A Flatlander's Ascent into Five Dimensions

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UKQCD Collaboration

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Chiral Fermions

- Conventions
  - We work in Euclidean space
    - γ matrices are Hermitian
  - We write $D = D_\mu \cdot \gamma_\mu$
  - We assume all Dirac operators are γ_5 Hermitian

$$D^\dagger = \gamma_5 D \gamma_5$$

On-shell chiral symmetry: I

- It is possible to have chiral symmetry on the lattice without doublers if we only insist that the symmetry holds on shell
  - Such a transformation should be of the form
    $\psi \to e^{i\alpha\gamma_5(1-aD)}\psi; \quad \bar{\psi} \to \bar{\psi} e^{i\alpha(1-aD)\gamma_5}$ *(Lüscher)*
    - $\bar{\psi}$ is an independent field from $\psi^\dagger$
    - $\bar{\psi}$ has the same Spin(4) transformation properties as $\psi^\dagger$
    - $\bar{\psi}$ does <u>not</u> have the same chiral transformation properties as $\psi^\dagger$ in Euclidean space (even in the continuum)

On-shell chiral symmetry: II

- For it to be a symmetry the Dirac operator must be invariant

$$D \to e^{i\alpha(1-aD)\gamma_5} D e^{i\alpha\gamma_5(1-aD)} = D$$

- For an infinitesimal transformation this implies that

$$(1-aD)\gamma_5 D + D\gamma_5(1-aD) = 0$$

- Which is the <u>Ginsparg-Wilson</u> relation

$$\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D$$

Neuberger's operator: I

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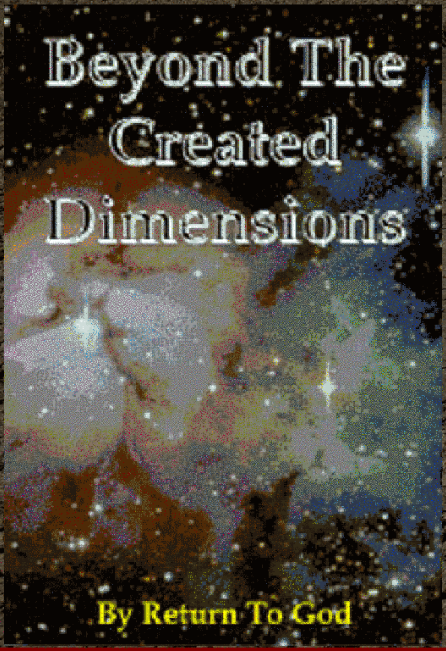
Aggressive · Creative · Persuasive

- We can find a solution of the Ginsparg-Wilson relation as follows
  - Let the lattice Dirac operator to be of the form
    $$aD = \tfrac{1}{2}\left[1+\gamma_5\hat{\gamma}_5\right];\ \hat{\gamma}_5^\dagger = \hat{\gamma}_5;\ aD^\dagger = \tfrac{1}{2}\left[1+\hat{\gamma}_5\gamma_5\right] = \gamma_5 aD\gamma_5$$
  - This satisfies the GW relation if $\hat{\gamma}_5^2 = 1$
  - And it must also have the correct continuum limit
    $$D \to \partial\!\!\!/ \Rightarrow \hat{\gamma}_5 = \gamma_5\left(2a\partial\!\!\!/ - 1\right) + O\left(a^2\right)$$
  - Both of these conditions are satisfied if we define
    $$\hat{\gamma}_5 = \gamma_5 \frac{D_W - M}{\sqrt{(D_W - M)^\dagger (D_W - M)}} = \operatorname{sgn}\left[\gamma_5 (D_W - M)\right] \quad \textit{(Neuberger)}$$

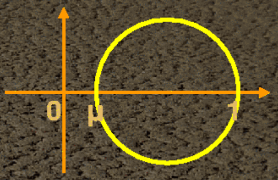
Into Five Dimensions



- H Neuberger hep-lat/9806025
- A Boriçi hep-lat/9909057, hep-lat/9912040, hep-lat/0402035
- A Boriçi, A D Kennedy, B Pendleton, U Wenger hep-lat/0110070
- R Edwards & U Heller hep-lat/0005002
- T-W Chiu hep-lat/0209153, hep-lat/0211032, hep-lat/0303008
- R C Brower, H Neff, K Orginos hep-lat/0409118

Neuberger's operator: II

$$D_N(\mu, H) = \frac{1}{2}\left[1 + \mu + (1-\mu)\gamma_5 \operatorname{sgn}(H)\right]$$



