

THE PHASE DIAGRAM OF LATTICE QCD IN THE STRONG COUPLING LIMIT AND AWAY FROM IT*

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The strong coupling limit of staggered lattice QCD has been studied for decades, both via Monte Carlo and mean field. In this model, the finite density sign problem is mild and the full phase diagram can be studied, even in the chiral limit. However, in the strong coupling limit the lattice is maximally coarse. Here, we propose a method to go beyond the strong coupling limit with first results and discuss the consequences on the QCD phase diagram in the μ - T plane, in particular the existence of chiral critical end point which is sought in heavy ion collisions. We explain how to construct an effective theory for non-zero lattice coupling, valid to $\mathcal{O}(\beta)$, and present Monte Carlo results incorporating these corrections.

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1. Introduction

It is one of the main goals of lattice QCD at finite temperature and density to map the phase boundary and the order of the transition as a function of the quark chemical potential μ and the temperature T . However, due to the sign problem of fermion determinant based Hybrid Monte Carlo, little progress has been made in this field. All the methods at hand are limited to small μ/T [1]. Here, we propose to study the phase diagram from a strong coupling perspective, where simulations are feasible also at finite chemical potential. The basic idea of strong coupling lattice QCD is to perform the link integrals analytically before integrating out the Grassmann variables, hence no fermion determinant arises. The sign problem does not

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pose a problem in practice, because at high temperatures or densities the sign problem vanishes and is still mild across the phase boundary. We adopt the staggered fermion discretization, where a reformulation in “dual variables” can be obtained ([2, 3], see also [4] for the dual variable approach in another model with chemical potential). The full QCD partition function is given by

$$Z_{\text{QCD}} = \int d\psi d\bar{\psi} dU e^{S_G + S_F}, \quad S_G = \frac{\beta}{2N_c} \sum_P \text{tr} [U_P + U_P^\dagger], \quad (1)$$

$$S_F = am_q \sum_x \bar{\psi}_x \psi_x \frac{1}{2} \sum_{x,\nu} \eta_\nu(x) \gamma^{\delta_{\nu 0}} \times \left[\bar{\psi}_x e^{a_t \mu \delta_{\nu 0}} U_\nu(x) \psi_{x+\hat{\nu}} - \bar{\psi}_{x+\hat{\nu}} e^{-a_t \mu \delta_{\nu 0}} U_\nu^\dagger(x) \psi_x \right] \quad (2)$$

with m_q the quark mass and $\mu = \frac{1}{3}\mu_B$ the quark chemical potential. The anisotropy in the Dirac couplings γ is introduced to vary the temperature continuously. At strong coupling, the ratio of spatial and temporal lattice spacing is $\frac{a}{a_t} \simeq \gamma^2(1 + \mathcal{O}(1/N_\tau))$ [5]. The action in the strong coupling limit is simply given by the fermionic action, as the lattice gauge coupling $\beta = 2N_c/g^2$ vanishes in the strong coupling limit $g \rightarrow \infty$. Since the link integration factorizes in the absence of the gauge action, the gauge links $U_\nu(x)$ can be integrated out analytically [6]. After performing the Grassmann integration, the final partition function, introduced in [2], is obtained by an analytic rewriting in terms of hadronic degrees of freedom (mesons and baryons)

$$Z_{\text{SC}} = \sum_{\{k,n,\ell\}} \prod_b \frac{(N_c - k_b)!}{N_c! k_b!} \prod_x \frac{N_c!}{n_x!} (2am_q)^{n_x} \prod_\ell w(\ell, \mu). \quad (3)$$

The mesons are represented by monomers $n_x \in \{0, \dots, N_c\}$ on sites x , and dimers $k_b \in \{0, \dots, N_c\}$ (with $b = (x, \mu)$ the bonds), whereas the baryons are represented by oriented self-avoiding loops ℓ . The weight $w(\ell, \mu) = (\prod_{b \in \ell} N_c!)^{-1} \sigma(\ell) e^{N_c N_\tau r_\ell a_\tau \mu}$ for a baryonic loop ℓ and its sign $\sigma(\ell) \in \{+1, -1\}$ depends on the loop geometry. The essential constraint on the admissible configuration $\{k, n, \ell\}$ is the Grassmann constraint

$$n_x + \sum_{\hat{\mu}=\pm\hat{0}, \dots, \pm\hat{d}} \left(k_{\hat{\mu}}(x) + \frac{N_c}{2} |\ell_{\hat{\mu}}(x)| \right) = N_c. \quad (4)$$

