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Hopping parameter expansion to all orders using the Complex Langevin equation

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We propose two novel formulations of the hopping parameter expansion for finite density QCD using Wilson fermions, while keeping the gauge action intact. We use the complex Langevin equation to circumvent the sign problem in the theory. We perform simulations at very high order of the expansion, such that convergence is directly observable. We compare results to the full QCD results, and see agreement at sufficiently high orders. These results provide support for the use of complex Langevin dynamics to study QCD at nonzero density, both in the full and the expanded theory, and for the convergence of the latter.

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1. Introduction

Non-perturbative calculations of the phases strongly interacting matter are hampered by the sign problem (for a review of different approaches see [1]).

In the past years, however, progress in complex Langevin (CL) dynamics [2, 3, 4, 5] has led to the hope that the full region of physical interest can be explored. In this study we support the complex Langevin simulations by exploring an alternative approach to lattice fermions at nonzero chemical potential: the hopping parameter expansion, which can be formulated as a systematic approximation to finite density QCD. The expansion is expected to converge at not too small quark masses.

Historically the hopping expansion was used in the form of the loop expansion (described in detail in Sec. 3). It was used by earlier studies at LO and NLO [6, 7, 8, 9] with the full Yang-Mills action, also to map the phase diagram in [10, 11]. In studies combined with strong coupling expansion it has been possible to calculate NNLO contributions as well [12, 13, 14], but it has proven quite difficult to further extend the expansion to higher orders.

Here we present an alternative way to introduce higher-order corrections in the hopping parameter expansion [15]. The approach allows calculations at very high orders (only limited by available computer power), while keeping the full Yang-Mills action, and without having to consider fermionic loops and their combinatorial factors at each new order.

We define the κ- and κ_s-expansions below, with slightly different properties. We improve on the convergence properties of the loop expansion where the effective expansion parameter is κN_τ with N_τ the temporal extent of the lattice.

In section 2, we briefly describe Complex Langevin simulations. In Section 3, we first review the loop expansion, then describe the new approaches we call κ- and κ_s-expansion, and discuss their implementation in the complex Langevin equation. In Section 4 we present numerical results gained using this approach. Finally, in Section 5 we conclude.

2. Complex Langevin Simulations

The Complex Langevin approach is based on the complexification of the Langevin equation [16, 17]. This also leads to the complexification of the field manifold. The resulting process is susceptible to numerical problems (runaway trajectories, solved by using adaptive step sizes [18]), as well as convergence to a wrong result. Recently it has been shown that convergence is guaranteed as long as some conditions are satisfied, such as the fast decay of field distributions and holomorphy of the action and the observables [2]. Note that there are several types of modifications possible to adapt the Langevin process for a given action, which one can use to get the process to satisfy convergence criteria [19]. The method has proven useful in other contexts with a complex action as well [20, 21, 22, 23, 24].

In lattice QCD the discretised Langevin equation is written as [25]

$$U_{x,\nu} \mapsto \exp\left\{\sum_a i\lambda_a(\varepsilon K_{x\nu a} + \sqrt{\varepsilon}\eta_{x\nu a})\right\} U_{x,\nu}, \tag{2.1}$$

where $K_{xva} = -D_{xva}S$ is the drift force, ε the (adaptive) stepsize, and η independent Gaussian noises satisfying $\langle \eta_{xva}\eta_{x'v'a'}\rangle = 2\delta_{aa'}\delta_{xx'}\delta_{vv'}$. A complex action leads to a complex drift K, and link variables take values in SL(3,$\mathbb{C}$), losing their unitarity.

The available configuration space is thus complexified, and loses compactness. For gauge theories this leads to an additional complication: the volume of gauge orbits corresponding to a configuration is infinite. To restrict the movement of the system along the infinite gauge orbits one has to modify the process, while respecting the gauge invariance of the action and observables. This can be very conveniently achieved with the gauge cooling [3] (see also the review [26]), which uses non-compact gauge transformations to force the process to stay near the unitary manifold. As a consequence the decay of the distributions is fast, as required for the convergence proof. Together with the adaptive stepsize this practically eliminates runaways.