- Four dimensional space of algorithms
  - Kernel $H = \gamma_5 D_W(-M)$
  - Approximation $\operatorname{sgn}(H) \approx \varepsilon_{n,m}(H) = \frac{P_n(H)}{Q_m(H)}$
  - Representation
  - Constraint

Kernel

- Wilson (Boriçi) kernel

$$H_W = \gamma_5 D_W(-M)$$

- Shamir kernel

$$H_S = \gamma_5 D_S; \quad D_S = \frac{D_W(-M)}{2 + a_5 D_W(-M)}$$

- Möbius kernel

$$H_M = \gamma_5 D_M; \quad D_M = \frac{(b_5 + c_5) D_W(-M)}{2 + (b_5 - c_5) D_W(-M)}$$

Approximation: tanh

- Pandey, Kenney, & Laub; Higham; Neuberger
- for even n (analogous formulæ for odd n)

$$\varepsilon_{n-1,n}(x) = \tanh\left(n \tanh^{-1} x\right) = \frac{1-\left(\frac{1-x}{1+x}\right)^n}{1+\left(\frac{1-x}{1+x}\right)^n}$$

$$= xn \frac{\prod_{k=1}^{\frac{n}{2}-1}\left(x^2+\tan^2\frac{k\pi}{n}\right)}{\prod_{k=1}^{\frac{n}{2}}\left(x^2+\tan^2\frac{\left(k+\frac{1}{2}\right)\pi}{n}\right)} = \frac{2x}{n}\sum_{k=1}^{\frac{n}{2}}\frac{1}{x^2\cos^2\left[\frac{\pi}{n}\left(k-\frac{1}{2}\right)\right]+\sin^2\left[\frac{\pi}{n}\left(k-\frac{1}{2}\right)\right]}$$

ω_j

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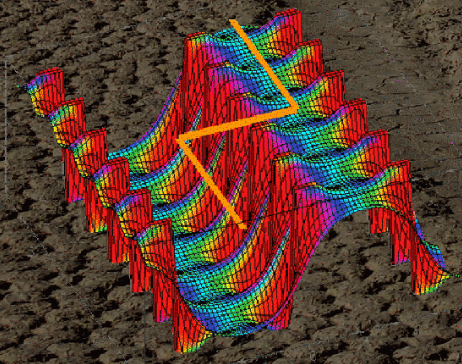
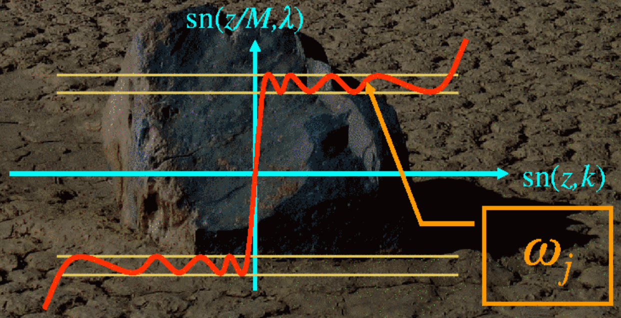
Approximation: Золотарев

$$\frac{\operatorname{sn}(z/M;\lambda)}{\operatorname{sn}(z;k)} = \frac{1}{M}\prod_{m=1}^{\lfloor n/2 \rfloor}\frac{1-\frac{\operatorname{sn}(z;k)^2}{\operatorname{sn}(2iK'm/n;k)^2}}{1-\frac{\operatorname{sn}(z;k)^2}{\operatorname{sn}\left(2iK'\left(m-\frac{1}{2}\right)/n;k\right)^2}}$$





