Improved Chiral Lattice Fermion Actions

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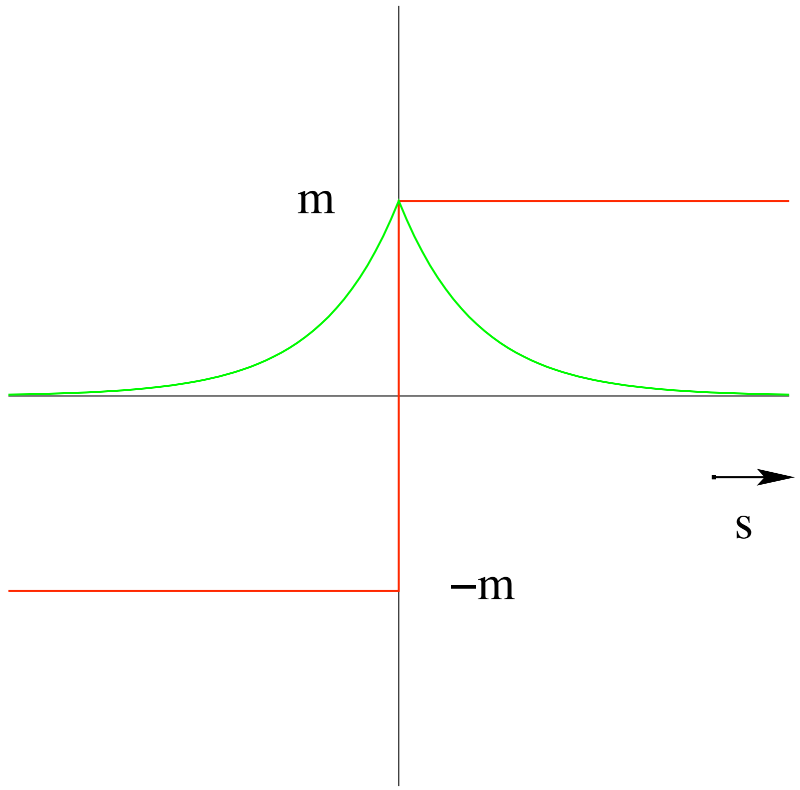
Summary

- Introduction:
  - Lattice Fermions and Chiral symmetry
  - Domain Wall Fermions
  - Overlap
  - “Perfect” Fermions
- The Ginsparg-Wilson relation
- Implementations
- Improvements on the implementation
  - Gauge actions
  - Mobius fermions
  - Continued Fraction
- What is the best thing to do?
- Conclusions and future

Kaplan's Fermions

Continuum 5D fermions:

$$\not{\partial}\psi(x,s) + \gamma_5 \partial_5 \psi(x,s) + m(s)\psi(x,s) = 0$$



The zero mode:

$$\psi_0 = \phi^{\pm}(s) u_{\pm} \qquad \gamma_5 u_{\pm} = \pm u_{\pm} \qquad [\pm\partial_5 + m(s)]\, \phi^{\pm}(s) = 0$$

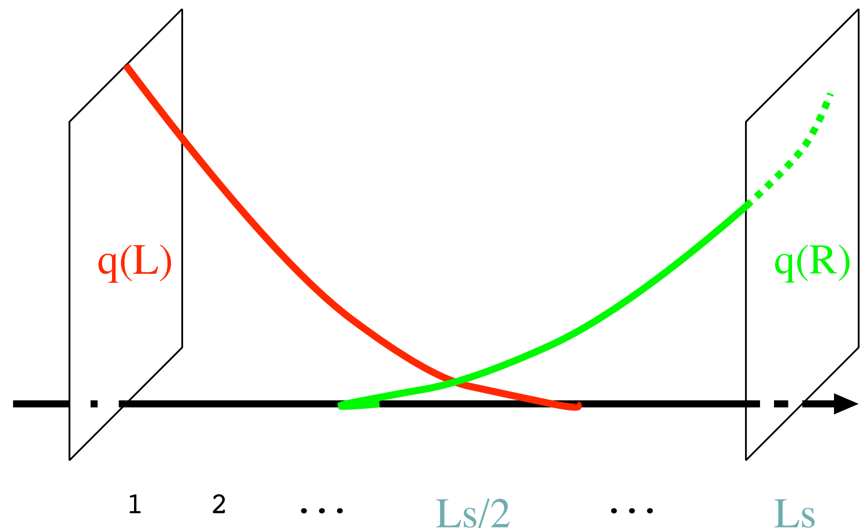
and

$$\phi^{+}(s) = e^{-m|s|}$$

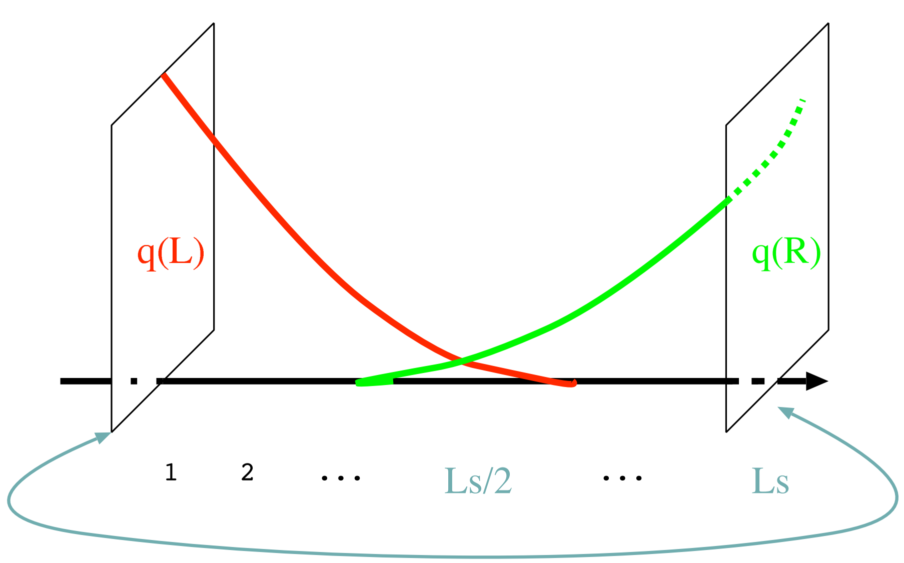
is the only normalizable state

Domain Wall Fermions for QCD

Formulate the 5D Wilson fermions with mass $M \neq 0$ in $s \,\epsilon\, [1, L_s]$



For $-2 < M < 0$, light chiral modes are bound on the walls.
Only one Dirac fermion without doublers remains.



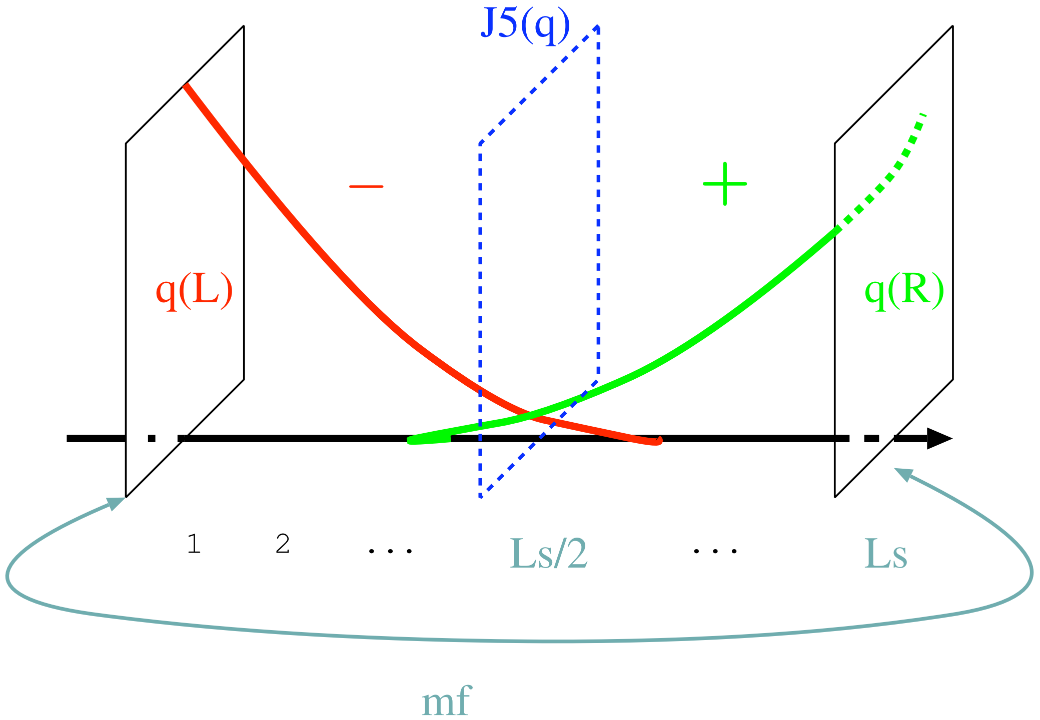
Fermion mass is introduced by explicitly coupling m_f of the walls. [Shamir,Furman & Shamir]

Ward Identity

$$q(x) = P_L\psi(x,0) + P_R\psi(x,L_s-1)$$
$$\bar{q}(x) = \overline{\psi}(x,L_s-1)P_L + \overline{\psi}(x,0)P_R$$

$$q_{mp}(x) = P_L\psi(x,\frac{L_s}{2}+1) + P_R\psi(x,\frac{L_s}{2})$$
$$\bar{q}_{mp}(x) = \overline{\psi}(x,\frac{L_s}{2})P_L + \overline{\psi}(x,\frac{L_s}{2}+1)P_R$$

$$P_{R/L} = \frac{1}{2}(1 \pm \gamma_5)$$



$$\Delta_\mu \langle \mathcal{A}^a_\mu(x)\mathcal{O}\rangle = 2\, m_f\, \langle J^a_5(x)\mathcal{O}\rangle + 2\langle J^a_{5q}(x)\mathcal{O}\rangle + i\langle \delta^a_x \mathcal{O}\rangle$$

$$J^a_5(x) = \bar{q}(x)\tau^a\gamma_5 q(x) \qquad J^a_{5q}(x) = \bar{q}_{mp}(x)\tau^a\gamma_5 q_{mp}(x) \qquad \mathcal{A}^a_\mu(x) = \sum_{s=0}^{L_s-1} \mathrm{sign}\left(s - \frac{L_s-1}{2}\right) j^a_\mu(x,s)$$

