One-Flavour Hybrid Monte Carlo with Wilson Fermions

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Abstract. The Wilson fermion determinant can be written as product of the determinants of two hermitian positive definite matrices. This formulation allows to simulate non-degenerate quark flavors by means of the hybrid Monte Carlo algorithm. A major numerical difficulty is the occurrence of nested inversions. We construct a Uzawa iteration scheme which treats the nested system within one iterative process.

1 Introduction

The strong interaction between the quarks is described by quantum chromodynamics (QCD), a constitutive part of the standard model of elementary particle physics. QCD develops a strong coupling constant at the hadronic mass scale and thus, perturbation theory cannot be applied. The only known non-perturbative ab-initio method is to simulate QCD on a 4-dimensional space-time lattice by use of Monte Carlo methods as known from statistical physics.

One would think that lattice simulations of QCD have to take into account virtual loops from all six quark flavors, up ($u$), down ($d$), strange ($s$), charm ($c$) bottom ($b$), and top ($t$). Their masses span a wide range from about 3 MeV to about 180 GeV. 1 The masses of the three heavy quarks lie above the momentum scale set by dynamical chiral symmetry breaking. The QCD Lagrangian is chirally symmetric for vanishing quark masses. Chiral symmetry is explicitly broken by the quark masses and spontaneously by the dynamics. For light quarks, ($u, d, s$), dynamical breaking dominates, as signaled by zero mass Goldstone bosons, i.e., the pion octet. Supposedly only the light quarks contribute with virtual loops; the contributions of the heavier ones are assumed to be negligible.

1 The light quark ($u, d, s$) masses are so-called “current” masses determined within the $\overline{\text{MS}}$ scheme at a renormalization scale $\mu = 2$ GeV. The masses of the heavy quarks ($c, b, t$) are “running” masses determined at $\mu = m_{c,b,t}$ in the $\overline{\text{MS}}$ scheme [1].
A straightforward lattice QCD simulation including u, d, and s is difficult: on one hand, u and d are very light. As we know from chiral perturbation theory, the square of the pion mass is proportional to the quark mass \(^2\). Therefore, the pion acquires a small mass, i.e. a large correlation length, \(\xi = \frac{1}{ma}\), for u and d masses approaching the chiral limit, \(m_u\) and \(m_d\) = 0. \(a\) denotes the lattice spacing. The lattice volume must be larger by more than one order of magnitude than possible today to reach physical parameter values for \(m_u\) and \(m_d\). Hence, one has to recourse to extrapolations using results of simulations at artificial parameters for \(m_u\) and \(m_d\) and small lattices, far off the chiral limit. These difficulties go along with an increasing condition number of the fermionic matrix \(M\), therefore its inversion suffers from critical slowing down approaching the chiral limit \([3,4]\).

On the other hand, until recently, the only exact simulation algorithm for QCD with dynamical fermions\(^2\) was the hybrid Monte Carlo algorithm (HMC) \([5,6]\). The benefits of HMC in reducing the computational complexity are achieved by treating the fermionic determinants as a stochastic estimate using Gaussian random fields \([7]\), with the advantage, that instead of computing the determinant, only the solution of a linear system is required. For this approach the fermion matrix \(M\) must be hermitian positive definite (hpd).

The Wilson fermion discretization of the fermionic sector of QCD describes single flavors \([8]\), in contrast to staggered fermions that represent four fermions, intermixed in spin-flavor space.\(^3\) Unfortunately, Wilson fermions must violate chiral symmetry, see Ref. \([9]\). As a consequence, the Wilson fermion matrix is complex non-normal and thus cannot be included in the HMC scheme. To avoid this problem, one usually simulates two mass degenerate light quarks, an approximation justified by the fact that both quarks, u and d, are light and close in mass compared to the next heavier one, s. The product of two mass degenerate determinants indeed amounts to an hpd matrix, that can be simulated by the HMC. The minor price to pay is that the two light quarks are mass-degenerate, the major price is that the s quark is not included in the simulation.

There are attempts to evaluate operators, that contain the s quark, by application of a “partially quenched analysis” \([10]\). The PQA extrapolates only one of the valence quarks towards the chiral limit and holds the other one at the mass of the s quark—of course within the light mass-degenerate u-d-sea. PQA, however, leads to inconsistencies: the so-called J-parameter does not acquire its physical value \([11,12]\).

One can try to employ an approximate one-flavor determinant representation. Such simulations, however, are plagued by systematic uncertainties, as one has to recourse to non-exact simulation algorithms like the hybrid molecular dynamics algorithm \([13,14]\).