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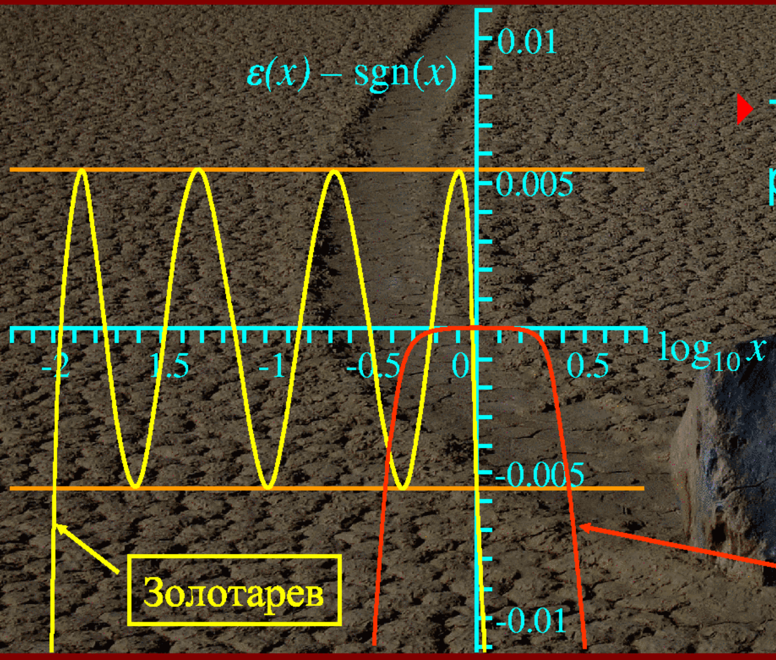
Approximation: Errors



- The fermion sgn problem
  - Approximation over $10^{-2} < |x| < 1$
  - Rational functions of degree (7,8)

Representation: Schur Complement

- Consider the block matrix
  - Equivalently a matrix over a skew field = division ring
  - It may be block diagonalised by an LDU factorisation (Gaussian elimination)

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \cdot \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \cdot \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix}$$

  - The bottom right block is the Schur complement
    - In particular $\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det\left(AD - ACA^{-1}B\right)$

Representation: Continued Fraction I

- Consider a five-dimensional matrix of the form
  - Compute its LDU decomposition

$$\begin{pmatrix} A_0 & 1 & 0 & 0 \\ 1 & A_1 & 1 & 0 \\ 0 & 1 & A_2 & 1 \\ 0 & 0 & 1 & A_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ S_0^{-1} & 1 & 0 & 0 \\ 0 & S_1^{-1} & 1 & 0 \\ 0 & 0 & S_2^{-1} & 1 \end{pmatrix} \cdot \begin{pmatrix} S_0 & 0 & 0 & 0 \\ 0 & S_1 & 0 & 0 \\ 0 & 0 & S_2 & 0 \\ 0 & 0 & 0 & S_3 \end{pmatrix} \cdot \begin{pmatrix} 1 & S_0^{-1} & 0 & 0 \\ 0 & 1 & S_1^{-1} & 0 \\ 0 & 0 & 1 & S_2^{-1} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

  - where $S_0 = A_0; \quad S_n + \frac{1}{S_{n-1}} = A_n$
  - then the Schur complement of the matrix is the continued fraction $S_3 = A_3 - \frac{1}{S_2} = A_3 - \frac{1}{A_2 - \frac{1}{S_1}} = A_3 - \frac{1}{A_2 - \frac{1}{A_1 - \frac{1}{A_0}}}$

Representation: Continued Fraction II

- We may use this representation to linearise our rational approximations to the sgn function

$$\varepsilon_{n-1,n}(H) = \beta_0 H + \cfrac{c_1}{c_1\beta_1 H + \cfrac{c_1 c_2}{c_2\beta_2 H + \ddots + \cfrac{c_{n-1}c_n}{c_n\beta_n H}}}$$

- as the Schur complement of the five-dimensional matrix

$$\begin{pmatrix} c_n^2\beta_n H & c_{n-1}c_n & 0 & & & \\ c_{n-1}c_n & -c_{n-1}^2\beta_{n-1}H & \ddots & 0 & & \\ 0 & \ddots & \ddots & & 0 & \\ & 0 & \ddots & c_2^2\beta_2 H & c_1c_2 & 0 \\ & & 0 & c_1c_2 & -c_1^2\beta_1 H & c_1 \\ & & & 0 & c_1 & \beta_0 H \end{pmatrix}$$

Representation: Partial Fraction

- Consider a five-dimensional matrix of the form *(Neuberger & Narayanan)*
  - Compute its LDU decomposition
  - its Schur complement is $R + \frac{p_1 x}{x^2+q_1} + \frac{p_2 x}{x^2+q_2}$
  - which allows us to represent the partial fraction expansion of our rational function as the Schur complement of a five-dimensional linear system

$$\begin{pmatrix} \frac{x}{p_1} & 1 & 0 & 0 & 1 \\ 1 & -\frac{p_1 x}{q_1} & 0 & 0 & 0 \\ 0 & 0 & \frac{x}{p_2} & 1 & 1 \\ 0 & 0 & 1 & -\frac{p_2 x}{q_2} & 0 \\ -1 & 0 & -1 & 0 & R \end{pmatrix}$$