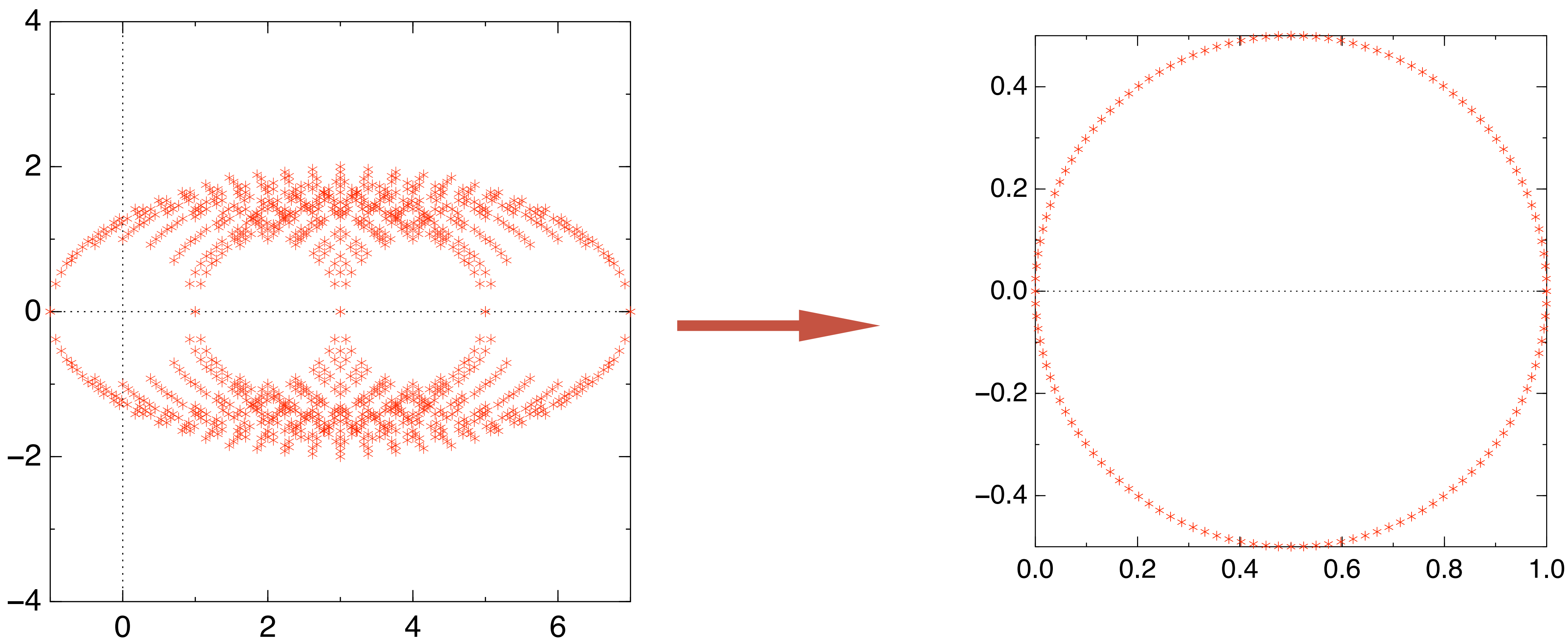
- $\lim_{L_s\to\infty} \langle J^a_{5q}(x)\mathcal{O}\rangle = 0$: Exact chiral symmetry at finite lattice spacing

Overlap Fermions

Narayanan - Neuberger

- Develop Kaplan's idea $\quad e^{-S(U)} = \langle 0_- | 0_+ \rangle$
- Derive the 4D effective action
- The overlap formula $\quad D^0_{ov} = \frac{1}{2} + \frac{1}{2}\gamma_5 \varepsilon[\gamma_5 D(M_5)]$ and $M_5 < 0$

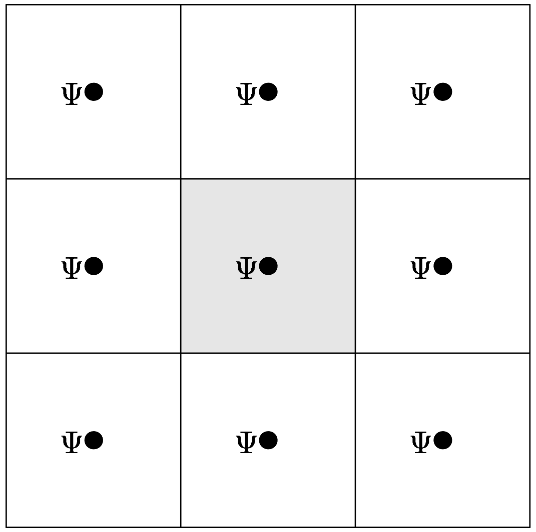
$$D^{Wilson}_{xy}(M_5) = (4+M_5)\delta_{x,y} - \frac{1}{2}[(1-\gamma_\mu)U_\mu(x)\delta_{x+\mu,y} + (1+\gamma_\mu)U^\dagger_\mu(y)\delta_{x,y+\mu}] \, ,$$



Ginsparg-Wilson Relation

Renormalization group transformation:

$$e^{-S'[\Phi]} = \int \mathcal{D}\phi \, e^{-S[\phi]-\mathcal{T}[\Phi;\phi]},$$



The fixed point operator satisfies (massless case):

$$\gamma_5 \, D \; + \; D \, \gamma_5 \; = \; 2 \, D \, \gamma_5 \, D$$

Luscher symmetry: $\delta\Psi = \gamma_5(1-2D)\Psi$ $\quad\quad \delta\bar{\Psi} = \bar{\Psi}\gamma_5$

- The overlap satisfies the GW relation
- What about the DWF?

Is the GW relation enough?

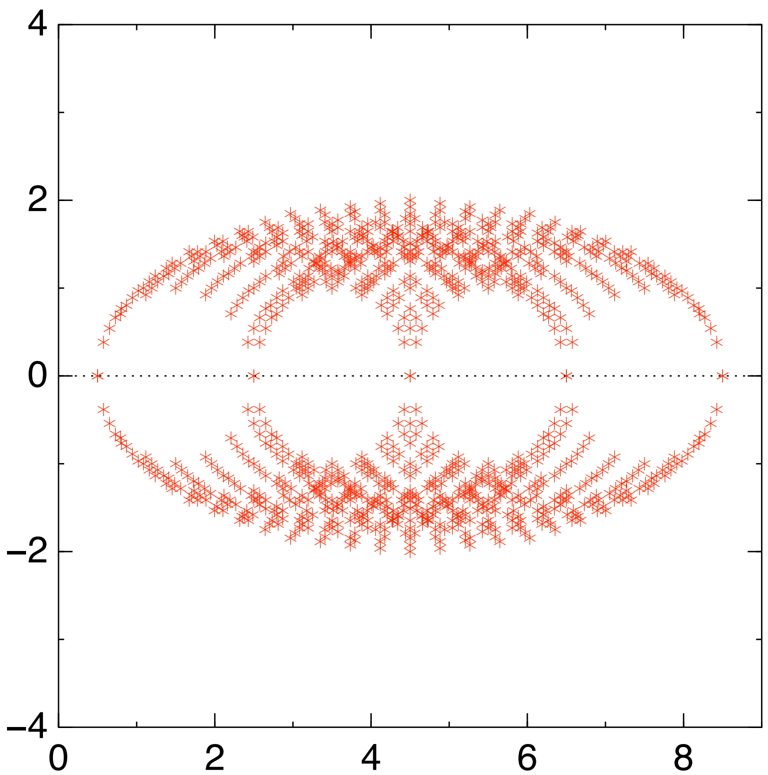
- Take the overlap formula with $M_5>0$

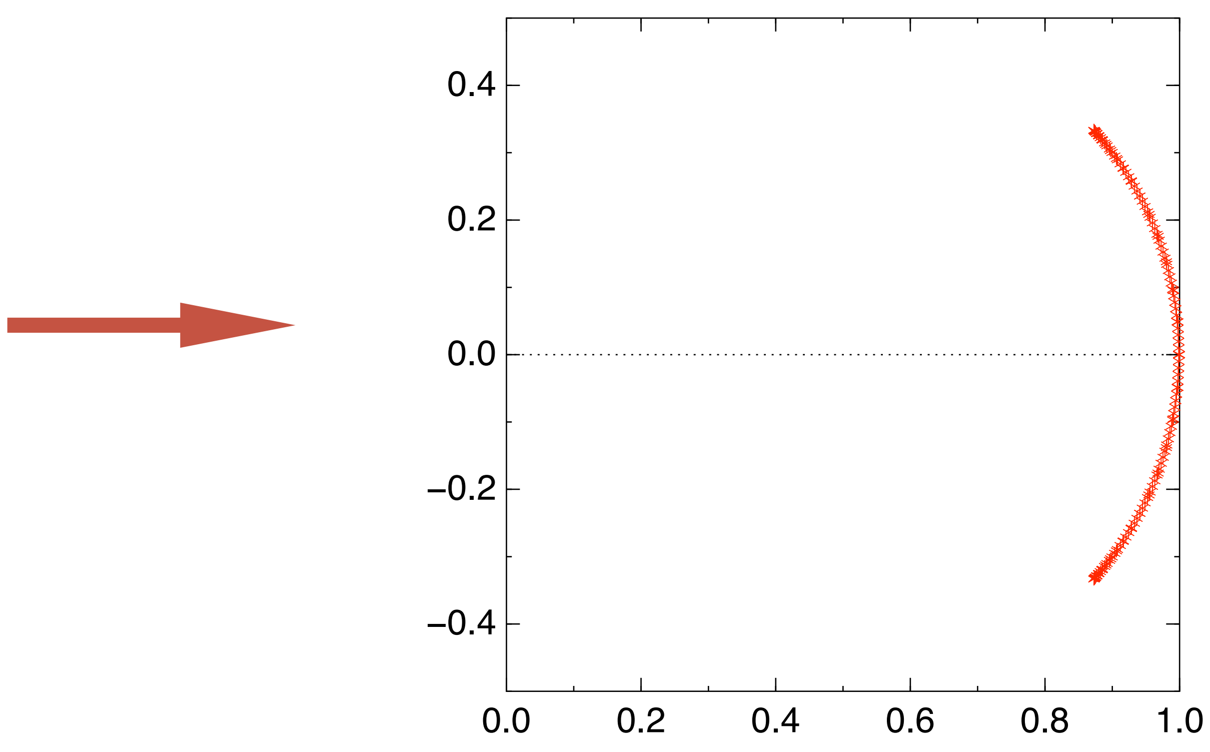
$$D^0_{ov} = \frac{1}{2} + \frac{1}{2}\gamma_5 \varepsilon[\gamma_5 D(M_5)]$$

- It satisfies the GW relation

$$\gamma_5 D + D \gamma_5 = \gamma_5 + \frac{1}{2}\varepsilon[\gamma_5 D(M_5)] + \frac{1}{2}\gamma_5 \varepsilon[\gamma_5 D(M_5)]\gamma_5 = 2 D \gamma_5 D$$

- It does not have chiral modes!





