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The Pseudocritical Line in the QCD Phase Diagram

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We report about ongoing work to determine the chiral transition line in 2+1 flavour QCD for small values of the light quark chemical potential. The curvature of this line can be derived from a scaling analysis of the chiral condensate and its derivative with respect to the chemical potential. We outline the method and show results as available.

1 Introduction

One of the central goals of the physics program of the present and future heavy ion colliders is the exploration of the phase diagram of Quantum Chromo Dynamics (QCD) the theory of the strong interactions of quarks and gluons. At high temperatures and/or baryon densities the theory undergoes a transition from a confined, hadron phase where chiral symmetries are spontaneously broken to the so-called quark gluon plasma which is characterised by deconfinement and restored chiral symmetries. The general picture of the phase diagram is such that at small densities the two regions are presumably separated by a second order phase transition line in the chiral limit of vanishing quark masses. For small quark masses the transition happens along a pseudocritical line and is a rapid crossover. At sufficiently large densities or, equivalently, chemical potentials the transition could turn into a first order phase transition. It is the aim of the work presented here to shed more light on the location and the properties of the transition lines and perhaps provide some means to study the Critical End Point separating the first order line from second order/crossover.

In the experimental studies of the QCD phase diagram mentioned above the analysis of conserved charge fluctuations, the correlation between fluctuations of different charges and their higher moments, play an increasingly important role; not the least because experiments start to be able to measure them with rising reliability. In particular higher order cumulants of net baryon number, net electric charge and net strangeness carry information on the phase structure of strong interaction matter as function of the corresponding chemical potentials. At present there are thus major on-going efforts undertaken to measure observables related to these higher-order non-Gaussian fluctuations in various heavy-ion collision experiments[1–5].

Cumulants of conserved charge fluctuations characterise the thermal conditions in a heavy ion collision at the time of freeze-out, i.e. at the time when partons have recombined again and formed hadrons and when inelastic scatterings have seized to change the particle decomposition of the expanded fireball. Large deviations of these fluctuation observables from a non-critical baseline model, e.g. the hadron resonance gas (HRG) model, will occur in the vicinity of a phase transition. The hope is that experiments may detect a non-monotonic behaviour of cumulants of charge fluctuations at zero or non-zero values of the chemical potentials which, on the one hand, would be indicative[6] for critical behaviour in the vicinity of the chiral phase transition at small μ_B and, on the other hand, would provide evidence for the existence of the QCD Critical End Point (CEP)[7–10] at non-zero chemical potential. While the former may be studied at the highest energies at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory as well as at the Large Hadron Collider (LHC) at CERN in its lead-lead collision mode, the latter may be found with the Beam Energy Scan (BES) program at RHIC.

This critical point, if it exists, is likely to be connected to the chiral phase transition at zero chemical potential for two degenerate light (l) and a strange (s) quark flavour. In fact, in the chiral limit the CEP will be a tri-critical point at which the line of second order chiral transitions turns into a line of first order transitions. An important aspect of the theoretical analysis of the chiral transition is the quantitative determination of the chiral transition line at moderate, non-zero values of the chemical potential. In this context, it is an important issue to determine the relation between the QCD transition temperature T_c at non-zero quark chemical potential μ_q, and the experimentally determined freeze-out curve because the experimental success may depend crucially on the relative position of these two lines.

The determination of the QCD phase diagram clearly is a non-perturbative problem. As such it invites to be tackled by a numerical evaluation of the QCD path integral on space time lattices i.e. lattice QCD. However, at non-vanishing baryo-chemical potential the QCD action becomes complex such that standard Monte Carlo methods to compute the path integrals stochastically don't work anymore. This is the famous sign problem. Various ways have been invented to by-pass this problem at least at small densities. Here, in order to determine the crossover transition line at non-zero chemical potential, we follow an approach that is based on Taylor expansion around $\mu_q = 0$ and a scaling analysis relating a pseudocritical line (crossover) at non-zero quark masses to the true critical line in the chiral limit.

2 The Method

A theoretically sound and attractive approach to determine the pseudocritical (crossover) line in the QCD phase diagram at nonvanishing quark masses is based on a scaling analysis which relates this line to a true critical line in the chiral limit. We have worked out this method[19] and sketch it in the following.

