

Dynamical simulations of QCD at finite temperature with a truncated perfect action

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The Hypercube operator determines a variant of the approximate, truncated perfect fermion action. In this pilot study we are going to report on first experiences in dynamical QCD simulations with the Hypercube fermions. We apply this formulation in an investigation of the finite temperature transition for two flavours. On lattices of size $8^3 \times 4$ we explore the phase diagram. Physical scales are estimated from pseudoscalar and vector meson masses obtained on $8^3 \times 16$ lattices. We observe the presence of a metastability region but do not find evidence for an Aoki phase. The Hypercube operator allows us to simulate at ratios of pseudoscalar to vector meson masses at least as small as 0.8 at the thermal crossover at $N_f = 4$, which renders this formulation cheaper than the Wilson like fermions.

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1. Motivation

There are infinitely many ways to discretize the fermionic action of QCD which give the same naive continuum limit. In the class of actions preserving flavour symmetry the most attractive choice from the implementation point of view is the Wilson operator. The application of the Wilson matrix on a spinor field is very cheap since only the nearest neighbours contribute to the fermion action. However when it comes to the physics results this choice may be not the optimal one. Dynamical simulations with two flavours of Wilson fermions revealed the Aoki phase [1] and a first order bulk transition [2, 3] on coarse lattices which are lattice artifacts disappearing in the continuum limit. Therefore sensible simulations have to be restricted to fine lattices. This automatically increases the cost of the operator and makes dynamical simulations at light pion mass with current computer resources and conventional algorithms prohibitively expensive. In particular finite temperature simulations at $N_t = 4$ revealed that the crossover to the high temperature phase occurs at parameters corresponding to heavy pion masses.

Another approach is the perfect action. The idea of the perfect action is based on the iterative application of the Wilson renormalisation group transformation to some given lattice formulation starting from a theory defined on a very fine lattice. After an infinite number of iterations one integrates out all higher modes of the theory beyond some cutoff and arrives at a fixed point which constitutes the perfect action. Quantities calculated with the perfect action are automatically free of any lattice artifacts i.e. they are in the continuum. Hasenfratz and Niedermayer developed the concept of the classically perfect action [4] where one approximates the Wilson renormalisation group transformation by a minimisation procedure. The resulting discretization also has to be truncated to render the formulation implementable. Still, it contains many more terms than the conventional ones like Wilson fermions and Wilson gauge action. Therefore the matrix multiplication will be much more expensive. However one may gain back by using it at a coarse lattice spacing which could render the formulation much cheaper in the end. In addition the classically perfect action obeys the Ginsparg-Wilson relation and thus it has an exact chiral symmetry which is absent for the conventional formulations [5].

It is complicated to realise – especially dynamically – the whole procedure of a truncated perfect action. Attempts to dynamically simulate the classically perfect action are reported in [6]. In this work we simulate a simplified version of a truncated perfect action, the Hypercube operator which was introduced by Bietenholz and Wiese [7]. To construct it one starts from free fermions where the perfect action can be found analytically. It still contains a vector term plus a scalar term

$$D_{\text{HF}}(x, y) = \gamma_\mu \rho_\mu(x - y) + \lambda(x - y). \quad (1.1)$$

Then in [8] a truncation to a unit Hypercube was introduced which would hopefully still not distort much the perfect properties of the theory. It has been shown that even a truncated version leads to an excellent agreement with the continuum Stefan-Boltzmann law already at $N_t = 4, 5$ which is by far better than with the Wilson fermions [8]. Next one proceeds to the interacting case with a simple ansatz of hyperlinks [8, 9, 10] and one uses the Wilson gauge action. This construction leads to a matrix multiplication which is around 15 times more expensive than with the conventional Wilson operator. However one can win back a factor of around 5 in the matrix inversion due to a smaller maximal eigenvalue, which is around 2, and hence a smaller condition number. Therefore one

is left with a computational overhead of a factor around 3 – 4 depending whether the matrix is inverted or the smallest eigenvalues of it are calculated.