DWF and the GW relation

- DWF are at hart the same as the overlap
- It's easy to show that

$$D_{ov}(m) = \frac{1+m}{2} + \frac{1-m}{2}\gamma_5 \mathcal{E}_{L_s}[\gamma_5 D(M_5)]$$

$$D(M_5) = \frac{a_5 D^W(M_5)}{2 + a_5 D^W(M_5)}$$

- The physical quark propagator is $\frac{1}{D_{eff}} \equiv \langle q\bar{q}\rangle = \frac{1}{1-m}\left(\frac{1}{D_{ov}} - 1\right)$
- This is just a particular approximation of the sign function

$$\mathcal{E}_{L_s}(x) = \frac{\prod_s^{L_s}(1+x) - \prod_s^{L_s}(1-x)}{\prod_s^{L_s}(1+x) + \prod_s^{L_s}(1-x)}$$

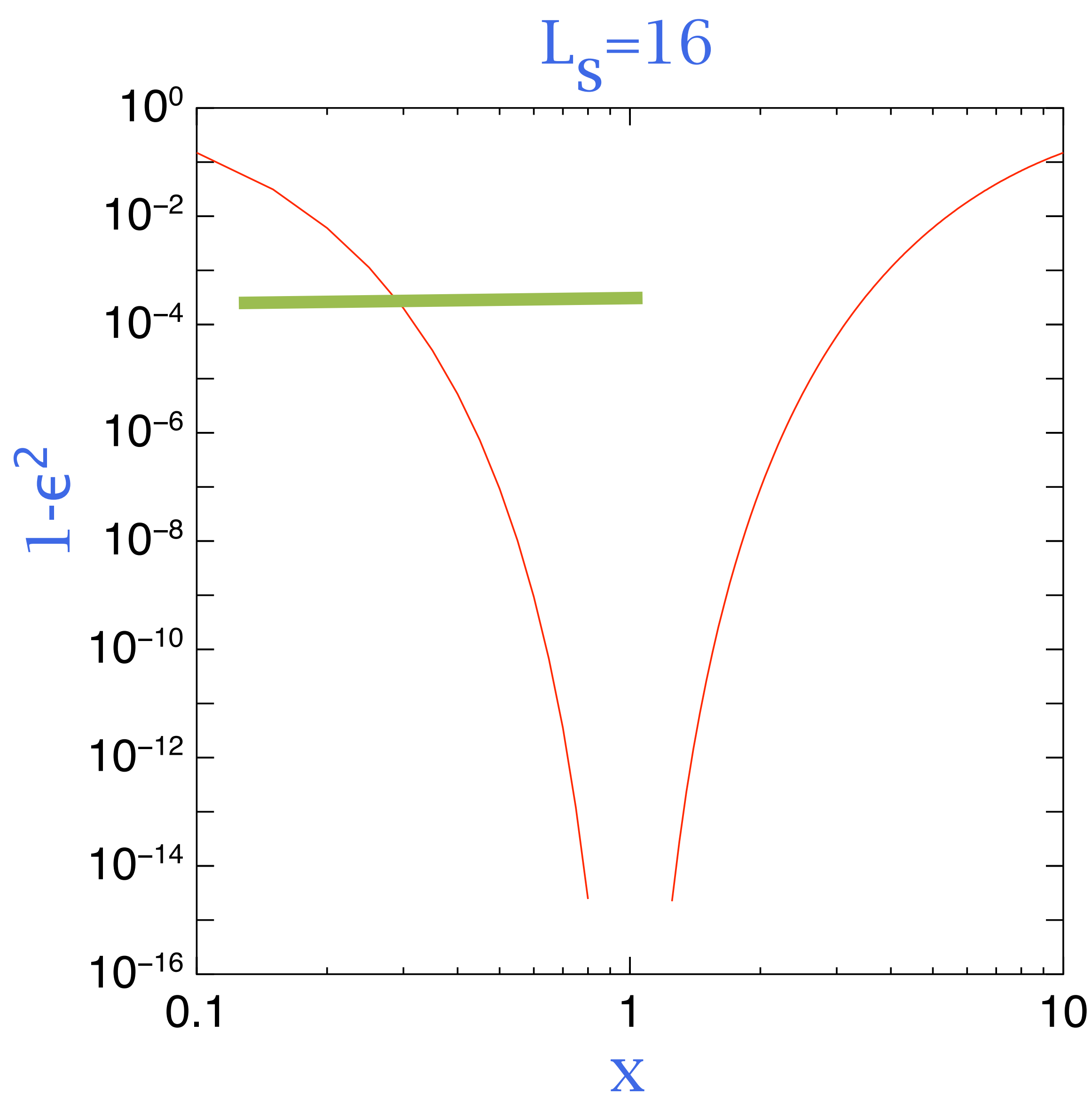
- The GW relation

$$2\gamma_5\Delta_L \equiv \gamma_5 \frac{1}{2}\left[1 - \mathcal{E}_{L_s}{}^2\right] = \gamma_5 D_{ov}^0 + D_{ov}^0\gamma_5 - 2D_{ov}^0\gamma_5 D_{ov}^0$$

- The violation is positive for L_s even

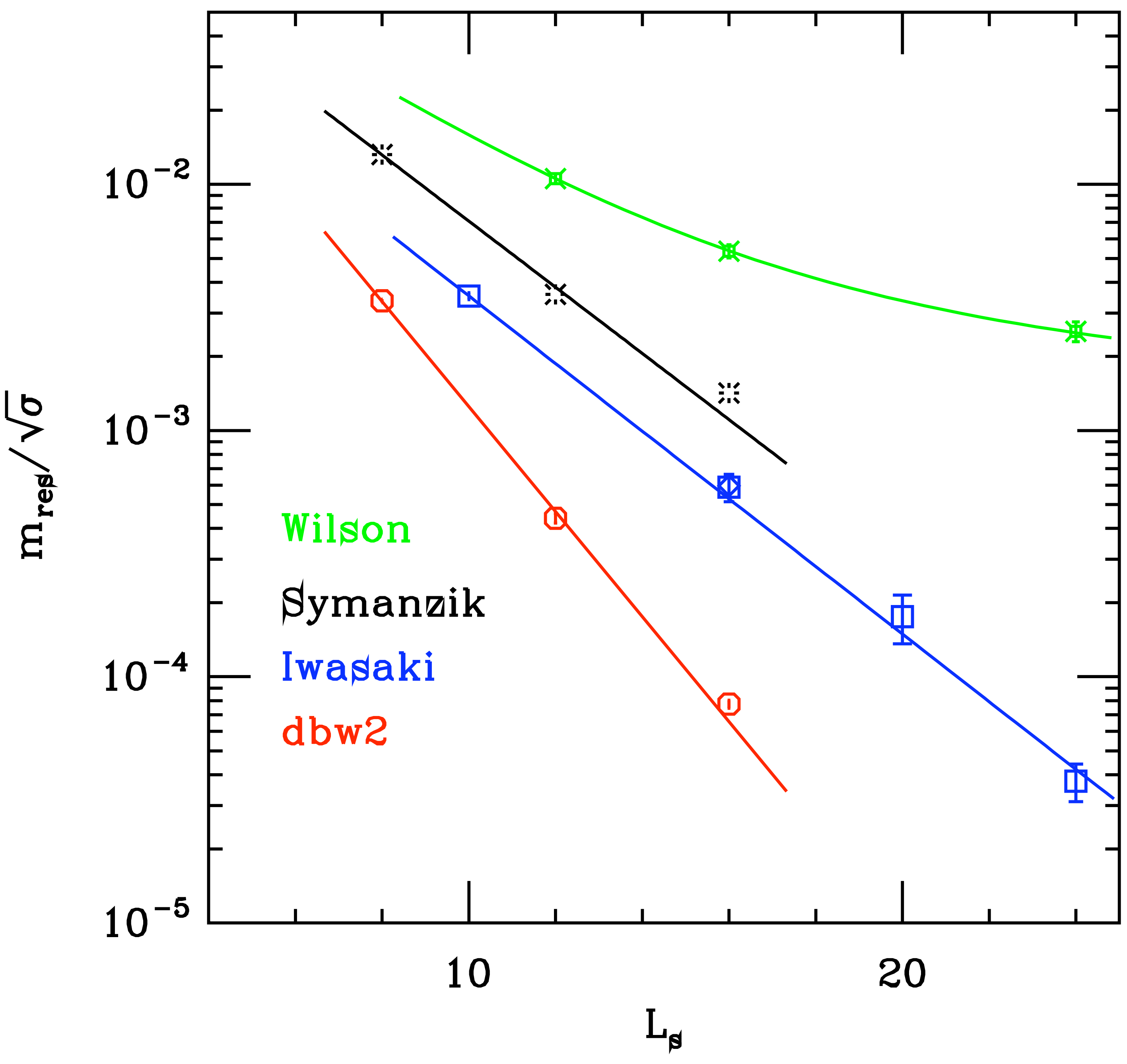
The DWF approximation

$$\varepsilon_{L_s}(x) = \frac{\prod_s^{L_s}(1+x) - \prod_s^{L_s}(1-x)}{\prod_s^{L_s}(1+x) + \prod_s^{L_s}(1-x)}$$



- No flexibility in the approximation
- Only L_s can be changed and hope for the best....

Changing the gauge action



- DBW2 gauge action works for quenched (2GeV cutoff)
- Dynamical with 1.7GeV cutoff only a factor of 2 better

Why do we still work with DWF?

- For the overlap it seems there are a lot of tricks one can play (Zolotarev, continued fractions, double pass, Nested iteration prec. etc.)
- The physical picture is compelling for DWF (Axial current)
- The 5D action is local. New algorithms can exploit this feature.
- Dynamical: Easy force computation. (other 5D methods have this feature too)
- Computing the inverse is easier than computing the matrix and then inverting!
- A little flexibility would not hurt!

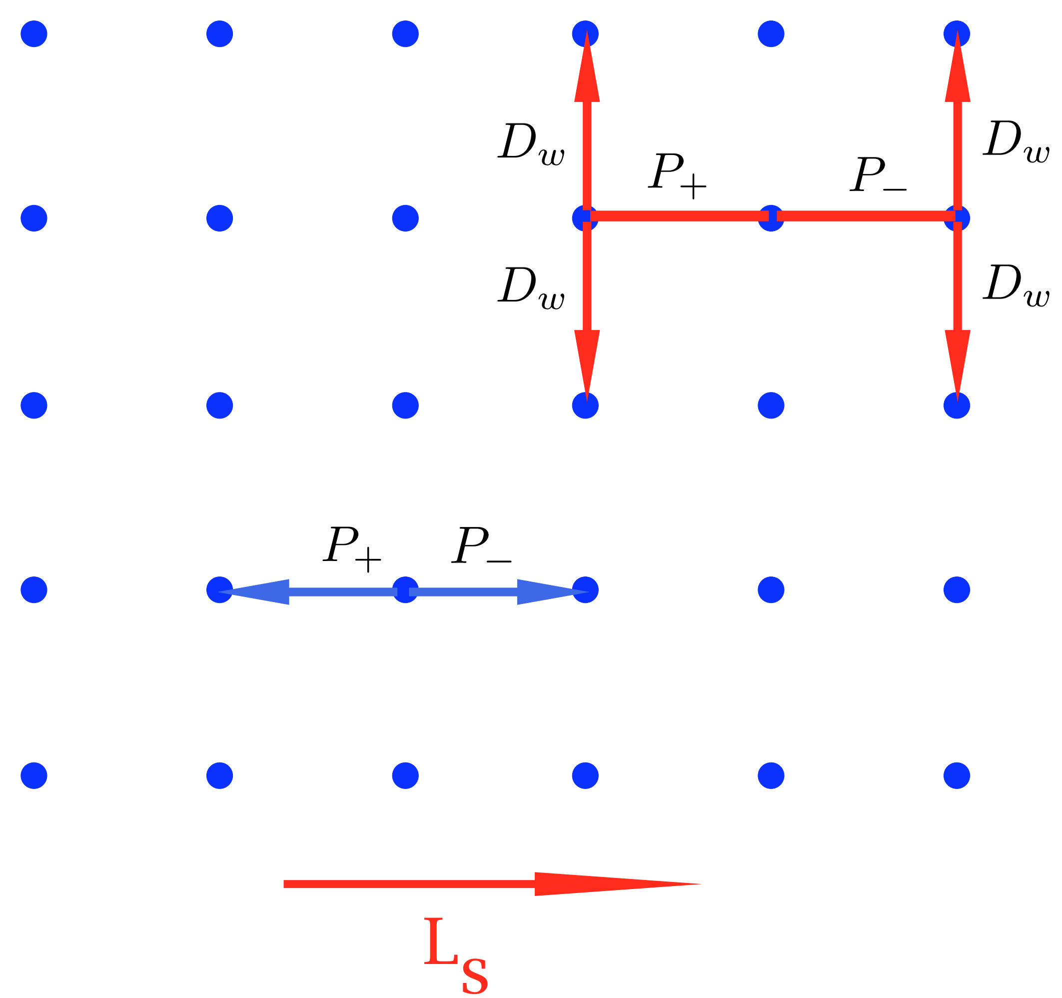
The Mobius Fermions

$$D^{(5)}_{dwf} = \begin{bmatrix} D_+ & -D_- P_- & 0 & \cdots & 0 & m\,D_- P_+ \\ -D_- P_+ & D_+ & -D_- P_- & 0 & \cdots & 0 \\ 0 & -D_- P_+ & D_+ & -D_- P_- & 0 & \cdots \\ \vdots & & & & & \vdots \\ m\,D_- P_- & 0 & \cdots & \cdots & -D_- P_+ & D_+ \end{bmatrix}$$

