A 3d effective lattice theory for phase transitions in Yang-Mills and heavy dense QCD

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Abstract. QCD thermodynamics is crucial for the physics of the early universe, heavy ion collisions and compact stars. However, predictions by lattice simulations are very costly or, in the case of finite baryon density, even impossible because of a sign problem. Starting from Yang-Mills theory, I review how to use strong coupling methods to construct a 3d effective theory which reproduces the deconfinement phase transition to about 10% accuracy. The generalisation to QCD, which is valid for heavy quarks, has only a mild sign problem in the case of finite density and can be simulated efficiently. Moreover, it allows to address the nuclear liquid gas transition in the cold and dense regime for the first time directly from QCD.

1. Introduction

The understanding of the different forms of nuclear matter under extreme conditions plays an increasingly important role for nuclear astrophysics, particle physics and heavy ion collisions. Unfortunately, the infamous "sign problem" of QCD, i.e. the fact that the fermion determinant becomes complex with real chemical potential for baryon number $\mu_B$, prohibits direct Monte Carlo simulations of QCD at finite matter density. Approximate methods are able to circumvent this problem only for small quark chemical potentials $\mu = \mu_B/3 \lesssim T$ [1]. So far, no sign of a critical point or a first order phase transition has been found in this controlled region. Complex Langevin algorithms do not suffer from the sign problem, but occasionally converge to incorrect answers and thus have their own problems. A lot of progress has been made recently, but no true phase transition has been reported in this approach either [2].

These difficulties have for a long time motivated the development of effective lattice theories, which can either be handled analytically or whose sign problem is mild enough to simulate the cold and dense region of QCD. Since the non-perturbative physics resides in the pure gauge sector, it is useful to first find an effective theory for Yang-Mills. Since the latter can be fully treated by Monte Carlo, it also serves as a testing ground to check the quality of effective theories. $SU(N)$ Yang-Mills theory in 4d is well-known to have a deconfinement transition at some critical temperature $T_c$, which corresponds to the breaking of the global $Z(N)$ centre symmetry. For the description of the electroweak phase transition within an $SU(2)$ Higgs model, perturbative dimensional reduction led to successful analytical [3] and numerical [4] descriptions. This approach is based on the existence of a scale hierarchy $g^2 T \ll g T \ll \pi T$, which allows perturbative integration over the hard modes to produce an effective theory which is then treated with non-perturbative methods. However, for the deconfinement transition this approach fails, even for weakly coupled theories, because the perturbative integration step explicitly breaks the...
centre symmetry which is then lost in the effective theory. A bottom up construction of an effective theory by writing down the most general centre symmetric Lagrangian and matching the couplings [5] has so far only been successful for $SU(2)$ [6].

In this contribution I summarise a solution to this problem in terms of a strong coupling expansion of the lattice Yang-Mills theory [7]. An extremely simple effective theory gives a correct description of the universality of the $SU(2), SU(3)$ transitions as well as their critical couplings and hence temperature within 10% accuracy, which can be systematically improved. Further, the effective theory can be extended to dynamical QCD with heavy quarks by a hopping expansion. Its sign problem is sufficiently mild to allow for a description of the thermal deconfinement transition at all baryon chemical potentials [8] as well as the cold and dense regime of nuclear matter [9, 10].

2. The effective theory for Yang-Mills

2.1. Derivation of the effective theory

Starting point is the (3+1)-dimensional Wilson lattice action at finite temperature $T = (aN_\tau)^{-1}$, and we now specialise to $SU(3)$. The partition function is

$$Z = \int [dU_0][dU_i] \exp \left[ \frac{\beta}{2N} \sum_p (\text{tr} U_p + \text{tr} U_p^\dagger) \right], \quad \beta = \frac{2N}{g^2}.$$ (1)