Due to this constraint, mesonic degrees of freedom (monomers and dimers) cannot occupy baryonic sites. This system has been studied both via mean field [7–10] and Monte Carlo methods [5, 11, 13]. In recent years, Monte

Carlo simulations of this system have undergone a revival due to the applicability of the Worm algorithm [5, 12, 13]. The idea is to violate the Grassmann constraint in order to sample the monomer two-point function $G(x, y)$ from which the chiral susceptibility is computed. These techniques have been applied to obtain all lattice data presented in this paper. In Fig. 1, we show the (μ, T) phase diagram in the strong coupling limit and for $m_q = 0$, where $\langle \bar{\psi}\psi \rangle$ is an exact order parameter for spontaneous chiral symmetry breaking. It is qualitatively similar to the expected phase diagram of QCD in the chiral limit: the transition is of second order at $a\mu = 0$, up to the tricritical point at $(a\mu_{\text{tcp}}, aT_{\text{tcp}})$, and turns to first order. At finite quark mass, the second order line turns into a crossover, the tricritical point into a second order critical end point. At low temperatures, in contrast to QCD, the chiral transition coincides with the nuclear transition. This is because above the critical chemical potential a baryonic crystal forms, which restores chiral symmetry. This saturation effect is a lattice artifact.

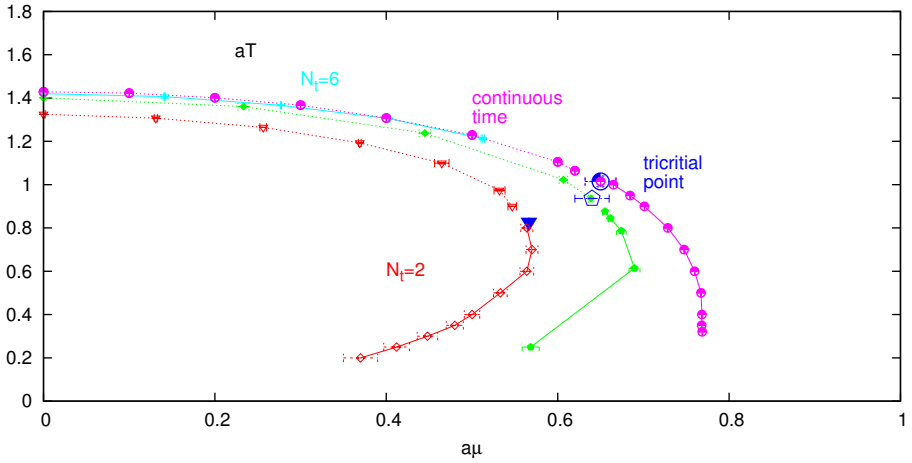


Fig. 1. SC phase diagram from Worm algorithm with identifications: $aT = \frac{\gamma^2}{N_\tau}$, $a\mu = \gamma^2 a_\tau \mu$. Note that the re-entrance at low temperatures vanishes in continuous time ($N_\tau \rightarrow \infty$).

Since strong coupling lattice QCD can be thought of as a one-parameter deformation of continuum QCD, an important question is how both phase diagrams are connected. Due to the sign problem, only the plane at $\mu = 0$ and the plane at $\beta = 0$ is known. The QCD phase diagram in the (μ, T) plane in the continuum limit is largely unknown. If the tricritical point persists in the continuum limit, this is strong evidence for the existence of a chiral critical end point in full QCD at physical quark mass. In order to go beyond the strong coupling limit, we derive a partition function valid at $\mathcal{O}(\beta)$, from

which we compute the slope of the chiral transition temperature. There are two questions we want to address: What is the slope of the tricritical line with respect to β , and do the chiral and nuclear transition split as expected? Two of various possible scenarios are sketched in Fig. 2.