$$D^{(5)}_{dwf} = \begin{bmatrix} D_+ & -P_- & 0 & \cdots & 0 & m\,P_+ \\ -P_+ & D_+ & -P_- & 0 & \cdots & 0 \\ 0 & -P_+ & D_+ & -P_- & 0 & \cdots \\ \vdots & & & & & \vdots \\ m\,P_- & 0 & \cdots & \cdots & -P_+ & D_+ \end{bmatrix}$$

$$D_+ = 1 + b_5 D_w$$
$$D_- = 1 - c_5 D_w$$

$$P_+ = \frac{1+\gamma_5}{2}$$
$$P_- = \frac{1-\gamma_5}{2}$$



The Mobius overlap

With a little high school algebra we get

$$\mathcal{P}^{-1}\frac{1}{D_{dwf}(1)}D_{dwf}(m)\mathcal{P} = \begin{bmatrix} D_{ov}(m) & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ -(1-m)T^{-L_s/2+1}\frac{1}{T^{-L_s/2}+T^{L_s/2}} & 1 & 0 & 0 & \cdots & \cdots & 0 \\ -(1-m)T^{-L_s/2+2}\frac{1}{T^{-L_s/2}+T^{L_s/2}} & 0 & 1 & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \cdots & \vdots \\ -(1-m)\frac{1}{T^{-L_s/2}+T^{L_s/2}} & 0 & \cdots & \cdots & 1 & 0 & \cdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ -(1-m)T^{L_s/2-1}\frac{1}{T^{-L_s/2}+T^{L_s/2}} & 0 & \cdots & \cdots & \cdots & 0 & 1 \end{bmatrix}$$

$$\mathcal{P} = \begin{bmatrix} P_- & P_+ & \cdots & 0 \\ 0 & P_- & P_+\cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & P_+ \\ P_+ & 0 & \cdots & P_- \end{bmatrix} \qquad L = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -T^{-L_s+1}M_+ & 1 & 0 & 0 & \cdots \\ -T^{-L_s+2}M_+ & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ -T^{-1}M_+ & 0 & \cdots & 0 & 1 \end{bmatrix}$$

$$M_- = P_- - m\,P_+ \qquad M_+ = P_+ - m\,P_-$$

$$T^{-1} = \frac{1+H_T}{1-H_T} \qquad H_T = \gamma_5 D$$

$$D_{ov}(m) = \frac{1+m}{2} + \frac{1-m}{2}\gamma_5 \mathcal{E}_{L_s}[\gamma_5 D(M_5)]$$

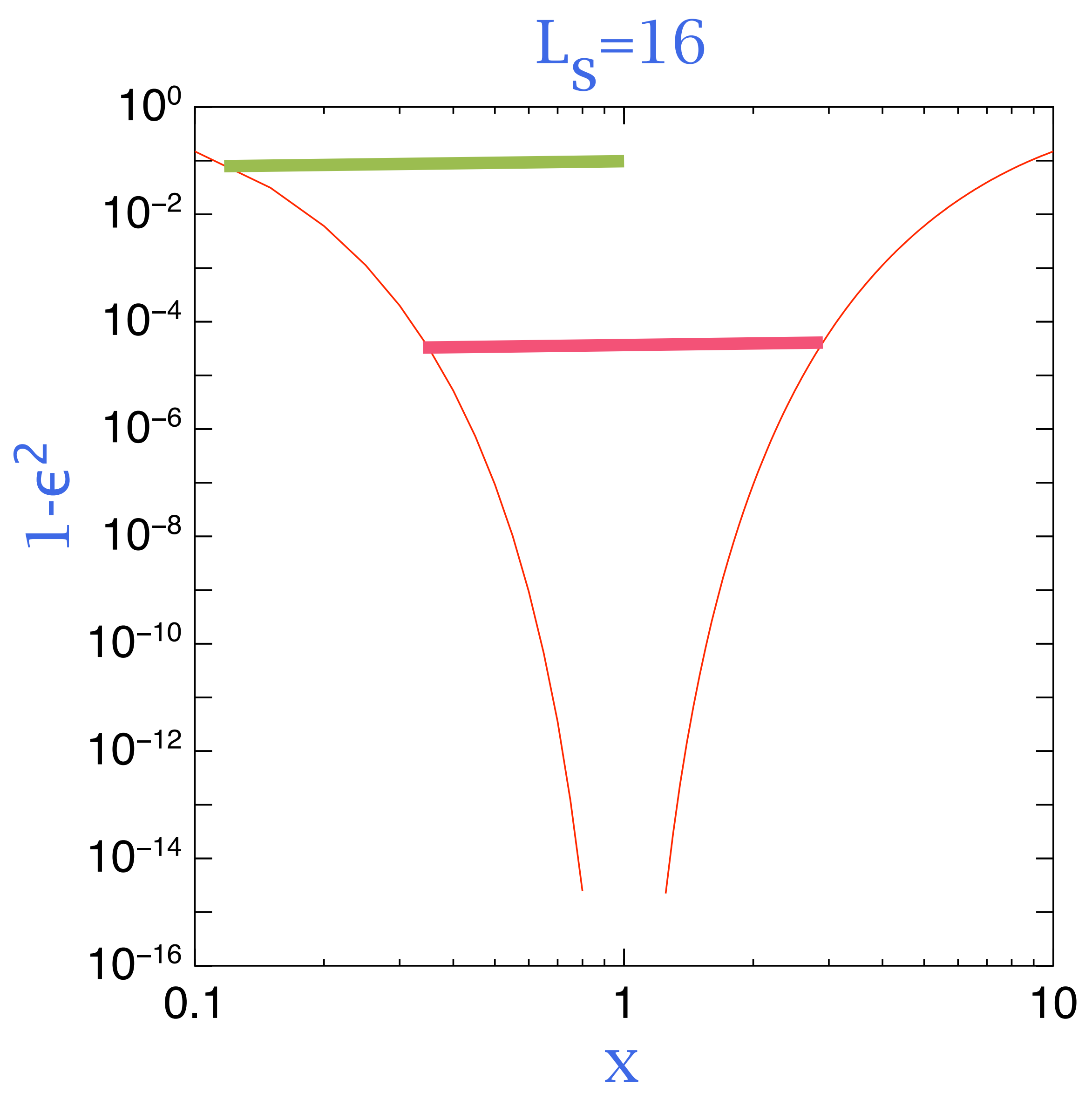
$$\varepsilon_{L_s} = \frac{T^{-L_s}-1}{T^{-L_s}+1} = \frac{(1+H_T)^{L_s}-(1-H_T)^{L_s}}{(1+H_T)^{L_s}+(1-H_T)^{L_s}}$$

$$D = (b_5+c_5)\frac{D_w}{2+(b_5-c_5)D_w} = \alpha\frac{D_w}{2+a_5 D_w}$$

- Overlap: $\alpha=2$, $a_5=0$ (Borici)
- DWF: $\alpha=1$, $a_5=1$ (Shamir)

What do we gain?

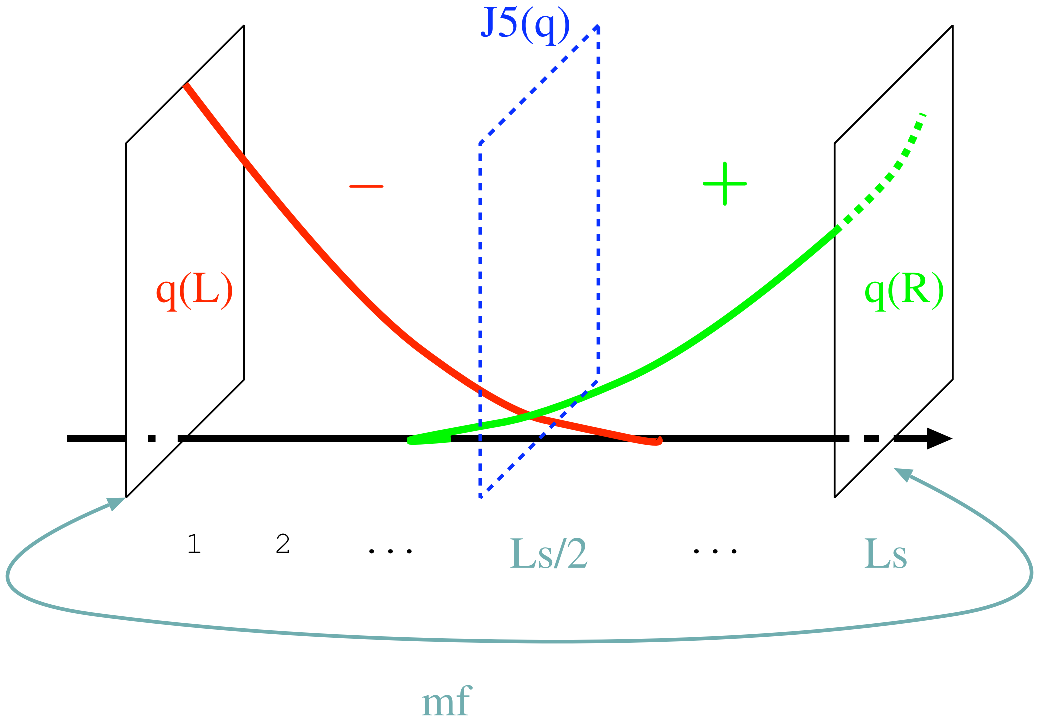
- Keep a_5 fixed
- Tune the scale α
- Shift the eigenvalues to better fit the approximation window