Finite temperature and the bosonic nature of the degrees of freedom imply the use of periodic boundary conditions in the time direction. Finer lattices correspond to larger $N_\tau$ for fixed physics. We now integrate out the spatial links and get schematically

$$Z = \int [dU_0] \exp[-S_{\text{eff}}];$$

$$-S_{\text{eff}} = \ln \int [dU_i] \exp \left[ \frac{\beta}{2N} \sum_p (\text{tr} U_p + \text{tr} U_p^\dagger) \right] \equiv \lambda_1 S_1 + \lambda_2 S_2 + \ldots$$ (3)

Note that, without truncations, the effective action is unique and exact. Since all spatial links, which are originally coupled by nearest neighbour interactions, were integrated over, the effective action has long-range interactions, irrespective of the way it is determined. It contains interactions of Polyakov lines at all distances and to all powers. For the effective theory to be practical, truncations are necessary. For non-perturbative ways to determine truncated theories, see [11, 12, 13] Here we consider the case where the Boltzmann factor is expanded in a strong coupling expansion about $\beta = 0$ so that all link integrations can be performed analytically. We arrange the effective couplings $\lambda_n(\beta, N_\tau)$ in increasing order in $\beta$ of their leading terms. Thus the $\lambda_n$ become less important the higher $n$. The interaction terms $S_n$ depend only on $Z(3)$-invariant combinations of Polyakov loops

$$L_j = \text{tr} \prod_{\tau=1}^{N_\tau} U_{0}(x_j, \tau).$$ (4)

Hence any truncation of the effective theory will still exhibit the $Z(3)$-invariance of full Yang-Mills. The simplest effective theory is the one with only nearest neighbour interaction terms, whose higher powers can be summed up in closed form to yield [7]

$$Z_{\text{eff}} = \prod_i dL_i e^{V_i} \prod_{(ij)} (1 + 2\lambda_1 \text{Re} L_i L_j^*), \quad V_i = \frac{1}{2} \ln(27 - 18|L_i|^2 + 8\text{Re}(L_i^3) - |L_i|^4).$$ (5)
Figure 1. A graphical representation of the contributions in the strong coupling expansion and the corresponding terms in the effective action. The first term is the interactions of two nearest neighbour Polyakov lines and the second one corresponds to the interaction of next-to nearest neighbours with distance $\sqrt{2}$ on the lattice. From [14].

Here $V_i$ is related to the Jacobian when transforming the measure $dU_0(i) \rightarrow dL_i$. Usually the effective couplings are exposed in terms of the fundamental character expansion coefficient $u = u(\beta) = \beta/18 + O(\beta^2)$, which shows better convergence. The relation between $u$ and $\beta$ can be computed to arbitrary precision, hence they can be used synonymously. The leading effective coupling has been computed to high orders,

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

(6)

Note that the next-to-nearest neighbour coupling starts only at $\lambda_2 \sim u^{2N_\tau+2}$ while the nearest neighbour coupling of adjoint loops is $\lambda_a \sim u^{2N_\tau}$. Figure 1 illustrates how higher order contributions arise in terms of additional contributions to the coupling constants of the nearest neighbour interaction and next to nearest neighbour interactions.

2.2. Numerical results for the one-coupling theory

The effective theory is 3d with complex scalars left as dynamical degrees of freedom, corresponding to a 3d continuous spin model. It is obvious that this accounts for a drastic reduction of numerical effort for the simulation. The effective theory exhibits an order-disorder phase transition corresponding to the spontaneous breaking of the centre symmetry as a function of its coupling, as shown in Figure 2 (left), which causes the Polyakov loop to rise. A finite size analysis shows that this rise develops into a discontinuous jump, signalling the first-order nature of the transition in the infinite volume limit, Figure 2 (right). This can also be seen in the distribution of the Polyakov loop variable in the critical region. Figure 3 shows the double-peak distribution of a first-order transition for $SU(3)$ (left), whereas a single Gaussian distribution moves smoothly as a function of the coupling for $SU(2)$ (right), which has a second-order continuous transition. Thus the effective theory in its simplest form correctly describes the order of the $SU(N)$ transition.

