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FIRST EXPERIENCES WITH HMC FOR DYNAMICAL OVERLAP FERMIONS

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Abstract. We describe[1] an HMC algorithm for dynamical overlap fermions which makes use of their good chiral properties. We test the algorithm in the Schwinger model. Topological sectors are readily changed even in the massless case.

1. HMC algorithm for overlap fermions for any number of flavors

Overlap fermions represent a lattice discretization of fermions with the same chiral properties as continuum fermions [1]. Properties of overlap fermions are reviewed in [2] (see also [3]). In this contribution we would like to describe a Hybrid Monte Carlo (HMC) algorithm for the dynamical simulation of overlap fermions, which exploits some of their chiral properties.

We denote by $H_o(\mu)$ the hermitian overlap Dirac operator $\gamma_5 D(\mu)$ and find $D^\dagger(\mu)D(\mu) = H_o^2(\mu)$. Since $[H_o^2(\mu), \gamma_5] = 0$ [2, 3] one can split $H_o^2(\mu)$ into two parts, each acting in one chirality sector only, $H_o^2(\mu) = H_{o+}^2(\mu) + H_{o-}^2(\mu)$ where, with $P_\pm = \frac{1}{2}(1 \pm \gamma_5)$,

$$H_{o\pm}^2(\mu) = \frac{1+\mu^2}{2}P_\pm \pm \frac{1-\mu^2}{2}P_\pm \epsilon(H_w)P_\pm. \tag{1}$$

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The non-zero eigenvalues of $H_o^2(\mu)$ are equal in both chirality sectors and hence also their contribution to the fermion determinant:

$$\det(H_{o+}'^2(\mu)) = \det(H_{o-}'^2(\mu)) > 0 \qquad (2)$$

The $'$ indicates that the zero modes have been left out.

For N_f dynamical flavors the fermion determinant is thus

$$[\det(D(\mu))]^{N_f} = \mu^{N_f|Q|}[\det(D'(\mu))]^{N_f} =$$
$$\mu^{N_f|Q|}[\det(H_o'^2(\mu))]^{N_f/2} = \mu^{N_f|Q|}[\det(H_{o\pm}'^2(\mu))]^{N_f}. \qquad (3)$$

We can use this rewriting to get a Hybrid Monte Carlo algorithm for dynamical overlap fermions for any number of flavors. For each flavor we introduce one pseudo-fermion of a single chirality:

$$\det(H_{o\pm}'^2(\mu)) = \int d\phi_\pm^\dagger \phi_\pm e^{-S_p} ; \qquad S_p = \phi_\pm^\dagger \left[H_{o\pm}'^2(\mu)\right]^{-1}\phi_\pm . \qquad (4)$$

The choice of the chirality is made such as to avoid zero modes: If the gauge configuration at the beginning of the trajectory has non-trivial topology, we choose the chirality that does not have an exact zero mode of the massless overlap Dirac operator. If the topology is trivial, we choose the chirality randomly. To take the zero mode contribution into account, we reweight to compute observables

$$\langle O \rangle = \langle \mu^{N_f|Q|}O \rangle_\pm / \langle \mu^{N_f|Q|} \rangle_\pm. \qquad (5)$$

Having introduced the pseudo-fermions, doing HMC is straightforward. We need the contribution from the pseudo-fermions to the force:

$$\frac{\delta S_p}{\delta U} = \mp \frac{1}{2}(1-\mu^2)\chi_\pm^\dagger \frac{\delta\epsilon(H_w)}{\delta U}\chi_\pm ; \qquad [H_{o\pm}^2(\mu)]^{-1}\phi_\pm = \chi_\pm. \qquad (6)$$

We use a rational polynomial approximation for $\epsilon(H_w)$ written as a sum over poles [4, 5]:

$$\epsilon(x) \leftarrow x\frac{P(x^2)}{Q(x^2)} = x\left(c_0 + \sum_k \frac{c_k}{x^2+b_k}\right). \qquad (7)$$