The Hypercube operator is not chirally symmetric and therefore a fine tuning is needed to approach the chiral limit. To do this one rescales the link variables like

$$U_{x,\mu} \rightarrow uU_{x,\mu}. \quad (1.2)$$

Increasing u towards its critical value corresponds to decreasing the current quark mass i.e. the tuning towards zero pion mass.

2. Simulation setup and results

In this study we simulated dynamically two flavour QCD with a truncated fermionic perfect action and the standard plaquette gauge action. The quarks obey periodic boundary conditions in spatial directions and antiperiodic ones in time. We used the Hybrid Monte Carlo algorithm with the exact fermionic force. As an integrator we chose the Sexton-Weingarten integration scheme with partially suppressed $\delta\tau^3$ errors [11].

We used the Polyakov loop and its susceptibility to monitor the thermal phase transition in simulations on an $8^3 \times 4$ lattice. As an example in Figure 1 we show histories of the Polyakov loop measured over 1000 trajectories at $\beta = 5.0$. We see that as we increase the value of u (i.e. decrease the current quark mass) we pass from the confined phase with zero expectation value of the Polyakov loop to the deconfined phase indicated by a non-zero Polyakov loop.

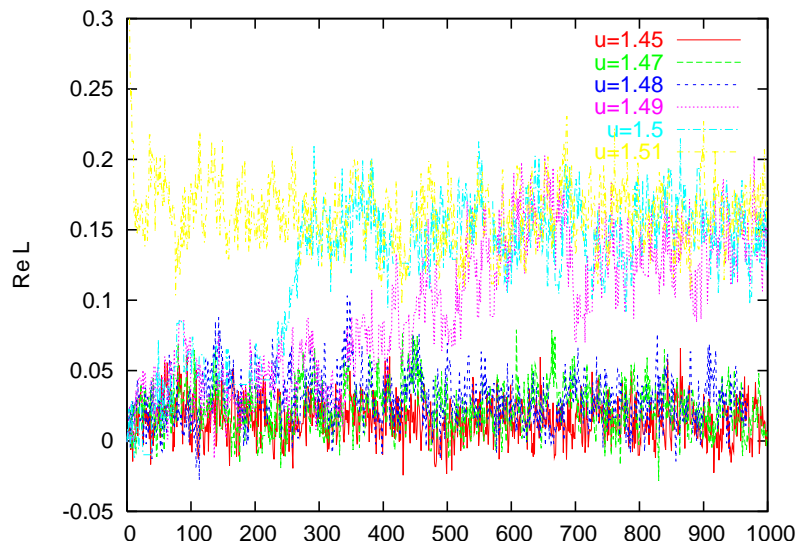


Figure 1: Histories of the Polyakov loop at $\beta = 5.0$. As the value of u is increased the system passes from the confined into the deconfined phase. The transition occurs somewhere between $u = 1.48$ and 1.49 .

In Figure 2 we show an example of the dependence on u of the mean value of the Polyakov loop and its susceptibility at $\beta = 5.0$. We see that the thermal crossover occurs somewhere between $u = 1.48$ and $u = 1.49$ as also seen from the histories at $\beta = 5.0$.