Next the location of the phase transition, i.e. the critical coupling $\lambda_c$, can be translated back to the lattice gauge coupling $\beta$ by inverting Equation (6) for every given $N_\tau$. The result is shown in Figure (4) (left) for different truncations of the series for the effective coupling. The computed orders are just about high enough for an appreciable convergence to set in. Note, that a single simulation of the effective theory provides the critical coupling $\lambda_c$, the predictions
Figure 2. Left: Distribution of $L$ for small and large $\lambda_1$. Right: Expectation value of $|L|$. The vertical line marks the infinite-volume transition.

Figure 3. Distribution of $L$ in the critical region for $SU(3)$ (left) and $SU(2)$ (right).

Figure 4. Left: The critical gauge coupling to different orders in $u$. Right: relative error of $\beta_c$ as estimated by the effective models compared to the Monte Carlo results.
for $\beta_c(N_\tau)$ all follow by analytic mapping from this single number. This is in contrast to the full theory, where of course every $N_\tau$-lattice has to be simulated anew. With the predictions for $\beta_c$ at hand, we can now compare with the corresponding ones from the full 4d Yang-Mills theory. Figure 4 (right) shows the relative deviation of the effective theory predictions from the true answer. For a large range of $N_\tau$ values the error is less than 10%, a remarkable achievement for so simple an effective theory. The figure also shows the corresponding predictions of two versions of two-coupling theories, one with a second coupling over lattice distance two and one with a second coupling for adjoint loops. These couplings were only evaluated to leading order, which gives a negligible contribution in particular with rising $N_\tau$, which parametrically suppresses it, with even smaller leading order contributions from other couplings. The same behavior with similar accuracy is found for $SU(2)$.

With the critical couplings at hand, we can convert them to critical temperatures using a beta-function as from [15], Figure 5. The error bars in the figure are purely systematic and give the difference of the results between the two highest orders of the effective coupling. Note again that all points are from a single effective theory simulation, with the $N_\tau$-dependence encoded in the mapping Equation (6). For larger $N_\tau$ the data enter the scaling regime with leading $1/N_\tau^2 \sim a^2$ corrections to the continuum result. Thus an extrapolation is feasible, which provides a continuum limit again within about 10% of the one obtained from full Yang-Mills theory.

2.3. Range of validity and limitations
One might wonder how such a simple model as the one-coupling effective theory reviewed here can possibly describe the complexities of Yang-Mills theory. Clearly there are limitations. Firstly, the effective theory has been derived by an analytic strong coupling expansion about $\beta = 0$. In the infinite volume limit, the critical coupling $\beta_c$ of the deconfinement transition marks a singularity and therefore the radius of convergence for the strong coupling series. Hence, the effective theory is valid in the confined phase up to the phase transition, but not in the deconfined phase. (Of course, the effective theory will have the same structure and terms there, but the couplings cannot be determined as a strong coupling series and may be ordered differently). Secondly, we have so far discussed only the phase transition. Consider now the free energy of a quark anti-quark pair in the plasma, which is extracted from the Polyakov loop correlation
Figure 6. Left: Free energy from the effective one-coupling theory at $T = 0.9T_c$ on $32^3 \times 4$ compared to full Yang-Mills. From [16] Right: Interaction measure $\Delta S = e^{-3p}$ computed as a strong coupling series, from the effective theory and in full Yang-Mills. From [16]

function

$$\langle L(R)L^\dagger(0) \rangle = e^{-F(R,T)/T} .$$  \hspace{1cm} (7)

In the confining phase up to the phase transition, the free energy rises linearly at long distance with an effective temperature-dependent "string tension", as shown in Figure 6 (left). The effective one-coupling theory shows the same qualitative behaviour, but the string tension is significantly overestimated. This easy to understand. A correct description of a correlation function over some fixed length scale requires the effective theory to contain all interactions over that length scale, which is clearly not the case for the one-coupling theory and with only a nearest neighbour interaction. Hence, quite generally this simplest version of effective theory is inappropriate to describe quantities defined by length or mass scales, such as the spectrum, screening masses etc.

