with 50 noise vectors for evaluation of quark traces. In all cases
FIG. 5: The diagonal QRC as a function of the temperature in $N_f = 2$ QCD within the Z scheme, for $a = 1/4T$ holding the renormalized quark mass fixed by fixing the bare mass to be $m/T_c = 0.1$. Pluses denote results obtained on $4 \times 8^3$ lattices, pentagons on $4 \times 12^3$ and circles on $4 \times 16^3$. The boxes represent the quenched QCD value.

FIG. 6: The off-diagonal QRC as a function of the temperature in $N_f = 2$ QCD within the Z scheme, for $a = 1/4T$ holding the renormalized quark mass fixed by fixing the bare mass to be $m/T_c = 0.1$. Pentagons represent results for $4 \times 12^3$, and circles for $4 \times 16^3$.

we used spatial sizes $N_s = 2N_t$. From the $T = 0$ runs described earlier, it can be seen that the size of the spatial box corresponds to over 5.5 pion Compton wavelengths (at $T = 0$) and hence finite size effects are under reasonable
control.

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. On all but the coarsest lattice, $N_t = 6$, the first expectation value was significantly smaller than the second. As a consequence $\chi_{ud}$ and $\chi_{uu}$ were equal within errors even at finite lattice spacing. As shown in Figure 4, $C_S^{20}$ also vanishes within errors in the continuum limit, showing that the vanishing of $\chi_{uu}$ is not an accident of the choice of the quark mass. The off diagonal QRC was consistent with zero at each $N_t$.

C. Dynamical staggered quarks

We report 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 $0.1T_c$, corresponding to $m_\pi/m_\rho = 0.36 \pm 0.01$ \cite{30}. Three lattice sizes were used in most of the simulations, namely $4 \times 8^3$, $4 \times 12^3$ and $4 \times 16^3$. The critical coupling $\beta_c$ for $N_t = 4$ was determined in \cite{31} and the setting of the temperature scale was performed by methods given in \cite{31}. The critical coupling for this quark mass was seen in the peaks of $\chi_\epsilon$, the Wilson line susceptibility, and even in autocorrelation times \cite{30, 31}. The critical coupling is also consistent with those found for neighbouring values of quark mass in \cite{30, 31, 32}.

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. The critical couplings at these $N_t$ were determined in \cite{33}. It is impossible to collect a sufficient number of statistically independent configurations on $N_t = 8$ lattices near $T_c$ with current computing resources due to a rapid increase in autocorrelation times, $\tau$. In all our simulations autocorrelations of local observables were monitored and the total run length was at least 50 times the longest, $\tau_{\text{max}}$, when measured self consistently over the history. The measurements used between 50 and 250 configurations, each separated by $\tau_{\text{max}}$. We work in the Z scheme since we are interested in the $T$ dependence of the derivatives.

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 \ref{fig:5}. For comparison, results from the quenched theory at the same bare quark mass are also shown. The $T$-dependence is
FIG. 8: The panels on top show the expected phase diagrams in the $T$-$\mu_0$ [8] and $T$-$\mu_3$ [8] planes for $m_R > 0$. The panels below show the expectations in the chiral limit, $m_R = 0$ [10, 11]. Thick lines denote second order transitions, the tri-critical point is marked with a fancy circle and the dotted line shows a part of the critical line which could be a model artifact [33]. Further interesting phases at large $\mu$ are not shown.

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 (see Figure 6) is 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.

The results of our preliminary investigation of the continuum limit with dynamical quarks are shown in Figure 7. 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. These completely fix the parameters of a linear extrapolation to the continuum. Error estimates were obtained by then taking the slope as this given parameter and estimating the error on the continuum value in the usual way. The resulting 1-$\sigma$ and 3-$\sigma$ error limits on the extrapolation are shown in Figure 7. Another estimate is to take the extrapolations of the upper end of one error bar and the lower end of the other. This lies within the 3-$\sigma$ band given. With all these caveats, our data currently points to a non-zero continuum extrapolation of renormalized $C_{S}^{20}$ at $T_c$.

IV. DISCUSSION

The chiral condensate is a derivative of the free energy density with respect to quark mass (eq. 11), and the latter requires renormalization. As a result, so does the condensate and its Taylor coefficients. We have defined two renormalization schemes for staggered quarks (eq. 12) in order to set up a well defined Taylor series expansion for the chiral condensate as a function of the chemical potential $\mu$ (eqs. 13 and 14). Diagrammatic rules for writing down the operators defining the Taylor coefficients have been given (Figure 1). The first order Taylor coefficient, $C_{S}^{1}$ vanishes by symmetry. The two QRCs are related through Maxwell relations and chiral Ward identities to all other second order
Taylor coefficients in the chiral sector (eqs. [15]). The diagonal QRC, $C_S^{20}$, has small errors and is easily measurable at the renormalized quark mass we used. We found that at finite lattice cutoff it is negative. Away from $T_c$, both in quenched and $N_f = 2$ QCD, the continuum limit of this quantity vanishes. We have presented evidence (Figure 7) that near $T_c$ in the $N_f = 2$ theory it does not vanish.