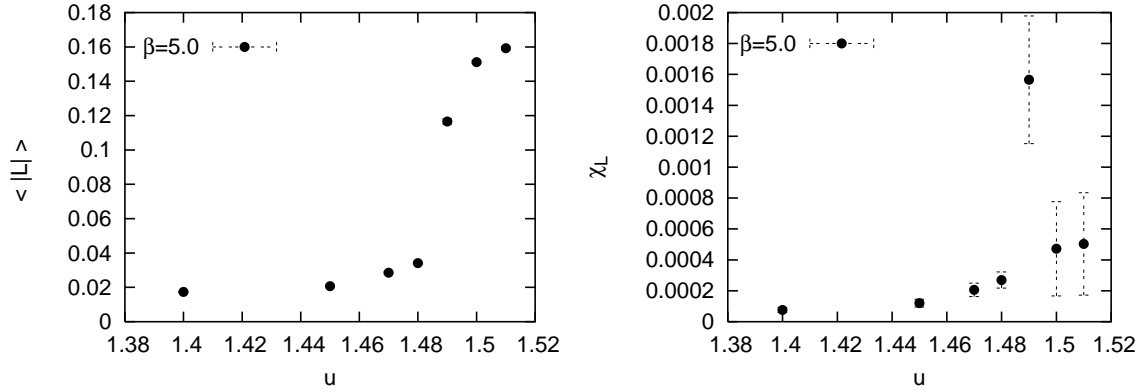


Figure 2: The mean value of the Polyakov loop (left) over about 1000 trajectories of length 1 and the susceptibility of the Polyakov loop (right).

We also considered the number of iterations required to invert the Hypercube operator in the course of the molecular dynamics. This number indicates how singular the Hypercube operator is i.e. how small the current quark mass is. In particular in the confined phase we found a nice linear dependence of the inverse number of iterations on the parameter u , see Figure 3, up to a u value where the inverse number of iterations increases linearly again. This point is nearly identical with the u value where the Polyakov loop susceptibility develops a peak. On the same lattice we

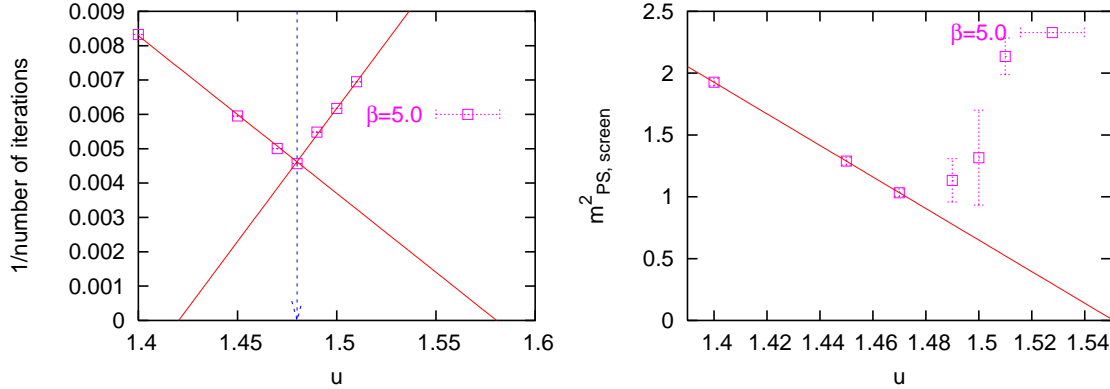


Figure 3: On the left plot we show the dependence of the inverse number of the iterations needed to invert the Hypercube operator in the course of the molecular dynamics. In particular we see a nice linear dependence on u in the confined and in the deconfined regions. This allows us to estimate both the thermal transition point and the critical point. On the right plot we show the dependence of the screening pion mass on u . This also allows us to estimate the critical point by an extrapolation from the confined region to zero.

estimated the critical line by extrapolating the inverse number of iterations to zero and for some parameters we also calculated the critical u by extrapolating the pseudoscalar screening mass to zero, see Figure 3. Obviously these two methods suffer from different systematic errors so that we

know only approximately the critical line.

We also performed zero temperature simulations on $8^3 \times 16$ lattices to estimate ratios of the pseudoscalar and the vector meson masses. Using an empirical formula

$$m_V = 756 \text{ MeV} + 450 \text{ MeV} \left(\frac{m_{\text{PS}}}{m_V} \right)^2. \quad (2.1)$$

also an estimate of the lattice spacing can be derived from this ratio. For example at $\beta = 5.0$ and $u = 1.48$ the ratio is around 0.80(1) and the corresponding inverse lattice spacing is 934 ± 11 MeV. This yields a critical temperature of $T_C = 234 \pm 3$ MeV. The errors are purely statistical, the systematic error due to Eq. (2.1) can be much bigger.