$$\varepsilon_{n-1,n}(H) = H \sum_{j=1}^{n} \frac{p_j}{H^2+q_j}$$

Representation: Cayley Transform I

- Consider a five-dimensional matrix of the form
  - Compute its LDU decomposition

$$\begin{pmatrix} 1 & -A_1 & 0 & 0 \\ 0 & 1 & -A_2 & 0 \\ 0 & 0 & 1 & -A_3 \\ -A_0 & 0 & 0 & C \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -A_0 & -A_0A_1 & -A_0A_1A_2 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & C-A_0A_1A_2A_3 \end{pmatrix} \cdot \begin{pmatrix} 1 & -A_1 & 0 & 0 \\ 0 & 1 & -A_2 & 0 \\ 0 & 0 & 1 & -A_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

  - so its Schur complement is $S_{\text{CT}} = C - A_0 A_1 \cdots A_n$
  - Set $C = c_+; A_0 = -c_- T_0; A_j = T_j$ where $c_\pm = \frac{1}{2}(1 \pm \gamma_5) + \frac{1}{2}(1 \mp \gamma_5)\mu$
  - then $S_{\text{CT}}(\mu) = \frac{1}{2}\left[(1+\mu) + (1-\mu)\gamma_5 \frac{1-T}{1+T}\right](1+T)$ with $T = T_0 \cdots T_n$

Representation: Cayley Transform II

- Hence the Neuberger operator is $D_{\mathrm{N}}(\mu, H) \approx \frac{S_{\mathrm{CT}}(\mu)}{S_{\mathrm{CT}}(1)}$
- if $T(x)$ is the Euclidean Cayley transform of $\varepsilon_{n,m}(x) \approx \mathrm{sgn}(x)$

$$\varepsilon(x) = \frac{1-T(x)}{1+T(x)}; \quad T(x) = \frac{1-\varepsilon(x)}{1+\varepsilon(x)}$$

- for an odd function we have $\varepsilon(-x) = -\varepsilon(x) \Leftrightarrow T(-x) = \frac{1}{T(x)}$

$$\varepsilon(0) = 0 \Leftrightarrow T(0) = 1 \qquad T_j(x) = \frac{\omega_j - x}{\omega_j + x}$$

  - In Minkowski space a Cayley transform maps between Hermitian (Hamiltonian) and unitary (transfer) matrices

Representation: Cayley Transform III

- Thus the Neuberger operator with a general Möbius kernel is the Schur complement of D_5

$$\begin{pmatrix} D_+^{(1)} & P_-D_-^{(2)} & 0 & \cdots & \mu P_+ D_-^{(n)} \\ P_+D_-^{(1)} & D_+^{(2)} & P_-D_-^{(3)} & & 0 \\ 0 & P_+D_-^{(2)} & D_+^{(3)} & \ddots & 0 \\ \vdots & & \ddots & \ddots & \\ \mu P_-D_-^{(1)} & 0 & 0 & P_+D_-^{(n-1)} & D_+^{(n)} \end{pmatrix} = P_+ \begin{pmatrix} D_+^{(1)} & 0 & 0 & \cdots & \mu D_-^{(n)} \\ D_-^{(1)} & D_+^{(2)} & 0 & & 0 \\ 0 & D_-^{(2)} & D_+^{(3)} & \ddots & 0 \\ \vdots & & \ddots & \ddots & \\ 0 & 0 & 0 & D_-^{(n-1)} & D_+^{(n)} \end{pmatrix} + P_- \begin{pmatrix} D_+^{(1)} & D_-^{(2)} & 0 & \cdots & 0 \\ 0 & D_+^{(2)} & D_-^{(3)} & & 0 \\ 0 & 0 & D_+^{(3)} & \ddots & 0 \\ \vdots & & \ddots & \ddots & \\ \mu D_-^{(1)} & 0 & 0 & 0 & D_+^{(n)} \end{pmatrix}$$