On the other hand, phase transitions and all bulk thermodynamic observables are derived from the partition function. The non-trivial quantity to compute in this case is the effective action, which is local in the sense that its couplings over larger distances are exponentially suppressed with the decay of Polyakov loop correlates, since the theory has a mass gap. Indeed, Figure 6 (right) shows the interaction measure computed in the effective theory compared to that of full Yang-Mills. We observe quantitative agreement up to the onset of the phase transition, which is shifted by about 10% in the effective theory as discussed before. Thus, a local effective action with the correct symmetries is capable to provide a good description of bulk thermodynamic quantities as well as phase transitions, even though it might be inaccurate for specific correlation functions or the spectrum of the theory. As a final remark, note how significantly the simulation of the strong coupling effective theory improves over a full strong coupling calculation of the interaction measure [17, 18, 19], which as a power series is incapable of describing the phase transition. On the other hand, since the effective coupling $\lambda_1$ is small, a perturbative evaluation of the effective partition function gives excellent results for the interaction measure, but as a power series of course also misses the phase transition.

3. QCD with very heavy quarks

After the successful test with Yang-Mills theory, let us now extend the effective theory to include fermions [8]. In order to arrive at a Polyakov loop effective theory again, these are also analytically integrated over using the hopping parameter expansion. The quark part of the action for $N_f$ mass-degenerate flavours with masses $M$ is then written as a power series in the
hopping parameter $\kappa$,

$$-S_q = -N_f \sum_{l=1}^{\infty} \frac{\kappa^l}{l} \text{tr} H[U]_l^l, \quad \kappa = \frac{1}{2aM + 8}, \quad H[U]_{y,x} = \sum_{\pm} \delta_{y,x+\delta}(1 + \gamma_{\nu}), \quad \gamma_{-\nu} = -\gamma_{\nu}. \quad (8)$$

Thus each hop to a neighbouring lattice site gives a power of the hopping parameter, which limits the validity of the effective theory to heavy quarks. The quark chemical potential $\mu$ is introduced as usual by a factor $e^{\mu\nu}(e^{-\alpha\mu})$ multiplying link variables in positive (negative) time direction. The effective theory is obtained from the full theory in the same way as for Yang-Mills,

$$Z = \int [dU_0][dU_1] \exp[-S_g - S_q] = \int [dU_0] \exp[-S_{\text{eff}}], \quad -S_{\text{eff}} = \ln \int [dU_1] \exp[-S_g - S_q]. \quad (9)$$

We now have a double expansion in $u(\beta)$ and $\kappa$, i.e. all effective couplings depend on both parameters and $N_\tau$. Furthermore, quarks of finite mass lead to terms in the action which explicitly break the $Z(3)$ symmetry present in the pure gauge case. We may arrange this as

$$-S_{\text{eff}} = \sum_{i=1}^{\infty} \lambda_i(u, \kappa, N_\tau) S_i^a - 2N_f \sum_{i=1}^{\infty} \left[ \hat{h}_i(u, \kappa, \mu, N_\tau) S_i^a + \hat{h}_i(u, \kappa, \mu, N_\tau) S_i^{a,\dagger} \right]. \quad (10)$$

The $\lambda_i$ are defined as the effective couplings of the $Z(3)$-symmetric terms $S_i^a$, whereas the $\hat{h}_i$ multiply the asymmetric terms $S_i^a$. The $h_i$ and $\hat{h}_i$ are related via $\hat{h}_i(u, \kappa, \mu, N_\tau) = h_i(u, \kappa, -\mu, N_\tau)$.