Another requirement for the proof of convergence is the holomorphy of the action, which is unfortunately not satisfied for QCD. This manifests in zeros of the measure, i.e. $\det M = 0$, leading to a meromorphic drift. Poles in the drift then might lead to wrong convergence of the process, as shown in nontrivial, soluble models [27], while in many cases the process gives correct results in spite of a non-holomorphic action, especially in the cases where the non-holomorphy is due to a Haar measure or Jacobian [19].

3. Hopping parameter expansions

3.1 Loop expansion

Recall the path integral formulation of QCD, where we use the plaquette action $S_{\rm YM}$ for the gauge fields

$$Z = \int DU\, \mathrm{e}^{-S}, \quad S = S_{\rm YM} - \log\det M, \tag{3.1}$$

with the Wilson fermion matrix M, the hopping term Q of which we split into spatial hopping terms S and temporal hopping terms R

$$M = 1 - \kappa Q = 1 - \kappa_s S - R, \tag{3.2}$$

with

$$\begin{aligned} S_{xy} &= 2\sum_{i=1}^{3}\left(\Gamma_{-i}U_{x,i}\delta_{y,x+a_i} + \Gamma_{+i}U^{-1}_{y,i}\delta_{y,x-a_i}\right), \\ R_{xy} &= 2\kappa\left(e^{\mu}\Gamma_{-4}U_{x,4}\delta_{y,x+a_4} + e^{-\mu}\Gamma_{+4}U^{-1}_{y,4}\delta_{y,x-a_4}\right), \end{aligned} \tag{3.3}$$

using the matrices $\Gamma_{\pm v} = (1 \pm \gamma_v)/2$. Note that these matrices are projectors satisfying $\Gamma^2_{\pm v} = \Gamma_{\pm v}$ and $\Gamma_{+v}\Gamma_{-v} = 0$. We then expand the fermionic part of the measure

$$\det M = \exp(\mathrm{Tr}\log(1-\kappa Q)) = \exp\left(-\mathrm{Tr}\sum_{n=1}^{\infty}\frac{\kappa^n}{n}Q^n\right), \tag{3.4}$$

which we can rewrite noticing that we can perform the sum for each loop built from hopping terms on the lattice separately, then resum the determinant for each loop (ignoring possible convergence

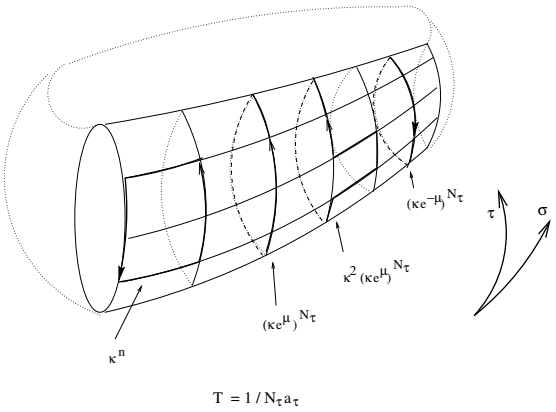

Figure 1: An illustration of the different loops contributing to the loop expansion of the fermion determinant.

problems)

$$\det M = \exp\left(-\mathrm{Tr}\sum_{C,s=1}^{\infty}\frac{\kappa^{l_C s}}{s}L_C^s\right) = \prod_C \det(1-\kappa^{l_C}L_c), \tag{3.5}$$

where C goes over all the possible loops on the lattice and l_C is the length of the loop. Since $\Gamma_{+\nu}\Gamma_{-\nu} = 0$, no loop that turns back on itself needs to be considered.

In the static limit, where $\kappa \to 0$, $\mu \to \infty$, $\zeta = 2\kappa\exp\mu = \text{const.}$, all contributions vanish except for the Polyakov loops. This is called the leading order of the loop expansion. Next to leading order (NLO) loops are gained by a decorating the Polyakov loop with two spatial hoppings, as illustrated in Fig. 1. NNLO contributions involve Polyakov loops with more decorations as well as the plaquette contribution.

