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Universal O(N) scaling and the chiral critical line in (2+1)-flavor QCD with small chemical potentials

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We show that for small values of the chemical potential the curvature of the phase transition line can be deduced from an analysis of scaling properties of the chiral condensate and its susceptibilities. We make use of a recent analysis of the magnetic equation of state in (2+1)-flavor QCD where a connection between the QCD parameters and the universal scaling fields could be established. The remaining dependence of the reduced temperature on the chemical potential can be fixed by an analysis of a mixed susceptibility, obtained from a derivative with respect to quark mass and chemical potential. We extract this dependence which describes the curvature of the phase transition line, at two values of the cut-off, $aT = 1/4$ and $1/8$. We find that cut-off effects are small for the curvature parameter and determine the transition line in the chiral limit to leading order in the light quark chemical potential. We obtain $T_c(\mu_B)/T_c(0) = 1 - 0.00656(66)(\mu_B/T)^2 + \mathcal{O}(\mu_B^4)$.

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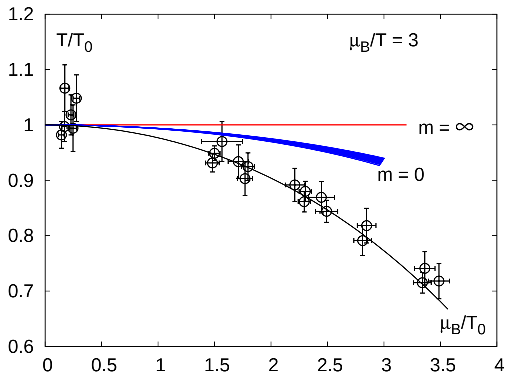

Figure 1: The curvature of the transition line in the (T,μ_B)-diagram for infinitely heavy quarks and – as the result of this paper – in the chiral limit. For comparison we also show the freeze-out data from heavy ion experiments, together with a parameterization for the freeze-out line from [11]. Units are normalized to the transition temperature at $\mu_B = 0$ (T_0).

1. Introduction and Summary

Extending lattice QCD calculations to non-zero baryon-chemical potential or, equivalently, to non-zero net baryon number density is known to be difficult in general. However, important information on the QCD phase diagram can be deduced for small values of the chemical potential by using well established numerical techniques such as reweighting [1], analytic continuation [2, 3] or Taylor expansion [4, 5]. At non-zero values of the chemical potential a phase boundary in the temperature and chemical potential parameter space of QCD is well defined only in the heavy quark limit or for vanishing quark masses. In the former case the phase transition line corresponds to the first order deconfinement transition in the pure gauge theory. At infinite values of the quark mass this transition is independent of the chemical potential and defines a straight line in the T-μ plane. For a large range of quark mass values the transition line is not unique. It characterizes a region of (rapid) crossover in thermodynamic quantities and a pseudo-critical temperature extracted from these observables may differ somewhat, depending on the observable that is used. In the chiral limit, however, the transition line is again well defined. For sufficiently large strange quark mass it defines a line of second order phase transitions in the universality class of three dimensional $O(4)$ symmetric spin models [6].

In a recent work [7] we have shown that the curvature of the phase transition line in the chiral limit can be obtained from an analysis of the universal scaling properties of a certain mixed susceptibility which is defined by the leading order Taylor expansion coefficient of the chiral condensate with respect to the light quark chemical potential. Numerical calculations have been performed for (2+1)-flavor QCD keeping the heavier strange quark mass close to its physical value and decreasing the two degenerate light quark masses towards the massless limit. We will make use of a recent scaling analysis [7, 8] of the chiral order parameter performed with an improved staggered fermion action. This study showed that the chiral order parameter is well described by a universal scaling function characteristic for a three dimensional, $O(N)$ universality class. As a result for the critical line in the chiral limit we find

$$T(\mu_B)/T(0) = 1 - 0.00656(66)(\mu_B/T)^2 + \mathscr{O}((\mu_B/T)^4) \,. \tag{1.1}$$

This curvature is about a factor two larger than the reweighting results obtained in (2+1)-flavor QCD [1]. It is however consistent with results obtained in calculations with imaginary chemical potentials. In fact it lies in between the 2-flavor [2] and 3-flavor [9] simulations performed with the standard staggered fermion formulation and also is consistent with results reported from (2+1)-flavor simulations with imaginary chemical potential performed with the action used also in this study (p4-action) [10]. The result is most relevant for comparison with the experimentally determined freeze-out curve as shown in Fig. 1. The parameterization found in [11] has a curvature that is about a factor 3-4 larger which suggests that (for sufficiently large values of the chemical potential) the freeze-out line does not follow the critical line. In the following two Sections we briefly review the scaling analysis of the order parameter and the mixed susceptibility.

