

Deconfinement critical point of heavy quark effective lattice theories

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Effective three-dimensional Polyakov loop theories derived from QCD by strong coupling and hopping expansions are valid for heavy quarks and can also be applied to finite chemical potential μ , due to their considerably milder sign problem. We apply the Monte-Carlo method to the $N_f = 1, 2$ effective theories up to $\mathcal{O}(\kappa^4)$ in the hopping parameter at $\mu = 0$ to determine the critical quark mass, at which the first-order deconfinement phase transition terminates. The critical end point obtained from the effective theory to order $\mathcal{O}(\kappa^2)$ agrees well with 4-dimensional QCD simulations with a hopping expanded determinant by the WHOT-QCD collaboration. We also compare with full QCD simulations and thus obtain a measure for the validity of both the strong coupling and the hopping expansion in this regime.

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1. Introduction

Significant effort in theory and experiment is dedicated to explore QCD under extreme conditions, such as high temperature (T) or baryon chemical potential ($\mu_B = 3\mu$). Despite considerable progress for zero and small chemical potential, the QCD phase diagram is still largely unknown, because the fermion sign problem prohibits Monte Carlo investigations with finite chemical potential, especially in the cold and dense region, which is central to astrophysics.

These difficulties have motivated the development of effective theories derived from lattice QCD by strong coupling and hopping parameter expansions, which are valid in the heavy quark regime. These can either be solved by fully analytic series expansion techniques known from statistical mechanics [1–3], or by numerical simulations if their sign problem is sufficiently mild [4, 5].

For the $SU(3)$ pure gauge theory, the deconfinement transition spontaneously breaks the global Z_3 center symmetry, and is of first order. The presence of dynamical quarks breaks the center symmetry explicitly, and leads to a weakening of the deconfinement transition with decreasing quark mass until it vanishes at a critical point in the 3D Ising universality class. For still lighter quark masses, the transition becomes an analytic crossover. This behavior is also inherited by the effective theory.

Here we update previous studies of three-dimensional effective theories at zero chemical potential in the heavy quark regime using standard Monte Carlo simulations. We calculate the deconfinement phase transition and its critical end point for $N_f = 1, 2$, for $N_t = 4, 6$ for different truncations of the three-dimensional effective theory up to order $\mathcal{O}(\kappa^4)$ in the hopping parameter. Our results are compared with simulations of four-dimensional QCD after hopping expansion [6], as well as with full QCD simulations [7].

2. 3D Effective lattice theories

First we briefly discuss the derivation of the effective action. For more detail, see for instance [4, 8]. The starting point is a $(3 + 1)$ -dimensional lattice with Wilson gauge and fermion action for N_f flavors. Integration over the fermion fields leads to a partition function of the form

$$Z = \int [dU_\mu] \exp[-S_g] \prod_{f=1}^{N_f} \det[D_f], \quad S_g = -\frac{\beta}{2N_c} \sum_p [\text{tr} U_p + \text{tr} U_p^\dagger], \quad (1)$$

where $\det[D_f]$ is the fermion determinant and S_g is the Wilson gauge action. The effective theory arises after integrating over the spatial link variables,

$$Z = \int [dU_0] \exp[-S_{\text{eff}}], \quad \exp[-S_{\text{eff}}] = \int [dU_i] \exp[-S_g] \prod_{f=1}^{N_f} \det[D_f]. \quad (2)$$

The effective action depends on temporal Wilson lines $W_{\vec{x}}$ only, whose traces are the Polyakov loops

$$L_{\vec{x}} = \text{tr } W_{\vec{x}} = \text{tr} \prod_{t=0}^{N_t-1} U_0(\vec{x}, t). \quad (3)$$