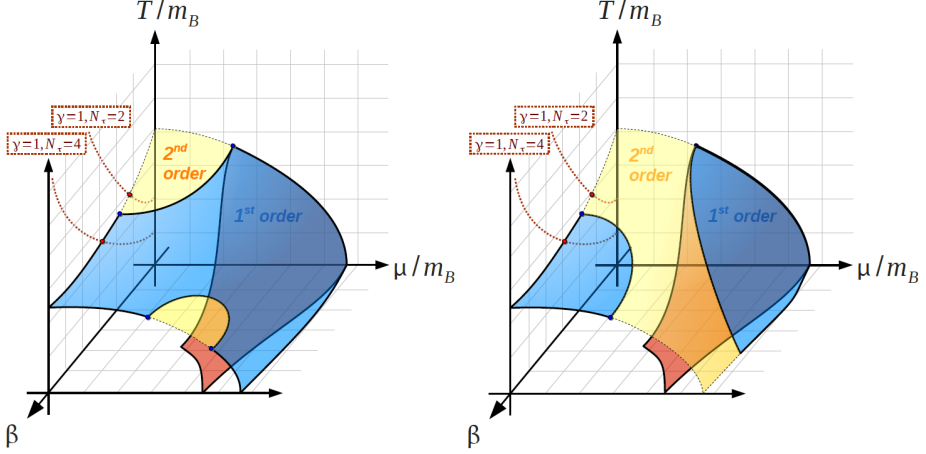


Fig. 2. Two scenarios of the extension of the chiral transition to finite β . It is expected that the chiral transition and the nuclear transition will split. The first and second order regions are separated by tricritical lines. Of special interest is whether the tricritical point at strong coupling will move to smaller (left) or larger (right) values of μ_c as a function of β .

2. Corrections to the strong coupling limit

To go beyond the strong coupling limit, a systematic expansion of the QCD partition function in β is needed. Here, we derive the effective action valid to the leading order $\mathcal{O}(\beta)$. The SC partition function including the gauge part can be written in terms of a fermionic path integral

$$Z_{\text{QCD}} = \int d\chi d\bar{\chi} dU e^{S_G + S_F} = \int d\chi d\bar{\chi} Z_F \langle e^{S_G} \rangle_{Z_F}, \quad (5)$$

where $Z_F = \int dU e^{-S_F}$ is the fermionic partition function, which is related to the strong coupling partition function via $Z_{\text{SC}} = \int d\chi d\bar{\chi} Z_F$. The gauge action can then be expressed as an expectation value which we linearize to obtain the $\mathcal{O}(\beta)$ contribution

$$\langle e^{S_G} \rangle_{Z_F} \simeq 1 + \langle S_G \rangle_U = 1 + \frac{\beta}{2N_c} \sum_P \left\langle \text{tr} [U_P + U_P^\dagger] \right\rangle_{Z_F}. \quad (6)$$

Evaluating the expectation value of the elementary plaquette $\text{tr}[U_P]$ in the strong coupling ensemble, we need to compute the link integrals with an additional gauge link coming from the plaquette. Before Grassmann integration, the plaquette is given by $P = J_{ij}J_{jk}J_{kl}J_{li}$ with the link integrals at the edge of an elementary plaquette [14–16]

$$J_{ij} = \sum_{k=1}^{N_c} \frac{(N_c - k)!}{N_c!(k-1)!} (M_\chi M_\varphi)^{k-1} \bar{\chi}_j \varphi_i + \frac{1}{N_c!(N_c-1)!} \epsilon_{ii_1 i_2} \epsilon_{jj_1 j_2} \bar{\varphi}_{i_1} \bar{\varphi}_{i_2} \chi_{j_1} \chi_{j_2} - \frac{1}{3} \bar{B}_\chi B_\phi \bar{\phi}_j \chi_i \quad (7)$$

with M and B representing the mesons and baryons. From these link integrals, we can compute the weight for inserting a plaquette or a Polyakov loop into the strong coupling configuration. At the corners of the plaquette, the Grassmann variables ϕ, χ are bound into baryons and mesons to fulfill a modified Grassmann constraint: here, the degrees of freedom add up to $N_c + 1$. For $N_c = 3$, there are 19 diagrams contributing to the plaquette P [16], one of them given in Fig. 3. We can summarize the generalized link weights w and site weights v as follows