This negative peak in $C_S^{20}$ (Figures 4 and 7) corresponds to a significant shift of the condensate, and hence $\chi_\pi$, with chemical potential. The implications for strangeness production have been pointed out in Section IIII. Here we discuss how measurements of the diagonal and off-diagonal QRCs, $C_S^{20}$ and $C_{S1}^{11}$, test current conjectures about the phase diagram of QCD at small $\mu$ based on the perturbative expansion or model computations [8, 11, 12, 13].

The location of $T_c$ is often identified through a peak in the scalar susceptibility $\chi_\pi$ (which is the same as the mass derivative of the chiral condensate through the Patel Ward identity [20]). In the chiral limit this is an unique definition, since the direction of spontaneous symmetry breaking at low $T$ makes this a massive particle, which becomes massless precisely at $T_c$. However, at finite quark mass the symmetry is explicitly broken, $\chi_\pi$ is finite throughout the low $T$ phase and there is a cross over instead of a critical point along the $T$ axis at $T_c$ [36, as shown in the top panel of Figure 5 (see however, [37]). The cross over temperature $T_c$ is usually not uniquely defined, in the following sense. At a phase transition different physical quantities give exactly the same estimate of $T_c$. This is no longer true at a cross over. Thus the slight shift in the peak of $C_S^{20}$ (Figure 5) compared to $T_c$ previously defined from peaks in $\chi_\pi$ and the Wilson line susceptibilities [30, 31] lends some support to the scenario of a cross over.

Furthermore, the observed negative peak in the quadratic response of the condensate shows that $\chi_\pi$ decreases at finite $\mu$, and hence pions cannot be the soft mode as one approaches the critical end point. To the best of our knowledge, this is the first such indication from lattice QCD. Unless $C_S^{20}$ changes sign in the continuum, this argument continues to hold. We have presented evidence that it does, because the diagonal QRC does not turn positive in the vicinity of $T_c$ (Figure 4). Thus support for the standard picture of the phase diagram for $m_R > 0$ is provided by $C_S^{20}$ in two different ways—by indicating that at $\mu = 0$ there could be a cross over, and by showing that pion fluctuations decrease as the baryon density increases.

It is interesting to see what else the QRCs can say about the phase diagram. For $m_R > 0$, as $T$ decreases, the Taylor series for $C_S$ will eventually hit the critical end point in an extrapolation in $\mu_0$. [8], and the critical line in $\mu_3$ [11, 12] (see upper panels in Figure 5). Therefore, at lower $T$ there must be differences in the two extrapolations. This can only happen if the off-diagonal QRC becomes significant. We have shown preliminary evidence for this in Figure 6. This should become easier to measure with decreasing $m_R$ since $m_\pi$ as well as the chemical potential at the critical end point are expected to decrease.

In the chiral limit the phase diagram in the $T-\mu_0$ plane is expected [8] to contain a critical line meeting the $T$ axis at a critical point $T_c$. It is also expected that this critical line ends in a tri-critical point where it meets a line of first order phase transitions emerging from the $\mu_0$ axis (see lower panels in Figure 5). The phase diagram in the $T-\mu_3$ plane has been explored in [11]. A second critical line is expected to emerge from the $T$ axis, curving down to eventually touch the $\mu_3$ axis [35]. Since there is a unique transition along the $T$-axis for $\mu_0 = \mu_3 = 0$, one expects both critical lines to start from $T_c$.

A Taylor expansion cannot be started at the critical point $T_c$, but it is possible to make such a series expansion immediately above and below, and thus track the curvature of the two critical lines. If the off-diagonal QRC vanishes, then the physics along these two lines is the same. However, one has massless pions, whereas the other does not. Also, at lower temperature, one series should give evidence of a tri-critical point on extrapolation, whereas the other should not. Thus, if the phase diagrams drawn above are accurate, then they should be reflected by a non-vanishing value of the off-diagonal QRC. Further, measurements of $C_S^{20} \pm C_{S1}^{11}$ would give information on the soft modes in these two directions.

Thus, there are several extensions of this study which would be interesting to perform in the future. First, the chiral extrapolation of $C_S^{20}$ and $C_{S1}^{11}$ obtained at fixed $N_t$ by varying $m_R$ would indicate whether the tri-critical point indeed appears at $m_R = 0$. If the standard picture does hold, then the chiral extrapolation of $C_S^{20} + C_{S1}^{11}$ and $C_S^{20} - C_{S1}^{11}$ at $T$ just below $T_c$ would give information on the soft modes along the two critical lines.

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Preliminary results for the bare Taylor coefficients of the condensate at lattice spacing $a = 1/4T$ in QCD with two flavours of quarks were presented in S. Choe et al., Nucl. Phys. B (Proc. Suppl.), 106 (2002) 462. The bare series for the condensate has been also been studied earlier in the NJL model in O. Miyamura et al., Phys. Rev., D 66 (2002) 077502.

In most literature on lattice QCD the sign of the condensate is chosen as in eq. (11), and $C_S$ is therefore positive. In translating our results to the convention with negative $C_S$, care must be taken to absorb the sign into the multiplicative renormalization constant, so that the renormalizations of mass and chiral condensate differ by a sign. Eq. (12) shows that this sign will not appear in the expansion of the condensate, but will then appear in the chiral Ward identities and the Maxwell relations.

In [11] this downward curvature of the critical line in the $T$-$\mu_3$ plane is due to a lattice artifact called saturation, which occurs when each lattice site contains the maximum number of allowed fermions. This is why the downward curve has been shown dotted in Figure 8.