Our investigation is based on truncated effective theories, where the spatial link integration is performed after a combined character (i.e. effectively resummed strong coupling) and hopping parameter expansion. For the Yang-Mills part, to leading order we obtain a nearest-neighbor two-point interaction

$$S_{\text{eff}}^g = - \sum_{\langle \vec{x}, \vec{y} \rangle} \log \left[1 + \lambda(u, N_t) (L_{\vec{x}} L_{\vec{y}}^* + L_{\vec{x}}^* L_{\vec{y}}) \right], \quad (4)$$

where the effective coupling reads

$$\lambda(u, N_t = 4) = u^4 \exp \left[4(4u^4 + 12u^5 - 14u^6 - 36u^7 + \frac{295}{2}u^8 + \frac{1851}{10}u^9 + \frac{1035317}{5120}u^{10}) \right], \quad (5)$$

$$\lambda(u, N_t \geq 6) = u^{N_t} \exp \left[N_t(4u^4 + 12u^5 - 14u^6 - 36u^7 + \frac{295}{2}u^8 + \frac{1851}{10}u^9 + \frac{1055797}{5120}u^{10}) \right]. \quad (6)$$

Here $u(\beta) = \beta/18 + \beta^2/216 + \dots \in [0, 1]$, is the coefficient of the fundamental representation character. It is a numerically known function over the entire range of lattice gauge couplings and constitutes the expansion parameter. Higher order interaction terms can be found in [9].

The contributions of the fermion determinant are computed by a hopping expansion. It is factored into temporal and spatial hops in forward and backward directions, $T = T^+ + T^-$ and $S = S^+ + S^-$,

$$\det[D_f] = \det[1 - T - S] = \det[1 - T] \det[1 - (1 - T)^{-1}S] = \det[D_{\text{stat}}] \det[D_{\text{kin}}].$$

To leading order the fermion determinant represents static quarks with only temporal hops, and can be reformulated in terms of Polyakov loops,

$$S_0 = - \log \det[D_{\text{stat}}] = - \log \left(\prod_{\vec{x}} [1 + h_1 L_{\vec{x}} + h_1^2 L_{\vec{x}}^* + h_1^3]^2 [1 + \bar{h}_1 L_{\vec{x}}^* + \bar{h}_1^2 L_{\vec{x}} + \bar{h}_1^3]^2 \right). \quad (7)$$

To leading order in the combined expansions, the coefficients are the heavy quark fugacities,

$$h_1(\mu) = (2\kappa e^{a\mu})^{N_t} = e^{\frac{\mu - m_q}{T}} = \bar{h}_1(-\mu). \quad (8)$$

In the strong coupling limit $\beta = 0$ the constituent quark mass is given by $am_q = -\log(2\kappa)$ [10]. The kinetic quark determinant is evaluated by further splitting D_{kin} into parts from positive and negative spatial hops, $P = \sum_i P_i = (1 - T)^{-1}S^+$ and $M = \sum_i M_i = (1 - T)^{-1}S^-$. Here the static quark propagator $Q_{\text{stat}}^{-1} = (1 - T)^{-1}$ enters, which is known to all orders in the hopping parameter.

Then the expansion of the kinetic quark determinant proceeds as

$$\begin{aligned}\det[D_{\text{kin}}] &= \det[1 - P - M] = \exp[\text{tr} \log(1 - P - M)] \\ &= \exp\left[-\text{tr} PM - \text{tr} PPMM - \frac{1}{2} \text{tr} PMPM + \mathcal{O}(\kappa^6)\right] \\ &= 1 - \text{tr} PM - \text{tr} PPMM - \frac{1}{2} \text{tr} PMPM + \frac{1}{2} (\text{tr} PM)^2 + \mathcal{O}(\kappa^6).\end{aligned}\quad (9)$$

In order to perform the spatial gauge integrals on $\det[D_{\text{kin}}]$, it is necessary to expand down the exponential as shown in equation (9). Further details of the derivation up to order $\mathcal{O}(\kappa^4)$ can be found in [4, 11]. The process of resummation is employed to obtain the exponential expression of the effective theory which then improves the convergence of the effective theory, since it includes an infinite number of higher-order graphs. Finally, the leading term of the kinetic determinant contributes to a two-point interaction and is of order κ^2 ,