Ward Identity

$$\begin{aligned} q(x) &= P_-\psi(x,0) + P_+\psi(x,L_s-1) \\ \overline{q}(x) &= \overline{\psi}(x,L_s-1)D_-P_- + \overline{\psi}(x,0)D_-P_+ \end{aligned}$$

$$\begin{aligned} q_{mp}(x) &= P_-\psi(x,\frac{L_s}{2}+1) + P_+\psi(x,\frac{L_s}{2}) \\ \overline{q}_{mp}(x) &= \overline{\psi}(x,\frac{L_s}{2})D_-P_- + \overline{\psi}(x,\frac{L_s}{2}+1)D_-P_+ \end{aligned}$$



$$\Delta_\mu\langle\mathcal{A}^a_\mu(x)\mathcal{O}\rangle = 2\,m_f\,\langle J^a_5(x)\mathcal{O}\rangle + 2\langle J^a_{5q}(x)\mathcal{O}\rangle + i\langle\delta^a_x\mathcal{O}\rangle$$

$J^a_5(x) = \bar{q}(x)\tau^a\gamma_5 q(x)$

$J^a_{5q}(x) = \bar{q}_{mp}(x)\tau^a\gamma_5 q_{mp}(x)$

- The axial current is now more complicated

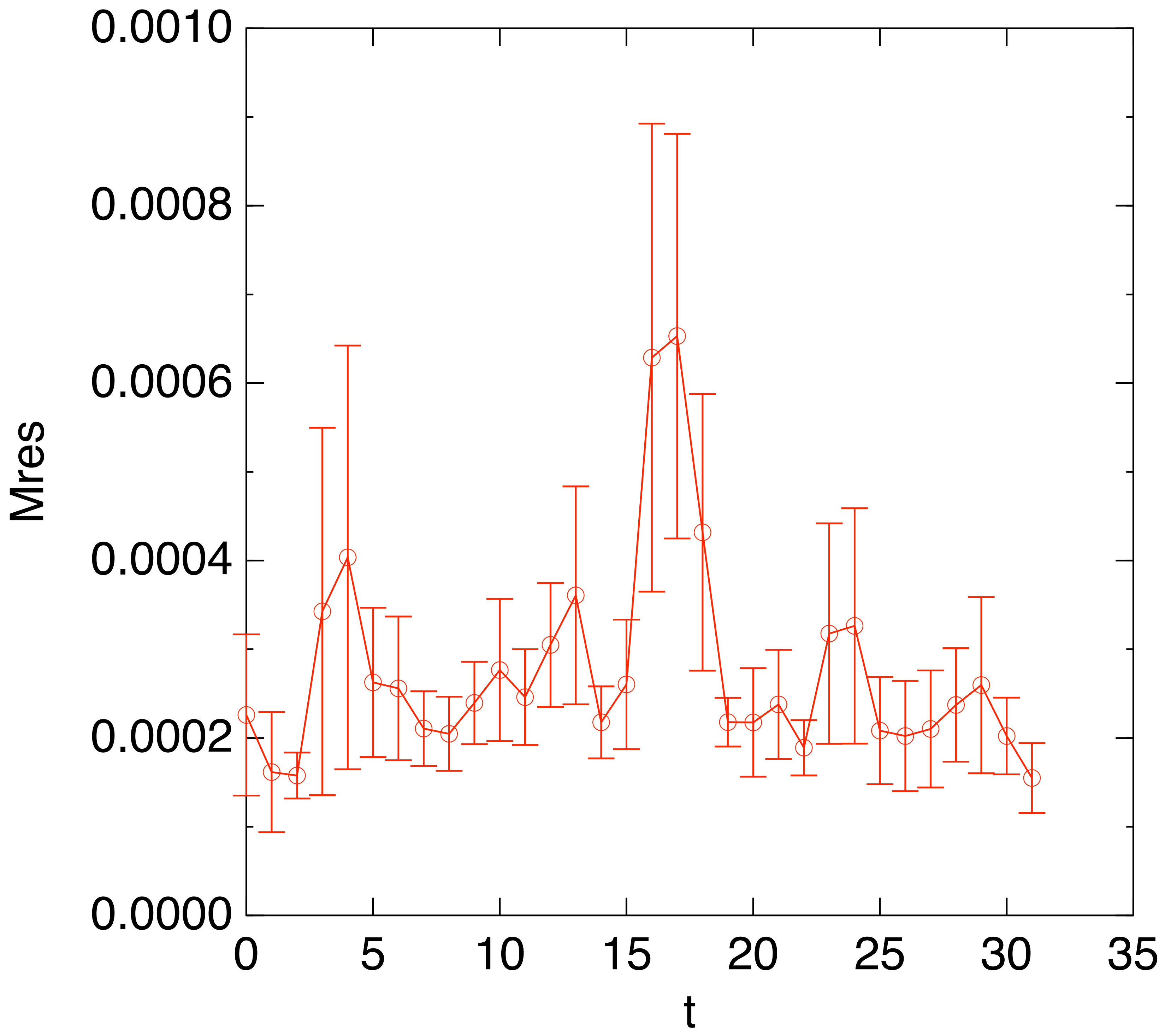
Chiral symmetry breaking

$$\Delta_\mu \langle \mathcal{A}^a_\mu(x)\mathcal{O}\rangle = 2\, m_f\, \langle J^a_5(x)\mathcal{O}\rangle + 2\langle J^a_{5q}(x)\mathcal{O}\rangle + i\langle \delta^a_x \mathcal{O}\rangle$$

- The size of $\langle J^a_{5q}(x)\mathcal{O}\rangle$ measures chiral symmetry breaking
- Let's use for the operator $\mathcal{O} = J^a_5(0)$
- Assume at long distances $J^a_{5q} \sim J^a_5$
- The proportionality constant is the residual mass

$$M_{\mathrm{res}} = \left.\frac{\sum_{x,y}\langle J^a_{5q}(y,t)J^a_5(x,0)\rangle}{\sum_{x,y}\langle J^a_5(y,t)J^a_5(x,0)\rangle}\right|_{t\geq t_{min}}$$

Residual Mass vs time



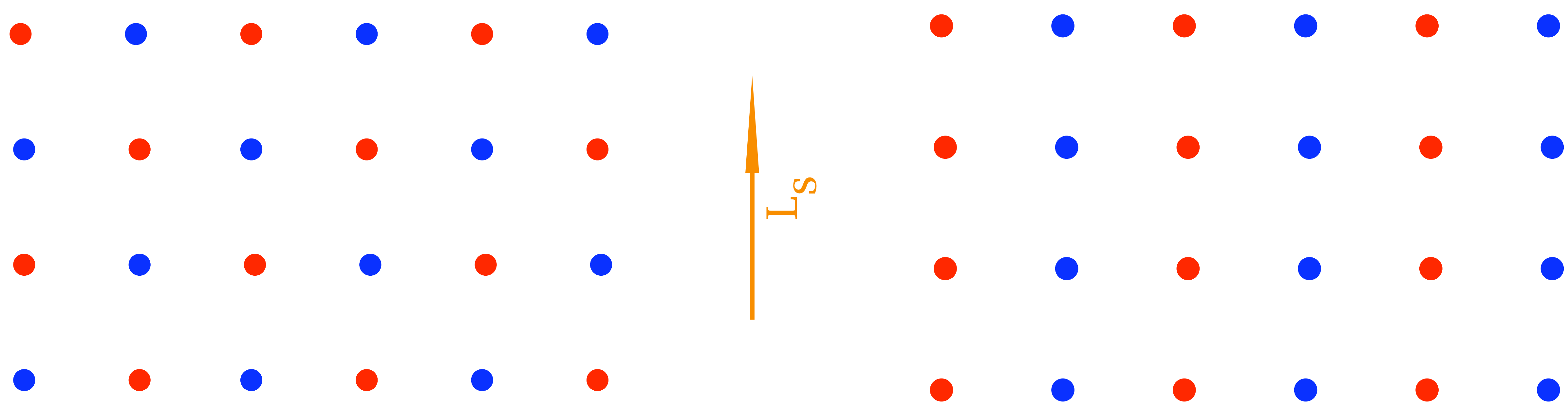
Residual mass and the GW

$$2\gamma_5\Delta_L \equiv \gamma_5\frac{1}{2}\left[1 - \varepsilon_{L_s}{}^2\right] = \gamma_5 D^0_{ov} + D^0_{ov}\gamma_5 - 2D^0_{ov}\gamma_5 D^0_{ov}$$

- The violation of the GW relation is related to the residual mass

$$M_{\rm res} = \frac{\sum_{x,y}\langle J^a_{5q}(y) J^a_5(x)\rangle}{\sum_{x,y}\langle J^a_5(y) J^a_5(x)\rangle} = \frac{{\rm Tr}\Delta_L \frac{1}{D^\dagger_{ov} D_{ov}}}{{\rm Tr} G_\pi}$$

