Lattice QCD with light dynamical quarks

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We report on the simulation of QCD with light dynamical quarks using the two-step multi-boson (TSMB) algorithm. In an exploratory study with two flavours of quarks at lattice spacing about 0.27 fm and with quark mass down to one sixth of the strange quark mass eigenvalue spectra and autocorrelations have been studied. Here we present results on the volume dependence as well as tests of possible algorithmic improvements.

1. INTRODUCTION

Predicting the low energy constants of the chiral effective Lagrangian from first principles in QCD is an exciting challenge for lattice gauge theories. This question has attracted a considerable attention in the last few years \cite{1,2,3}. However, existing unquenched simulations are typically done in a region where the light quarks are not light enough, in most cases – especially with Wilson-type quarks – with two light quark flavours (\(u\) and \(d\)) having masses larger than half of the strange quark mass (\(m_{ud} > \frac{1}{2}m_s\)). Since the quark mass dependence in the chiral Lagrangian is explicit, it is not necessary to perform simulations at the physical value of the \(u\)- and \(d\)-quark masses, which remains a too hard task for the foreseeable future. Nevertheless, in order to keep the systematic errors under control, three dynamical quarks should be simulated and, according to \cite{4}, the masses of the light ones should satisfy at least \(m_{ud} \leq \frac{1}{3}m_s\).

Simulating light dynamical quarks is a difficult task for numerical computations because all known algorithms for QCD have a substantial slowing down towards small quark masses. The present status has been summarized at the Berlin lattice conference \cite{5}. Inspired by that discussion, in a recent paper \cite{6} we parametrized the cost of an unquenched QCD simulation in two different ways:

\[
C = F \left( r_0 m_\pi \right)^{-z_\pi} \left( \frac{L}{a} \right)^{z_L} \left( \frac{r_0}{a} \right)^{z_a}, \quad (1)
\]

\[
C_U = F_U \left( \frac{m_\pi}{m_\rho} \right)^{-z_{\pi\rho}} \left( \frac{L}{a} \right)^{z_L} \left( \frac{r_0}{a} \right)^{z_a}. \quad (2)
\]

Here \(r_0\) is the Sommer scale parameter \cite{7}, \(m_\pi\) the pion mass, \(L\) the lattice extension and \(a\) the lattice spacing. The powers \(z_{\pi,\pi\rho,L,a}\) and the overall constants \(F, F_U\) are empirically determined. The value of the constants \(F, F_U\) depends on the definition of “cost”. Of course, when the quark masses are very light and the decay \(\rho \to \pi\pi\) is possible, the first parametrization is preferable. Typical values of the parameters can be taken from Ukawa’s contribution \cite{5}: \(F_U = 5.9 \cdot 10^6\) flop, \(z_{\pi\rho} = 6, z_L = 5, z_a = 2\). Other estimates are in reasonable agreement. However most of the simulations, whereon such estimates are based, were performed at quite large quark masses. This is a reason of concern because, as experienced already by several collaborations \cite{8}, at small quark masses new phenomena appear, especially for algorithms based on molecular dynamics integrators.

Given the compelling need of simulations at lighter quarks, we performed algorithmic studies in the regime of very light quark masses (though on very rough lattices) \cite{6} using the two-step
multi-boson algorithm [8]. Here we give an update of the cost analysis. We also include a preliminary study of the volume dependence and a test of a possible improvement of the algorithm.

2. COST OF THE SIMULATIONS

2.1. Algorithm

Let us first briefly summarize the main features of TSMB. The quark determinant of \( N_f \) degenerate flavours is represented as

\[
\left| \det(\tilde{Q}) \right|^{-N_f} \simeq \frac{1}{\det P_{n_1}(Q^2) \det P_{n_2}(Q^2)}. \tag{3}
\]

\( \tilde{Q} \) is the hermitian Wilson-Dirac fermion matrix. The polynomials \( P^{(1)} \) and \( P^{(2)} \) satisfy

\[
\lim_{n_2 \to \infty} P^{(1)}_{n_1}(x)P^{(2)}_{n_2}(x) = x^{-N_f/2}, \quad x \in [\epsilon, \lambda]. \tag{4}
\]

The interval \([\epsilon, \lambda]\) covers the spectrum of \( \tilde{Q}^2 \) on a typical gauge configuration. The first polynomial \( P^{(1)} \) of order \( n_1 \) is a crude approximation and is realized by the multi-boson representation. The second polynomial \( P^{(2)} \) of order \( n_2 \gg n_1 \) gives a better approximation. It is taken into account in the updates by a global noisy Metropolis correction step. Since for fixed \( n_2 \) (and outside the interval \([\epsilon, \lambda]\)) the approximation \( P^{(1)}P^{(2)} \) is not exact, a final correction step is performed by reweighting the gauge configurations which are considered for the evaluation of the expectation values. This is done with a sufficiently high order polynomial \( P^{(2)}_{n_2} \). For more details about the algorithm in this context we refer to [8].