$$\begin{aligned}-S_2 &= -\int [dU_j] \sum_i \text{tr} P_i M_i = \sum_i \int [dU_j] \text{tr} [Q_{\text{stat}}^{-1} S_i^+ Q_{\text{stat}}^{-1} S_i^-] \\ &= -2h_2 \sum_{i, \vec{x}} \left[\left(\text{tr} \frac{h_1 W_{\vec{x}}}{1 + h_1 W_{\vec{x}}} - \text{tr} \frac{\bar{h}_1 W_{\vec{x}}^\dagger}{1 + \bar{h}_1 W_{\vec{x}}^\dagger} \right) \left(\text{tr} \frac{h_1 W_{\vec{x}+\hat{i}}}{1 + h_1 W_{\vec{x}+\hat{i}}} - \text{tr} \frac{\bar{h}_1 W_{\vec{x}+\hat{i}}^\dagger}{1 + \bar{h}_1 W_{\vec{x}+\hat{i}}^\dagger} \right) \right].\end{aligned}\quad (10)$$

To re-express the trace over a rational function containing temporal Wilson lines in terms of Polyakov loops, we use the generating function

$$G(\alpha, \beta) = \log \det(\alpha + \beta h_1 W), \quad (11)$$

from which

$$W_{nm} = \text{tr} \frac{(h_1 W)^m}{(1 + h_1 W)^n} = \frac{(-1)^{n-1}}{(n-1)!} \frac{\partial^{n-m}}{\partial \alpha^{n-m}} \frac{\partial^m}{\partial \beta^m} G(\alpha, \beta) \Big|_{\alpha=\beta=1}. \quad (12)$$

The contribution to order κ^4 is

$$-S_4 = \int [dU_j] \left(-\text{tr} PPMM - \frac{1}{2} \text{tr} PMPM + \frac{1}{2} (\text{tr} PM)^2 \right) \quad (13)$$

and after complete evaluation is too long to be printed here. For explicit expressions, see [4, 11]. The effective action to $\mathcal{O}(\kappa^4)$ used in our simulations is then

$$S_{\text{eff}} = S_{\text{eff}}^g + S_0 + S_2 + S_4. \quad (14)$$

Note that moving away from the strong coupling limit leads to corrections to the fermion couplings h_i coming from mixed graphs with contributions from non-vanishing gauge coupling as well. Our

	Crossover	first-order triple	Tricritical	3D Ising
$B_4(\kappa_c, \infty)$	3	1.5	2	1.604
ν	-	1/3	1/2	0.6301(4)
γ	-	1	1	1.2372(5)

Table 1: Critical values for ν , γ and B_4 for different phase transitions [12].

effective couplings including corrections for $N_t \geq 4$ are

$$h_1(u, \kappa, N_t) = (2\kappa e^{a\mu})^{N_t} \exp \left[6N_t \kappa^2 u \left(\frac{1 - u^{N_t-1}}{1 - u} + 4u^4 - 12\kappa^2 + 9\kappa^2 u + 4\kappa^2 u^2 - 4\kappa^4 \right) \right], \quad (15)$$

$$h_2(u, \kappa, N_t) = \frac{\kappa^2 N_t}{N_c} \left(1 + 2 \frac{u - u^{N_t}}{1 - u} + 8u^5 + 16\kappa^2 u^4 \right), \quad (16)$$

$$h_3^1(u, \kappa, N_t) = \frac{N_t(N_t - 1)\kappa^4}{N_c^2} \left[1 + \frac{8}{3}(u + u^2 + 4u^5 + 8\kappa^3 u^4) \right], \quad \text{for } N_t = 4, \quad (17)$$

$$h_3^2(u, \kappa, N_t) = \frac{\kappa^4 N_t}{N_c^2} \left[1 + 4 \frac{u - u^{N_t}}{1 - u} + 16u^5 + 32\kappa^3 u^4 \right], \quad (18)$$

$$h_3^3(u, \kappa, N_t) = \frac{\kappa^4 N_t^2}{N_c^2} \left[1 + 4 \frac{(1 - u^{N_t})(u - u^{N_t})}{(1 - u)^2} + 16u^5 + 32\kappa^3 u^4 \right], \quad (19)$$

$$h_3^4(u, \kappa, N_t) = \frac{\kappa^4 u N_t}{2N_c^3} \left[1 + 4u^4 + 16\kappa^3 u^4 \right], \quad (20)$$

where h_3^1, \dots, h_3^4 are effective couplings of S_4 coupled to κ^4 graphs with different gauge corrections.