Next we looked at eigenvalues of the Hypercube operator at parameters (β, u) near to the thermal crossover. We see that the branches of the eigenvalues are very broad which signals poor chiral properties at coarse lattices, with lattice spacing around 0.25 – 0.35 fm. This however improves as one proceeds closer to the critical line where the lattice spacing is decreased.

So far we do not observe the Aoki phase which otherwise would be signalled by the vanishing pseudoscalar mass in some domain of the parameter space and result in a singular Hypercube operator and eventual breakdown of the molecular dynamics. There is however another potential problem, namely, the occurrence of a bulk phase transition. To monitor this transition we compare runs from hot and cold starts of the Markov chain. In the vicinity of a first order phase transition e.g. plaquettes level out at different values. Our present simulations indicate such a two state signal at $(\beta, u) = (4.8, 1.56)$ and $(5.0, 1.5)$ in simulations on an $8^3 \times 16$ lattice, while it is absent at $(4.8, 1.5)$, $(5.0, 1.48)$, $(5.2, 1.44)$ and $(5.3, 1.33)$, see Figure 4. However these results are obtained with limited statistics and may be therefore influenced by insufficient thermalisation. Also at $\beta = 5.0, u = 1.5$ the number of CG iterations along the plateau which originated from the hot start is around 500 whereas it drops to 350 when started from a unit configuration. This may suggest that there may be a difference in the pion mass for these two phases. We also note that on the finite temperature lattice, $8^3 \times 4$, the meta stability signal has disappeared at $\beta = 5.0, u = 1.5$. From this one may conclude that if present the first order phase transition becomes softer and is shifted in the direction of smaller current quark mass respectively larger u when the temperature is raised. The presence of a meta stability region sets a lower bound on the pion mass below which one cannot relate the results at given values of β and u to the correct universality class of the physical theory. Otherwise one could go to quite small pion masses in the region below $\beta = 5.0$.

In Figure 5 we conjecture the structure of the lattice phase diagram $\{\beta, u\}$ for an $8^3 \times 4$ lattice based on the current data. The red line denotes the crossover from the confined into the deconfined phases, blue line shows approximately where the critical line is and the shaded region indicates meta stability.

3. Conclusions

We simulated two flavours of dynamical fermions with a truncated perfect action implementing the exact fermionic force in the Hybrid Monte Carlo. For the gauge action we used the conventional plaquette action. So far we do not observe the Aoki phase at the investigated parameters. Instead, we observe some indications for the existence of a meta stable region in our simulations on an

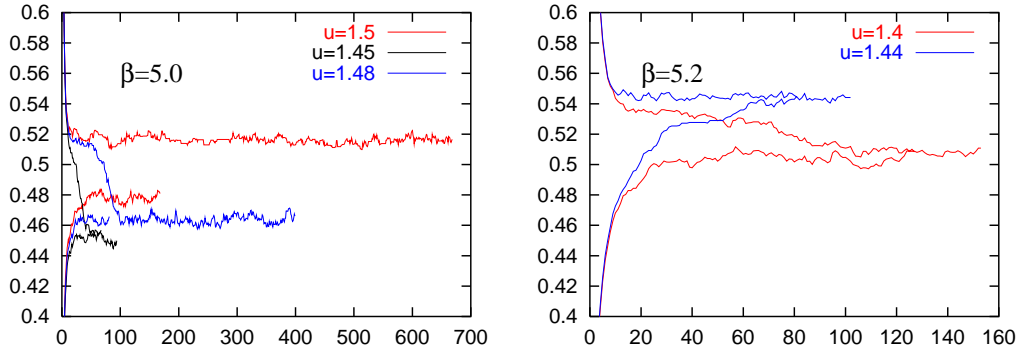


Figure 4: On the left plot we show histories of the plaquette at $\beta = 5$, $u = 1.45$ and $u = 1.5$ in simulations on an $8^3 \times 16$ lattice. We see a two-state signal of meta stability at $u = 1.5$ which is absent at $u = 1.48$. At $\beta = 5.2$ we so far do not observe such meta stability as shown on the right.