Keeping the leading fermionic coupling $h_1$ only and summing up all fermion loops winding multiple times around the torus produces a determinantal expression in the effective theory,

$$Z_{\text{eff}} = \int \left( \prod_i dL_i \ e^{V_i Q_i^N_f(1/h_1)} \right) \prod_{<ij>} (1 + 2\lambda_1 \text{Re} L_i L_j^*). \quad (11)$$

with

$$Q_i(h_1, \hat{h}_1) = \left[(1 + h_1 L_i + h_2^2 L_i^* + h_3^2)(1 + \hat{h}_1 L_i^* + h_2^2 L_i + \hat{h}_3^2)\right]^2, \quad (12)$$

Figure 7. Left: Order of the QCD phase transition as a function of quark masses at $\mu = 0$ (schematic). Right: Calculated phase boundary with critical endpoint.
| $N_f$ | $M_c/T$ | $\kappa_c(N_f = 4)$ | $\kappa_c(4)$, Ref. [20] |
|-------|---------|----------------------|-----------------------------|
| 1     | 7.22(5) | 0.0822(11)           | 0.0783(4)                   |
| 2     | 7.91(5) | 0.0691(9)            | 0.0685(3)                   |
| 3     | 8.32(5) | 0.0625(9)            | 0.0595(3)                   |

Table 1. Location of the critical point for $\mu = 0$ and $N_f = 4$. The first two columns report our results, the last compares with existing literature.

Figure 8. Left: The deconfinement critical surface with heavy quarks. Right: Phase diagram for $N_f = 2$ calculated on $N_f = 6$ lattices. Above the surface the theory is deconfined. The line of critical end points (dashed) separates the crossover (light) from the first order transitions (dark).

4. The deconfinement transition

As a first application we investigate the deconfinement transition of QCD with heavy quarks as a function of quark mass and chemical potential. We begin by considering the case of zero baryon density, shown schematically in Fig. 7 (left). In the pure gauge limit in the upper right corner, the deconfinement transition is of first order. Dynamical quarks at any fixed $N_f$ break the global $Z(3)$ symmetry of the QCD action explicitly. As a consequence, the phase transition weakens with decreasing quark masses until it vanishes at a critical point. For still lighter quarks the deconfinement transition is an analytic crossover. This behaviour is inherited by the effective theory. For a given $N_f$ and $\mu = 0$, we have $h = \bar{h}$ and the effective theory has two couplings, $(\lambda_1, h_1)$. The first-order phase transition of the one-coupling theory extends to a first-order line with a weakening transition as $h_1$ increases. Eventually the transition vanishes at a critical point.

The resulting phase boundary between the ordered and disordered phase is shown in Fig. 7 (right) and found to be linear in the small coupling $h_1$. In order to locate the critical endpoint we study the scaling of the fourth order Binder cumulant along the phase boundary and find $\lambda_{1c} = 0.18672(7), h_{1c} = 0.000731(40)$. The location of the critical endpoint is marked in Fig. 7 (right). As in the case of pure gauge theory, this can be mapped back analytically to predict $\kappa_c(N_f)$ for the 4d lattice theory, which can then be compared to full 4d simulations. For $N_f = 4$ the results are specified in Table 1, with an accuracy of 5% or better.

With this test passed, it is now easy to switch on chemical potential. In this case $\bar{h}_1 \neq h_1$ and the sign problem enters. However, the sign problem is comparatively mild. The theory can be simulated both by complex Langevin or ordinary Monte Carlo with agreeing results. This allows for a complete determination of the deconfinement transition as a function of quark or pion mass and chemical potential as shown in Fig. 8. The left plot shows the heavy quark (upper right) corner of Fig. 7 (left) extended to real and imaginary chemical potential. The deconfinement critical surface has been computed for all chemical potentials, shown is the result for $N_f = 6$ lattices. Note that the $\mu$-dependence of the surface follows the tricritical scaling dictated by the tricritical line at imaginary chemical potential as predicted in [21].
5. The nuclear liquid gas transition