$$v_M = (N_c - 1), \quad v_B = N_c!, \quad w_{D_k} = \frac{(N_c - k)!}{N_c!k!} k, \\ w_{B_0} = \frac{1}{N_c!}, \quad w_{B_1} = \frac{1}{N_c!(N_c - 1)!}, \quad w_{B_2} = \frac{(N_c - 1)!}{N_c!}, \quad (8)$$

where at v_B the external leg is baryonic, whereas at v_M the external leg is mesonic, B_1 is an oriented link where one quark flux is replaced by a gauge flux and B_2 the link state of a baryon dressed with oppositely oriented gauge and quark flux. We can insert a new set of variables, the plaquette occupation numbers $q_p \in \{0, 1\}$ (and derived from it a bond-plaquette number $q_b \in \{0, 1\}$), to include a Metropolis update allowing to sample the partition function

$$Z = \sum_{\{k,n,q,\ell\}} \prod_x w_x \prod_b w_b \prod_\ell w_\ell \prod_P w_P, \\ w_x = \frac{N_c!}{n_x!} (2am_q)^{n_x} v_i(x), \quad w_b = \frac{(N_c - k_b)!}{N_c!(k_b - q_b)!}, \\ w_\ell = \prod_\ell w_{B_i}(\ell) \sigma(\ell) e^{3N_\tau r_\ell a_\tau \mu}, \quad w_P = \left(\frac{\beta}{2N_c} \right)^{-2q_p} \quad (9)$$

at finite β . Qualitatively new aspects of the $\mathcal{O}(\beta)$ contributions are (1) that mesons and baryons are now allowed to interact and (2) that baryons become

extended objects, in contrast to their pointlike nature in the strong coupling limit. There is no strict decomposition of the lattice into mesonic and baryonic sites due to the plaquettes. The $\mathcal{O}(\beta)$ corrections allow to measure the zero-th order of gauge observables (average plaquette, Polyakov loop), and the first order of fermionic observables (slope of the chiral susceptibility, baryon density).

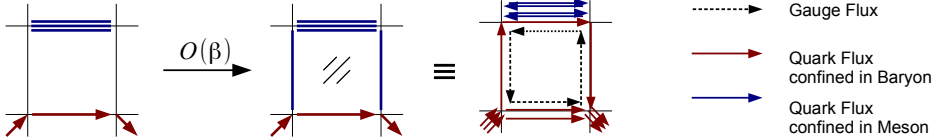


Fig. 3. Illustration of reweighting from the strong coupling ensemble: insertion of two parallel dimers produces one of the 19 plaquette diagrams. The dimer and flux variables adjacent to the plaquette are composed of quark flux and gauge flux: black/blue lines represent mesonic content, gray/red lines represent baryonic content. The baryon becomes an extended object.

3. Gauge observables

We obtain gauge observables via reweighting from the strong coupling ensemble, instead of sampling at finite β . This is because the average plaquette, given by

$$\langle P \rangle = \frac{2}{Vd(d-1)} \frac{\partial}{\partial \beta} \log(Z) = \frac{1}{\beta} \langle n_P \rangle, \quad n_P = \frac{2}{Vd(d-1)} \sum_P q_P \quad (10)$$

is very noisy for small β due to the division of two small numbers. In Fig. 4 we show a detailed comparison of the strong coupling algorithm (making use of both the worm algorithm and reweighting in the plaquette number, abbreviated SC-algorithm) with conventional hybrid Monte Carlo (HMC). Both the Polyakov loop and the average plaquette are consistent in the whole parameter space in quark mass and temperature. In Fig. 5 the volume dependence of the Polyakov loop and average plaquette is shown, both are sensitive to the chiral transition. This cusp-like behaviour should not be interpreted as deconfinement, but is an imprint of the chiral transition. We have reported this finding for U(3) gauge theory in [17], and similar behaviour is also found in the opposite limit of non-confining models, discussed in [18].

