Dynamical Overlap

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with

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and

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Outline

- The overlap Dirac operator.
- Hybrid Monte Carlo.
- Eigenvalue Crossings (Changing topological charge/index).
- Small Masses
- Small Kernel Eigenvalues
- Our simulations.

The overlap operator

- The overlap operator is:

$$D = (1 + \mu) + \gamma_5 (1 - \mu)\epsilon(Q).$$

- The Hermitian overlap operator is $H = \gamma_5 D$.
- Q is the Hermitian Wilson operator $Q = \gamma_5 D_W$ with a negative mass (and stout smearing).
- ϵ is the matrix sign function.
- bare fermion mass $\propto \mu/(1 - \mu)$.

The matrix sign function

1. Exact: $\epsilon(Q) = \sum_i |\psi_i\rangle \langle\psi_i| \, \text{sign}(\lambda_i)$.
2. Approximate: $\epsilon(Q) \sim \sum a_n Q^{2n+1}$ (Chebechev).
3. Approximate: $\epsilon(Q) \sim \frac{D(Q)}{N(Q)} = \sum \frac{\omega_i Q}{Q^2+\zeta_i}$ (Zolotarev).
4. Approximate: Lanczos method $\epsilon(Q) \sim L\epsilon(q)R$ (Borici).
5. Approximate: 5 Dimensional representations (Domain Wall, Kennedy).

- Method (1) numerically impractical.
- Use method 2-5, and have approximate chiral symmetry.
- Use methods 2-5, but treat the small eigenvectors exactly using (1).

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- Use methods 2-5, but treat the small eigenvectors exactly using (1).
- For the rest of this talk, I will use method (1).

The Overlap operator - why we want to use it

- It satisfies the Ginsparg Wilson chiral symmetry exactly.
- No additive mass renormalisation.
- No wrong chirality mixing.
- Automatic O(a) improvement.
- No exceptional configurations - no critical slowing down: Can (in principle) simulate at small mass.
- Well defined index theorem $Q_f = \frac{1}{2}\mathrm{Tr}(\gamma_5 D)$ (=topological charge in continuum limit), account for the anomaly.
- "Easy" non-perturbative renormalisation.
- (Nearly) essential for any studies of topology, χSB, low eigenvalue distributions ...
- From a physics point of view, it is the best lattice Dirac operator in our arsenal.
- If we had an infinite amount of computing power, we would all be using overlap fermions. It will be the method of choice in some years time (unless someone invents a better alternative).

The Overlap operator - why we don't want to use it.

- It is slow.
- It is difficult changing topological sectors (especially at low mass).
- There are few technical problems to overcome.

Dynamical overlap fermions.

- Now is the optimum time to develop algorithms for dynamical overlap fermions.
- Three groups have published work on this topic:
  - Z. Fodor, S. Katz, K. Szabo, G.Egri (Wuppertal/Budapest).
  - N. Cundy, Thomas Lippert, S. Krieg (Wuppertal/Jülich).
  - T. DeGrand, S. Schäfer (Colorado).

Hybrid Monte Carlo.

- Start with the gauge action $S_g(U)$.
- Approximate the fermion determinant using a heat-bath:

$$\det D^\dagger D = \int d\phi d\phi^\dagger \exp(\phi^\dagger H^{-2} \phi)$$

- We want to generate ensembles according to the probability distribution

$$W_c(U) = \int d\phi d\phi^\dagger \exp(-S_g(U) - \phi^\dagger H^{-2} \phi)$$

- Any update with satisfies the detailed balance condition will do the job:

$$P([U] \leftarrow [U'])W_c(U') = P([U'] \leftarrow [U])W_c(U)$$

Hybrid Monte Carlo.

- We use an update

$$P([U'] \leftarrow [U])W_c[U] = \int d\Pi d\Pi' d\phi d\phi^\dagger d\phi' d\phi'^\dagger e^{-\frac{1}{2}\Pi^2 - \phi^\dagger H^{-2}\phi - S_g[U]}$$
$$\delta([U', \Pi', \phi'] - T([U, \Pi, \phi])) \min(1, \exp(\Delta))$$

where

$$E = \frac{1}{2}\Pi^2 + S_g[U] + \phi^\dagger (H)^{-2}\phi$$
$$J = \frac{\partial[U, \Pi, \phi]}{\partial[U', \Pi', \phi']}$$
$$\Delta = E - E' + \log J$$

- Thanks to A. Borici.

Hybrid Monte Carlo.

- This satisfies the detailed balance condition as long as T is reversible ($T^{-1}T = 1$)
- Most HMC simulations use an area conserving T ($\log J = 0$).
- We want to choose T so that $E - E' + \log J$ is as small as possible (for as little work as possible) to get a high acceptance in the metropolis step.

Differentiation of eigenvectors

- To calculate the fermionic force, we need to differentiate the eigenvalues and eigenvectors of Q:

$$Q\,|\psi\rangle = \lambda\,|\psi\rangle$$

$$(Q + \delta Q)(|\psi\rangle + |\delta\rangle) = (\lambda + \delta\lambda)(|\psi\rangle + |\delta\rangle)$$

$$\delta\lambda = \langle\psi|\,\delta Q\,|\psi\rangle$$

$$|\delta\rangle = \frac{1}{Q - \lambda}(1 - |\psi\rangle\,\langle\psi|)\delta Q\,|\psi\rangle$$

Differentiation of sign function

$$\frac{d}{d\tau}\epsilon(Q) = \sum_{i,j\neq i} |\psi_i\rangle \langle\psi_i| \dot{Q} |\psi_j\rangle \langle\psi_j| \frac{\text{sign}(\lambda_i) - \text{sign}(\lambda_j)}{\lambda_j - \lambda_i}$$
$$+ \sum_i |\psi_i\rangle \langle\psi_i| \frac{d}{d\tau}\text{sign}(\lambda_i)$$

