Dynamical overlap fermions, results with HMC algorithm

Kálmán Szabó
Universität Wuppertal

Z. Fodor, S. D. Katz, K. Szabo hep-lat/0311010

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overlap Dirac operator Neuberger '98

$$D = m_0[1 + \gamma_5 \mathrm{sgn}(H_W)]$$

- exact chiral symmetry through GW Ginsparg, Wilson '82

$$\gamma_5 D + D\gamma_5 = \frac{1}{m_0} D\gamma_5 D$$

- chance to define lattice topology

$$Q = n_L - n_R$$

- no problem with extreme low ev's of D at finite mass:

$$D(m) = \left(1 - \frac{m}{2m_0}\right) D + m \Rightarrow |\lambda| \geq m$$

only quenched investigations in overlap QCD:

- quenching effects unknown
- no topological susceptibility results at low masses

Wilson and staggered fermions: UKQCD '01, CP-PACS '01, MILC '03

Approximating the sgn function

$\text{sgn}(x)$ is approximated by a rational series:

$$\text{sgn}(x) \approx \varepsilon_n(x) = x(x^2 + c_{2n}) \sum_{l=1}^{n} \frac{b_l}{x^2 + c_{2l-1}} \quad \text{in} \quad [1, x_{max}]$$

b_l, c_l optimal choice $\longrightarrow$ Zolotarev van den Eshof et al ’02, Chiu et al ’02

approximated overlap Dirac operator:

$$D = m_0[1 + \gamma_5 \varepsilon_n(h_W)] \qquad\qquad h_W = H_W / |\lambda_{\min}|$$

fortunately we do not need $n\ H_W^2$ inversions for one multiplication with D $\Rightarrow$ multishift CG Frommer et al ’95, Jegerlehner ’96 $\longrightarrow$ even-odd precondition lost

projecting out low-lying eigenmodes to speed up inversions

$$H_W|\lambda_i\rangle = \lambda_i|\lambda_i\rangle \qquad P_i = |\lambda_i\rangle\langle\lambda_i| \qquad Q = 1 - \sum_i P_i$$

it can help two ways:

a. $\text{sgn}(h_W)|\psi\rangle \approx \sum_i \text{sgn}(\lambda_i) P_i |\psi\rangle + Q\varepsilon_n(h_W) Q|\psi\rangle$

b. to get $Q\varepsilon_n(h_W)Q|\psi\rangle$ we can project out further vectors

HMC for the overlap 1.

Duane et al '87

introduce pseudofermions

$$\det(D^\dagger D) = \int d\phi^\dagger d\phi \exp(-S_p) \qquad \text{with} \qquad S_p = \phi^\dagger (D^\dagger D)^{-1} \phi$$

gauge configurations are generated by classical motion

$$\mathscr{H} = \frac{1}{2}\langle P,P\rangle + S_{\text{gauge}}[U] + S_{\text{p}}[U,\phi] = \frac{1}{2}\langle P,P\rangle + S[U,\phi]$$

equations of motions

$$\frac{dU}{dt} = PU \quad \text{and} \quad \frac{dP}{dt} = T * (U\frac{dS}{dU}) = \text{gf.} + \text{ff.}$$

numerically solved by leapfrog integration:

- area preserving $[dU][dP] = [dU'][dP']$
- reversible

$\Rightarrow$ detailed balance at finite stepsize using $p = \min(1, \exp(-\Delta\mathscr{H}))$

- $\mathscr{O}(\tau^3)$ errors $\rightarrow$ resource demands grow only with $V^{5/4}$

HMC for the overlap 2.

fermionic force $\quad \text{ff.} = -\psi^\dagger \frac{dD^\dagger D}{dU}\psi \qquad \text{with} \qquad \psi = (D^\dagger D)^{-1}\phi$

- time consuming nested inversions for ψ
- for PFE straightforwardly calculated Liu '98
- include contribution of projected modes Narayanan, Neuberger '00

$$\frac{dP_i}{dU} = \frac{d|\lambda_i\rangle}{dU}\langle\lambda_i| + |\lambda_i\rangle\frac{d\langle\lambda_i|}{dU} \qquad \frac{d|\lambda_i\rangle}{dU} = \frac{1-P_i}{\lambda_i - H_W}\frac{dH_W}{dU}P_i$$

first experiences in Schwinger model Bode et al '99

separate zero modes of D and use $[D^\dagger D(m), \gamma_5] = 0$

$$\det(D^\dagger D) = m^{2Q}\det(D^\dagger D') = m^{2Q}\det(D^\dagger D'_+)^2$$

do simulations without zero modes $\longrightarrow$ finally reweighting

simultaneous investigations in overlap HMC

$\longrightarrow$ N. Cundy's talk S. Krieg's poster Cundy et al hep-lat/0311025, hep-lat/0405003