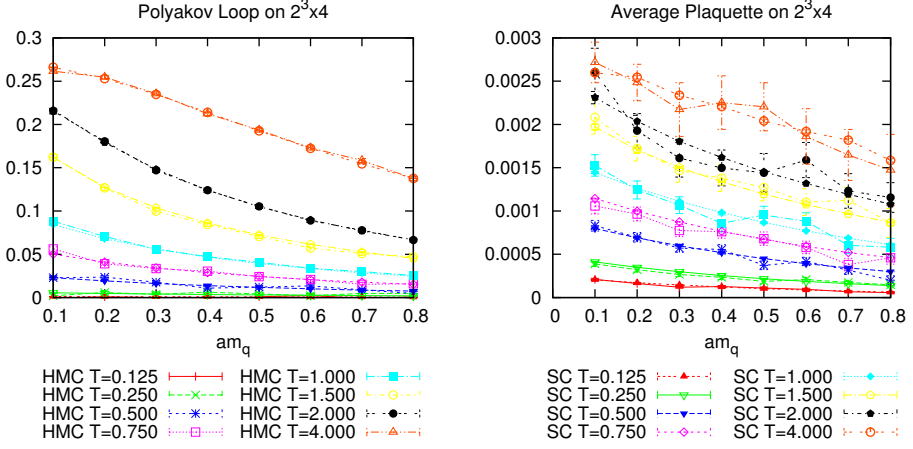


Fig. 4. Comparison of gauge observables measured both with SC-algorithm and Hybrid Monte Carlo. Perfect agreement is found for the Polyakov loop (left). The average plaquette (right) is very noisy in HMC, but in good agreement with the results from the SC-algorithm.

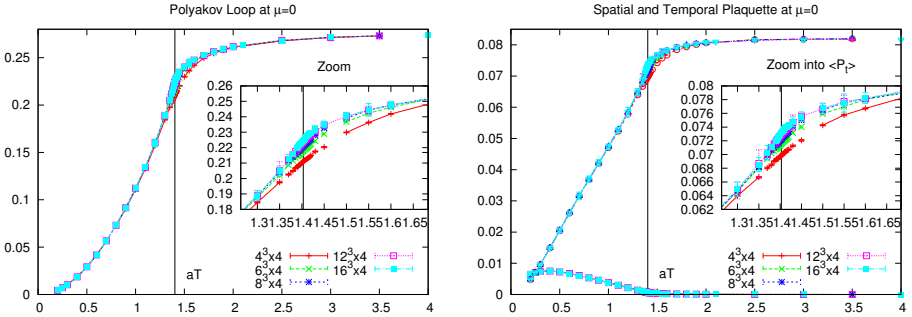


Fig. 5. Volume dependence of gauge observables: both the Polyakov loop (left) and the average plaquette (right) show an L -dependence at the transition region, close to $aT_c = 1.402(1)$.

4. Phase diagram as a function of β

For fermionic observables, such as the chiral susceptibility or the baryon density, we can extract the leading order corrections (the slope with respect to β). This allows us to compute the gauge corrections to the strong coupling phase diagram. We now address the chiral susceptibility, which in terms of the monomer number N_M is given by

$$\chi = \frac{1}{(2am_q)^2 L^3 N_t} \left(\langle N_M^2 \rangle - \langle N_M \rangle^2 - \langle N_M \rangle \right). \quad (11)$$

In the following, we consider the chiral limit, where $\langle N_M \rangle = 0$ due to the finite system size. The worm algorithm samples the 2-point correlation function in the 2-monomer sector, its integral is

$$\chi = \frac{1}{V} \sum_{x_1, x_2} G(x_1, x_2) \equiv \langle (\bar{\psi}\psi)^2 \rangle. \quad (12)$$

The leading order Taylor coefficient of χ is given by the derivative of the chiral susceptibility w.r.t. β .

$$\begin{aligned} \chi(\beta) &= \chi_0 + c_\chi \beta + \mathcal{O}(\beta^2), \\ c_\chi &= \frac{\partial}{\partial \beta} \langle (\bar{\psi}\psi)^2 \rangle = N_s^3 N_t \left(\langle (\bar{\psi}\psi)^2 P \rangle - \langle (\bar{\psi}\psi)^2 \rangle \langle P \rangle \right). \end{aligned} \quad (13)$$