At leading order in the quark chemical potential μ_q the variation of the transition temperature with chemical potential is parametrised in terms of the constant κ_q

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

Here T_c is the phase transition temperature in the chiral limit. This constant κ_q can be determined by analysing the dependence of the light quark, chiral condensate $\langle\bar{\psi}\psi\rangle_l$ on the quark chemical potential. Of course, at vanishing light quark mass one would simply determine the temperature at which $\langle\bar{\psi}\psi\rangle_l$ vanishes. At non-zero but small values of the quark mass this information is encoded in scaling functions.

Scaling functions arise from the partition function or, equivalently, the free energy density f. In the vicinity of a critical point regular contributions f_r to the partition functions become negligible in higher order derivatives and the singular behaviour of response functions will generally be dominated by contributions coming from the singular part f_s of the free energy density[a]

$$f(T,m_l,m_s,\mu_q) = f_s(T,m_l,m_s,\mu_q) + f_r(T,m_l,m_s,\mu_q) \ . \tag{2}$$

The singular part of the free energy density depends on the parameters of the QCD Lagrangian, e.g. the quark masses, and the external control parameters, temperature and chemical potentials, enter only through two relevant couplings. These scaling variables, t and h, control deviations from criticality, $(t,h) = (0,0)$, along the two relevant directions, which in the case of QCD characterise fluctuations of the energy and chiral condensate, respectively. 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 quark chemical potential

$$\begin{aligned} t &\equiv \frac{1}{t_0}\left(\frac{T-T_c}{T_c} + \kappa_q\left(\frac{\mu_q}{T}\right)^2\right) \ , \\ h &\equiv \frac{1}{h_0}\frac{m_l}{m_s} \ , \end{aligned} \tag{3}$$

The curvature parameter κ_q appearing in the above expression for t is the same as in Eq. 1 as the (pseudo) critical line $T_c(\mu_q)$ is determined by $t = 0$. Note that the strange quark mass has been chosen to render the magnetic field like parameter h dimensionless, and t_0, h_0 are non-universal scale parameters.

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

$$f_s(t,h) = h^{1+1/\delta} f_s(z,1) \equiv h^{1+1/\delta} f_s(z) \ . \tag{4}$$

where β, δ are known critical exponents of the three-dimensional $O(N)$ universality class[21,22], $\beta = 0.349$ and $\delta = 4.780$ for three-dimensional $O(2)$ models and $\beta = 0.380$ and $\delta = 4.824$ for $O(4)$, respectively. All parameters entering the definition of t and h, *i.e.* t_0, h_0 and T_c may depend on the strange quark mass, but are otherwise unique in the continuum limit of (2+1)-flavour QCD. Just like the transition temperature T_c, however, also t_0 and h_0 are cut-off dependent and will need to be extrapolated to the continuum limit.

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

$$M(t,h) \ = \ h^{1/\delta} f_G(z) \ . \tag{5}$$

[a]For systems belonging to the 3-dimensional $O(2)$ or $O(4)$ universality classes this does not hold for the thermal response function (specific heat) as the relevant critical exponent α is negative in these cases.

Also 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[21].

To extract information about the curvature κ_q it suffices to consider the leading order Taylor expansion coefficient of the chiral condensate,

$$\frac{\langle\bar{\psi}\psi\rangle_l}{T^3} = \left(\frac{\langle\bar{\psi}\psi\rangle_l}{T^3}\right)_{\mu_q=0} + \frac{\chi_{m,q}}{2T}\left(\frac{\mu_q}{T}\right)^2 + \mathcal{O}((\mu_q/T)^4)\ , \tag{6}$$

the mixed susceptibility $\chi_{m,q}$

$$\frac{\chi_{m,q}}{T} = \frac{\partial^2\langle\bar{\psi}\psi\rangle_l/T^3}{\partial(\mu_q/T)^2} = \frac{\partial\chi_q/T^2}{\partial m_l/T} \tag{7}$$

which may also be viewed as the quark mass derivative of the light quark number susceptibility (χ_q). By means of the scaling relations the mixed susceptibility is immediately proportional to κ_q,

$$\frac{\chi_{m,q}}{T} = \frac{2\kappa_q T}{t_0 m_s} h^{-(1-\beta)/\beta\delta} f'_G(z)\ , \tag{8}$$

where $f'_G(z) \equiv \mathrm{d}f_G(z)/\mathrm{d}z$ is easily obtained from $f_G(z)$ by using the parametrisations for the latter given in Refs. 21, 23. The way to proceed thus is to compute $\chi_{m,q}$ as a function of T and m_l numerically and extract κ_q, exploiting the knowledge on β, δ etc..