Even-odd preconditioning



Even - Odd preconditioning

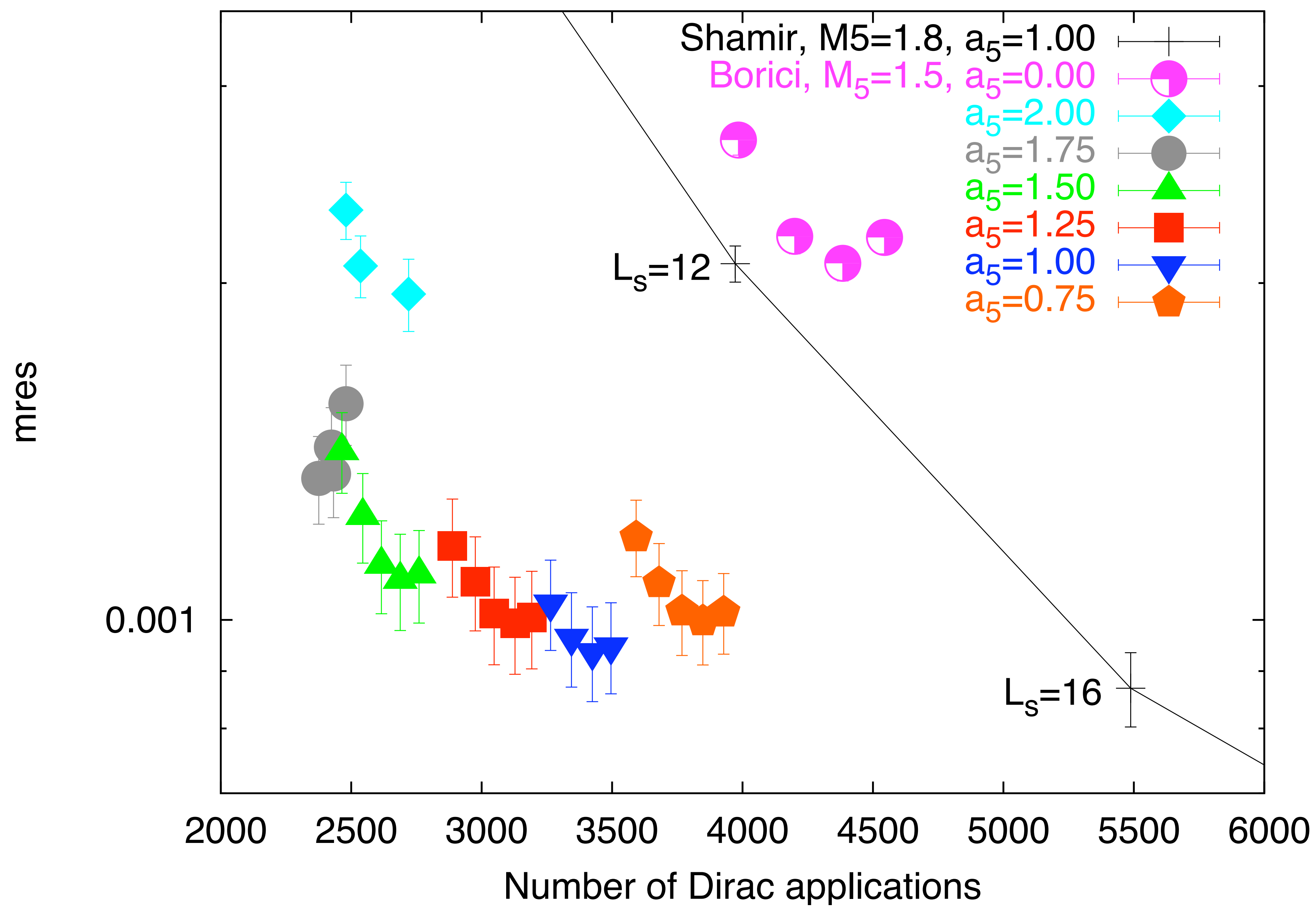
4D Even - Odd preconditioning

$$\mathbf{Q}_{DWF} = \begin{pmatrix} \mathbf{Q}_{ee} & \mathbf{Q}_{eo} \\ \mathbf{Q}_{oe} & \mathbf{Q}_{oo} \end{pmatrix} = \begin{pmatrix} \mathbf{Q}_{ee} & 0 \\ 0 & \mathbf{Q}_{oo} \end{pmatrix} \times \begin{pmatrix} 1 & 0 \\ \mathbf{Q}_{oo}^{-1}\mathbf{Q}_{oe} & 1 \end{pmatrix} \times \begin{pmatrix} 1 & 0 \\ 0 & 1 - \mathbf{Q}_{oo}^{-1}\mathbf{Q}_{oe}\mathbf{Q}_{ee}^{-1}\mathbf{Q}_{eo} \end{pmatrix} \times \begin{pmatrix} 1 & \mathbf{Q}_{ee}^{-1}\mathbf{Q}_{eo} \\ 0 & 1 \end{pmatrix}$$

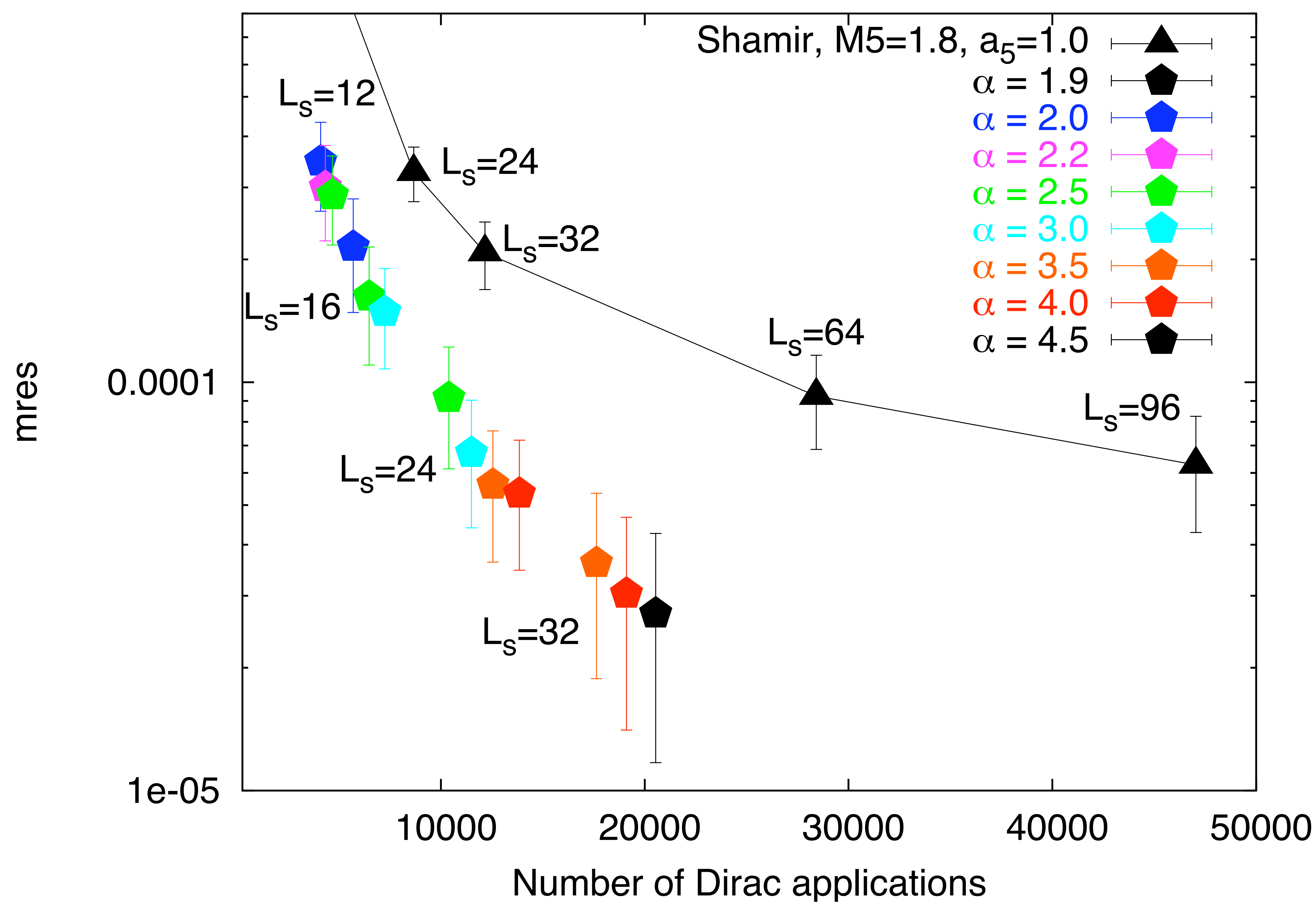
- The mobius extra terms do not allow 5d even-odd preconditioning

For the 4d preconditioning the even-even and odd-odd are non-trivial they do not depend on the gauge fields and can be inverted with few extra flops

Residual Mass: Quenched



- Quenched 2GeV cutoff
- Almost 40% speedup



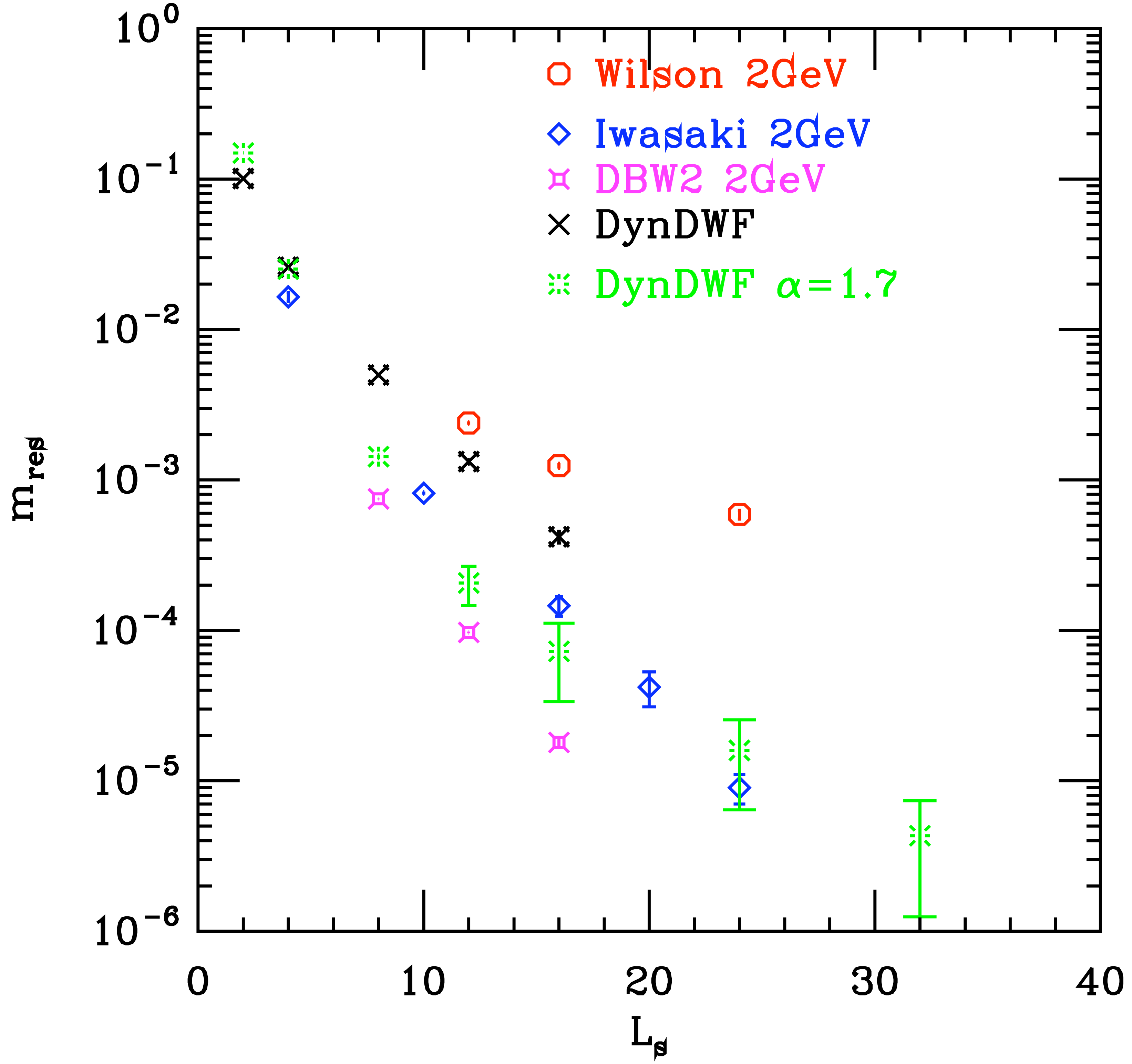
- Change the scale as we change L_s
- Speed up approaches a factor of infinity!