\(^2\) “Dynamical” in contrast to “quenched” simulations that neglect fermionic loops.

\(^3\) The naive discretization of the Dirac operator yields, in addition to the true mode, 15 “doublers”.

On the other hand, in the framework of the multi-boson algorithm [15], one can define an exact single flavor simulation scheme for Wilson fermions [16–18]. Here many additional bosonic auxiliary fields are required, and it is not clear if the method would be well suited for more complicated actions or allows to exploit sophisticated preconditioning.

In this paper, we propose to include the Wilson fermion determinant into HMC such that a single quark can be described. We show that the fermionic determinant can be written as a product of the determinants of two \( \text{hpd} \) matrices. This is achieved by the representation of the fermion matrix via its Schur complement. Both determinants can be treated by the hybrid Monte Carlo in the standard manner. There are, however, some caveats: one of the two matrices involves the inverse of the other one. As a consequence, a nested inversion must be carried out. We propose to use a Uzawa-like inverter which allows to solve the nested system within one iterative process. A second difficulty stems from the initialization of the fermion action in the HMC algorithm: since we have a single flavor system, we have to compute a square root at the beginning of a HMC trajectory.

The paper is organized as follows: in section 2 we introduce the basics of lattice QCD and will discuss the difficulties simulating single flavors of Wilson fermions by the HMC. In section 3 we give the transformation of the fermion matrix using the Schur complement, in section 4 we present the non-mass-degenerate HMC for Wilson fermions along with a discussion of numerical problems. In section 5, we introduce an algorithm that can compute the nested inversion in one iterative process. Finally, we summarize and give an outlook.

2 Numerical Problem

The action of lattice QCD is the sum of a gauge part (which is not relevant for the following) and a fermionic part:

\[
S[U, \bar{\psi}, \psi] := S_g[U] + \sum_{x,y,a,b,\alpha,\beta} \bar{\psi}_x^a \, M_{x,y}^{a,b} \, \psi_y^b.
\]  

(1)

\( V \) is 4-dimensional volume in Euclidean space. The full matrix is a tensor product with \( 3 \times 3 \) SU(3) matrices \( U \) (color) and four \( 4 \times 4 \) matrices \( \gamma_\mu \) (Dirac spin), hence

\[
M \in \mathbb{C}^{12V \times 12V}.
\]  

(2)

Here the indices \( x,y \) stand for the 4-dimensional coordinates, \( a \) and \( b \) denote color space and \( \alpha \) and \( \beta \) Dirac space indices.

The fermion fields \( \psi_x \) are Grassmann variables. Therefore, the Grassmann integral of the exponential of the fermionic part of the action, i.e., the
fermionic part of the path integral, can be carried out,
\[
\int [d\psi][d\bar{\psi}] e^{-\bar{\psi} M \psi} = \det(M),
\]  
(3)
to yield the determinant of \(M\) for arbitrary complex \(M\).

Wilson fermions are defined by the interaction matrix
\[
M = 1 - \kappa D, \quad M \in \mathbb{C}^{12V \times 12V},
\]
\[
D_{x,y} = \sum_{\mu=1}^{4} (1 - \gamma_{\mu}) U_{\mu}(x) \delta_{x,y-\mu} + (1 + \gamma_{\mu}) U_{\mu}^\dagger(x - \mu) \delta_{x,y+\mu}.
\]  
(4)

The Dirac matrices in Euclidean space satisfy the anti-commutator relations
\[
\gamma_{\mu} \gamma_{\nu} + \gamma_{\nu} \gamma_{\mu} = 2 \delta_{\mu\nu}.
\]  
(5)

It is important for the following considerations to work with the chiral representation of the Dirac matrices, as given in the appendix A. In this representation, \(\gamma_5\), defined as the product \(\gamma_5 = \gamma_4 \gamma_1 \gamma_2 \gamma_3\), is diagonal.

\(M\) is a complex non-hermitian matrix which moreover is not normal, i.e.,
\[
MM^\dagger \neq M^\dagger M.
\]  
(6)

Thus \(M\) cannot be diagonalized by a unitary transformation. At most, it might be diagonalizable by a similarity transformation. However, \(M\) exhibits the so-called \(\gamma_5\)-symmetry or \(\gamma_5\)-hermiticity:
\[
M \gamma_5 = \gamma_5 M.
\]  
(7)

Therefore, the matrix
\[
Q := \gamma_5 M
\]  
(8)
is hermitian. We can immediately read off the chiral representation of the Dirac matrices, see the appendix, that, for \(\kappa = 0\), \(Q\) exhibits an equal number of positive and negative eigenvalues. In general, \(Q\) is indefinite.