3.2 κ expansion and κ_s expansion

To define an expansion which can be conveniently included in the Langevin equation, we go back to the first step in the loop expansion

$$\det M = \exp(\mathrm{Tr}\log(1-\kappa Q)) = \exp\left(-\mathrm{Tr}\sum_{n=1}^{\infty}\frac{\kappa^n}{n}Q^n\right). \tag{3.6}$$

In the sum only even powers of the hopping matrix contribute, as a trace is present. The expression is straightforwardly generalized to $N_f > 1$ flavors. We call this expansion the κ-expansion. The fermionic observables can then be expressed in terms of the expansion as

$$\langle\bar\psi\psi\rangle = \frac{2\kappa N_f}{\Omega}\sum_{n=0}^{\infty}\kappa^n\langle\mathrm{Tr}\,Q^n\rangle, \tag{3.7}$$

$$\langle n\rangle = -\frac{N_f}{\Omega}\sum_{n=1}^{\infty}\kappa^n\left\langle\mathrm{Tr}\left(\frac{\partial Q}{\partial\mu}Q^{n-1}\right)\right\rangle, \tag{3.8}$$

for the chiral condensate $\langle\bar\psi\psi\rangle$ and baryonic density n, using $\Omega = N_s^3 N_\tau$ the lattice volume.

Alternatively, we can rewrite the fermion matrix using the identity

$$M = (1-R)\left(1 - \frac{1}{1-R}\kappa_s S\right). \tag{3.9}$$

before expanding to gain the following expansion:

$$\det M = \det(1-R)\exp\sum_{n=1}^{\infty} -\frac{\kappa_s^n}{n}\mathrm{Tr}\left(\frac{1}{1-R}S\right)^n. \tag{3.10}$$

Since the matrix $(1-R)^{-1}$ is diagonal in spatial indices (and dense in temporal indices) and S describes spatial hoppings, again only even powers contribute in the sum. The first factor of the expansion $\det(1-R)$ describes the LO contribution in the static limit, also known as the HDQCD approximation. This simplification happens only for Wilson fermions, as backtracking is forbidden, hence the only possible loop built from temporal hoppings is the Polyakov loop. In this case the determinant and the inverse of the matrix can be calculated analytically as follows. The inverse of the matrix can be written as

$$(1-R)^{-1} = (1-R^+)^{-1} + (1-R^-)^{-1} - 1 \tag{3.11}$$

with $R^+ + R^- = R$, $R^+R^- = 0$ and R^+ (R^-) containing hoppings in positive (negative) temporal directions. We can then find the inverse of the two terms by the simple expansion (omitting spatial coordinates)

$$(1-R^+)^{-1}_{xy} = \sum_{n=0}^{\infty}\left(2\kappa e^{\mu}\Gamma_{-4}U_{x,4}\delta_{y,x+a_4}\right)^n, \tag{3.12}$$

Separating the parallel transporter between x and y, we can easily resum the remaining factor to give

$$\begin{aligned}(1-R^+)^{-1}_{xy} &= 1 - \Gamma_{-4}\frac{(2\kappa e^{\mu})^{N_\tau}P(x)}{1+(2\kappa e^{\mu})^{N_\tau}P(x)} \quad \text{if } x=y \\ &= \Gamma_{-4}(2\kappa e^{\mu})^{y-x}\frac{1}{1+(2\kappa e^{\mu})^{N_\tau}P(x)}W(x,y) \quad \text{if } y>x \\ &= -\Gamma_{-4}(2\kappa e^{\mu})^{N_\tau+y-x}\frac{1}{1+(2\kappa e^{\mu})^{N_\tau}P(x)}W(x,y) \quad \text{if } y<x\end{aligned} \tag{3.13}$$

where $W(x,y)$ is the parallel transporter between x and y built from positive hoppings, $P(x)$ is the untraced Polyakov loop starting from site x (that is $P(x) = W(x,x)$). The inverse of $(1-R^-)$ is calculated similarly. Similar formulas were derived in Refs. [14] in an effort to develop an effective theory for Polyakov-loops, also utilizing the strong coupling expansion for the Yang-Mills action.

The observables in the κ_s expansion can be recovered using the defining equations such as $\langle n\rangle = \partial \ln Z/\partial\mu$ in straightforward calculations to yield formulas similar to (3.7).