2. Magnetic equation of state

In general we can separate two kinds of contributions to the free energy density, a part (f_s) that will generate singularities in higher order derivatives of the partition function and a regular part (f_r), we have

$$f(T,m_l,m_s,\mu_q,\mu_s) = f_s(T,m_l,m_s,\mu_q,\mu_s) + f_r(T,m_l,m_s,\mu_q,\mu_s) \,. \tag{2.1}$$

In addition to the temperature T, light (m_l) and strange (m_s) quark masses we also allow for a dependence of the free energy density on the quark chemical potentials. Close to the chiral phase transition temperature at vanishing chemical potential the singular part f_s will give rise to universal scaling properties of response functions. This has been exploited to analyze basic universal features of the QCD phase diagram close to criticality [12]. Although f_s depends on many parameters of the QCD Lagrangian, the universal behavior can be expressed in terms of only two relevant scaling variables t and h, that control deviations from criticality at $(t,h) = (0,0)$. To leading order the scaling variable h depends only on parameters that break chiral symmetry in the light quark sector, while t depends on all other couplings. In particular, t will depend on the light quark chemical potential while h remains unaffected by this in leading order,

$$\begin{aligned} t &\equiv \frac{1}{t_0}\left(\frac{T-T_c}{T_c} + \kappa_q\left(\frac{\mu_q}{T}\right)^2\right) \,, \\ h &\equiv \frac{1}{h_0}\frac{m_l}{m_s} \,, \end{aligned} \tag{2.2}$$

where T_c is the phase transition temperature in the chiral limit and t_0, h_0 are non-universal scale parameters (as is T_c). While the combination $z_0 = h_0^{1/\beta\delta}/t_0$ is unique for a given theory, the values of t_0 and h_0 will change under rescaling of the order parameter [8]. Just like the transition temperature T_c also t_0 and h_0 are cut-off dependent and will need to be extrapolated to the continuum limit.

The singular part of the free energy, f_s, is a homogeneous function of its arguments. This can be used to rewrite it in terms of the scaling variable $z = t/h^{1/\beta\delta}$ as

$$f_s(t,h) = h^{1+1/\delta} f_s(z,1) \equiv h^{1+1/\delta} f_s(z) \,. \tag{2.3}$$

where $\beta,\ \delta$ are critical exponents of the three dimensional $O(N)$ universality class [13].

The universal critical behavior of the order parameter, $M \sim \partial f/\partial m_l$, is controlled by a scaling function f_G that arises from the singular part of the free energy density after taking a derivative with respect to the light quark mass,

$$M(t,h) \;=\; h^{1/\delta} f_G(z)\;. \tag{2.4}$$

The scaling function $f_G(z)$ is well-known for the $O(2)$ and $O(4)$ universality classes through studies of three dimensional spin models [14]. This so-called magnetic equation of state, Eq. (2.4), has been analyzed recently for (2+1)-flavor QCD using an improved staggered fermion formulation (p4-action) on lattices with temporal extent $N_\tau = 4, 8$ [7, 8] and light quark masses as small as $m_l/m_s = 1/80$, which corresponds to a pion mass that is about half its physical value. It could be shown that the chiral order parameter can be mapped onto a universal $O(2)$ scaling curve [1] and the scale parameters $t_0,\ h_0,\ T_c$ could be extracted. The scaling analysis has been performed for two order parameters, that are multiplicatively renormalized by multiplying the chiral condensate with the strange quark mass, but differ in handling additive divergences, linear in the quark mass[2],

$$\begin{aligned} M_b &\equiv \frac{m_s}{T^4}\langle\bar\psi\psi\rangle_l\;, \\ M &\equiv \frac{m_s}{T^4}\left(\langle\bar\psi\psi\rangle_l - \frac{m_l}{m_s}\langle\bar\psi\psi\rangle_s\right)\;. \end{aligned} \tag{2.5}$$

All resulting fit parameters from fits with and without a regular contribution are summarized in Table 1. Note that for $N_\tau = 8$ only fits including a regular contribution have been possible, since the smallest available mass in this case has been $m_l/m_s = 1/20$.

3. Curvature of the critical line

At leading order the light quark chemical potential only enters the reduced temperature t, as introduced in Eq. (2.2). Also at non-vanishing values of the quark chemical potential the phase transition point is located at $t = 0$. The variation of the transition temperature with chemical potential therefore is parameterized in terms of the constant κ_q introduced in Eq. (2.2),

$$\frac{T_c(\mu_q)}{T_c} = 1 - \kappa_q\left(\frac{\mu_q}{T}\right)^2 + \mathcal{O}\left(\left(\frac{\mu_q}{T}\right)^4\right)\;. \tag{3.1}$$

To determine the chiral phase transition line in the T-μ plane we thus need to determine the proportionality constant κ_q. This is, in fact, the only left over free parameter in universal scaling functions that needs to be determined.