- with $P_\pm = \frac{1}{2}(1 \pm \gamma_5)$ and

$$D_+^{(j)} = b_5^j D_W(-M) + 1; \quad D_-^{(j)} = c_5^j D_W(-M) - 1$$

$$b_5^j + c_5^j = \frac{b_5 + c_5}{\omega_j}; \quad b_5^j - c_5^j = b_5 - c_5$$

Representation: Cayley Transform IV

- Cyclically shift the right-handed part $\tilde{D}_5 = \wp D_5$ where

$$\wp = P_+ \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ \vdots & & & \ddots & \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} + P_- \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & & & \ddots & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\tilde{D}_5 = P_- \begin{pmatrix} D_+^{(1)} & D_-^{(2)} & 0 & \cdots & 0 \\ 0 & D_+^{(2)} & D_-^{(3)} & & 0 \\ 0 & 0 & D_+^{(3)} & \ddots & 0 \\ \vdots & & \ddots & \ddots & \\ \mu D_-^{(1)} & 0 & 0 & & D_+^{(n)} \end{pmatrix} + P_+ \begin{pmatrix} D_-^{(1)} & D_+^{(2)} & 0 & \cdots & 0 \\ 0 & D_-^{(2)} & D_+^{(3)} & & 0 \\ 0 & 0 & D_-^{(3)} & \ddots & 0 \\ \vdots & & \ddots & \ddots & \\ \mu D_+^{(1)} & 0 & 0 & & D_-^{(n)} \end{pmatrix}$$

Constraint: I

- So, what can we do with the Neuberger operator represented as a Schur complement?
  - Consider the five-dimensional system of linear equations

$$D_5 \begin{pmatrix} \tilde{\phi}_1 \\ \tilde{\phi}_2 \\ \vdots \\ \tilde{\phi}_{n-2} \\ \tilde{\phi}_{n-1} \\ \psi \end{pmatrix} = LDU \begin{pmatrix} \tilde{\phi}_1 \\ \tilde{\phi}_2 \\ \vdots \\ \tilde{\phi}_{n-2} \\ \tilde{\phi}_{n-1} \\ \psi \end{pmatrix} = LD \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{n-2} \\ \phi_{n-1} \\ \psi \end{pmatrix} = L \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \chi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \chi \end{pmatrix}$$

  - The bottom four-dimensional component is $D_{n,n}\psi = D_N\psi = \chi$

Constraint: II

- Alternatively, introduce a five-dimensional pseudofermion field $\Phi = \begin{pmatrix} \phi_1 & \phi_2 & \cdots & \phi_{n-1} & \psi \end{pmatrix}$
  - then the pseudofermion functional integral is

$$\int d\Phi^\dagger d\Phi \, e^{-\Phi^\dagger D_5^{-1}\Phi} \propto \det D_5 = \det LDU = \det D = \prod_{j=1}^{n} \det D_{j,j}$$

  - So we also introduce n-1 "Pauli-Villars" fields

$$\prod_{j=1}^{n-1} \int d\xi_j^\dagger d\xi_j \, e^{-\xi_j^\dagger D_{j,j}\xi_j} \propto \left[\prod_{j=1}^{n-1} \det D_{j,j} \right]^{-1}$$

  - and we are left with just $\det D_{n,n} = \det D_N$

Matrix-vector applications

	M	$M^\dagger$	$M^\dagger M$	Relative cost per CG iteration compared to DWF
DWF (Shamir/Möbius)	n	n	$2n$	1
Continued Fraction (H_W)	n	n	$2n$	1
Continued Fraction (H_S)	$2n+1$	$n+1$	$3n+2$	$\frac{3}{2}+\frac{1}{n}$