The matrix \(M^\dagger M\) is hpd. Since the determinant of \(M^\dagger M\) represents two mass degenerate fermion flavors,
\[
\det (M^\dagger M) = \det (M) \det (M),
\]  
(9)

the two flavor situation is ideal for HMC simulations. Being unitary diagonalizable it can be represented by a Gaussian integral over complex fields \(\phi\):
\[
\det (M) \det (M) = \left(\frac{1}{2\pi}\right)^{12V} \int [d\phi][d\phi^\ast] e^{-\phi^\dagger (M^\dagger M)^{-1} \phi}. \]  
(10)
For the single flavor $M$, such a simple construction fails even for the situation $\kappa < \kappa_c$ where $M$ is positive definite, because the Jacobian of the similarity transform—if the diagonalization is feasible at all—is not equal to 1.

On the other hand,

$$\det (M) = \det (Q).$$

But, $Q$ is indefinite. Therefore, a Gaussian integral representation for its determinant does not exist.

We conclude that so far there is no direct way to include individual flavors within the HMC algorithm.

### 3 Schur Complement of $Q$

Let’s consider the hermitian matrix $Q$ with the Dirac matrices given in the chiral representation of appendix A. The explicit form of $Q$ in the chiral representation is given by

$$Q_{11} = \left( \begin{array}{cc} \frac{1}{1 - \kappa D_{11}} & -\kappa D_{12} \\ -\kappa D_{12}^\dagger & -1 \left( 1 - \kappa D_{11} \right) \end{array} \right).$$

Here, the bold face 1 represents a unit matrix in $2 \times 2$ spin space. $D_{11}$ does not carry spin indices while $D_{12}$ consists of $2 \times 2$ blocks in spin space,

$$D_{11} = \sum_{\mu=1}^{4} U_{\mu}^\dagger(x) \delta_{x,x+\mu} + U_{\mu}(x-\mu) \delta_{x,x-\mu},$$

$$D_{12} = \sum_{\mu=1}^{4} \eta_{\mu} \left[ U_{\mu}(x) \delta_{x,x+\mu} - U_{\mu}^\dagger(x-\mu) \delta_{x,x-\mu} \right],$$

with

$$\eta_1 = i\sigma_1, \quad \eta_2 = i\sigma_2,$$

$$\eta_3 = i\sigma_3, \quad \eta_4 = -1.$$  \hspace{1cm} (14)

The Schur complement of a $2 \times 2$ block matrix with non-singular block $A$ is given by

$$\left[ \begin{array}{cc} A & B \\ C & D \end{array} \right] = \left[ \begin{array}{cc} 1 & 0 \\ CA^{-1} & 1 \end{array} \right] \left[ \begin{array}{cc} A & 0 \\ 0 & D - CA^{-1}B \end{array} \right] \left[ \begin{array}{cc} 1 & A^{-1}B \\ 0 & 1 \end{array} \right].$$

Hence

$$\det(Q) = \det \left( \frac{1}{1 - \kappa D_{11}} \right) \det \left( 1 - \kappa D_{11} \right) + \kappa^2 D_{12} \left[ 1 - \kappa D_{11} \right]^{-1} D_{12}^\dagger.$$  \hspace{1cm} (16)
The minus sign of the $Q_{22}$ term cancels as the rank of the matrix is even. From Eq. 13 we know that the first matrix is diagonal in Dirac space. Therefore its determinant can be written as follows:

$$\det(Q) = \det(1(1 - \kappa D_{11})) = \det(1 - \kappa D_{11})^2 = \det(1 - \kappa D_{11})^2,$$

where $Q_{ww}^2 = (1 - D_{11})^2$ is $hpd$ for any $\kappa$. $Q_w$ carries no spin index.

The second matrix

$$Q_{sc} = 1(1 - \kappa D_{11}) + \kappa^2 D_{12}[1(1 - \kappa D_{11})]^{-1} D_{12}^\dagger,$$

the Schur complement, is hermitian, as it is the sum of hermitian matrices. For $\kappa = 0$, it is $hpd$, thus there exists some value of $\kappa, \kappa_{sc}^c$, for which it becomes indefinite. For $\kappa < \kappa_{sc}^c$, $Q_{sc}$ is $hpd$.