3 Some Technical Remarks

As pointed out in the previous section the first task is to determine the non-universal parameters t_0, h_0 and T_c at a given value for the lattice spacing, a, from the scaling properties of the chiral order parameter. For QCD this order parameter is (related to) the chiral quark condensate. However, owing to QCD being a Quantum Field Theory, the order parameter receives multiplicative as well as, at non-vanishing quark masses, additive renormalisations. The multiplicative renormalisation can be taken care of by using the renormalisation group invariant quantity

$$M_b = m_s\langle\bar{\psi}\psi\rangle_l. \tag{9}$$

The quadratically divergent additive correction $\sim m_l$ can in addition be subtracted according to

$$M = m_s\left(\langle\bar{\psi}\psi\rangle_l - m_l/m_s\langle\bar{\psi}\psi\rangle_s\right). \tag{10}$$

Multiplication by N_τ^4, where N_τ is the lattice extent in the temporal direction related to temperature by $aT = 1/N_\tau$, renders both quantities dimensionless. The difference between those two definitions becomes irrelevant in the chiral limit. Alternatively it can be accounted for by scaling correction terms.

On the lattice the quark condensate is obtained from the inverse of the Dirac matrix M_f for a given quark flavour f,

$$\langle\bar{\psi}\psi\rangle_f = \frac{1}{4}\frac{1}{N_\sigma^3 N_\tau}\langle\mathrm{Tr}M_f^{-1}\rangle \tag{11}$$

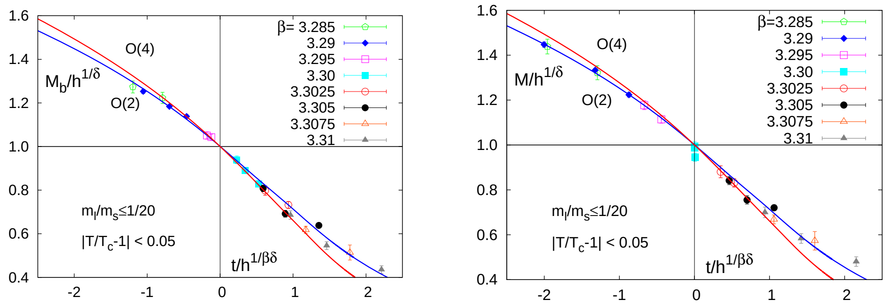

Figure 1. Fit of the $O(2)$ scaling function to numerical results for the light quark condensate. This analysis has been performed within the p4 discretisation with light quark masses $m_l/m_s \leq 1/20$ on $N_\tau = 4$ lattices. From Ref. 18.

by taking the trace Tr over Dirac and space-time indices. Similarly, the mixed susceptibility is obtained from traces over expressions involving M_l,

$$\frac{\chi_{m,q}}{T} = \frac{1}{N_\sigma^3} \left(\langle \mathcal{C}_2 \rangle + 2 \langle \mathcal{C}_1 \mathcal{D}_1 \rangle + \langle \mathcal{C}_0 \mathcal{D}_2 \rangle + \left\langle \mathcal{C}_0 \mathcal{D}_1^2 \right\rangle - \langle \mathcal{C}_0 \rangle \left(\langle \mathcal{D}_2 \rangle + \left\langle \mathcal{D}_1^2 \right\rangle \right) \right) \tag{12}$$

where

$$\mathcal{C}_n = \frac{1}{4} \frac{\partial^n \mathrm{tr} M_l^{-1}}{\partial \hat{\mu}^n} \bigg|_{\hat{\mu}=0} \quad , \quad \mathcal{D}_n = \frac{1}{2} \frac{\partial^n \ln \det M_l}{\partial \hat{\mu}^n} \bigg|_{\hat{\mu}=0} \quad , \tag{13}$$