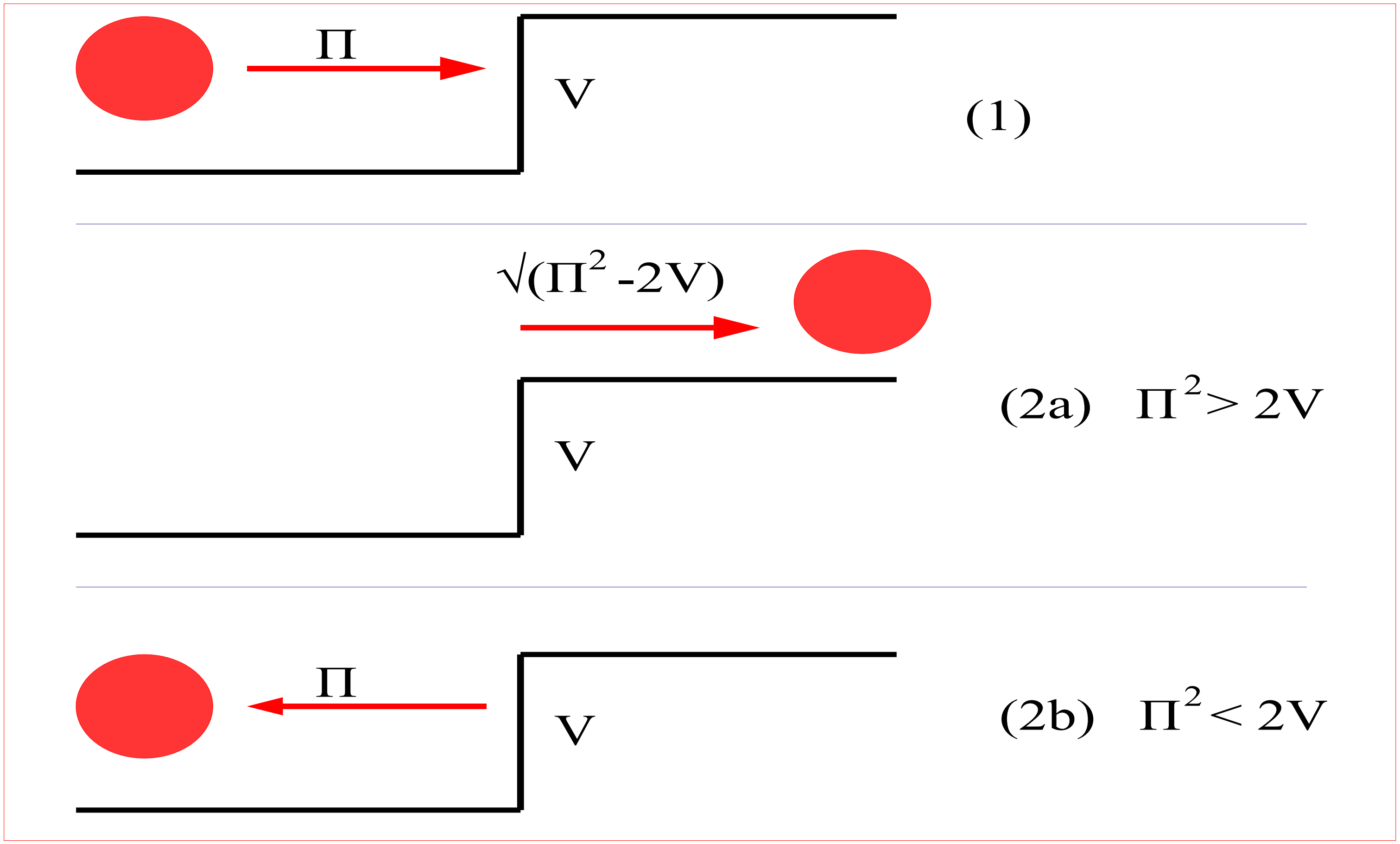
- Only mixings of eigenvectors with eigenvalues having different signs contribute to the fermionic force.
- Only small eigenvectors contribute to the fermionic force.
- For most eigenvector pairs, the fermionic force is small.
- But sometimes we will have a large force.
- It can be infinite.

The effect of the crossing.

- The Dirac delta function in the fermionic force will introduce a discontinuity in the momentum in an exact integration, but will not in a numerical integration procedure.
- We have to introduce the discontinuity by hand.
- Notation: a $-$ superscript indicates a computer time just before the eigenvalue crossing, a $+$ superscript indicates just after. τ_c computer time at which the eigenvalue is zero.

$$\frac{dE}{d\tau} = \frac{1}{2}\frac{d}{d\tau}\Pi^2 + \text{continuous term} + (1-\mu^2)\langle\phi|\frac{1}{(H^+)^2}\left\{\gamma_5, \frac{d}{d\tau}\epsilon(\lambda)|\psi\rangle\langle\psi|\right\}\frac{1}{(H^-)^2}|\phi\rangle$$

Eigenvalue crossings



Calculating the energy shift.

- Integrating the fermionic force gives us

$$(\Pi^+)^2 - (\Pi^-)^2 = -2V$$

$$V = 2(1-\mu^2) \langle\phi| \frac{1}{(H^+)^2} \left\{\gamma_5, \epsilon(\lambda^-) |\psi\rangle \langle\psi|\right\} \frac{1}{(H^-)^2} |\phi\rangle$$

- Calculating the discontinuity in the pseudo-fermion energy gives:

$$\Delta E = \phi^\dagger \frac{1}{(H^+)^2} \left((H^-)^2 - (H^+)^2\right) \frac{1}{(H^-)^2} \phi$$
$$= V$$

The General Philosophy.

Fodor *et al.* hep-lat/0311010, Cundy *et al* hep-lat/0502007.

- Update the gauge field to the crossing point $U \rightarrow e^{i\tau_c \Pi^-} U$.
- Update the momentum $\Pi^- \rightarrow \Pi^+$
- Return to the original gauge field $U \rightarrow e^{-i\tau_c \Pi^+} U$.
- Continue as normal

$$
\begin{aligned}
u_c =& u + \tau_c \pi^- \\
\tau_c =& \frac{(u_c - u, \eta)}{\pi^-, \eta} \\
\frac{\partial \tau_c}{\partial \pi_k} =& \tau_c \frac{\partial \tau_c}{\partial u_k} = -\tau_c \frac{\eta_k}{(\pi, \eta)}
\end{aligned}
$$

- η is a unit vector normal to the topological sector wall.