At finite temperature, we need in fact to measure both spatial and temporal plaquette expectation values as well as their joint expectation value with $(\bar{\psi}\psi)^2$. This results in two Taylor coefficients, c_s , c_t . However, c_s is largely suppressed with temperature, just as the spatial plaquette itself (see Fig. 5), so that we did not need to consider any anisotropy in the gauge coupling β_s/β_t at the phase boundary. We determine the chiral transition temperature via critical scaling with $3d$ $O(2)$ critical exponents γ , ν

$$\chi_L(T, \beta)/L^{\gamma/\nu} = A + BtL^{1/\nu}, \quad t = \frac{T - T_c(\beta=0)}{T_c(\beta=0)} \quad (14)$$

that is the chiral susceptibility collapses on a universal scaling function when rescaled in this way, which is almost linear in the scaling window with non-universal coefficients $A \simeq 1.001(1)$ and $B \simeq -0.982(1)$ for $SU(3)$ at zero density. Our strategy is to determine the shift in aT_c induced by a finite value of β . For this to be the case, the Taylor coefficient also has to obey critical scaling. We indeed find that c_χ can well be fitted by a linear function in t

$$\frac{c_\chi}{\chi} \simeq c_1 + c_2 L^{1/\nu} + c_3 t, \quad (15)$$

with $c_2 = -0.397(2)$ for $SU(3)$ at $\mu = 0$. The coefficient c_3 drops out since the term is of higher order in β . The slope of the critical temperature is

$$s \equiv \left. \frac{d}{d\beta} aT_c(\beta) \right|_{\beta=0} = -aT_c \frac{A}{B} c_2. \quad (16)$$

For SU(3), where $aT_c = 1.402(1)$ at $\mu = 0$, we obtain $s = -0.446(7)$, as shown in Fig. 6, so we indeed find that the transition temperature drops. The slope can be compared to the mean field result of Miura *et al.* [19], who get $s \approx 0.4$, which is quite compatible

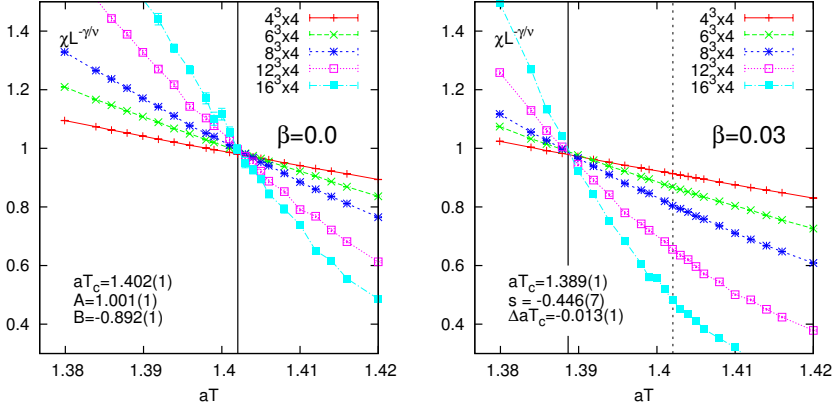


Fig. 6. The transition temperature from critical scaling of the chiral susceptibility. Left: for $\beta = 0$, $aT_c = 1.402(1)$. Right: for $\beta = 0.03$, the transition temperature shifts to $aT_c = 1.389(1)$.

The drop in aT_c is expected since the lattice spacing $a(\beta)$ shrinks as β is increased. Also, in the strong coupling limit, the ratio $\frac{T_c(\mu=0)}{3\mu_c(T=0)} \approx \frac{1.403}{1.71} = 0.82$ is much too large compared to the continuum result (in the chiral limit) $\frac{T_c}{3\mu_c} \approx \frac{154 \text{ MeV}}{0.93 \text{ GeV}} = 0.165$. Hence it is expected that the phase boundary at small μ decreases more drastically with β than at large μ . Due to the mild sign problem of the dimer representation, our method to determine the slope of aT_c can be readily extended to finite density. Numerical results for the phase boundary as a function of β will be presented in a forthcoming publication.

5. Conclusion

We have presented a method to compute gauge corrections to the QCD phase diagram at strong coupling. The correct average plaquette and Polyakov loop are reproduced at $\beta = 0$ and can be measured at high precision. This allows us to obtain the leading order gauge corrections to the chiral susceptibility via reweighting. Via a second order scaling analysis we were able to get the slope of the chiral transition temperature $\frac{d}{d\beta} aT_c$, which is in good agreement with the expected value.

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