with the shorthand notation $\hat{\mu} = \mu_q a$ for the chemical potential expressed in units of the lattice spacing. The different traces are obtained from stochastic estimators: given vectors of random numbers satisfying $\langle r_i^* r_j \rangle = \delta_{ij}$ in the average over the random vectors, one repeatedly solves $MX = r$ to obtain e.g. the quark condensate as $\langle r_j^* X_j \rangle$. Recycling the solutions X and applying them as part of the right hand side in e.g. $MY = M'X$ where $M' = \partial M / \partial \hat{\mu}$ delivers $\mathcal{C}_1 \sim \mathrm{Tr} M^{-1} M' M^{-1}$ as $\langle r_j^* Y_j \rangle$. Thus, quite a few right hand sides are needed to obtain all requested traces so that deflating the Krylov space of the Conjugate Gradient inverter[25] from $\mathcal{O}(100)$ pre-calculated low eigenmodes of M is applied.

4 Results

The analysis path sketched in Sec. 2 has been suggested and worked out by us in Ref. 19. As a proof of principle of the method it was applied there to lattice regularised QCD in the p4 discretisation scheme. As a prerequisite, in Ref. 18 we had studied the scaling behaviour on $N_\tau = 4$ lattices down to a light to strange quark mass ratio of $m_l/m_s = 1/80$. With the strange quark mass at its physical value this corresponds to a Goldstone pion as low as 75 MeV. As can be read off Fig. 1 the data is in agreement with $O(N)$ scaling in the chiral order parameter. Here we show results for both definitions of the parameter, Eqs. 9 and 10, for light quark masses smaller than 1/20 of the strange quark mass. The figure further reveals that on the basis of the condensate $O(2)$ is not distinguishable from $O(4)$.

It turned out that the scaling region was entered already at $m_l/m_s = 1/10$. At this and larger light quark mass values besides the singular part two regular terms were needed to obtain a good fit. As a byproduct this study provides evidence for the Goldstone effect in QCD at high temperature which consists of a $1/\sqrt{m_l}$ divergence of the disconnected susceptibility $\chi_m \sim \partial\langle\bar{\psi}\psi\rangle_l/\partial m_l$ in the chirally broken phase, giving further support that the scaling machinery works consistently. In Ref. 19 we added the analysis of $N_\tau = 8$ configurations, yet only light quark masses down to $m_l/m_s = 1/20$ were available. We found again agreement with scaling also at this finer lattice. A separate scaling fit for only the lightest quark masses was beyond the scope of this paper, and the non-universal scaling parameters were determined from a combined fit to all data in this case.

While these results are based on the p4 discretisation, in Ref. 20 we applied successfully the $O(N)$ scaling relation to HISQ configurations, an action with the smallest taste violations of all known staggered type actions, and obtained very good descriptions of the data on chiral observables. These were used subsequently in chiral interpolations of the quark condensate in order to determine the pseudocritical temperature T_c.

Whereas in all these studies agreement with $O(N)$ critical behaviour was observed, we want to stress that the nature of the chiral phase transition is not a question settled yet; other scenarios e.g. suggest a first order transition, see Ref.[26] for a recent paper. Thus, in the ongoing project we are carrying out a dedicated scaling analysis within the HISQ discretisation, with quark masses reaching down to values that lead to smaller than physical pion masses. The scaling parameters are then input to the combined analysis of the transition line.

Once the results on the non-universal scaling parameters t_0, h_0 are at hand, the curvature constant κ_q can be extracted from the mixed susceptibility, Eq. 8. This is shown in Fig. 2 taken from our pilot study. Note that κ_q is the only free parameter and the fit is completely fixed otherwise. As far as the value for κ_q is concerned a phenomenologically motivated approach[12] has obtained a result very close to our value from that study while a recent analysis based on simulations at imaginary chemical potential[27] suggests a larger curvature. It is the aim of the present project to reduce the systematic errors and greatly improve the prediction of that curvature at real chemical potentials.

5 Concluding Remarks

We have sketched a procedure to determine the curvature of the chiral transition line of QCD in the temperature - chemical potential plane at small baryon densities by means of numerical simulations of lattice QCD. This method is based on the analysis of the scaling behaviour of QCD in the vicinity of the chiral transition. We have demonstrated the feasibility of this procedure by providing quantitative results for the curvature in a pilot study. The present project is aiming at establishing these results at decreased systematic uncertainties.