Calculating the Jacobian.

$$u^{+} = u^{-} + \tau_c(\pi^{-} - \pi^{+}); \qquad (\pi^{+}, \pi^{+}) = (\pi^{-}, \pi^{-}) + G(\pi^{-}, U(\tau_c))$$

$$J = \begin{bmatrix} \frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} & \frac{\partial \pi_i^{+}}{\partial u_k^{-}} \\ \frac{\partial u_i^{+}}{\partial \pi_k^{-}} & \frac{\partial u_i^{+}}{\partial u_k^{-}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} & \frac{\partial \pi_i^{+}}{\partial u_k^{-}} \\ \tau_c \delta_{ik} + \frac{\partial \tau_c}{\partial \pi_k^{-}}(\pi_i^{-} - \pi_i^{+}) - \tau_c \frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} + \tau_c \frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} & \delta_{ik} + \frac{\partial \tau_c}{\partial u_k^{-}}(\pi_i^{-} - \pi_i^{+}) - \tau_c \frac{\partial \pi_i^{+}}{\partial u_k^{-}} + \tau_c \frac{\partial \pi_i^{+}}{\partial u_k^{-}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} - \tau_c \frac{\partial \pi_i^{+}}{\partial u_k^{-}} & \frac{\partial \pi_i^{+}}{\partial u_k^{-}} \\ 0 & \delta_{ik} + \frac{\eta_k}{(\eta, \pi)}(\pi_i^{+} - \pi_i^{-}) \end{bmatrix}$$

$$= \left[\left(\frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} \right)_{\tau_c} \right] \left[\delta_{ik} + \frac{\eta_k}{(\eta, \pi^{-})}(\pi_i^{+} - \pi_i^{-}) \right] = \left[\left(\frac{\partial \pi_i^{+}}{\partial \pi_k^{-}} \right)_{\tau_c} \right] \frac{(\eta, \pi^{+})}{(\eta, \pi^{-})}$$

The momentum update.

- Split the momentum into components parallel to η and perpendicular to η, and treat them seperately:

$$(\pi^+, \eta)^2 = (\pi^-, \eta)^2 + G_\eta((\pi^-, \eta), \tau_c)$$

- Then the detailed balance condition reads

$$\begin{aligned} e^{-G\eta/2-V}\frac{1}{\pi^+}\left((\pi^-, \eta) + \frac{1}{2}\frac{\partial G_\eta}{\partial((\pi^-, \eta))}\right)\frac{(\pi^+, \eta)}{(\pi^-, \eta)} =& 1 \\ e^{(\pi^-,\eta)^2/2}\frac{\partial}{\partial((\pi^-, \eta)^2/2)}\left(e^{-(\pi^-,\eta)^2/2-G\eta/2-V}\right) =& -1 \\ e^{-(\pi^+,\eta)^2/2} - e^{-(\pi^-,\eta)^2/2+V} - A(|V|)(1-e^V) =& 0 \end{aligned}$$

The momentum update.

- For momentum components perpendicular to η:
- Can establish a differential equation similar to above.
- Can solve it in any number of dimensions. Solution will be a sum of Gaussians and error functions.
- Two dimensional case:

$$\begin{aligned}(r^{\pm})^2 =& (\pi_1^{\pm})^2 + (\pi_2^{\pm})^2 \\ e^{-(r^{+})^2/2} =& e^{-(r^{-})^2/2-2d} + A(|V|)(1-e^{V})\end{aligned}$$

- Perpendicular to η, the probability of transmission is independant of the update we use.
- Parallel to η, it is a function of the integration constant A: maximum for $A = 1$.

Reflection and transmission.

- $0 \leq e^{-(r^-)^2/2} \leq 1$.
- $A \leq e^{-(r^+)^2/2} \leq e^{2d} + A$
- Fodor et al. suggested reflecting when $(r^+)^2$ is out of range:

$$\pi_\eta^+ = -\pi_\eta^-$$

- Important to keep the transmission rate as high as possible to decrease autocorrelation.

Energy conservation.

- The change in the energy for the correction step is

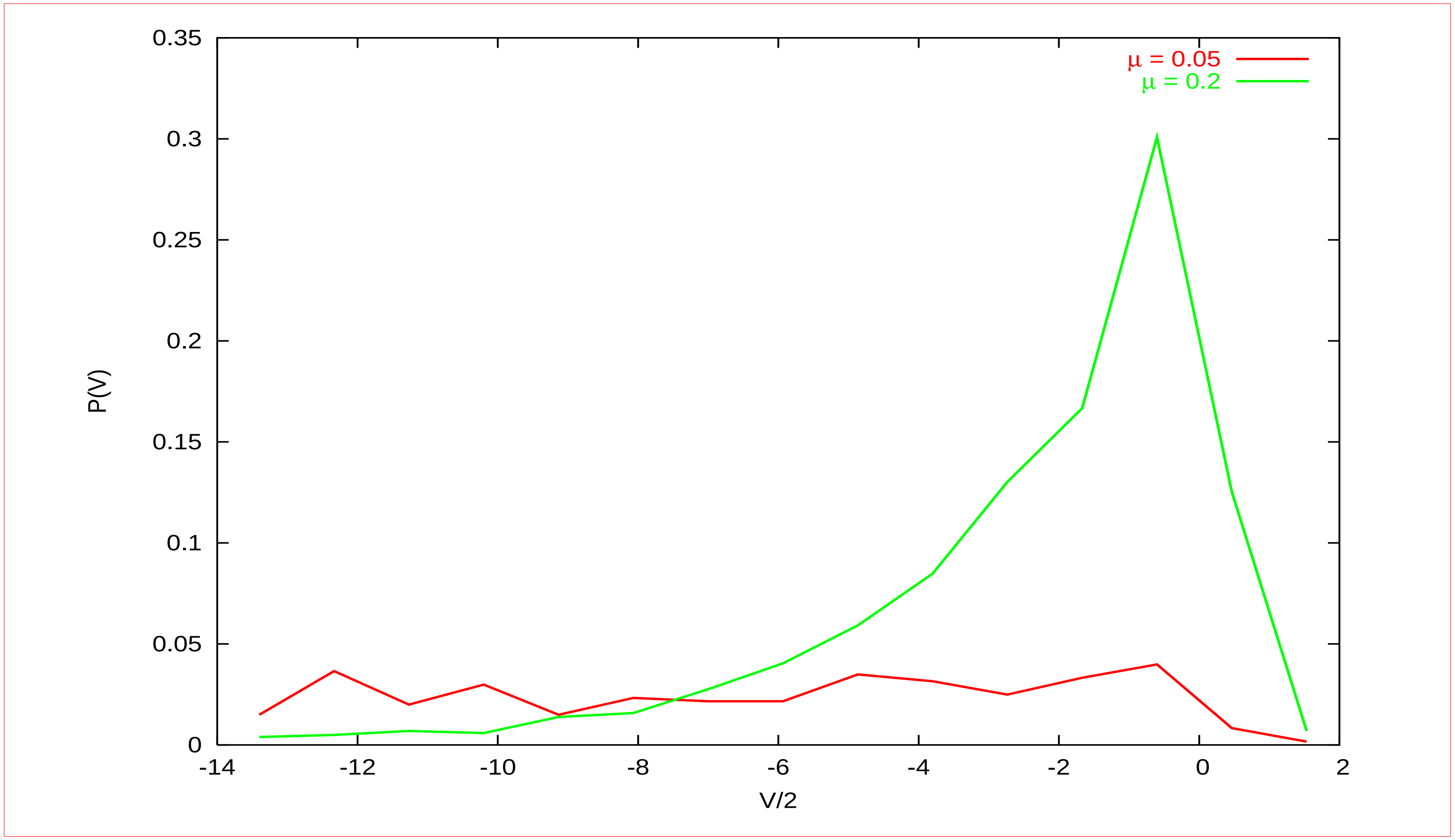
$$\Delta E = \tau_c(F^+, \Pi^+) - \tau_c(F^-, \Pi^-)$$