2.2. Parameters and the definition of cost

The Monte Carlo simulations have been done near the \( N_t = 4 \) thermodynamical cross-over line. We tuned the gauge coupling \( \beta \) and the hopping parameter \( \kappa \) in order to explore a range of the quark mass going from \( 2m_u \) to \( \frac{1}{2}m_s \) while keeping \( r_0/a \) roughly constant between \( r_0/a = 1.7 \) and \( r_0/a = 1.9 \), which implies \( a \simeq 0.27 \) fm. Most of the analysis is performed on lattices of size \( 8^3 \cdot 16 \) implying a physical lattice extension \( L \simeq 2.2 \) fm. For the study of finite volume effects we used \( 12^3 \cdot 24 \) and \( 16^3 \) lattices.

The cost of a simulation can be measured in units of the floating point operations (flop) which are necessary to produce a new decorrelated configuration (starting from a thermalized configuration). The decorrelation quantified by the integrated autocorrelation length \( \tau_{int} \) depends on the quantity whose autocorrelation is observed. We consider the average plaquette, the lowest eigenvalue of the fermion matrix, the pion correlator at some fixed distance and the pion mass. Instead of the number of flops the integrated autocorrelations can also be quoted by the necessary number of fermion-matrix vector multiplications (MVM’s). We always count multiplications by the fermion matrix \( \tilde{Q} \). In this way the dependence on the computer architecture is reduced. For TSMB we have the following approximate formula for the total amount of MVM’s needed for one update cycle:

\[
N \simeq 6(n_1N_B + N_U) + 2(n_2 + n_3)N_C + I_GF_G. \tag{5}
\]

Here \( N_B \) is the number of local bosonic sweeps per update cycle, \( N_U \) the number of local gauge sweeps, \( N_C \) the number global Metropolis accept-reject correction steps, and \( I_G \) and \( F_G \) give the number of MVM’s and frequency of the global quasi heatbath. \( n_3 \) is the order of an auxiliary polynomial \( P^{(3)} \). Of course, the number of MVM’s can easily be converted to flops by noting that the number of flops per lattice point (in our code) is 1344. The quantity in \([9]\) is reported for the runs considered here in the columns 7 and 5 of tables \([10]\) and \([11]\) respectively.

2.3. Results about the costs

In \([10]\) power fits have been given for the dependence of the integrated autocorrelations on the quark mass parameter \( M_r \equiv (r_0m_u)^2 \). For instance, in case of the average plaquette a good fit is

\[
\tau_{int}^{plaq} = c_{plaq}M_r^{z_{plaq}},
\]

\[
c_{plaq} = 7.92(68), \quad z_{plaq} = -2.02(10), \tag{6}
\]

if the cost is counted in MVM’s (= 10⁶ fermion-matrix vector multiplications). This corresponds to \( z_n \simeq 4 \) in \([10]\). A reasonable fit of \( \tau_{int}^{plaq} \) can also be found in the form \([9]\) with \( z_{\pi\rho} \simeq 6 \) if the heaviest quark mass point is omitted.

Another interesting quantity is the pion correlator and/or the pion mass. For instance, the cost
for the pion correlator at timeslice distance \( d = 5 \) is shown together with two power fits in figure 1. The fit to all points gives a power similar to \( z_{\text{plaq}} \):

\[
c_5 = 2.68(35) \ , \ z_5 = -1.96(17) \ .
\]

However, if the point at \( M_r \simeq 3 \) is omitted from the fit we obtain a lower power:

\[
c_5 = 2.99(22) \ , \ z_5 = -1.15(28) \ .
\]

Fitting the cost for obtaining the pion mass, the result is:

\[
c_m = 1.99(16) \ , \ z_m = -1.47(16) \ .
\]

(The data and the fit is shown in figure 2). This corresponds to \( z_\pi \simeq 3 \) in (1), similarly to the result for the minimal eigenvalue of the squared hermitean fermion matrix:

\[
c_{\text{min}} = 5.36(80) \ , \ z_{\text{min}} = -1.48(25) \ .
\]

It is remarkable that the pion mass has a substantially lower cost than, for instance, the average plaquette. In fact, at \( M_r \simeq 0.5 \) the cost ratio is already almost 10 in favour of the pion mass. This is partly due to the intrinsic fluctuation present in the pion propagator which is originated from the freedom of randomly choosing the position of the source.

2.4. Analysis with correction factors

The importance of the final correction step by the reweighting factors depends on the choice of the second polynomial \( P^{(2)} \). For good enough \( P^{(2)} \) the reweighting is negligible. In this case this has been the case for all but one runs. (The run where the reweighting was not completely negligible has the index (i).) Of course, at very small quark masses \( P^{(2)} \) becomes good enough only for a very large order \( n_2 \). In such a case it is a question whether it would be more advantageous to keep \( n_2 \) smaller and tolerate a non-trivial reweighting.

The consequences of a poor \( P^{(2)} \) at small quark masses could, however, be rather unpleasant. An example has been shown in figure 2: in run (i) at \( M_r \simeq 0.6 \) one of the four parallel runs had a serious fluctuation with exceptionally small eigenvalues and, as a consequence, very small correction factors in a substantial part of the run (see figure 2 in [3]). In this part of the run also a few negative eigenvalues of the fermion matrix have been observed. The smallness of the corresponding reweighting factors implies that with a better second polynomial \( P^{(2)} \) such fluctuations could have been suppressed.