These two expansions can be very conveniently implemented in Langevin simulations, as detailed in the next subsection, but they have different strengths and weaknesses. We consider a truncated version of the expansion to order N^qLO, in which terms up to κ^{2q} are kept. We keep also

the terms proportional to $\exp(-\mu)$, although their contribution is suppressed at large μ, but they lead to the determinant satisfying the symmetry:

$$\det M(\mu) = (\det(M(-\mu^*))^* \tag{3.14}$$

The κ expansion is very cheap to calculate, but its convergence properties at nonzero chemical potential are not optimal, as Q has terms proportional to $\kappa\exp(\mu)$. The action truncated to some order is holomorphic, so proofs of convergence (requiring also fast decaying distributions) apply [2]. In the κ expansion one needs to go to order κ^4 in order to see any κ dependence, as the first closed loop (the plaquette) can be formed at this order. Similarly, one needs to go to order κ^{N_τ} in order to see μ dependence (using the Polyakov loop), since for shorter loops the dependence cancels. As we will demonstrate below calculating high orders is easy in this setup, so this drawback is not a serious one.

In our second scheme, the κ_s-expansion the main part of the μ dependence is dealt with analytically, therefore one expects better convergence properties at high μ, and this is indeed satisfied, see in Section. 4. The price to pay is the slightly higher numerical cost and the non-holomorphic action.

3.3 κ- and κ_s expansion in Langevin simulations

It is useful to consider the expanded determinant (3.6) as part of the action. Note that the resulting effective action is holomorphic. It has then a contribution to the drift term of the Langevin equation (2.1)

$$K_{xva} = -\sum_{n=1}^{\infty} \kappa^n \mathrm{Tr}\left(Q^{n-1} D_{xva} Q\right). \tag{3.15}$$

Note that this contribution is non-real, therefore we have to complexify the theory and use complex Langevin dynamics. (At $\mu = 0$ real Langevin simulations are possible by taking the real part of the fermionic drift terms.)

This contribution to the drift term can be estimated using a random vector η_i (where i represents space-time, colour and Dirac indices), with the properties $\langle \eta_i \rangle = 0$, $\langle \eta_i^* \eta_j \rangle = \delta_{ij}$ as

$$K_{xva} = \langle \eta^* (D_{xva} Q) s \rangle, \qquad s = -\sum_n \kappa^n Q^{n-1} \eta. \tag{3.16}$$

The calculation of this term at $N^q LO$ thus requires $2q$ multiplications with the sparse matrix Q in every timestep, when the random vector is refreshed. In the case of the κ_s-expansion, the drift term has contributions from several places. The $\ln\det(1-R)$ term has contributions to the drift identical to the HDQCD, as calculated in [28]. The contribution of the expansion is

$$\begin{aligned} K_{xia} &= -\sum_{n=1}^{\infty} \kappa_s^n \mathrm{Tr}\left(\frac{1}{1-R}(D_{xia} S)\left[\frac{1}{1-R} S\right]^{n-1}\right), \\ K_{x4a} &= -\sum_{n=1}^{\infty} \kappa_s^n \mathrm{Tr}\left(\frac{1}{1-R}(D_{x4a} R)\left[\frac{1}{1-R} S\right]^{n}\right), \end{aligned} \tag{3.17}$$

for spatial and temporal links, correspondingly. These contributions are estimated using noise vectors similarly to (3.16). The numerical effort of the κ_s expansion involves also multiplications with $(1-R)^{-1}$, calculated according to (3.13), as well as multiplications with the sparse S matrix.