Being of high interest on its own, the curvature result obtained so far has been used to compare the chiral transition line in the $T - \mu$ QCD phase diagram with the freeze-out curve, see Fig. 3. Here, for the first time the freeze-out parameters T^f and μ_B^f were obtained by comparing experimental results from heavy ion collisions on fluctuations and correlations of conserved quantum numbers with lattice computations of the same quantities[14]. While in such comparisons care must be taken that effects of conservation laws due to finite system sizes, acceptance cuts etc. do not invalidate grand canonical statistics, an

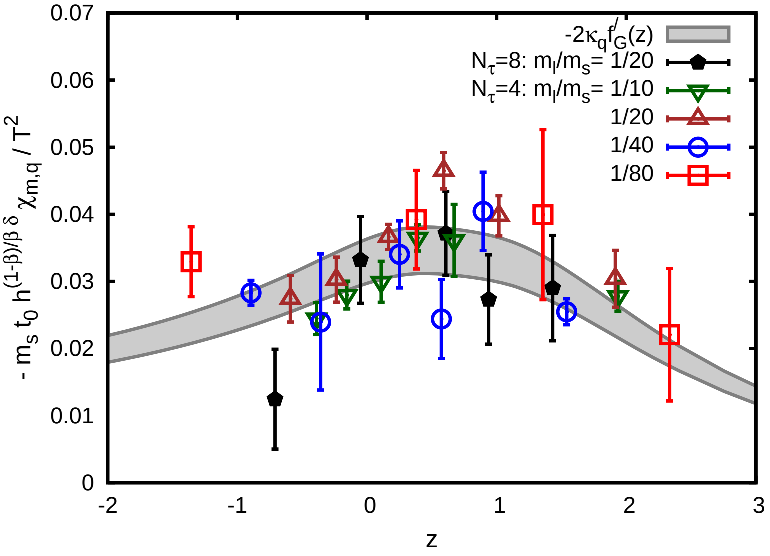

Figure 2. The scaled mixed susceptibility as function of the scaling variable $z = t/h^{1/\beta\delta}$. The data from simulations with the p4 action are compared to the $O(2)$ scaling curve. The band shows a 10% error on this curve which arises from statistical errors on the calculated observables as well as from the errors on the scaling parameters t_0 and z_0. From Ref. 19.

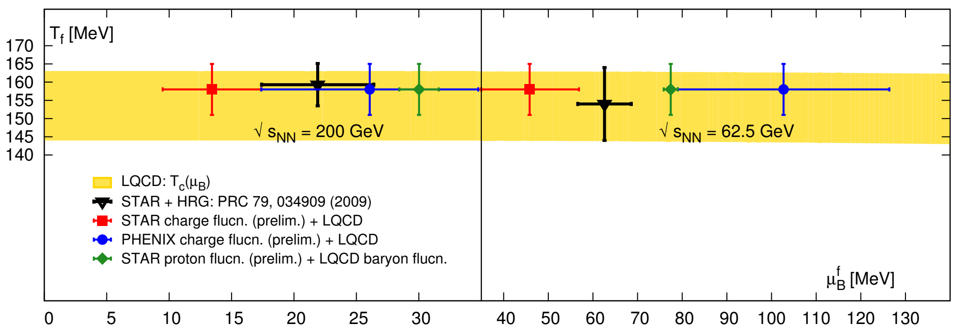

Figure 3. Freeze-out temperatures T^f and baryon chemical potentials μ_B^f obtained through direct comparisons between lattice calculations and the preliminary STAR and PHENIX data for cumulants of net charge and net proton fluctuations at two different beam energies $\sqrt{s_{NN}} = 200$ GeV and 62.5 GeV. The shaded region indicates the present lattice results[19,15] for the pseudocritical temperature T_c as a function of μ_B. From Ref. 24.

approach which does not rely on model assumptions certainly deserves further work. At present it is very interesting that the results for the freeze-out line $T^f(\mu_B^f)$ are close to the chiral/deconfinement crossover, raising the hope that the collision experiments may signal the presence of criticality in the phase diagram.

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