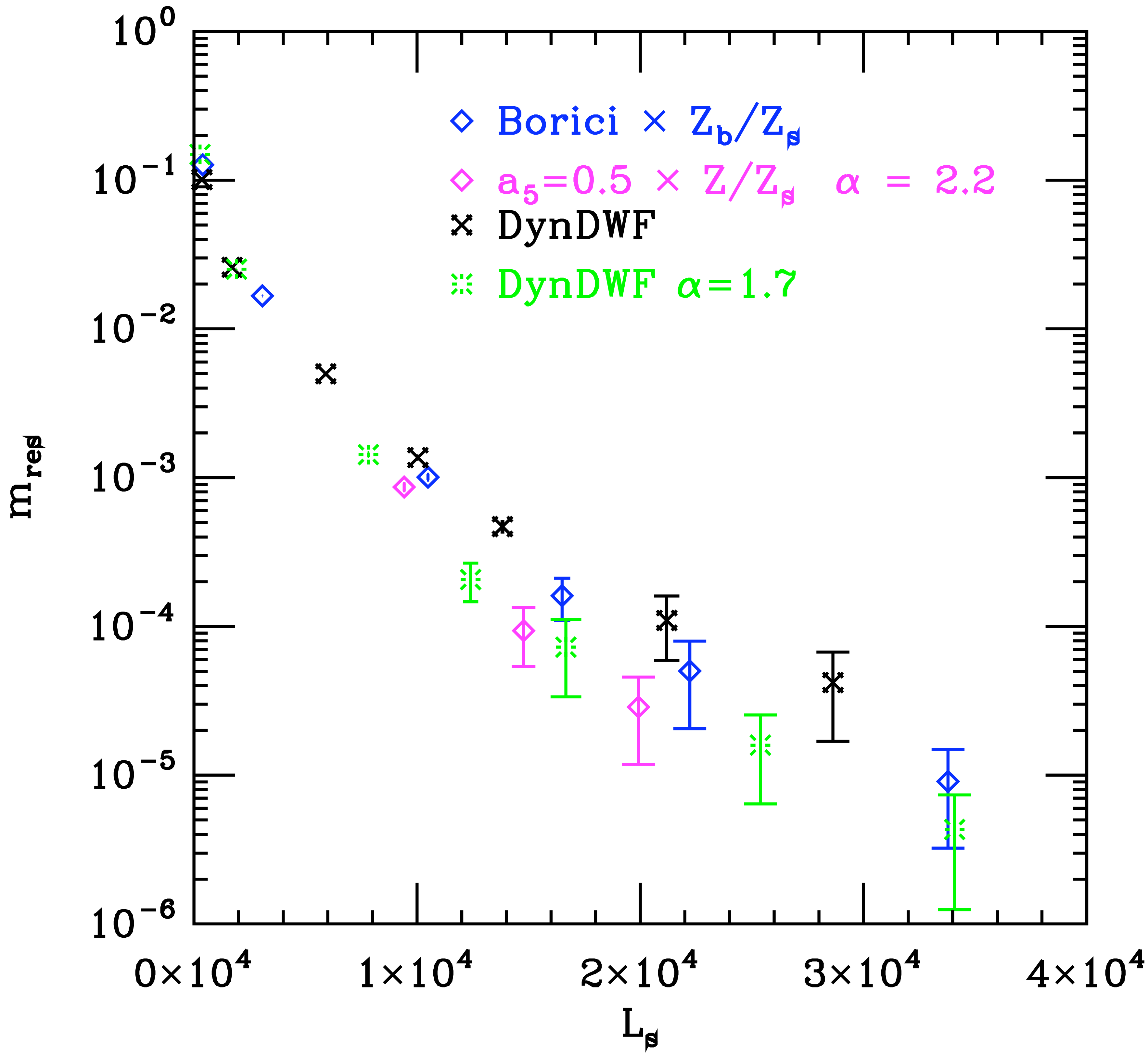
What's best for Dynamical

with R. Brower, R. Edwards, B. Joo, T. Kennedy, H. Neff and U. Wenger

- Define a metric for efficiency
- Ask: What is the cost for given residual mass
- Tested Mobius and Continued Fraction 5D algorithms
- Use RBC dynamical light mass configurations (25cnfs M_{π}~500MeV)
- Open question: How small chiral symmetry can we tolerate?
- We do not have to have exact chiral symmetry to do QCD

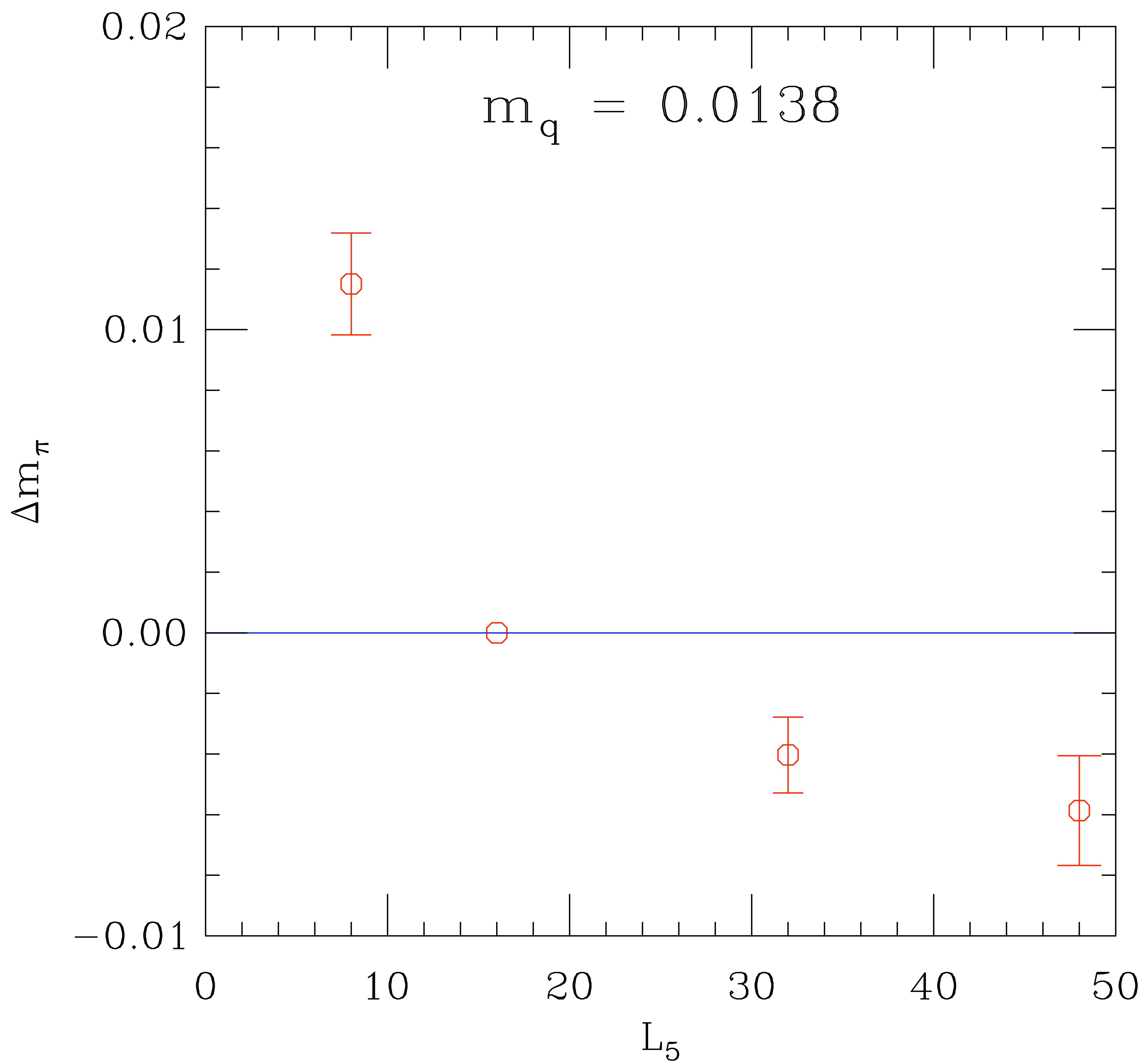
Residual Mass: dynamical



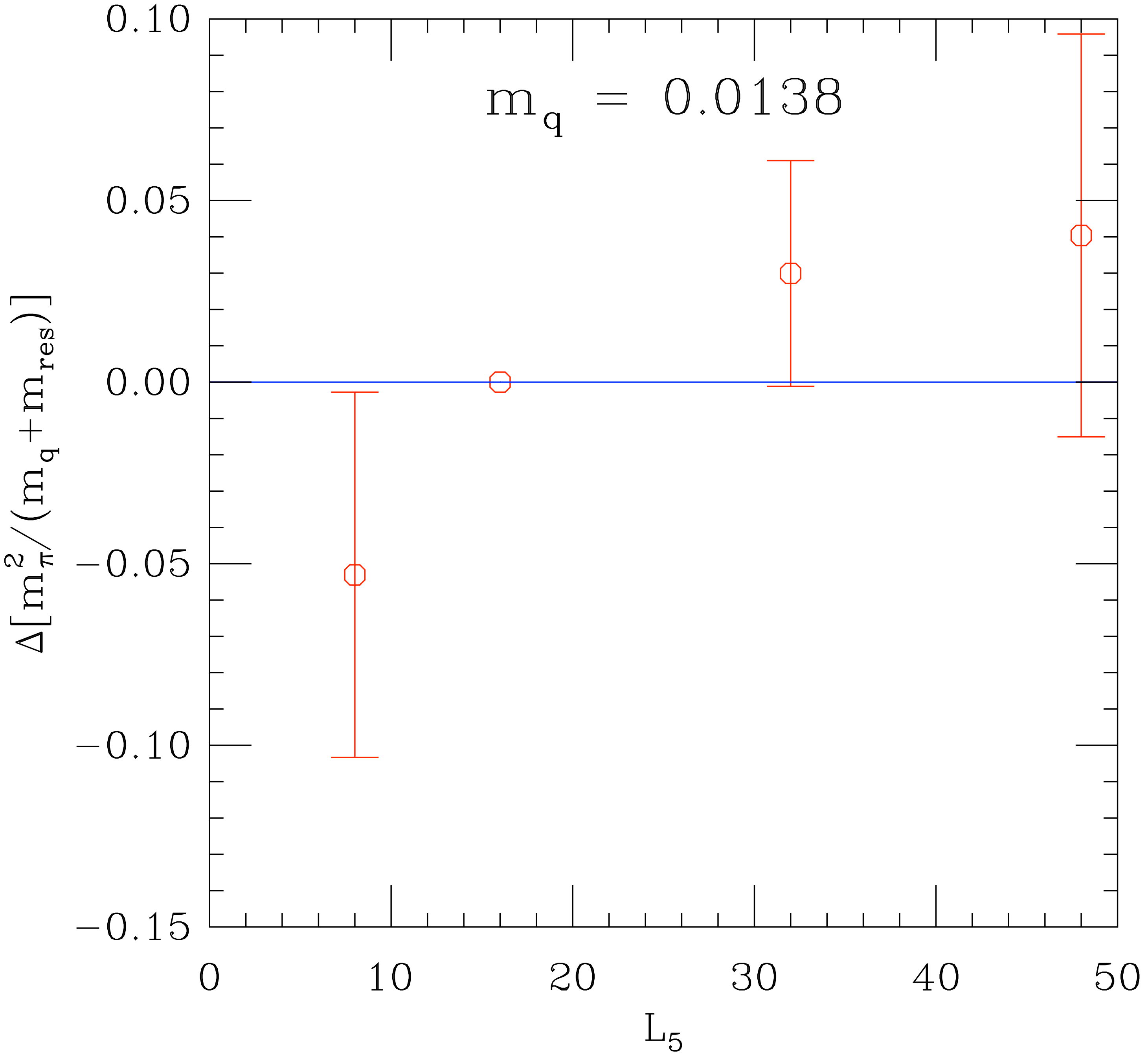


Borici × Z_b/Z_s
a_5=0.5 × Z/Z_s α = 2.2
DynDWF
DynDWF α=1.7
m_res
L_s
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
0×10^4
1×10^4
2×10^4
3×10^4
4×10^4