- This is O($\Delta\tau$). Unless we get this down to O($\Delta\tau^2$) we will have no acceptance on large lattices without an unfeasibly large time step.
- We can add a term $F^+ - F^- - \eta(\eta, F^+ - F^-)$ to the momentum update. We now have

$$\Delta E = \tau_c(F^+, \Pi^+) - \tau_c(F^-, \Pi^-)$$

- We can get rid of this last O(τ_c) term by adding this difference to the momentum jump perpendicular to η. Instead of correcting for an energy difference V we correct for a difference $V + \Delta E$.

Small masses.



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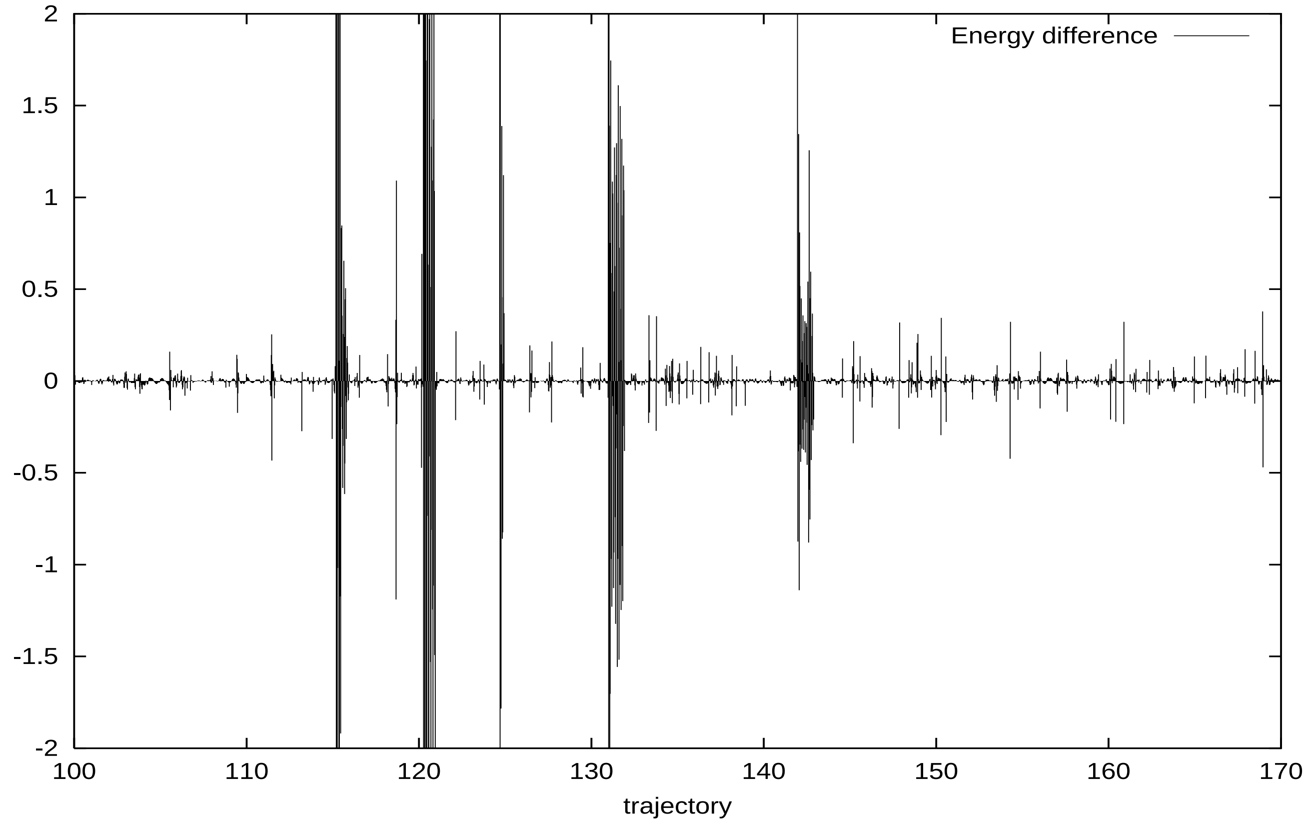

Small masses.

- We had

$$V = 2(1-\mu^2)\langle\phi|\frac{1}{(H^+)^2}\left\{\gamma_5, \epsilon(\lambda^-)|\psi\rangle\langle\psi|\right\}\frac{1}{(H^-)^2}|\phi\rangle$$

- This is (approximately) independent of the volume.
- This is (approximately) $\propto \mu^{-2}$.
- We will have no topological charge changes at small mass.

Small masses.

lattice size	β	μ	$< V >$	$< V > \mu^2$
4^4	7.5	0.2	1.10	0.044
12^4	7.5	0.1	3.25	0.033
4^4	7.5	0.05	17.96	0.045

One topological sector simulations.

- Z. Fodor suggested (lattice 2005, hep-lat/0510117) working in one topological sector (we always reflect).
- In this method we need to get the weighting of the various topological sectors
- The expectation value of an observable is

$$\langle O \rangle = \frac{\sum_{Q_f} Z_{Q_f} \langle O \rangle_{Q_f}}{\sum_{Q_f} Z_{Q_f}} = \left(\sum_{Q_f} \frac{Z_{Q_f}}{Z_0} \langle O \rangle_{Q_f} \right) \Big/ \left(\sum_{Q_f} \frac{Z_{Q_f}}{Z_0} \right)$$

$$\langle O \rangle_{Q_f} = \frac{1}{Z_Q} \int [\mathcal{D}U]_{Q_f} O[U] \det H^2 \exp(-S_g)$$

- We need to find the ratio of the weights Z_{Q_f+1}/Z_{Q_f}.