### 4 One Flavor HMC

We have shown that

$$\det(M) = \det(Q) = \det(Q_w) \det(Q_{sc}),$$

for $Q_{11}$ being non-singular. If $\kappa < \kappa_{sc}$, both matrices are $hpd$ and can be represented by Gaussian integrals. Let $\phi \in \mathbb{C}^{3V}$ and $\chi \in \mathbb{C}^{6V}$:

$$\det(Q_w) \det(Q_{sc}) = \left(\frac{1}{2\pi}\right)^{3V} \left(\frac{1}{2\pi}\right)^{6V} \int [d\phi[|d\phi^*][d\chi]|d\chi^*] e^{-\phi^\dagger(Q_w)^{-2}\phi - \chi^\dagger(Q_{sc})^{-1}\chi}.\tag{20}$$

The fermionic part of the path integral being expressed in terms of the pseudo-fermion degrees of freedom $\phi$ and $\chi$, the HMC algorithm can proceed as usual [19], see the $\Phi$-algorithm in Ref. [6]. The heat bath for the $\phi$ fields is trivial like in the previous case of mass-degenerate QCD. Let $R \in \mathbb{C}^{3V}$ be Gaussian distributed. With

$$\phi = Q_w^\dagger R,$$

$$R^\dagger R = \phi^\dagger(Q_w)^{-2}\phi,$$

and

$$(2\pi)^{3V} \det(Q_{ww}^2) = \int [d\phi]|d\phi^*| e^{-\phi^\dagger(Q_w)^{-2}\phi}.\tag{23}$$

The refreshment of the $\chi$ fields causes more trouble, however. In order to generate the required distribution, we have to solve a linear system involving the square root of $Q_{sc}$. Let $R \in \mathbb{C}^{6V}$ be Gaussian distributed:

$$\chi = Q_{sc}^{\frac{1}{2}} R.$$
Then

\[ R^\dagger R = \chi^\dagger (Q_{sc})^{-1} \chi \]  

(25)

and

\[ (2\pi)^{6V} \det(Q_{sc}) = \int [d\chi][d\chi^*] e^{-\chi^\dagger (Q_{sc})^{-1} \chi} \]  

(26)

Even though the solution of Eq. 25 is only required at the beginning of a trajectory, it is particularly expensive as we must cope with the internal inversion of \( Q_{11} \). The implications of this issue are not clarified yet. As an alternative, we might include the dynamics of the \( \chi \) fields into HMC avoiding the expensive heat bath step for \( Q_{sc} \), similar to the \( R \)-algorithm of Ref. [6].

### 5 Inexact Uzawa Iterations

The nested inversion within the solution of

\[ Q_{sc} X = \chi \]  

(27)

has to be carried out at each molecular dynamics time step of HMC as well as in the computation of the action. By Uzawa iterations [20] we avoid the solution of the linear system represented by \( Q_w \) within each iteration step of the \( Q_{sc} \) iteration.

The problem to solve is given by:

\[ (Q_w + D_{12} Q_w^{-1} D_{12}^\dagger) X = \chi, \]  

(28)

with \( X, \psi \in \mathbb{C}^{6V} \).

Let’s consider the Jacobi iteration for \( Q_{sc} \),

\[ X^{(i+1)} = \chi + \kappa D_{11} X^{(i)} - D_{12} Q_w^{-1} D_{12}^\dagger X^{(i)}. \]  

(29)

The fixed-point solution \( X \) of Eq. 29, defined by

\[ ||X^{(i+1)} - X^{(i)}|| < \epsilon, \quad \epsilon \to 0 \]  

(30)

solves equation Eq. 28, as can be easily verified.

Next we transform the simple Jacobi iteration into the Uzawa iteration:

\[ X^{(i+1)} = \chi + \kappa D_{11} X^{(i)} - D_{12} Y^{(i)} \]

\[ Y^{(i+1)} = Q_w^{-1} D_{12}^\dagger X^{(i)}. \]  

(31)

At this stage, the Uzawa scheme would certainly not offer an advantage as still we need to carry out an inversion in each iteration step. Let’s turn towards the inexact Uzawa iteration. Choose

\[ P_w \approx Q_w \]  

(32)
as a preconditioner for $Q_w$ which is easily invertible.

$$\begin{align*}
X^{(i+1)} &= \chi + \kappa D_{11} X^{(i)} - D_{12} Y^{(i)} \\
Y^{(i+1)} &= Y^{(i)} + P_w^{-1}(D_{12}^\dagger X^{(i)} - Q_w Y^{(i)}) \quad (33)
\end{align*}$$