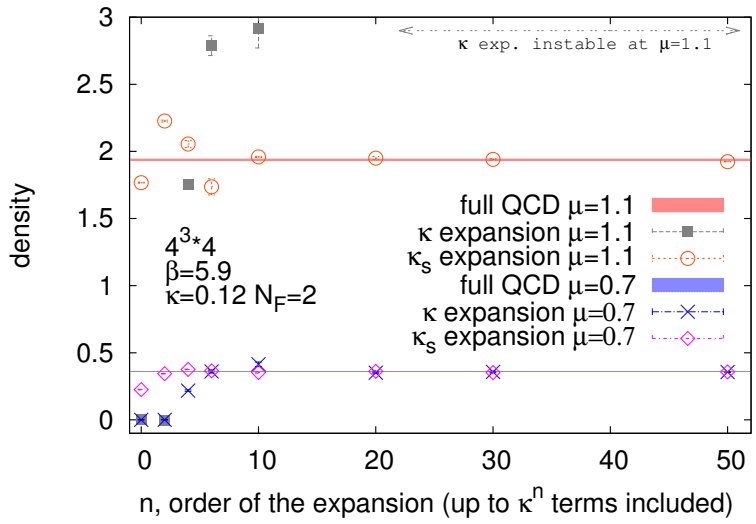

Figure 2: Dependence of the quark density (in lattice units) on the order of the truncation of the κ- and κ_s-expansions, for $\mu = 0.7$ and 1.1, on a 4^4 lattice with $\beta = 5.9$, $\kappa = 0.12$, and $N_f = 2$. The region where the κ-expansion breaks down for $\mu = 1.1$ is indicated. The lines show the result for full QCD. Saturation density is $n_{\rm sat} = 2N_cN_f = 12$.

4. Numerical results

We have used simulations on small 4^4 lattices to examine the convergence properties of the expansions. We have used two flavors of Wilson fermions with $\beta = 5.9$ and $\kappa = \kappa_s = 0.12$, for several μ values. We compare results with full QCD, obtained by complex Langevin simulations, extending the previous results available for staggered fermions [4] to Wilson fermions. Since the full QCD result is also obtained with Wilson fermions there is no need to renormalize the results, already the bare quantities of the expansions in lattice units should converge to their full QCD values. We plot results in lattice units. The lattice spacing is measured using the gradient flow, as proposed in Ref. [29]. The lattice spacing depends weakly on the mobility of the fermions for the heavy quark masses that we are using. For HDQCD we find that $\beta = 5.9$ and $\kappa = 0.12$ corresponds to $a \simeq 0.12$ fm, while for full QCD we find $a \simeq 0.114$ fm.

In Fig. 2 we show the quark number density as a function of the order of the κ- and κ_s-expansions for two different μ values, comparing to the full QCD result. We see that at the smaller chemical potential $\mu = 0.7$ both expansions behave similarly, with convergence around the κ^{10} order. At the higher chemical potential value, the κ expansion breaks down, as expected.

We observe good convergence of the series to the full QCD values. This is a non-trivial agreement which supports both the expansion and the full QCD. This means in particular in the case of the κ expansion, that we must obtain the correct value also in full QCD. This apparently means that the non-holomorphicity of the action for full QCD is not a problem (at least for the case where the κ expansion converges).

In Fig. 3 we see similar behavior for the chiral condensate and the spatial plaquette average.

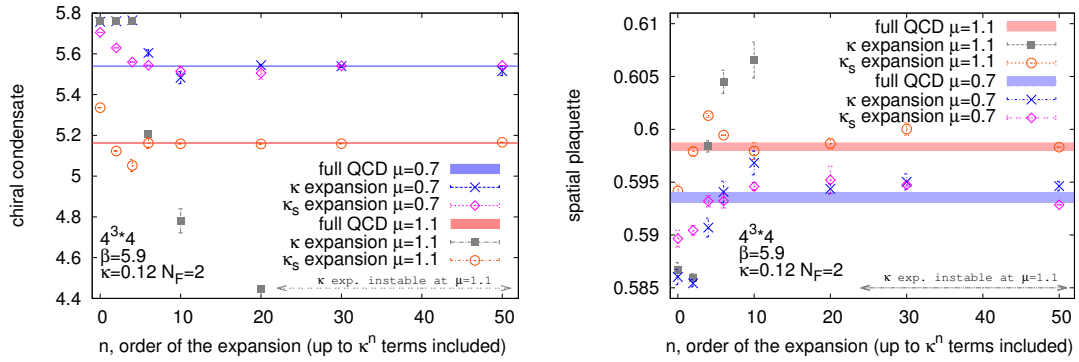

Figure 3: Dependence of the chiral condensate and the spatial plaquette average (in lattice units) on the order of the truncation of the κ- and κ_s-expansions, for $\mu = 0.7$ and 1.1, on a 4^4 lattice with $\beta = 5.9$, $\kappa = 0.12$, and $N_f = 2$. The region where the κ-expansion breaks down for $\mu = 1.1$ is indicated. The lines show the result for full QCD.

