Dynamical overlap fermions, results with HMC algorithm

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We present results of a hybrid Monte-Carlo algorithm for dynamical, $n_f = 2$, four-dimensional QCD with overlap fermions. The fermionic force requires careful treatment, when changing topological sectors. The pion mass dependence of the topological susceptibility is studied on $6^4$ and $12 \cdot 6^3$ lattices. The results are transformed into physical units.

1. HMC FOR THE OVERLAP

It is a great numerical challenge to make dynamical QCD simulations with Ginsparg-Wilson fermions, which have exact chiral symmetry at finite lattice spacing. We present an exploratory study for overlap fermions, which have the Dirac operator:

$$D = m_0(1 + \gamma_5 \text{sgn}(H_W)),$$

where $H_W$ is the hermitian Wilson-operator with $-m_0$ mass \cite{1}. The bare mass is introduced by:

$$D(m) = m + (1 - m/(2m_0)) D.$$

We use the Zolotarev rational series to approximate the sign function:

$$\text{sgn}(x) \approx \epsilon_n(x) = x(x^2 + c_{2n}) \sum_{l=1}^{n} \frac{b_l}{x^2 + c_{2l-1}},$$

for $b_l, c_l$ see \cite{2}. The evaluation of the inverse of the shifted Wilson-matrices is done by multishift conjugate gradient algorithm \cite{3}. To speed up the inversions one can project out the low-lying eigenmodes of the Wilson kernel:

$$\text{sgn}(H_W) \approx \sum_{i} \text{sgn}(\lambda_i) |\lambda_i\rangle \langle \lambda_i| + T \epsilon_n(H_W),$$

where $H_W |\lambda_i\rangle = \lambda_i |\lambda_i\rangle$ and $T = 1 - \sum_i |\lambda_i\rangle \langle \lambda_i|$ projects to the orthogonal subspace.

We use the HMC algorithm to generate dynamical configurations for $n_f = 2$ flavors. Thus we need the expression of the microcanonical energy:

$$\mathcal{H} = \frac{1}{2} \langle \mathbf{P}, \mathbf{P} \rangle + S_g[U] + \phi^\dagger (D^\dagger D)^{-1} \phi,$$

which governs a classical motion in the space of link variables. $\phi$ is the pseudofermion field, whereas $P$ is the canonical momenta, which is randomized at the beginning of each trajectory. For the classical motion we need the gauge derivative of pseudofermionic action, namely the fermion force. For the fermion force one needs to invert the overlap operator on the $\phi$ field:

$$\text{force} = -\psi^\dagger \frac{dD^\dagger D}{dU} \psi,$$

thus one ends up with a nested inversion procedure, which is the most time consuming part of the algorithm. The gauge derivative of the rational approximation is straightforwardly calculated, furthermore it is easy to include the contribution of the projected eigenmodes exactly in the force \cite{4}. Then one can solve the equations of motion with a reversible and area conserving integration procedure (usually it is a simple leapfrog).

2. FERMION FORCE

With the naive application of the above results one faces a further problem. The pseudofermionic action has a discontinuity across the surface, where $H_W$ matrix has a zeromode, which means a presence of a Dirac-delta type singularity in the force.
A finite stepsize integration of the equations of motion practically never notice it. This means that it drastically violates energy conservation. Finally one ends up with a very bad acceptance ratio, since the accept/reject step depends exponentially on the energy-conservation violation. We have observed that already on a $6^4$ lattice there were no accepted configurations at all.

These eigenvalue crossings are easily connected with the topological sector change, since topological charge $Q$ changes whenever a $\lambda_i$ crosses zero:

$$
\Delta Q = \frac{1}{2m_0} \Delta \text{Tr}(\gamma_5 D) = \frac{1}{2} \Delta \left[ \sum_i \text{sgn}(\lambda_i) \right] = \pm 1.
$$

We cure the problem by considering a classical trajectory, when it reaches the zero eigenvalue surface. Let the jump in the action on the surface be $\Delta S$, whereas the normalvector of the surface is $N = \langle \lambda | dH_W / dU | \lambda \rangle$. If the momentum is not large enough to climb the jump ($P^2 < 2\Delta S$), the trajectory will be reflected off from the surface, its new momentum will be:

$$
P' = P - 2N \langle N, P \rangle.
$$

If there is enough kinetic energy ($P^2 > 2\Delta S$), then the system will move into the other topological sector with a new momentum:

$$
P' = P - N \langle N, P \rangle + N \langle N, P \rangle \sqrt{1 - 2\Delta S / \langle N, P \rangle^2}.
$$

One should modify the standard leapfrog algorithm to accomodate the above momentum change. The eigenvalue crossing can happen only in the half step, when the gauge fields are updated. We propose to replace this step with three other ones (corrected leapfrog step):

1. Evolve the gauge fields just to the eigenvalue surface ($\tau_1$ is the time, which is needed for this).
2. Decide whether reflection or refraction happened, and modify the momentum according to the above rules.
3. Update the gauge fields in the remaining time ($\tau/2 - \tau_1$) with the new momenta.

The algorithm is reversible, preserves area and conserves energy only up to $O(\tau_1)$. It is an important goal of future algorithm developments to improve on this behaviour.

The stepsize should be small enough to keep track the evolution of eigenvalues, and to avoid of the problem of having 2,3 or more crossing eigenvalues in one microcanonical step.

Fig. 1 compares the evolution of the energy and lowest $\lambda$ for the usual and for the corrected leapfrog. In the uncorrected case there is a huge energy jump at the crossing, whereas in the modified case a reflection happens, and $\mathcal{H}$ is much better conserved.

3. NUMERICAL RESULTS

We have checked our code by a brute force approach on $2^4$ and $4^4$ lattices: we have weighted a quenched ensemble with the exactly calculated determinant. A complete agreement was found. On $4 \cdot 6^3$ lattices there is a sharp increase in the Polyakov loop at $\beta = 5.7$, this value of the coupling was used for measuring the topology on $6^4$ lattices. The negative quark mass was set to $m_0 = 1.6$, the bare fermion mass was in the range $m = 0.1 \ldots 1.15$, the stepsize was $\tau = 0.025$ in average. At each bare mass roughly 800 trajectories were generated.

The results are plotted on Fig. 2. The up-

![Figure 1. Comparison of the uncorrected (triangles) and corrected (boxes) leapfrogs. Upper part is the energy, lower part is the lowest mode of $H_W$.](image-url)
Figure 2. Topology on $N_s = 6$ lattices. See text. per panel shows the charge history. The average topological charge is consistent with zero for the total mass range (middle panel). 12 · $6^3$ lattices were used to fix the scale using $r_0$ from Wilson-loops. The result is $a \sim 0.25$ fm for small masses. Pion masses were also measured and $m_\pi^2 = Am$ with $A \approx 1$ is found in lattice units. Using the scale and the pion mass, it is possible to get the topological susceptibility in physical units (lower panel of Fig. 2). $\chi(m)$ tends to zero for small quark masses. One can compare these results with the continuum expectation in the chiral limit (solid line of the figure):

$$\lim_{m \to 0} \chi(m) = \lim_{m \to 0} \frac{\langle Q^2 \rangle_V}{V} = \frac{f_\pi^2 m_\pi^2}{2n_f}.$$ 

Caution is needed, when interpreting the results. There are obvious problems such as small volume and rough lattice. Furthermore there can be doubts about the locality of the theory at these rather large couplings [5].

A detailed description of the algorithm can be found in [6], whereas for an independent study see [7].

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