One topological sector simulations.

- Assume that we can construct an observable F_{Q_f} which is only non-zero on the topological sector wall, and

$$\int [\mathcal{D}U]_{Q_f} F[U] \det H^2 \exp(-S_g) = \int [\mathcal{D}U]_{Q_f+1} F[U] \det H^2 \exp(-S_g)$$

- Then

$$\frac{Z_{Q_f+1}}{Z_{Q_f}} = \frac{\langle F \rangle_{Q_f}}{\langle F \rangle_{Q_f+1}}$$

One topological sector simulations.

- The ratio of the determinants at the topological sector wall is

$$e^{-\Delta S} = \frac{\det H_+^2}{\det H_-^2} = \Big(1 - 2\text{sign}(\lambda_0^-)(1-\mu)\langle\psi_0|\, H_+^{-1}\,|\psi_0\rangle\Big)^{-2}$$

- Why not use this as our observable?

$$\frac{Z_{Q_f+1}}{Z_{Q_f}} = \frac{\langle \delta_{Q_f,Q_f+1}\min(1,e^{-\Delta S})\rangle_{Q_f}}{\langle \delta_{Q_f+1,Q_f}\min(1,e^{\Delta S})\rangle_{Q_f+1}}$$

- We can show that

$$\Big\langle \delta_{Q_f,Q_f+1}\min(1,e^{-\Delta S})\Big\rangle_{Q_f} = \left\langle \frac{1}{|\frac{d}{d\tau}\lambda_0|}\min(1,e^{-\Delta S})\right\rangle_{Q_f,\lambda_0=0}$$

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- Ergodicity? This assumes that each topological sector is connected.

One flavour simulations

- The overlap operator has an exact chiral symmetry.
- Can we split the overlap operator into left and right handed components?

One flavour simulations

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- Can we split the overlap operator into left and right handed components?

$$
\begin{aligned}
&2+\gamma_5\epsilon(Q)+\epsilon(Q)\gamma_5 = \\
&\left[\frac{1}{2}(1+\gamma_5)+\alpha\frac{1}{2}(1-\gamma_5)+\frac{1}{4}(1+\gamma_5)\epsilon(Q)(1+\gamma_5)\right]\times \\
&\left[\frac{1}{2}(1-\gamma_5)+\alpha\frac{1}{2}(1+\gamma_5)-\frac{1}{4}(1-\gamma_5)\epsilon(Q)(1-\gamma_5)\right]\frac{2}{\alpha}
\end{aligned}
$$

One flavour simulations

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\end{aligned}
$$

- Only really useful at large masses.
- Easy 2+1 or 2+1+1 flavour simulations.
- Can deal with zero mores by using pseudo-fermion terms like $1 \pm \nu\epsilon(Q)$.

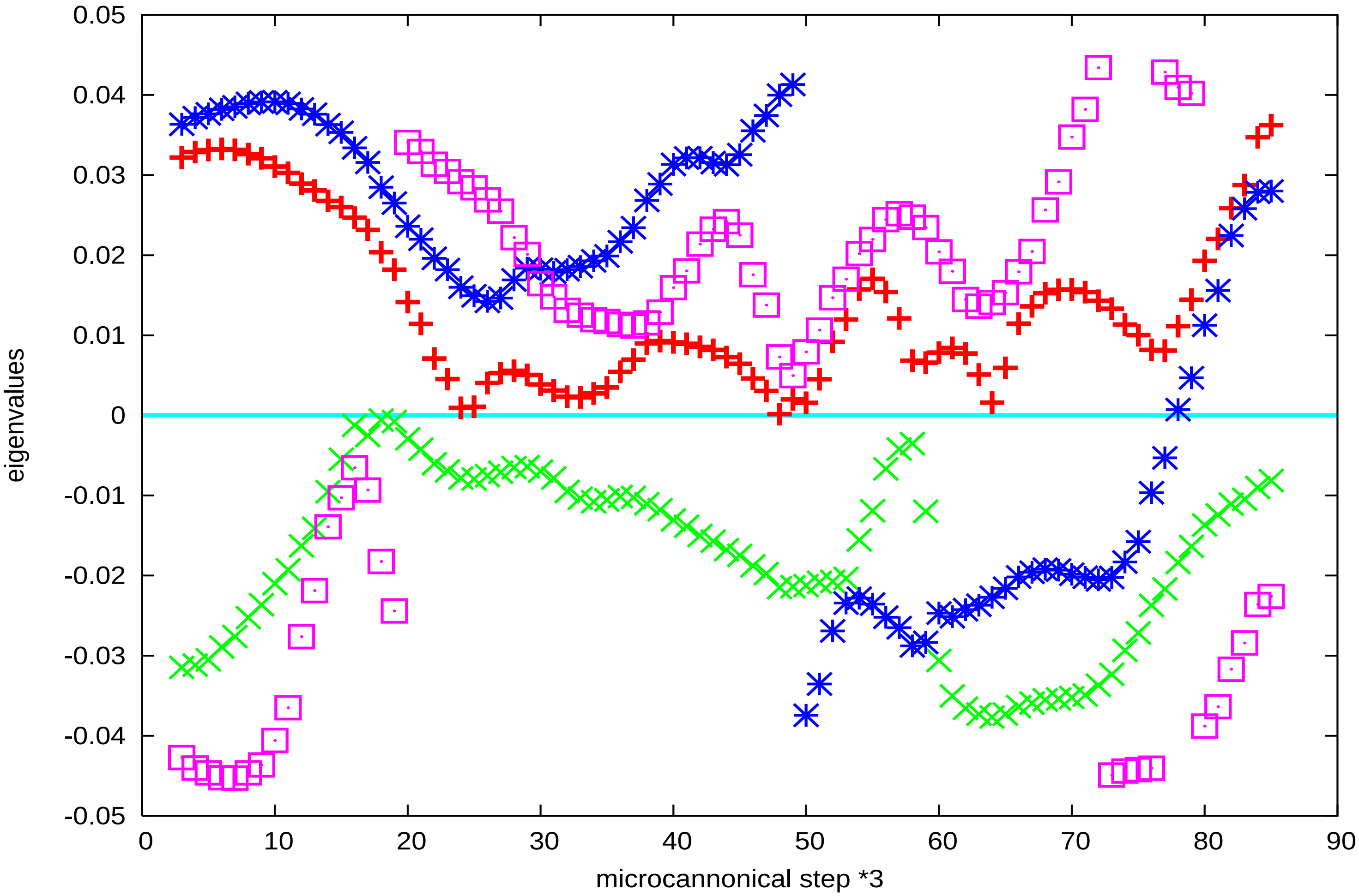
Mixing of small Eigenvalues (1)