The fixed-point solution of Eq. 33, defined by

$$
\begin{align*}
||X^{(i+1)} - X^{(i)}|| < \epsilon, \\
||Y^{(i+1)} - Y^{(i)}|| < \epsilon'.
\end{align*} \quad (34)
$$

for $\epsilon, \epsilon' \to 0$, solves Eq. 28. Using the second relation, one finds

$$0 = P_w^{-1}(-Q_w Y + D_{12}^\dagger X),$$

$$\Leftrightarrow Y = Q_w^{-1}D_{12}^\dagger X. \quad (35)$$

As a cheap preconditioner we can use a truncated Neumann series for $Q_w^{-1}$:

$$P_w^{-1} = (1 - \kappa D_{11})^{-1} = 1 + \kappa D_{11} + \ldots \quad (36)$$

One has to find the optimal length of this series compared to the convergence of the outer iteration. In our implementation we have chosen the simple first-order approximation.

$$P_w^{-1} = 1 + \kappa D_{11}. \quad (37)$$

We have made first tests of the Uzawa iteration in comparison to a conjugate gradient (CG) for the inversion of Eq. 28. We used a quenched $16^4$ configuration at $\beta = 6.0$ at a moderate $\kappa$-value of $\kappa = 0.12$. The outer CG took about 240 iterations while the inner iteration took about 50 steps. The Uzawa iteration required about 610 steps in comparison. The overall improvement for this setting is about a factor of 10. Of course, these results are very preliminary and have to be confirmed for other values of $\kappa$ and $\beta$ with realistic HMC simulations. It would also be desirable to implement the Uzawa scheme within Krylov subspace solvers.

For free theory ($U = 1$), one can diagonalize $D_{11}$ by Fourier transformation. As in the case of Wilson fermions, one finds $\kappa_c = \frac{1}{2}$. We have, so far, investigated the lowest lying eigenvalues of $Q_w$ for the interacting case: on a $16^3 \times 32$ configuration, taken from the SESAM ensembles at $\beta = 5.6$ and $\kappa_{sea} = 0.1575$, we found for the inverse of the critical eigenvalue of $D_{11}$, $1/\lambda_{min} = 0.144$. The critical $\kappa$ of $D_{11}$ is reached for a $\kappa$-value being smaller than the critical $\kappa$ value of the Wilson matrix. Therefore, the singularity might be a barrier screening the approach to the chiral limit. These questions have to be clarified in an actual HMC simulation with one-flavor QCD.
6 Summary and Outlook

The determinant of the Wilson fermion matrix is equivalent to the product of the determinants of two hermitian positive definite matrices. This formulation allows to simulate quark flavors with individual mass values by means of the HMC algorithm. The solution of the ensuing linear system is hampered by a nested inversion problem. However, it can be treated by use of Uzawa iterations.

Currently we perform a feasibility study to gain first experiences with the new method. In particular, we are interested in the analytic structure of $Q_w$ and $Q_{sc}$. Furthermore, we construct an efficient heat-bath for the refreshment of the pseudo-fermions for $Q_{sc}$ based on the polynomial representation of the square root of a truncated polynomial that represents $Q_{sc}$.

We have presented the method for standard Wilson fermions. The Schur decomposition can as well be applied to improved Wilson fermions with clover term. Work on this line is in progress.

Acknowledgments

I thank B. Bunk for important discussions that motivated the present work. I am happy to work with A. Frommer, B Medeke, and K. Schilling from Wuppertal university who contributed with interesting ideas. In particular I thank H. Neff who has kindly performed the eigenvalue computations. I am grateful to M. Peardon and Ph. de Forcrand who pointed out important simplifications of the method during my talk at the workshop.
A Chiral Dirac Matrices

Euclidean Dirac matrices in the chiral representation:

\[
\gamma_1 = \begin{pmatrix}
0 & 0 & 0 & -i \\
0 & 0 & -i & 0 \\
i & 0 & 0 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = i \begin{pmatrix}
0 & 0 \\
0 & -\sigma_1 \\
\sigma_1 & 0 \\
0 & 0
\end{pmatrix}
\]

\[
\gamma_2 = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
i & 0 & 0 & 0 \\
-1 & 0 & 0 & 0
\end{pmatrix} = i \begin{pmatrix}
0 & 0 \\
0 & -\sigma_2 \\
\sigma_2 & 0 \\
0 & 0
\end{pmatrix}
\]

\[
\gamma_3 = \begin{pmatrix}
0 & 0 & i & 0 \\
i & 0 & 0 & 0 \\
0 & i & 0 & 0 \\
0 & 0 & 0 & i
\end{pmatrix} = i \begin{pmatrix}
0 & 0 \\
0 & -\sigma_3 \\
\sigma_3 & 0 \\
0 & 0
\end{pmatrix}
\]

\[
\gamma_4 = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix} = \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\]

\[
\gamma_5 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}
\]

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