$8^3 \times 16$ lattice. This artifact may disappear at the same parameter values on an $8^3 \times 4$ lattice, which would signal that this region may be shifted in the direction of smaller pion masses once the temperature is increased. The presence of the meta stable region may prevent us from studying the critical temperature at small pion masses. Hopefully this problem will soften as one applies a different gauge action, see e.g. [12, 13], or uses some variants of the smearing in the fermionic action, see e.g. [14]. Also one may consider to simulate an approximate overlap operator with the kernel of the Hypercube operator. The smallest confirmed ratio of the pseudoscalar mass to the vector meson mass at the crossover line at $N_t = 4$ is around 0.8. Here the estimate for the critical temperature is about 234 ± 3 MeV which roughly agrees with the world data at this pion mass. Given the fact that this ratio is realised at $N_t = 4$ the Hypercube operator is still cheaper than the Wilson operator where such ratio was reported only at $N_t = 8$ using the plaquette gauge action, see e.g. [15].

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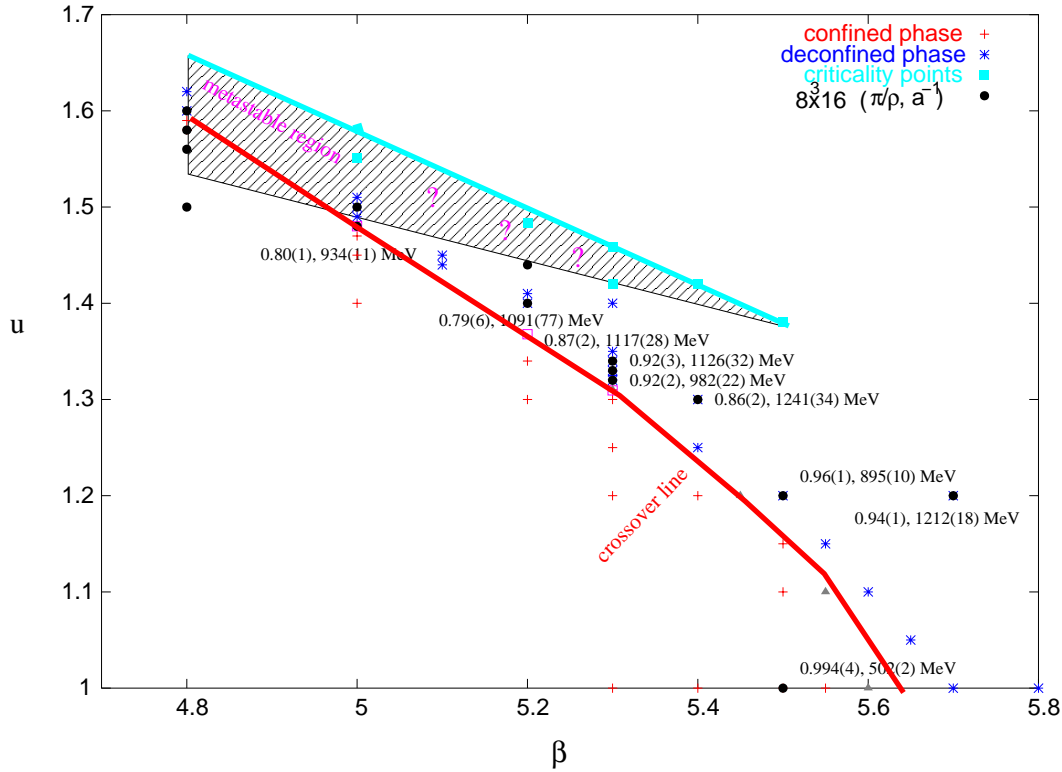


Figure 5: Conjectured phase diagram determined by inspecting the Polyakov loop and the inverse number of iterations required by a CG solver in the course of the molecular dynamics is shown. In particular the position of the critical line, the thermal crossover line and the region where meta stability may occur is shown. The black dots indicate simulations on $8^3 \times 16$ lattices together with the ratio of the pseudoscalar and the vector meson mass and an estimated inverse lattice spacing. The error bars are purely statistical.

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