Dependence on Ls



LHPC data on MILC lattices



- Checks if $m_\pi^2 = C(m_q + m_{\text{res}})$

LHPC data on MILC lattices

Mobius and Zolotarev

- An other approximation to the sign function

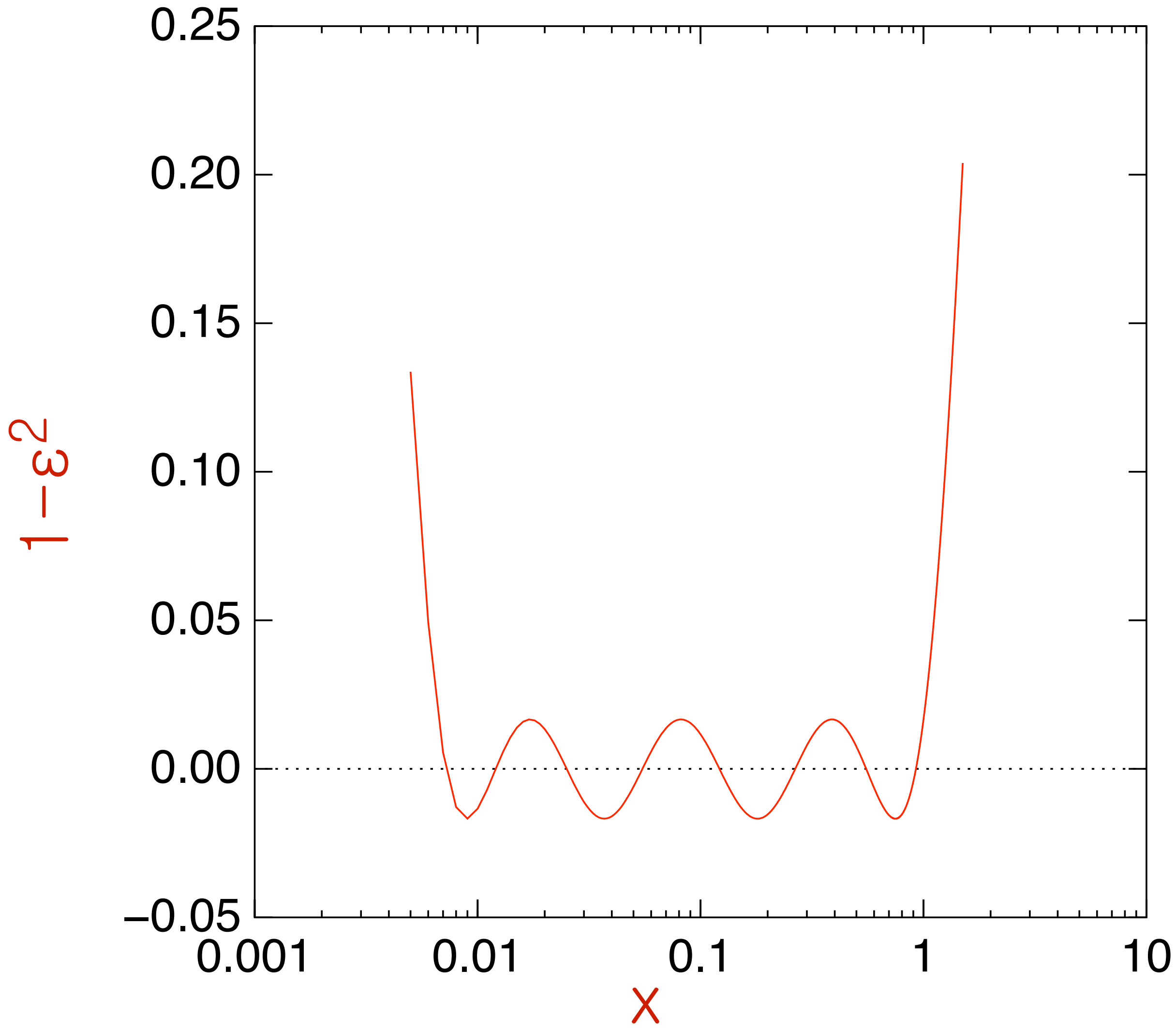
$$\varepsilon_{L_s}(x) = \frac{\prod_s^{L_s}(1+\alpha_s x) - \prod_s^{L_s}(1-\alpha_s x)}{\prod_s^{L_s}(1+\alpha_s x) + \prod_s^{L_s}(1-\alpha_s x)}$$

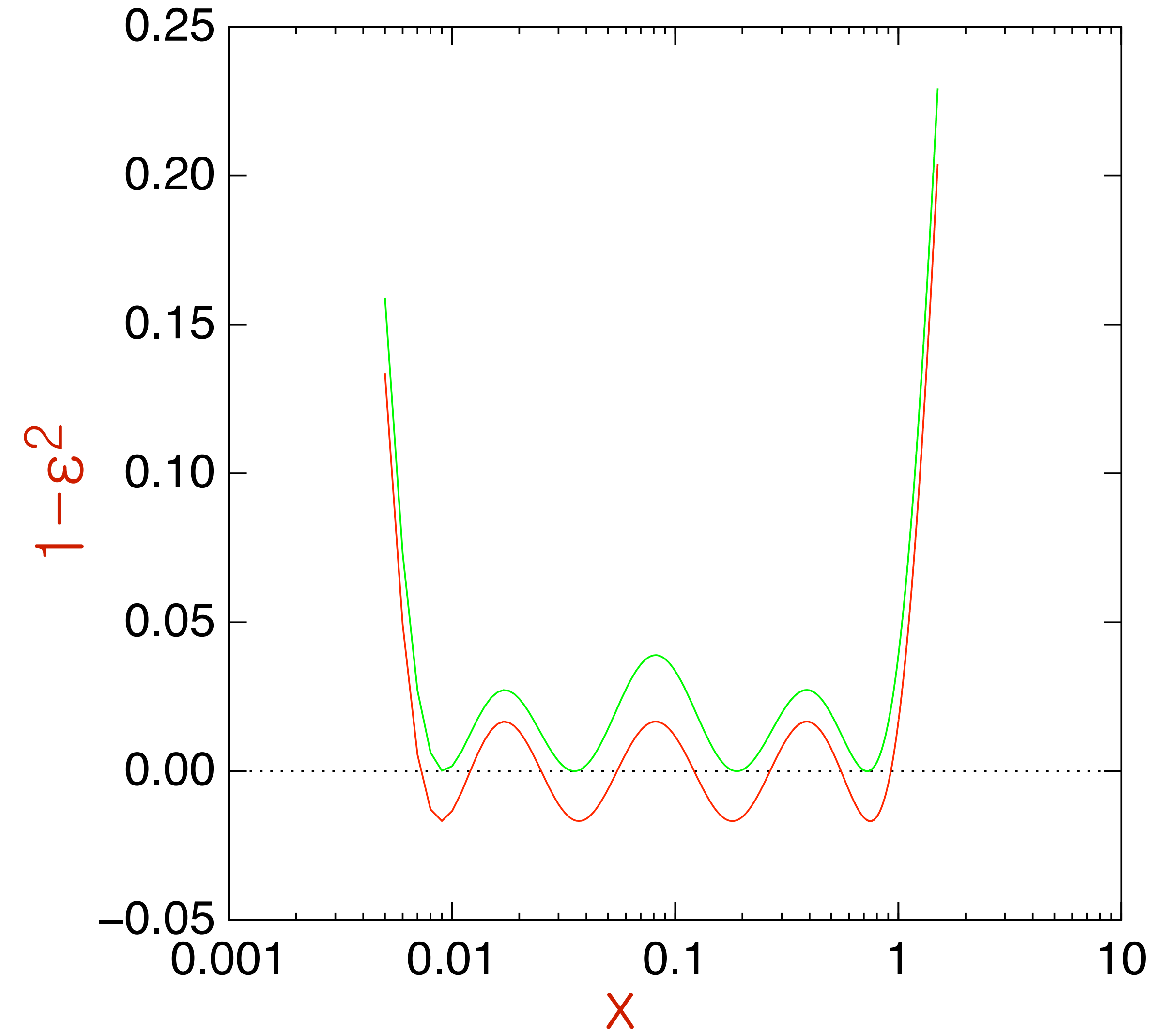
- The error in the approximation

$$\frac{1}{4}[1-\varepsilon_{L_s}^2(x)] = \frac{\prod_s^{L_s}(1+\alpha_s x)\prod_s^{L_s}(1-\alpha_s x)}{\left[\prod_s^{L_s}(1+\alpha_s x) + \prod_s^{L_s}(1-\alpha_s x)\right]^2}$$

- The error is zero for $x=\mp 1/\alpha_s$

- Zolotarev: Find α_s so that the approximation is optimal in a given interval





- Single zeros produce negative error.
- The residual mass is not positive!
- Possibility of exceptional configurations for m>0
- The problem can be fixed: Use double zeros

No free lunch theorem

- The Zolotarev Mobius operator is badly conditioned
- The cost of the calculation explodes if any of the $\alpha_s > 5$
- Zolotarev is impractical for Mobius
- We need to find a preconditioner that solves the problem
- We do have some ideas we are exploring....

Improved HMC for DWF

Two objectives:

- Achieve good accuracy of chiral symmetry
  - Increasing L_s also causes acceptance problems
  - HMC scales with $V_{5d}^{\frac{5}{4}}$
- Avoid critical slowing down as we approach the chiral limit
  - This seems most important

Current algorithms

What has been done?

- Fleming - Vranas and RBC (old)

$$detD_{ov}^{\dagger}D_{ov} = \int d\phi_0 \cdots d\phi_{L_s-1} d\phi_0^{pv} \cdots d\phi_{L_s-1}^{pv} e^{-\phi^{\dagger}\mathcal{P}^{\dagger}\frac{1}{D_{dwf}^{\dagger}}\frac{1}{D_{dwf}}\mathcal{P}\phi \; - \; \phi^{pv\dagger}\mathcal{P}^{\dagger}D_{pv}^{\dagger}D_{pv}\mathcal{P}\phi^{pv}}$$

- Dawson and RBC (new)

$$detD_{ov}^{\dagger}D_{ov} = \int d\phi_0 \cdots d\phi_{L_s-1} e^{-\phi^{\dagger}\mathcal{P}^{\dagger}D_{pv}^{\dagger}\frac{1}{D_{dwf}^{\dagger}}\frac{1}{D_{dwf}}D_{pv}\mathcal{P}\phi}$$

New HMC algoritms

Try to accelerate the approach to the chiral limit

$$det[M^\dagger M] = det[M_p^\dagger M_p] \times det\left[M^\dagger \frac{1}{M_p^\dagger}\frac{1}{M_p} M\right] = \int \mathcal{D}\phi\mathcal{D}\psi e^{-\phi^\dagger \frac{1}{M_p^\dagger}\frac{1}{M_p}\phi - \psi^\dagger M_p \frac{1}{M^\dagger}\frac{1}{M} M_p \psi}$$

- Luscher SAP algorithm
- Hasenbusch algorithm
- Hopefully new DWF preconditioners can be found...

Conclusions

- Dynamical chiral fermions with good chiral symmetry require enormous resources

- We need every possible algorithmic trick we can get

H. Nueberger: My main message in this paper is that in the context of dynamical fermion simulations there are many alternatives and tricks that have not been yet explored, and it might be a waste to exclusively focus on the most literal numerical implementations of the recent theoretical advances on the topic of chiral symmetry on the lattice.

- We are working on improving HMC and preconditioners for the DWF operators

- Future looks promising!