3. Numerical results

Since the effective theory depends only on the Polyakov loops, the numerical investigation for the effective theory can be performed directly with Metropolis updates of the temporal links, which live on a three-dimensional lattice. The bare fermion mass am is controlled via the hopping parameter $\kappa = (2(am + 4))^{-1}$. Finite temperature on the lattice is given by the inverse temporal extent of the original lattice, $T = 1/a(\beta)N_t$. We will work with $N_f = 1, 2$, and at fixed $N_t = 4, 6$ for the effective theory up to order $\mathcal{O}(\kappa^2)$, and at $N_t = 4$ for the $\mathcal{O}(\kappa^4)$ effective theory. This work aims to map the phase structure of heavy QCD at zero chemical potential, i.e., in the (u, κ) parameter space, for different approximations of the effective theory.

The observable used in this work is the Polyakov loop, $\mathcal{O} \equiv |L|$, which is a true order parameter of QCD in the limit $m_q \rightarrow \infty$, and signals a phase transition. We then construct the susceptibility, the skewness and the kurtosis as

$$\chi = N_s^3(\langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2), \quad B_3 = \frac{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^3 \rangle}{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle^{3/2}}, \quad B_4 = \frac{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^4 \rangle}{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle^2}. \quad (21)$$

The statistical error of these quantities are determined by a jackknife analysis. A true non-analytic phase transition can only exist in the infinite volume limit, therefore to extract this transition from

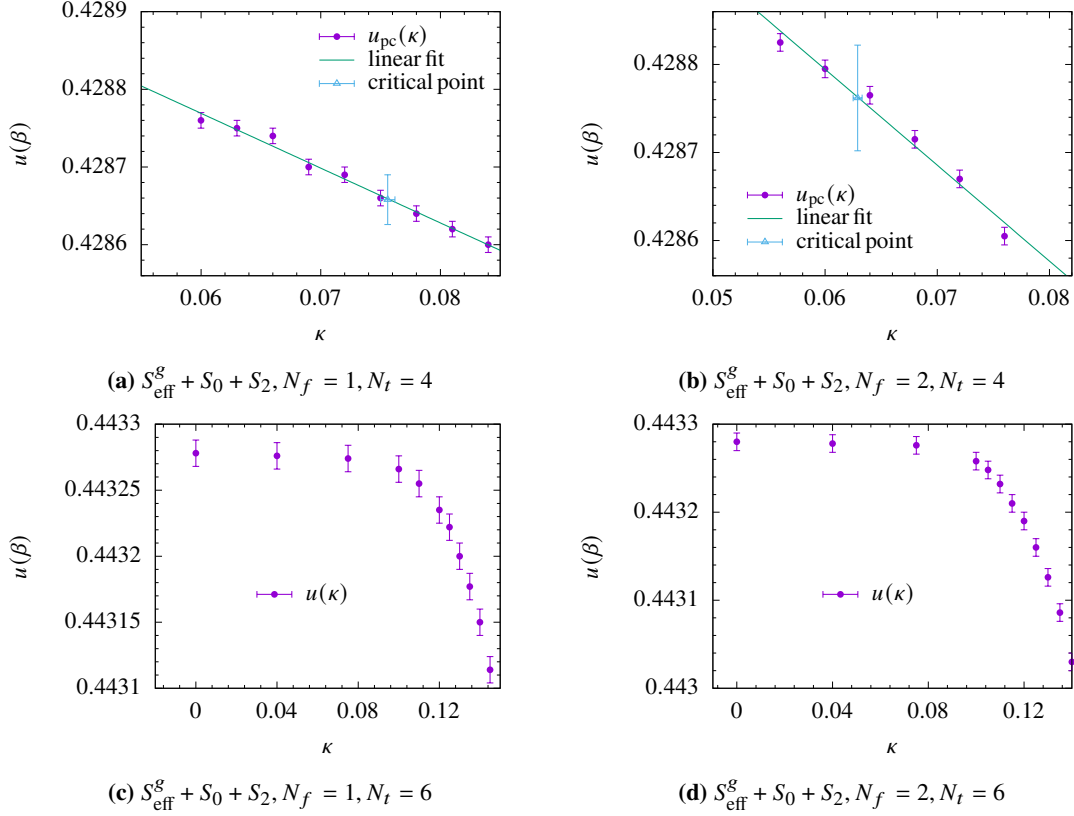


Figure 1: The pseudo-critical line for the next-to-leading order effective theory with $N_f = 1, 2$, $N_t = 4, 6$ and $N_s = 24$. A linear fit was performed for $N_t = 4$ according to equation (23).