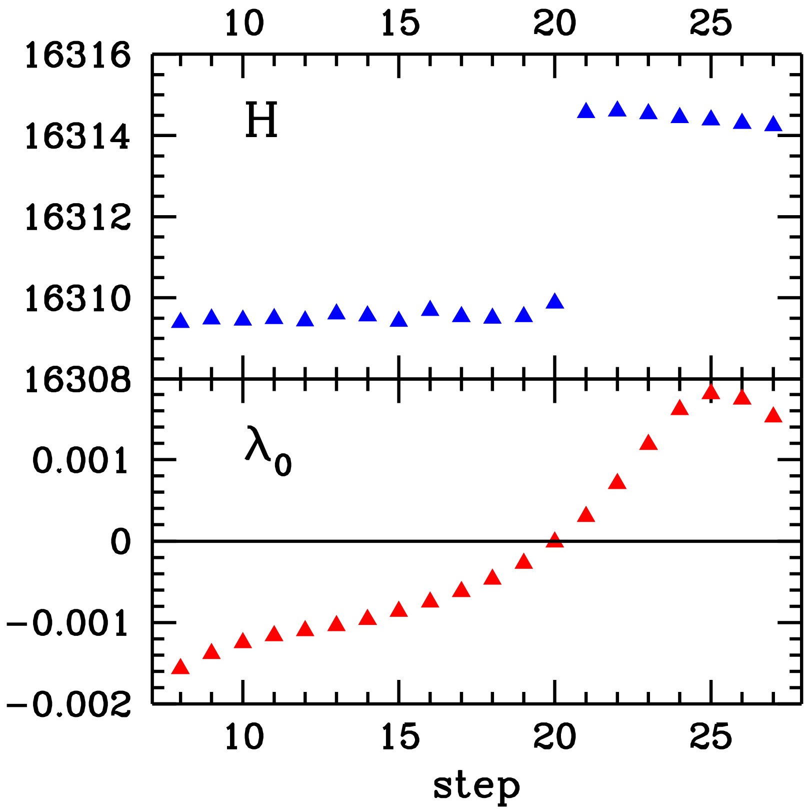
Problem with the fermionic force 1.

topological sector change $\equiv$ one of ev's of H_W crosses 0

$$\Delta Q = (1/2)\Delta[\mathrm{Tr}(\gamma_5 D)] = (1/2)\Delta[\sum_i \mathrm{sgn}(\lambda_i)] = \pm 1$$

step in the pf. action = Dirac-delta in the fermionic force

finite stepsize integration will miss it



the acceptance goes to 0 already on 6^4

Problem with the fermionic force 2.

N normal vector of surface, ΔS step in the action

trajectory reaches the ev surface

if $\langle N,P\rangle^2 < 2\Delta S$, then reflection:

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

if $\langle N,P\rangle^2 > 2\Delta S$, then refraction:

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

modify the leapfrog to be sensitive to the jump

originally:

$$U \xrightarrow{P} U_{\tau/2} \qquad P \xrightarrow{U_{\tau/2}} P_\tau \qquad U_{\tau/2} \xrightarrow{P_\tau} U_\tau$$

crossing can happen in the first or the last step, replace:

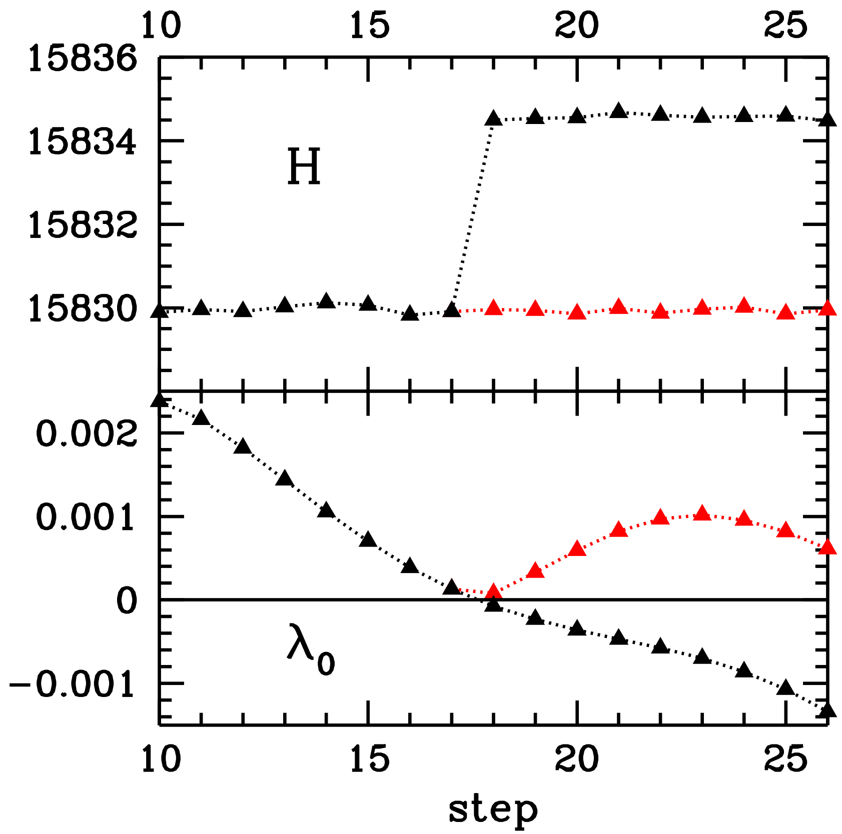
$$U \xrightarrow{P} U_{\tau_1} \qquad P \xrightarrow{N,\Delta S} P' \qquad U_{\tau_1} \xrightarrow{P'} U_{\tau/2}$$

τ_1 time to reach the surface

Problem with the fermionic force 3.

easy to see its reversibility

area preserving much harder to prove (τ_1 depends on the link, Haar measure)



delicate questions:

- $\mathscr{O}(\tau_1)$ error in $\mathscr{H}$ $\rightarrow$ small stepsize needed
- crossing identification (which ev goes to which)
- 2,3,. . . crossing in one step

Numerical results 1.

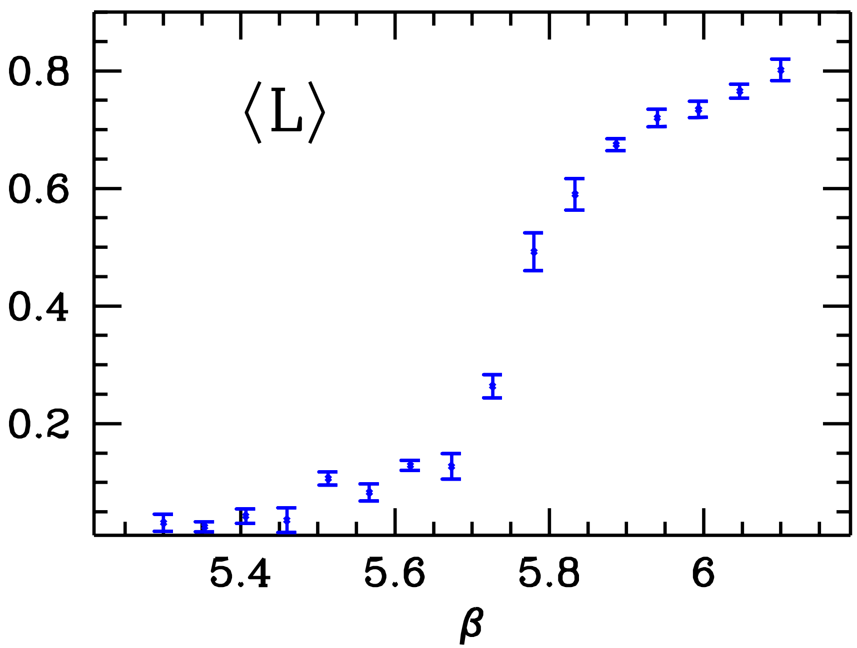
in collaboration with T. Kovacs

most time consuming: projecting eigenmodes, nested iterations

consistency check by brute force on 2^4 and 4^4:

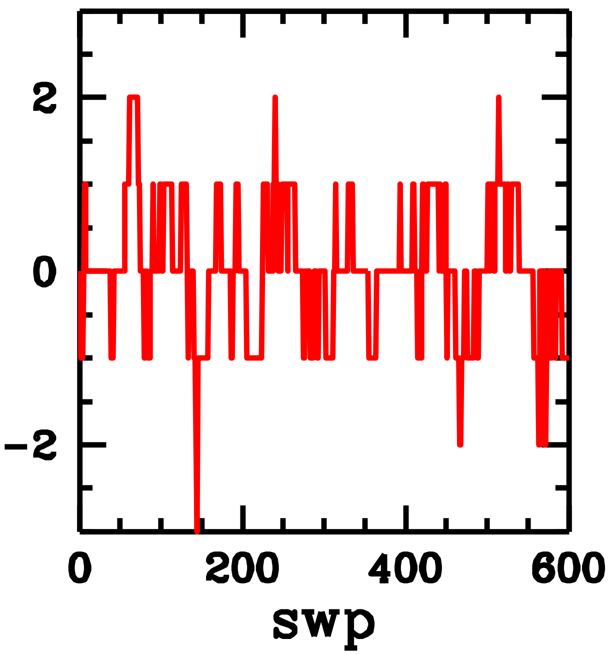
generate quenched confi gurations and weight them with exact determinant

finite T phase transition on $4 \cdot 6^3$



Numerical results 2.

topology on 6^4, $\beta = 5.7$, $\Delta\tau = 0.025$, $m = 0.1 - 1.15$

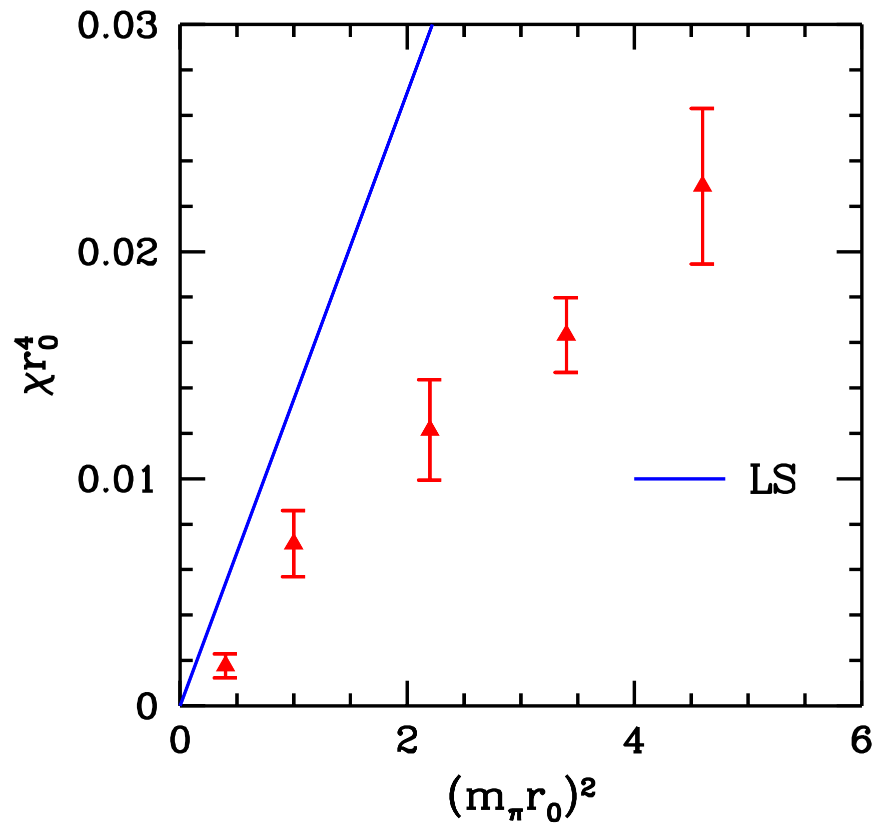


charge is consistent with 0

susceptibility goes to zero for small m

Numerical results 3.

setting the scale ($a \approx 0.26$fm), measure the pion mass



Leutwyler-Smilga limit, finite V corrections

$$\lim_{m \to 0} \frac{\langle Q^2 \rangle}{V} = \frac{f_\pi^2 m_\pi^2}{2N_f}$$

Summary, outlook

- HMC code for overlap fermions: Zolotarev approximation, projecting lowest modes of H_W
- modify the leapfrog to notice the singularity in the fermionic force, when changing topological sectors
- measuring charge, susceptibility on 6^4 lattices and setting the scale

- search for new integration schemes to have better V dependence
- decide whether it is worth separating the zero modes in the simulations