The constant κ_q can be determined by analyzing the dependence of the chiral condensate on the light quark chemical potential. To extract information about the dependence of the scaling

[1] As we are working with staggered fermions $O(2)$ is expected to be the relevant universality class at finite lattice spacing. We find, however, that fits to the $O(4)$-symmetric model work equally well.

[2] At finite value s of the cut-off these terms are, of course, finite and may be viewed as a specific contribution to the regular part that will not alter the scaling properties for sufficiently small values of the quark mass.

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N_τ	M_i	t_0	h_0	$T_c(0)$ [MeV]	z_0
fit using the scaling term only					
4	M_b	0.0037(2)	0.0022(3)	194.5(4)	6.8(5)
	M	0.0048(5)	0.0048(2)	195.6(4)	8.5(8)
fit using scaling and regular terms					
4	M_b	0.00407(9)	0.00295(22)	194.9(2)	7.5(3)
	M	0.00401(9)	0.00271(20)	194.8(2)	7.2(3)
8	M_b	0.00271(21)	0.00048(9)	174.1(8)	3.8(5)
	M	0.00302(22)	0.00059(10)	175.1(8)	3.8(4)

Table 1: Scale parameters determined from the scaling fits on lattices of temporal extent $N_\tau = 4$ and 8. The last column gives $z_0 \equiv h_0^{1/\beta\delta}/t_0$. We give the results for parameters entering the definition of scaling functions for M_b and the subtracted order parameter M as defined in Eq. (2.5). Only the former has been used in the analysis of the mixed susceptibilities. Note that fits including regular terms, give consistent determinations of the parameters of the scaling functions determined from M_b and M, respectively.

variable t on κ_q it suffices to consider the leading order Taylor expansion coefficient of the chiral condensate,

$$\frac{\langle\bar\psi\psi\rangle_l}{T^3} = \left(\frac{\langle\bar\psi\psi\rangle_l}{T^3}\right)_{\mu_q=0} + \frac{\chi_{m,q}}{2T}\left(\frac{\mu_q}{T}\right)^2 + \mathscr{O}((\mu_q/T)^4)\ , \tag{3.2}$$

where

$$\frac{\chi_{m,q}}{T} = \frac{\partial^2\langle\bar\psi\psi\rangle_l/T^3}{\partial(\mu_q/T)^2} = \frac{\partial\chi_q/T^2}{\partial m_l/T}\ . \tag{3.3}$$

The mixed susceptibility $\chi_{m,q}$ is proportional to the leading order coefficient of the Taylor expansion of the chiral condensate, which has been introduced in [15, 16]. It may also be viewed as the quark mass derivative of the light quark number susceptibility (χ_q).

In the vicinity of the critical point the mixed susceptibility can be expressed in terms of the scaling function $f_G'(z) \equiv \mathrm{d} f_G(z)/\mathrm{d}z$,

$$\frac{\chi_{m,q}}{T} = \frac{2\kappa_q T}{t_0 m_s} h^{-(1-\beta)/\beta\delta} f_G'(z)\ . \tag{3.4}$$

The scaling function $f_G'(z)$ is easily obtained from $f_G(z)$ by using the implicit parameterization for the latter given in Ref. [14]. We also note that $\chi_{m,q}$ diverges as function of the light quark mass at $t = 0$, *i.e.* at the chiral phase transition temperature. In contrast to the chiral susceptibility, $\chi_m \sim \partial M/\partial m_l$, which stays finite in the chiral limit only for $t > 0$, the mixed susceptibility is finite for all $t \neq 0$. For small values of the light quark mass numerical results for the mixed susceptibilities $\chi_{m,q}$ may be compared to the right hand side of Eq. (3.4). Here all parameters that enter $f_G'(z)$ are known and the only undetermined parameter is κ_q. Using a subset of the data samples that have been used for the scaling analysis of the order parameter [7, 8], we calculated the mixed susceptibility $\chi_{m,q}$ on lattices with temporal extent $N_\tau = 4$ for several values of the quark mass. For this analysis we used data sets separated by 50 trajectories. For the lightest quark mass ratio, $m_l/m_s = 1/80$, we selected 4 and for the three heavier quark mass ratios, $m_l/m_s = 1/10,\ 1/20,\ 1/40$, we choose 6