simulations of finite volumes, an extrapolation with a finite size scaling is needed. One way is to use the kurtosis B_4 for approaching the infinite volume limit. The critical value of B_4 in the thermodynamic limit for different orders of the phase transition is given in table 1. The leading finite size corrections are obtained by performing a Taylor expansion about a critical point in infinite volume, to which we fit our data,

$$B_4(\kappa, N_s) = B_4(\kappa_c, \infty) + a_1(\kappa - \kappa_c)N_s^{1/\nu} + \dots \quad (22)$$

Our investigation proceeds in two steps: first, the pseudo-critical line $u_{pc}(\kappa)$ is mapped, subsequently its critical point (u_c, κ_c) is located. The pseudo-critical line is found by fixing values of κ and performing a u -scan at $N_s = 16, 20, 24$, identifying the maximum of the susceptibility and minimum B_4 . Results on $N_s = 24$ are shown for $N_f = 1$ in figure 1a and for $N_f = 2$ in 1b. Due to the smallness of κ , the entire line can be parametrised as [13]

$$u_{pc}(\kappa) = u_0 - a_1\kappa, \quad (23)$$

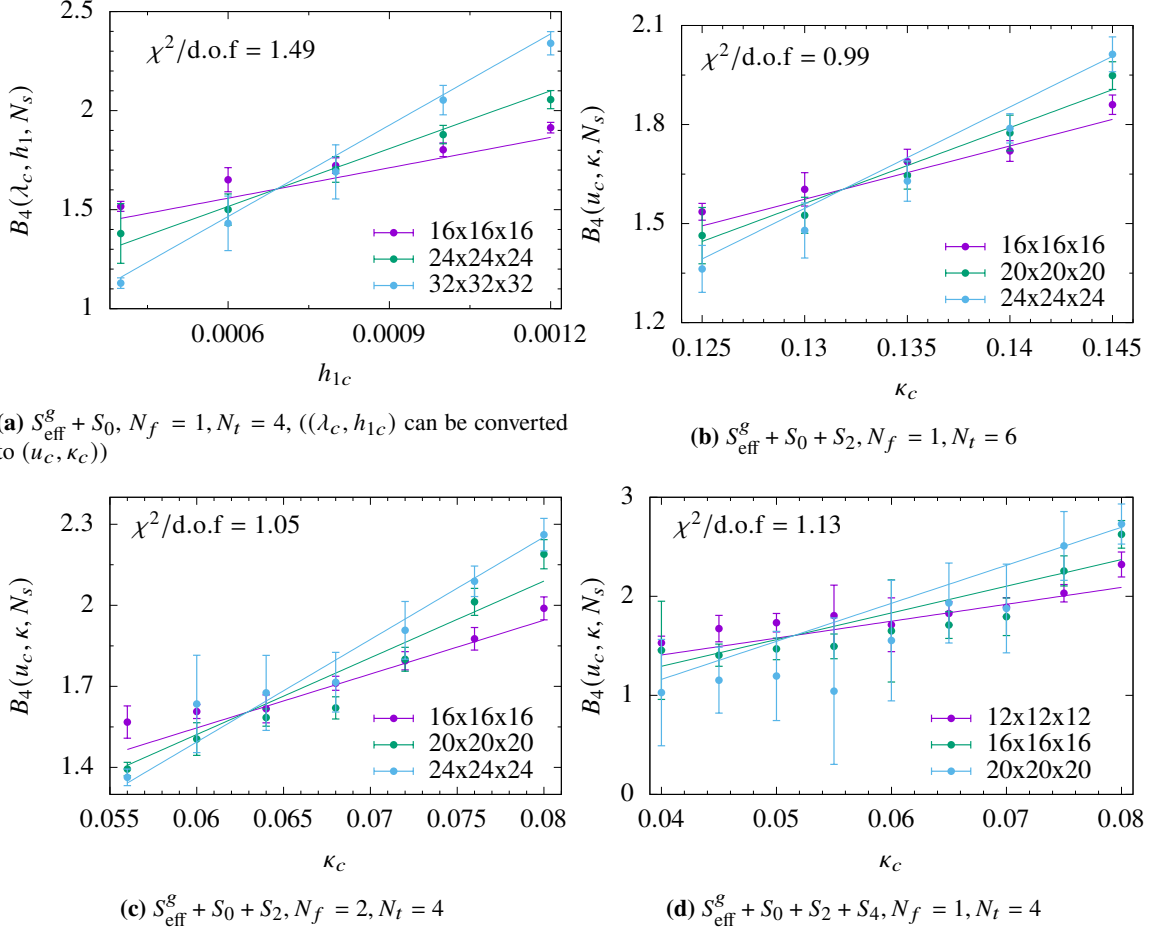


Figure 2: Example plots of the kurtosis for different orders of the effective theory.

with the following fit results,

$$a_1 = 0.0071(3), \quad u_0 = 0.429192(22), \quad \chi^2/\text{d.o.f} = 0.49, \quad \text{for } N_f = 1, \quad (24)$$

$$a_1 = 0.0109(8), \quad u_0 = 0.429448(52), \quad \chi^2/\text{d.o.f} = 1.74, \quad \text{for } N_f = 2. \quad (25)$$

However, the linearity does not hold for $N_t = 6$ and $N_f = 1, 2$ as illustrated in figure 1c and 1d.

Next, we find the location of the critical end point on the phase boundary. We plot the minimum values of B_4 against the couplings h, κ for several volumes, see figure 2, and perform a linear fit to equation (23). The $\chi^2/\text{d.o.f}$ values of the four fits are between 0.99 – 1.49, indicating good fit qualities. With the same analysis, we estimate the critical values κ_c also for the κ^2 -action at $N_t = 6$ and for the κ^4 -action at $N_t = 