Chiral Symmetry Breaking

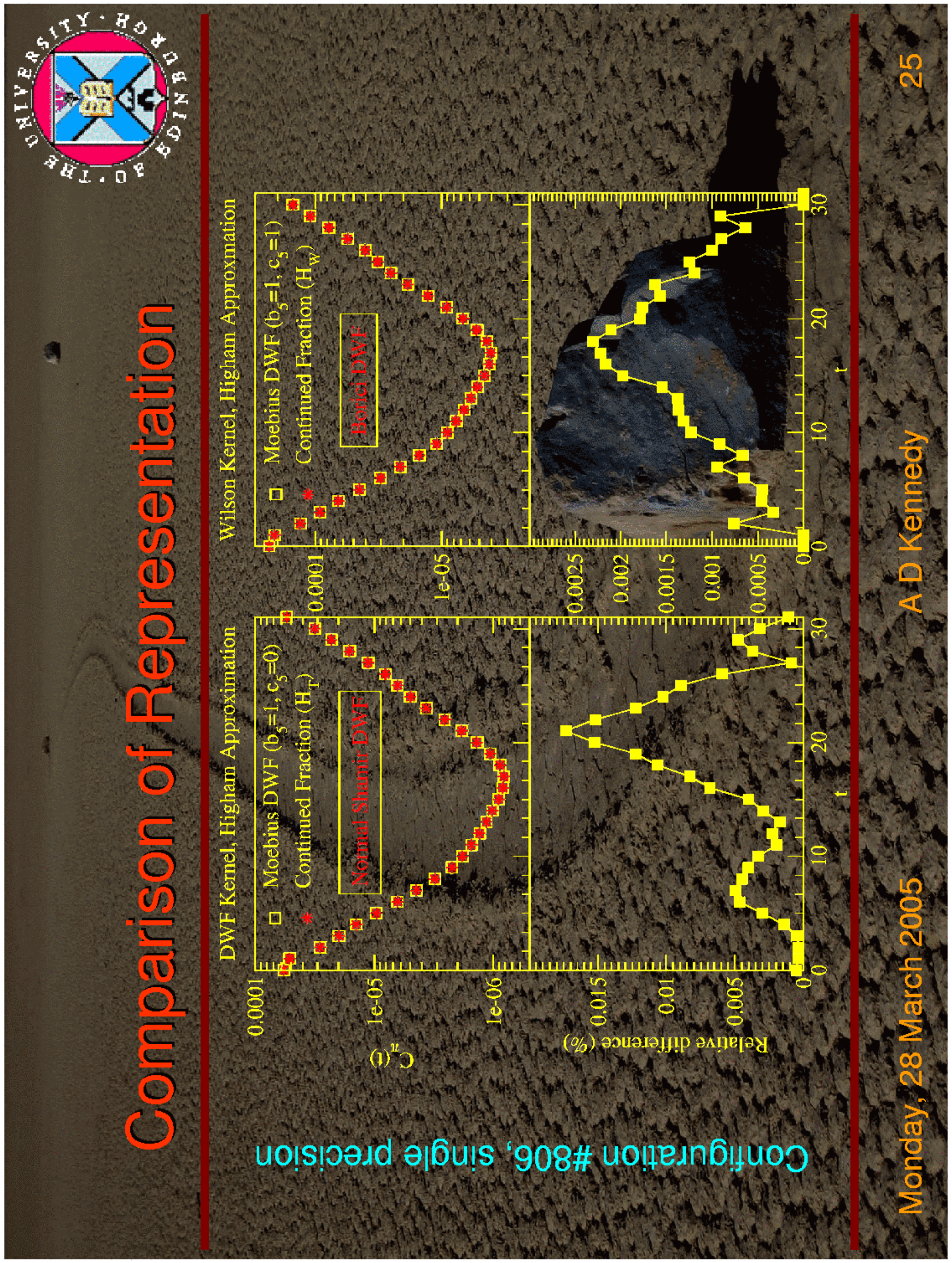
- Ginsparg-Wilson defect $\gamma_5 D + D\gamma_5 - 2aD\gamma_5 D = \gamma_5 \Delta_L$
  - using the approximate Neuberger operator $aD = \frac{1}{2}\left[1 + \gamma_5 \varepsilon(H)\right]$
  - Δ_L measures chiral symmetry breaking $a\Delta_L = \frac{1}{2}\left[1 - \varepsilon^2(H)\right]$
  - The quantity $m_{\text{res}} = \frac{\langle \operatorname{tr} G^\dagger \Delta_L G \rangle}{\langle \operatorname{tr} G^\dagger G \rangle}$ is just the usual domain wall residual mass *(Brower et al.)*
    - G is the π propagator
    - m_{res} is just one moment of Δ_L

Numerical Studies

- Used 15 configurations from the RBRC dynamical DWF dataset

$$V = 16^3 \times 32 \quad n = L_s = 12 \quad n_f = 2$$
$$\beta = 0.8 \quad M = -1.8 \quad \mu = 0.02$$

- Matched π mass for Wilson and Möbius kernels
- All operators are even-odd preconditioned
- Did not project eigenvectors of H_W