- Fermionic force:

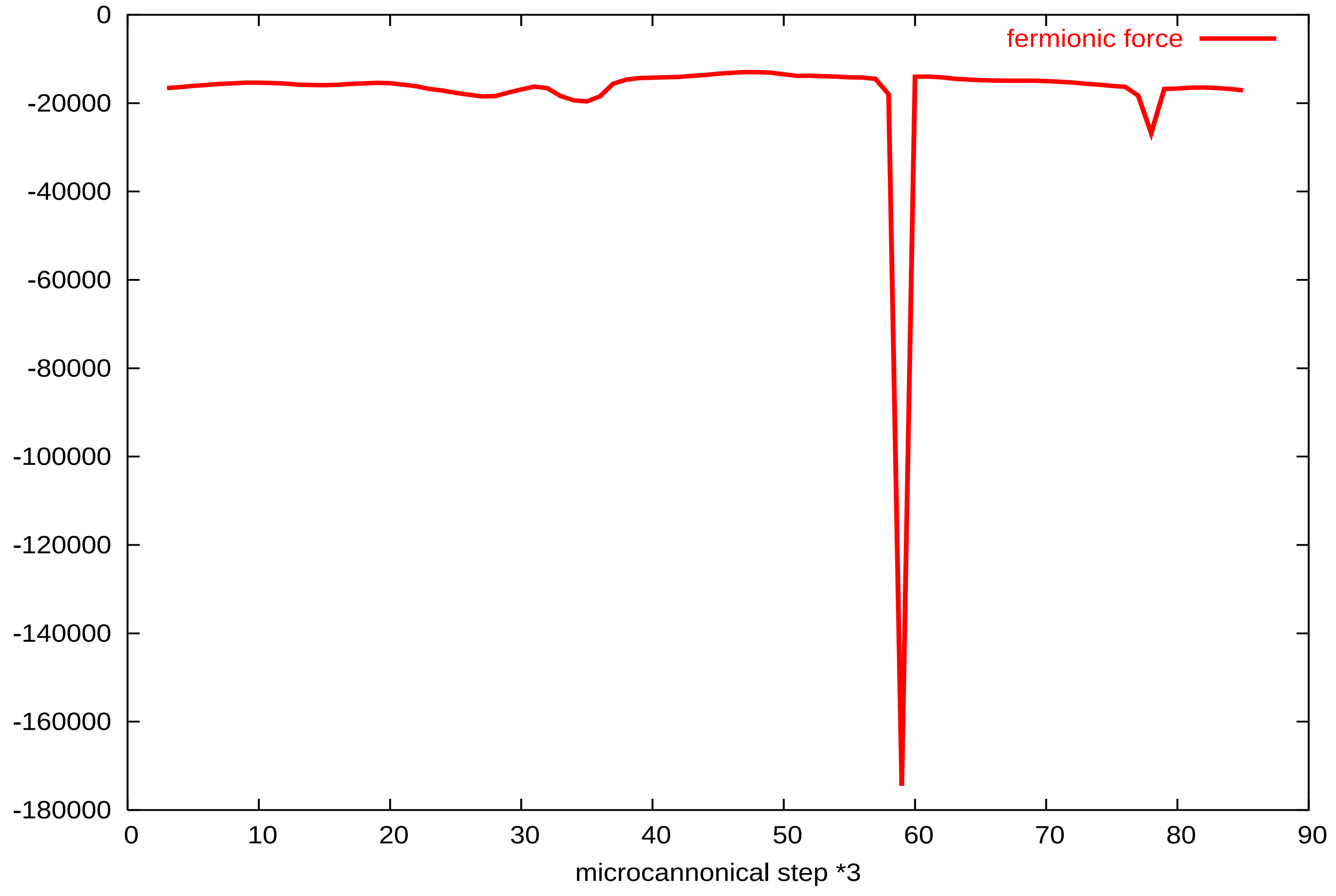
$$\frac{d}{dt}\epsilon(Q) = \sum_{i,j\neq i} |\psi_i\rangle \langle\psi_i| \dot{Q} |\psi_j\rangle \langle\psi_j| \frac{\text{sign}(\lambda_i) - \text{sign}(\lambda_j)}{\lambda_j - \lambda_i}$$

$$+ \sum_i |\psi_i\rangle \langle\psi_i| \frac{d}{d\tau}\text{sign}(\lambda_i)$$

- What happens when we have two small eigenvalues of the Wilson operator which have opposite signs and large mixing between them?



0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
eigenvalues
0
10
20
30
40
50
60
70
80
90
microcannonical step *3