It is now exciting to also apply this effective theory to cold and dense conditions [9, 10]. First, consider the static and strong coupling limits, as in this case the partition function factorises into one-site integrals that can be solved analytically. In the zero temperature limit for $N_f = 1$,

$$Z(\beta = 0, \kappa = 0) \xrightarrow{T \to 0} [1 + 4C N_c + C^2 N_c]^{N_s^3}.$$ (13)

The quark number density is now easily evaluated

$$n = \frac{T}{V} \frac{\partial}{\partial \mu} \ln Z = \frac{1}{a^3} \frac{4N_cN_c^2 + 2N_c^2C^2}{1 + 4C N_c + C^2 N_c}, \quad \lim_{T \to 0} a^3 n = \begin{cases} 0, & \mu < m, \\ 2N_c, & \mu > m. \end{cases}$$ (14)

and at zero temperature exhibits a discontinuity when the quark chemical potential equals the mass. Note that this reflects the silver blaze property of QCD, i.e. the fact that the baryon number stays zero for small $\mu$ even though the partition function explicitly depends on it. Once the baryon chemical potential is large enough to make a baryon ($m_B = 3M$ in the static strong coupling limit), a transition to the lattice saturation density happens. Note that saturation density here is $2N_c$ quarks per flavour and lattice site and reflects the Pauli principle once the lattice is full. This is a discretization effect disappearing in the continuum limit.

Next, we switch on the gauge coupling as well as the fermionic couplings $h_1, h_2$ through order $\kappa^2$, where the latter also includes $L_i L_j$ terms and hence quark-quark-interaction (for explicit expressions, see [9]). To keep our truncated series in full control, we choose $\beta = 5.7, \kappa = 0.0000887, N_x = 116$ corresponding to $M = 20$ GeV, $T = 10$ MeV, $a = 0.17$ fm. The silver blaze property as well as lattice saturation are observed also in the interacting case, but the step function is now smoothed, Figure 9 (left). Note that the Polyakov loop as well as its conjugate get screened in the presence of a baryonic medium, and hence rise. The ensuing decrease is due to saturation which forces all $Z(3)$ states to be occupied. Figure 9 (right) shows the continuum extrapolated results for the baryon density as a function of chemical potential, each point being extrapolated from results for 4-7 lattice spacings [10]. We observe the silver blaze property followed by the onset of nuclear matter, which is steeper for $N_f = 2$ than for $N_f = 1$ as expected. Note that the onset transition happens at $\mu_c \lesssim m_B$, due to the binding energy between the nucleons. Note also that the onset transition here is a smooth crossover, in contrast to the first-order phase transition for physical QCD in nature. This is due to the fact that the binding energy decreases strongly as function of quark masses and for the heavy quarks studied here is smaller than the temperature realized in Figure 9. It was confirmed in [10] that the a first-order behavior indeed results for sufficiently small quark masses, but in that mass range the effective theory is not yet converging and terms of higher order in $\kappa$ are necessary to faithfully reproduce QCD.

6. Conclusions

It was shown how a 3d effective lattice theory of Polyakov loops can be derived from lattice QCD via combined strong coupling and hopping expansions. The deconfinement phase transition of Yang-Mills theory and QCD with heavy quarks is described to within 10% accuracy compared to the full theory, but allows for an extension to all quark chemical potentials. In addition, the effective theory for the first time allows for a description of the cold and heavy dense regime of nuclear matter directly from QCD. It remains a challenging task to extend the effective theory to be valid also for light quarks.
Figure 9. Left: Baryon density, Polyakov loop and conjugate Polyakov loop obtained from Monte Carlo ($N_f = 3$), complex Langevin ($N_f = 6$) and the static strong coupling limit, respectively. Right: Baryon density extrapolated to the continuum.

Acknowledgments
This presentation is based on work in various collaborations with G. Bergner, M. Fromm, J. Langelage, M. Neuman and S. Lottini. The work is supported by the German BMBF, No. 06FY7100 as well as Helmholtz International Center for FAIR within the LOEWE program of the State of Hesse.

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