4$. All results are summarized in table 2. One observes that the value of κ_c for $N_f = 2$ of the same order effective theory is smaller than those of $N_f = 1$. This is because the explicit center symmetry breaking is stronger with more fermion fields. The same argument can also be used to explain the decrease of κ_c as the order in the hopping expansion in the effective theory increases.

N_t	action	eff. theories (preliminary)		hopping expanded-QCD [6]		Full QCD [7]
		$N_f = 1$	$N_f = 2$	$N_f = 1$	$N_f = 2$	$N_f = 2$
4	$S_{\text{eff}}^g + S_0$	0.0810(4)	-	0.0783(12)	0.0658(10)	-
	$S_{\text{eff}}^g + S_0 + S_2$	0.0756(6)	0.0629(4)	0.0753(11)	0.0640(10)	-
	$S_{\text{eff}}^g + S_0 + S_2 + S_4$	0.0515(16)	0.0443(34)	-	-	-
6	$S_{\text{eff}}^g + S_0 + S_2$	0.1319(6)	0.1210(5)	0.1326(21)	0.1202(19)	0.0877(9)

Table 2: Comparison of the κ_c -values for the deconfinement critical point obtained by different approximations to lattice QCD with Wilson quarks.

4. Conclusions

In table 2, we also compare our results with those obtained from 4-dimensional QCD simulations in the heavy quark region, in one case with a hopping expanded fermion determinant, in the other case with no approximations. We see that the phase structure of the 4-dimensional full QCD is reproduced by the effective theories on a semi-quantitative level, so that their application to the cold and dense regime can be trusted. Regarding quantitative accuracy, the comparison with either hopping expanded or full QCD allows for detailed conclusions regarding the strong coupling and hopping expansions separately: the 3D effective theory agrees almost quantitatively with the hopping expanded 4D QCD, while both exhibit larger differences with full QCD as N_t grows. This means that the character expansion shows good convergence behavior and is sufficient for thermodynamical applications up to $N_t = 6$, while higher order corrections are necessary in the hopping expansion already at $N_t = 6$.

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