fermionic force
0
-20000
-40000
-60000
-80000
-100000
-120000
-140000
-160000
-180000
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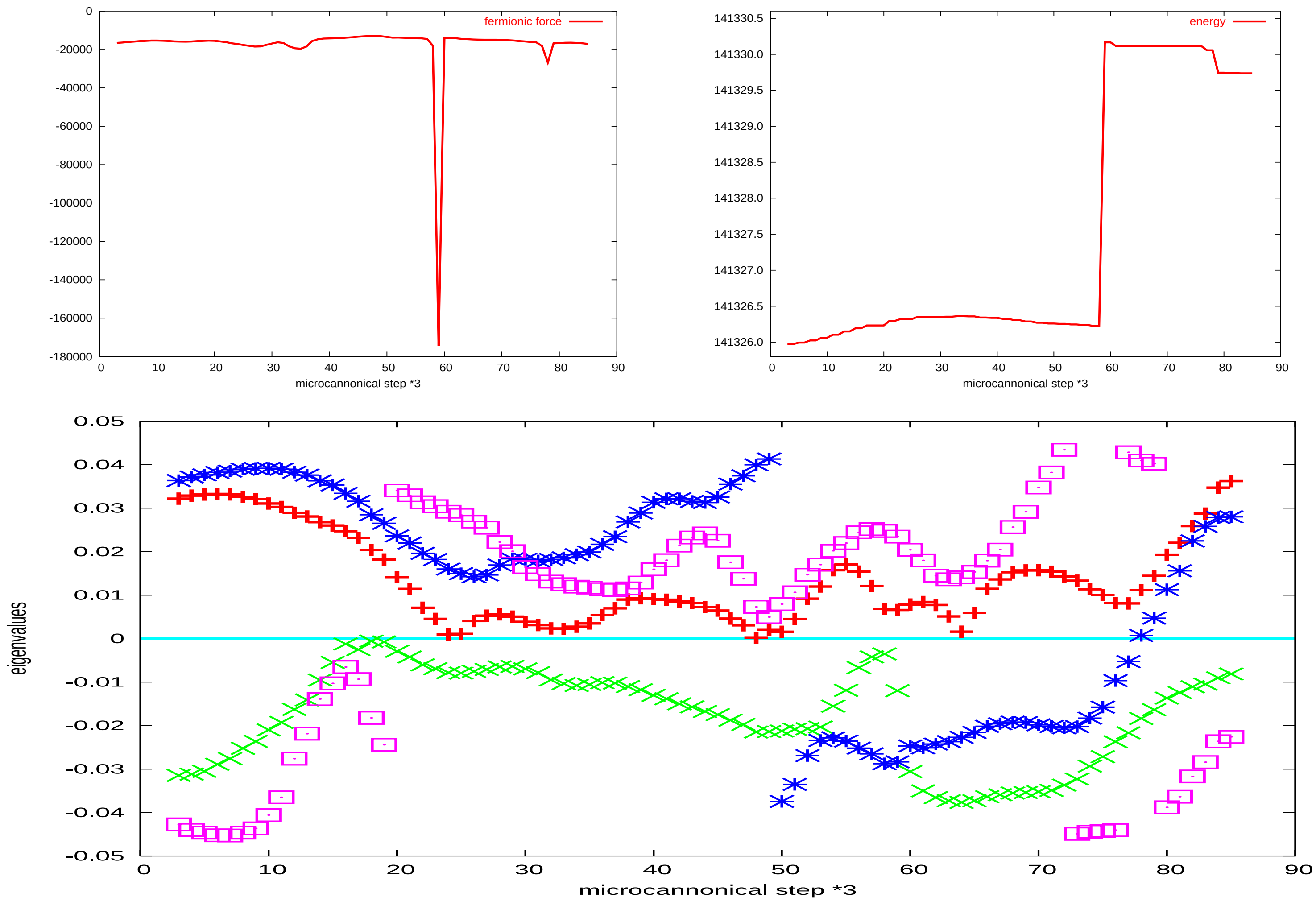
70
80
90
microcannonical step *3


fermionic force
0
-20000
-40000
-60000
-80000
-100000
-120000
-140000
-160000
-180000
0 10 20 30 40 50 60 70 80 90
microcannonical step *3
energy
141330.5
141330.0
141329.5
141329.0
141328.5
141328.0
141327.5
141327.0
141326.5
141326.0
microcannonical step *3
eigenvalues
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
microcannonical step *3

Stout Smearing

- Modify the links in the Dirac operator:

$$U_\mu(x) \rightarrow e^{iS_\mu(x)} U_\mu(x)$$
$$S = \sum_\nu \rho_{\mu\nu} U_{\mu\nu}(x)$$

- Smooths out the gauge field, improves locality of overlap operator, and reduces number of small eigenvalues.
- Fewer small eigenvalues = fewer crossings? Longer autocorrelation?
- We can't smear too much.

Improved Kernel operator

- DeGrand and Schaefer use an improved Kernel operator:

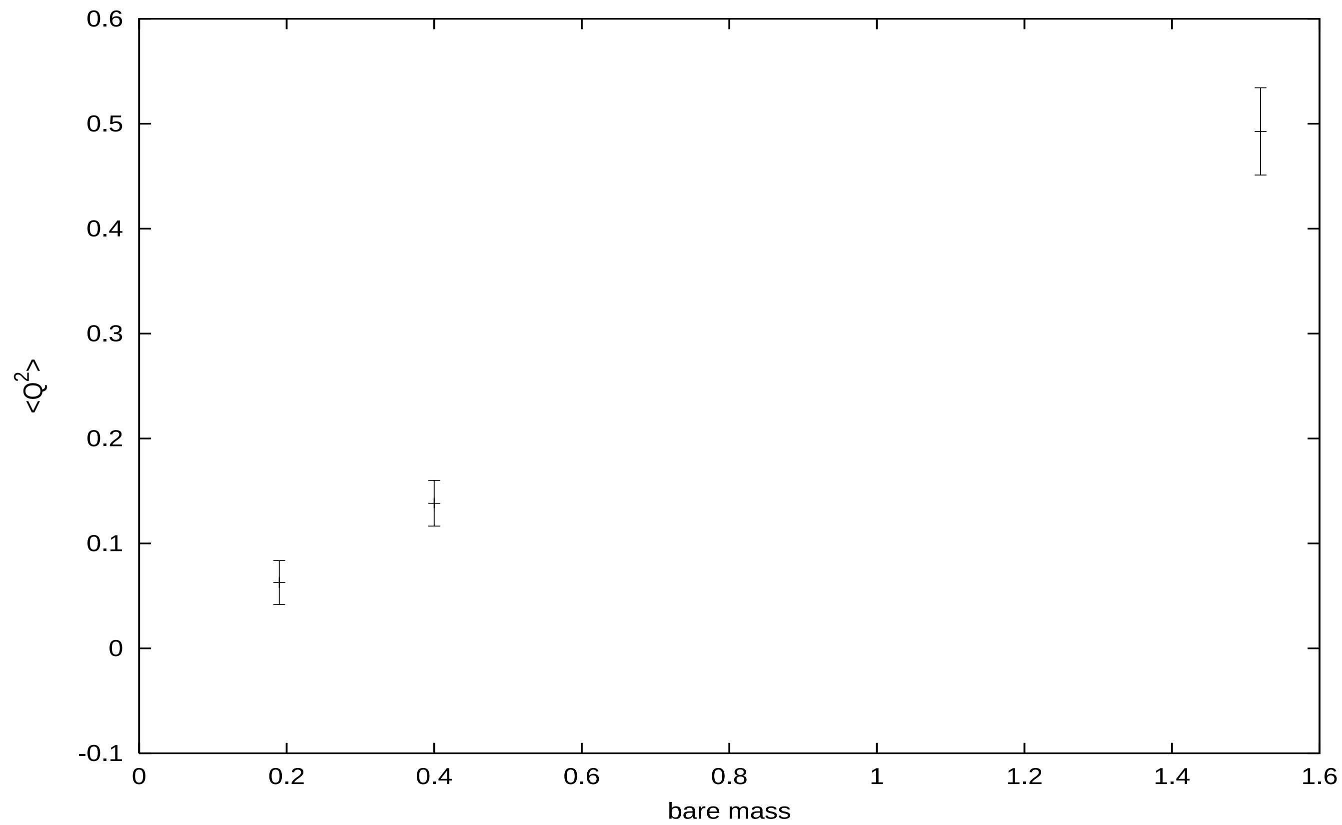
$$S = \sum_{x,r} \overline{\psi}(x)[\zeta(r) + i\gamma_\mu \rho_\mu(r)]\psi(x+r) - \frac{iaC_{SW}}{4}\overline{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}\psi(x)$$