Straightforward algebra then gives (see also [6])

$$\chi_\pm^\dagger \frac{\delta\epsilon(H_w)}{\delta U}\chi_\pm \leftarrow c_0\chi_\pm^\dagger \frac{\delta H_w}{\delta U}\chi_\pm + \sum_k c_k b_k \chi_{k\pm}^\dagger \frac{\delta H_w}{\delta U}\chi_{k\pm}$$
$$- \sum_k c_k \chi_{k\pm}^\dagger H_w \frac{\delta H_w}{\delta U}H_w \chi_{k\pm}. \qquad (8)$$

where we introduced

$$\chi_{k\pm} = [H_w^2 + b_k^2]^{-1}\chi_\pm. \qquad (9)$$

The computation of the force requires thus one additional multi-shift "inner" CG inversion to obtain the $\chi_{k\pm}$.

A few remarks are in order: (1) We anticipate that a straightforward HMC for dynamical overlap fermions will suffer even more than with staggered fermions from difficulties in changing topology due to the existence of exact zero modes. By working only in one chiral sector, a change of topology is possible, unimpeded by the fermions, as long as the number of zero modes changes only in the opposite chirality sector. (2) Accuracy of the approximation of $\epsilon(H_w)$ can be enforced by projecting out the lowest few eigenvectors of H_w, and adding their correct contribution exactly [2]. The molecular dynamics evolution of the eigenvector projectors $P_\pm$ in Eq. (1) can be included using ordinary first order perturbation theory. However, we have not included projections in our dynamical fermion code yet. (3) The approximation of $\epsilon(H_w)$ used in the molecular dynamics steps need not be the same as the approximation of $\epsilon(H_w)$ for the Metropolis accept/reject step. E.g. an approximation, which is smooth around the origin, can be used for the HMD part and the more accurate optimal rational approximation with projection for the accept/reject step.

2. Testing in the Schwinger model

We tested our HMC algorithm in the $N_f = 1$ and 2 Schwinger model. We first look at time histories of the topological charge Q, determined via the number of exact zero modes. We see (Fig. 1) that the topological charge changes, even in the massless case.

We compared our HMC results with fiducial results, obtained by a brute force approach (exact diagonalization, and then reweighting with the fermion determinant of quenched gauge fields). We notice that the acceptance rate does not drop rapidly and the number of CG iterations does not diverge as $\mu \to 0$.

3. Conclusions

The non-zero eigenvalues of $H_o^2(\mu)$ in each chirality sector contribute identically to the overlap fermion determinant. Utilizing this fact, and separating the contribution from the fermion zero modes in non-trivial gauge fields, we devised an HMC algorithm for any number of flavors of overlap fermions, with changes of topology possible even in the massless limit. The trick consists in working in the chirality sector without exact zero modes.
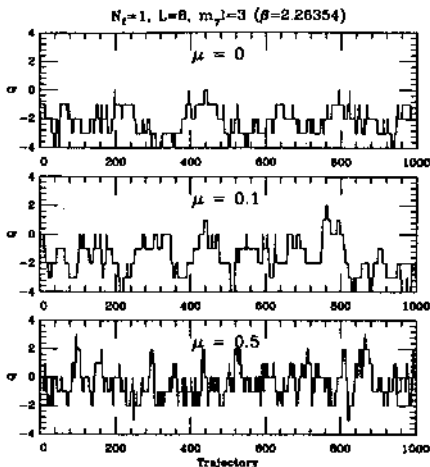
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Figure 1. Time history of Q in the 1 flavor model for several quark masses.

Preliminary tests in the $N_f = 1$ and 2 Schwinger model show that the algorithm works. The topological charge changes. The algorithm works even in the massless case. The acceptance rate does not go to zero or the CG count to infinity. Further tests on larger systems and in four dimensions are needed to better judge the usefulness of the algorithm for realistic dynamical simulations.

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