Comparison of Representation
DWF Kernel, Higham Approximation
Moebius DWF (b_5=1, c_5=0)
Continued Fraction (H_T)
Normal Shamir DWF
Wilson Kernel, Higham Approximation
Moebius DWF (b_5=1, c_5=1)
Continued Fraction (H_W)
Borici DWF
$C_\pi(t)$
Relative difference (%)
t
Configuration #806, single precision
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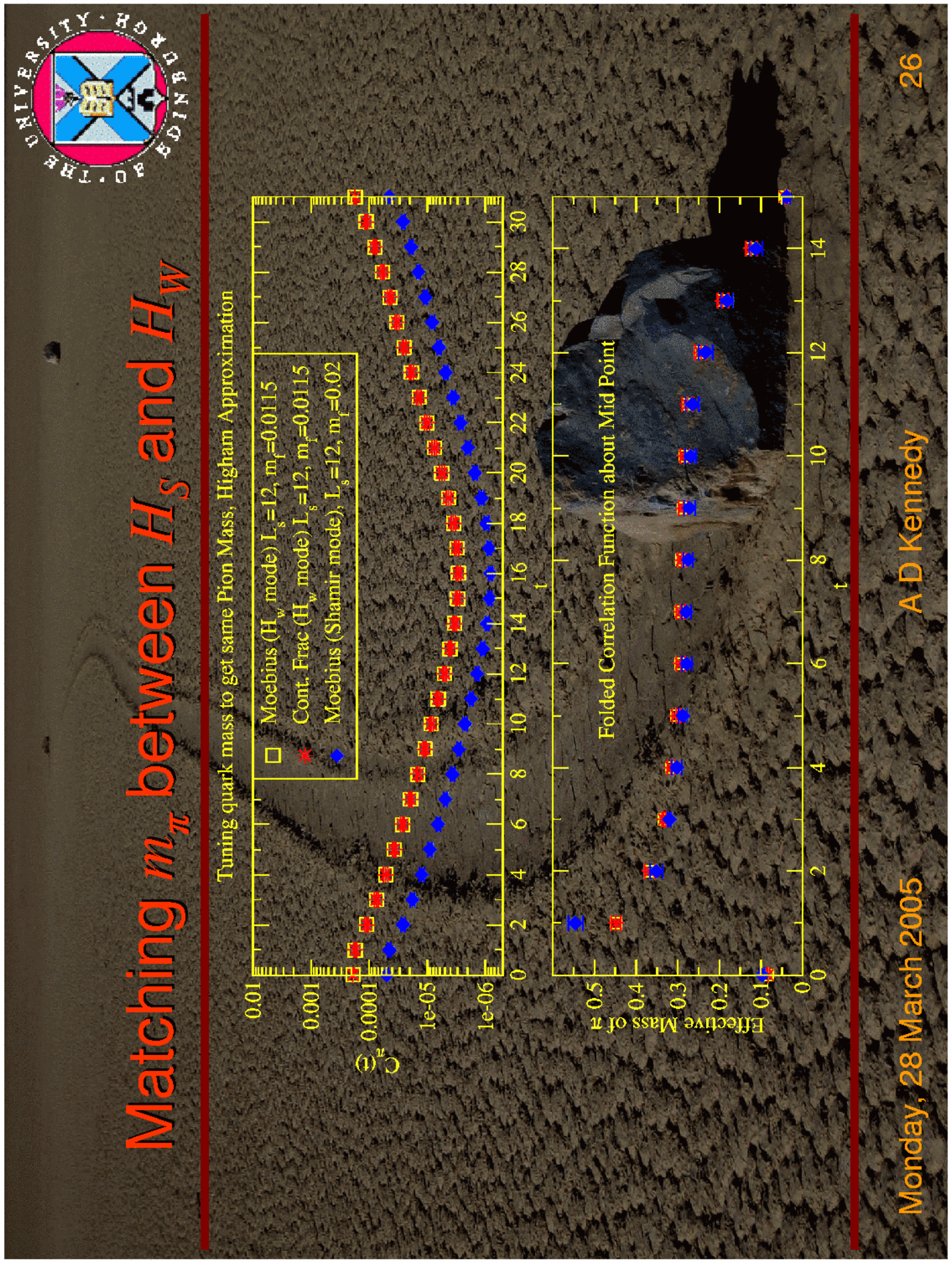
Matching m_π between H_S and H_W
Tuning quark mass to get same Pion Mass, Higham Approximation
Moebius (H_w mode) L_s=12, m_f=0.0115
Cont. Frac (H_w mode) L_s=12, m_f=0.0115
Moebius (Shamir mode) L_s=12, m_f=0.02