- r extends over the original site, nearest neighbours, and diagonal neighbours.
- Can choose the parameters ρ and ζ to get the correct continuum limit etc.
- This again improves the locality, reduces the number of small eigenvalues, etc.

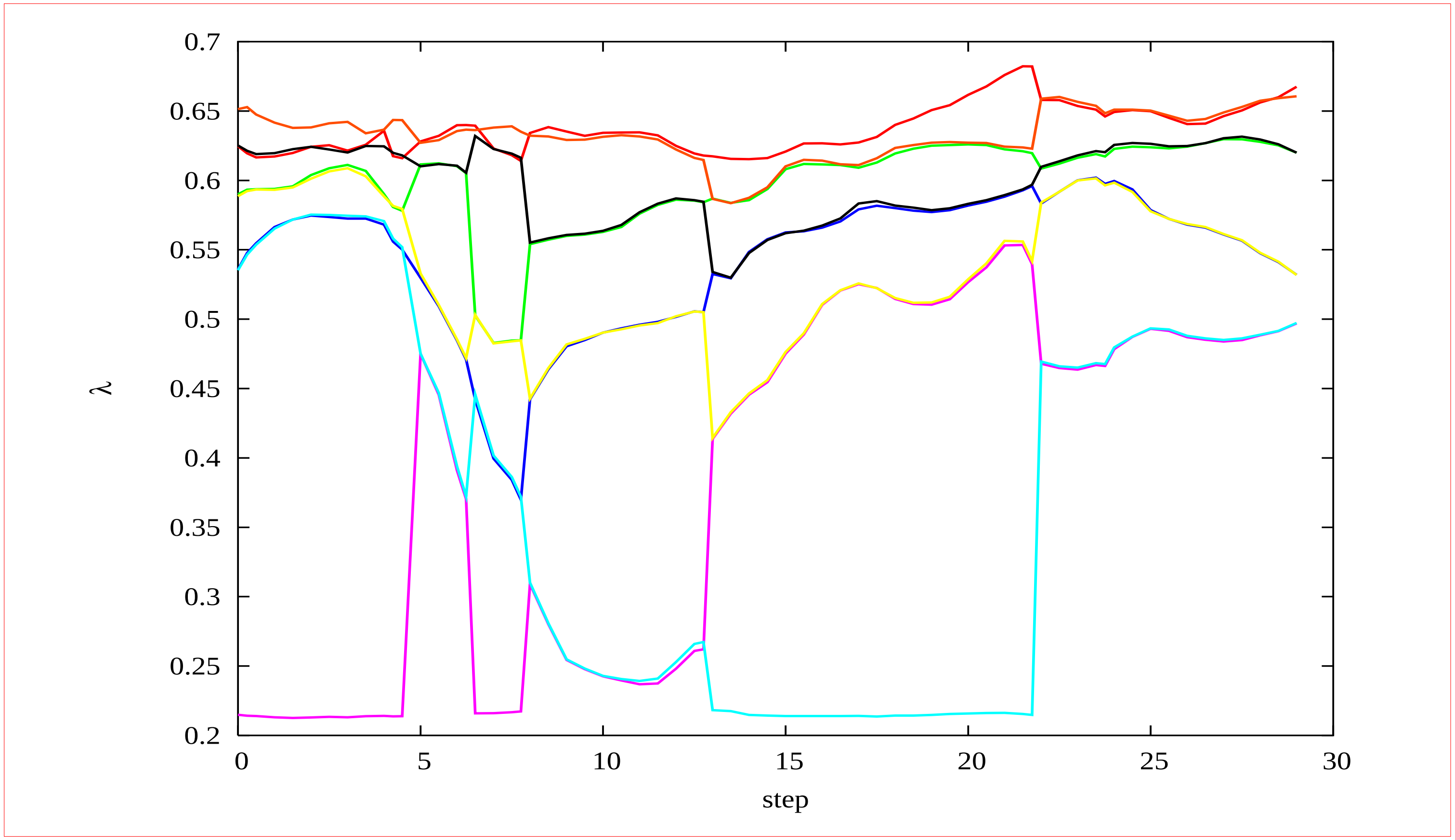
Volume dependence of algorithm.

- DeGrand+Schaefer say algorithm O(V^2):
  1. Get O(V) small eigenvalues.
  2. Number of eigenvalue crossings: O(V)
  3. Eigenvalue crossing correction: O(V)
  4. Algorithm O(V^2)
- Me: No - small eigenvalues repel - it's more like O($V^{3/2}$).
- We need to study this.

Topological susceptibility



Chiral Symmetry breaking



Outlook

size	μ	β	a	time
4^4	0.05-0.5	5.4(W), 7.5 LW	?	
6^4	0.1-0.3	5.4(W)	?	
8^4	0.025-0.1	7.5-8.3	2.5-1.5	2 hour/trajectory
$8^3 32$	0.01-0.05	8.3	1.5	7 hours/trajectory
12^4	0.05-0.1	8.3	∼1.5	
$12^3 32$	0.1	8.3	∼1.5	
$16^3 32$	0.1	8.3	∼1.5	

Conclusions

- We will soon have lattice QCD simulations with an exact lattice chiral symmetry.
- The discontinuity in the matrix sign function gives us some unique problems.
- We have solved some of them.
- Not quite there yet.
- First Physics results coming in (N. Cundy lattice 2005).