The question is, what is the consequence of such a fluctuation on the integrated autocorrelations and on the related magnitude of statistical errors. This can be investigated, for instance, by considering the linearized deviation of effective pion masses which appears in the linearization method for determining the autocorrelations of functions of primary averages [10]. For an illustration see the case of the effective mass between timeslice distances \( d = 3 \) and \( d = 7 \) after including the reweighting factors in the above mentioned run of [6] (figure 3). As this figure shows, the exceptionally small eigenvalues and the corresponding small reweighting factors are accompanied by a large downwards fluctuation of the effective mass \( m^{\text{eff}}_\pi \). This implies that in this run the average value of \( m^{\text{eff}}_\pi \) is smaller than in the “normal” runs and at the same time its error is larger. This pulls down the overall mass estimate: the average of all four parallel runs gives for this effective mass \( m^{\text{eff}}_\pi = 0.4160(103) \). For the three other runs the result is: \( m^{\text{eff}}_\pi = 0.4298(63) \). Our
conclusion is that it is probably better to suppress the kind of fluctuations in figure 3 by sufficiently improving $P^{(2)}$.

3. VOLUME DEPENDENCE

The physical volume of the lattices in [6] is such that strong finite volume effects are not expected. For checking this and for observing the behaviour of our algorithm in increasing volumes new simulations were performed on a $12^3 \cdot 24$ and a $16^4$ lattices (see (f12) and (e16) in table 1). In order to hold all the quantities fixed, except for the volume, run (f12) has the same value of $\beta$ and $\kappa$ as run (f) and run (e16) the same as run (e). The lattice extensions deduced from $r_0/a$ are collected in the last column of table 1.

When going to a larger lattice one has to adjust in TSMB the first polynomial order $n_1$. Assuming no large finite volume effects the interval given by $\epsilon$ and $\lambda$ remains unchanged. Therefore it is not needed to change $n_2$ and $n_3$. This is true for the runs (e) and (e16). For run (f) the lower boundary $\epsilon$ was not optimal therefore we used a better (i.e. smaller) one in run (f12). Consequently, $n_2$ and $n_3$ had to be increased there.

4. DETERMINANT BREAKUP

Inspired by [11] (see also [12]) we tried to improve autocorrelations by “determinant breakup”. In our case this means, for instance, that simulating two flavours separately should be more effective than two degenerate flavours together. In general, one can write the determinant as

$$\left| \det(\tilde{Q}) \right|^{N_f} = \left\{ \left| \det(\tilde{Q}) \right|^{N_f/N_b} \right\}^{N_b},$$

with an arbitrary positive integer $N_b$ and use the polynomial approximation (3) for the individual factors on the right hand side.

For tests we have chosen run (b) in [6] where $M_r \simeq 3$ (close to the strange quark mass). Results are shown in table 2. (Note that $r_{\text{int}}^{m_\pi}$ are
obtained here from effective masses with the linearization method for autocorrelations and errors and therefore are slightly different from [6].) Tests at smaller quark masses and/or in larger volumes will be done later.

Choosing some breakup of the flavours we fixed \( n_1 \) by requiring a constant acceptance rate of 50-60%. The higher polynomial orders \( n_2 \) and \( n_3 \) were fixed by keeping the relative deviation at the interval ends roughly constant. We found that the autocorrelation measured in update cycles is reduced when breaking up the determinant in more pieces. However the costs per update cycles is increasing. It is remarkable that the total number of iterations in the determinant breakup almost a factor of two when splitting up two flavours in two pieces.

### 5. Eigenvalues

The study of the low lying modes of the Wilson-Dirac operator \((Q)\) is interesting both physically and algorithmically. It is an interesting question how the qualitative features of the spectrum change with increasing volume. As described in [6], we used the implicitly restarted Arnoldi method [3] to compute a portion of the eigenvalues of the non-hermitean Wilson-Dirac fermion matrix \(Q\). Typically we computed the eigenvalues with lower real part of the matrix \(Q\) and those with smallest modulus of the preconditioned matrix \(Q\) (as defined in [6]). By use of the analytical relations in [6] we had access to a reasonable part of the spectrum of \(Q\) around the origin.

In figure 4 we plot \(O(200)\) eigenvalues from 10 configurations thermalized at point (f) on the \(8^3\cdot16\) lattice. The portion of spectrum to which we have access is that inside the dashed circle and to the left of the dashed vertical line. In figure 5 we plot again \(O(200)\) eigenvalues from 10 configurations thermalized at point (f12) on \(12^3\cdot24\) lattice, which has the same parameters as (f) except for the volume. As expected, the lowest border of the spectrum does not essentially move, even if the density of eigenvalues is higher (and as a consequence, the portion of spectrum that we can cover is smaller).

### 6. Conclusion

In conclusion, the cost increase with the lattice volume is quite acceptable because it is close to the trivial volume factor. In case of the autocorrelation of the pion mass the observed increase
turns out to be even smaller.

The determinant breakup is an easy and effective method to speed up the gauge field update.

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