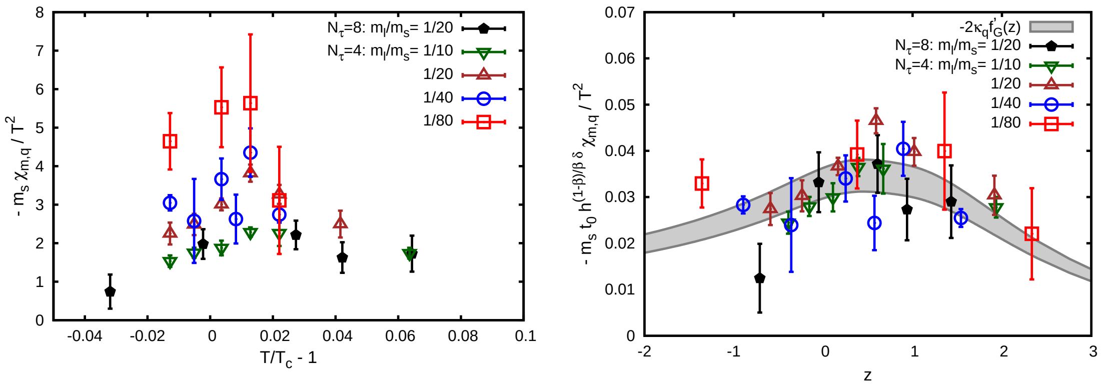

Figure 2: The mixed light quark number susceptibility as a function of the reduced temperature, $(T-T_c)/T_c$ (left) and the scaled mixed susceptibility as function of the scaling variable $z = t/h^{1/\beta\delta}$ (right). Shown are results obtained at two values of the cut-off, $N_\tau = 4$ (open symbols) and $N_\tau = 8$ (filled symbols), and for several values of the light to strange quark mass ratio. On the right hand side, the data is compared to the $O(2)$ scaling curve.

values of the gauge coupling in a narrow temperature interval close to the chiral phase transition temperature T_c, *i.e.* $-0.02 \le (T-T_c)/T_c \le 0.06$. Typically this involved about 500 to 950 gauge field configurations per parameter set, except for the lightest quark mass ratio where we analyzed about 350 gauge field configuration. On each gauge field configuration we calculated the various operators necessary to construct $\chi_{m,q}$.

The calculation of the various operators required inversions of the staggered fermion matrix with a large set of random noise vectors. We used 500 noise vectors on each gauge field configuration and constructed unbiased estimators for the various traces that need to be calculated. All these calculations could be performed very efficiently on a GPU cluster.

Results obtained for the mixed light quark number susceptibility, $\chi_{m,q}$, on lattices with temporal extent $N_\tau = 4$ are shown in Fig. 2 (left). We clearly see that $\chi_{m,q}$ increases in the transition region with decreasing values of m_l/m_s. Using the scaling relation given in Eq. (3.4) we can rescale the data and obtain a unique scaling curve. This scaling curve can be mapped onto the $O(2)$ scaling function $f'_G(z)$ with a simple multiplicative rescaling factor, $2\kappa_q$. The resulting scaling plot is shown in Fig. 2 (right). To check for possible contributions from scaling violating terms we have analyzed the data separately for quark mass ratios $m_l/m_s = 1/10,\ 1/20$ and $m_l/m_s = 1/40,\ 1/80$. These fits agree within statistical errors. We then determine the curvatures κ_q from fits to the complete data set. Results of these fits are summarized in Table 2.

The scaling analysis performed for the mixed susceptibility on lattices with temporal extent $N_\tau = 4$ suggests that the determination of the curvature parameter κ_μ can be reliably performed with quark masses $m_l/m_s \lesssim 1/10$. This is in accordance with the scaling analysis of the order parameter itself [7, 8]. It thus seems to be safe to extract the curvature parameter also at smaller values of the lattice spacing, *i.e.* from our $N_\tau = 8$ data set, by using the smallest quark mass ratio available there, $m_l/m_s = 1/20$. We have performed calculations at five values of the temperature using gauge field configurations on $32^3 \times 8$ lattices generated by the HotQCD collaboration [17]. For

N_τ	m_l/m_s	κ_q	χ^2/dof
4	1/10, 1/20	0.0598(26)	3.5
	1/40, 1/80	0.0573(29)	1.5
8	1/20	0.0559(35)	0.4
4, 8	all	0.0591(17)	2.1

Table 2: Determination of the curvature of the critical surface of the chiral phase transition in $(2+1)$-flavor QCD as function of the light quark chemical potential μ_q. The table summarizes fits performed separately for two lighter and two heavier quark mass sets as well as the combined data set.

these parameter sets we have analyzed 300 to 600 gauge field configurations, which were separated by 100 trajectories. Again we used 500 noise vectors for the calculation of all relevant operators on each of the gauge field configurations. The result of this analysis is shown in Fig. 2 with filled symbols. As can be seen they agree well with results obtained on coarser lattices.

When rescaling data obtained for $\chi_{m,q}$ to the $O(2)$ scaling curve $f'_G(z)$ we need to take into account errors on the scaling parameters t_0 and z_0 (or h_0). This leads to a 10% error for the determination of the curvature terms. Performing a combined fit to all results obtained for different quark mass values and lattice spacings we obtain $\kappa_q = 0.059(2)(4)$ or equivalently $\kappa_B = 0.00656(22)(44)$.

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