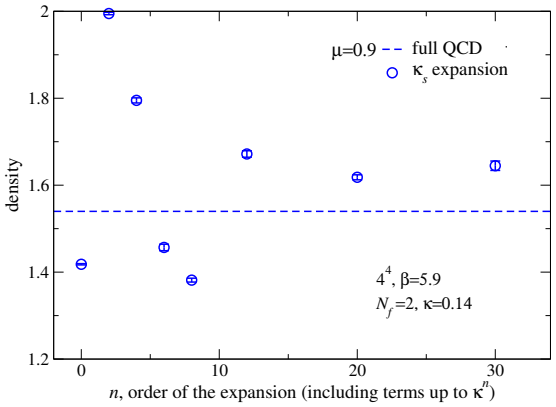

Figure 4: The density at $\kappa = 0.14$ on a 4^4 lattice for the κ_s-expansion and full QCD.

While the convergence appears quite quick at $\kappa = 0.12$, at larger κ this might not be the case, see Fig. 4 where we show the performance of the κ_s expansion at $\kappa = 0.14$. These results suggest that the convergence radius of the κ_s expansion is below $\kappa = 0.14$ at $\mu = 0.9$. The convergence radius seems to be independent of the lattice size, however. In Fig. 5 we show the convergence of the density on a 8^4 lattice. This lattice system has a temperature below the deconfinement transition. We see that density grows about a factor of 3 as one changes the chemical potential from $\mu = 0.7$ to $\mu = 0.8$, which is a sign of the rapid onset transition. One observes that the κ_s expansion still performs well in this region.

5. Conclusions

In this study we have presented the novel implementations of the hopping expansion for the complex Langevin equation which are called κ- and κ_s expansion. They allow calculations at very high, previously impossible orders. This allows the direct observation of the convergence of

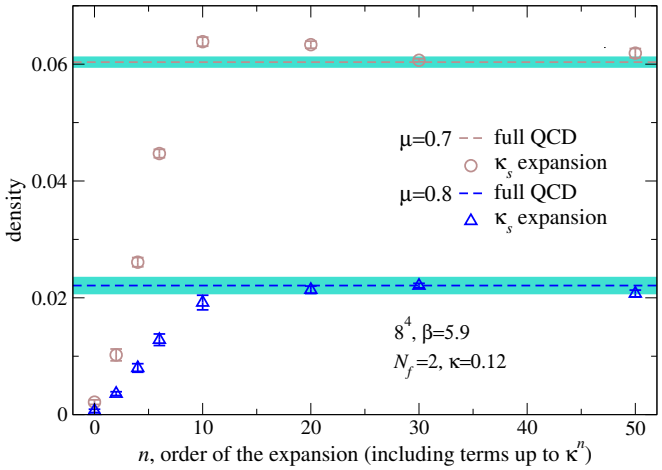

Figure 5: The density at $\kappa = 0.12$ on a 8^4 lattice for the κ_s-expansion and full QCD for chemical potential $\mu = 0.7$ and $\mu = 0.8$.

the series to the full QCD result. We use the complex Langevin equation to circumvent the sign problem of these theories at finite chemical potential. We use no further approximation other than the hopping expansion, the gauge action is kept intact in particular, thus our method can also be used as a test ground for other effective models.

Our expansions have different merits: the κ expansion is cheap and has a holomorphic action, but its convergence properties are bad at large chemical potentials. The κ_s expansion is slightly more expensive numerically, but has improved convergence properties also at high chemical potentials.

We performed simulations of the expansions and observed good convergence to full QCD at not too high κ parameters. This convergence supports both the expanded and the full theory, as the agreement shows that the non-holomorphy of the full theory has apparently no impact on the results, at least in the parameter range where the convergence is observed.

The first results indicate that at least the onset transition might be within the reach of this method in the cold and dense region of the QCD phase diagram, but further studies are required at low temperatures on large lattices.

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