$C_\pi(t)$
Folded Correlation Function about Mid Point
Effective Mass of π
t
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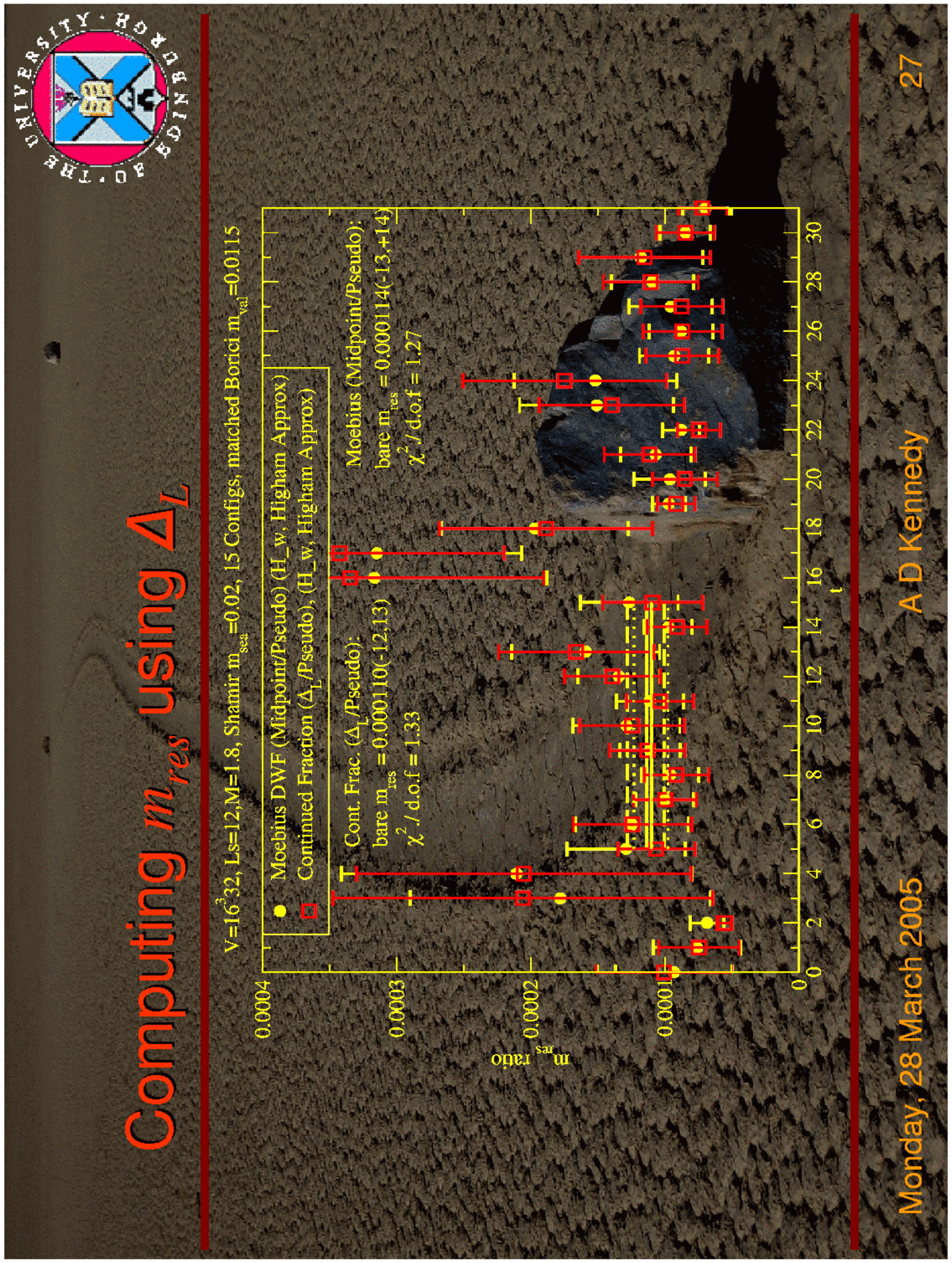
Computing m_{res} using Δ_L
V=16^3 32, Ls=12,M=1.8, Shamir m_sea=0.02, 15 Configs, matched Borici m_val=0.0115
Moebius DWF (Midpoint/Pseudo) (H_w, Higham Approx)
Continued Fraction (Δ_L/Pseudo), (H_w, Higham Approx)
Cont. Frac. (Δ_L/Pseudo):
bare m_res = 0.000110(-12,13)
χ² / d.o.f = 1.33
Moebius (Midpoint/Pseudo):
bare m_res = 0.000114(-13,+14)
χ² / d.o.f = 1.27
m_res ratio
t
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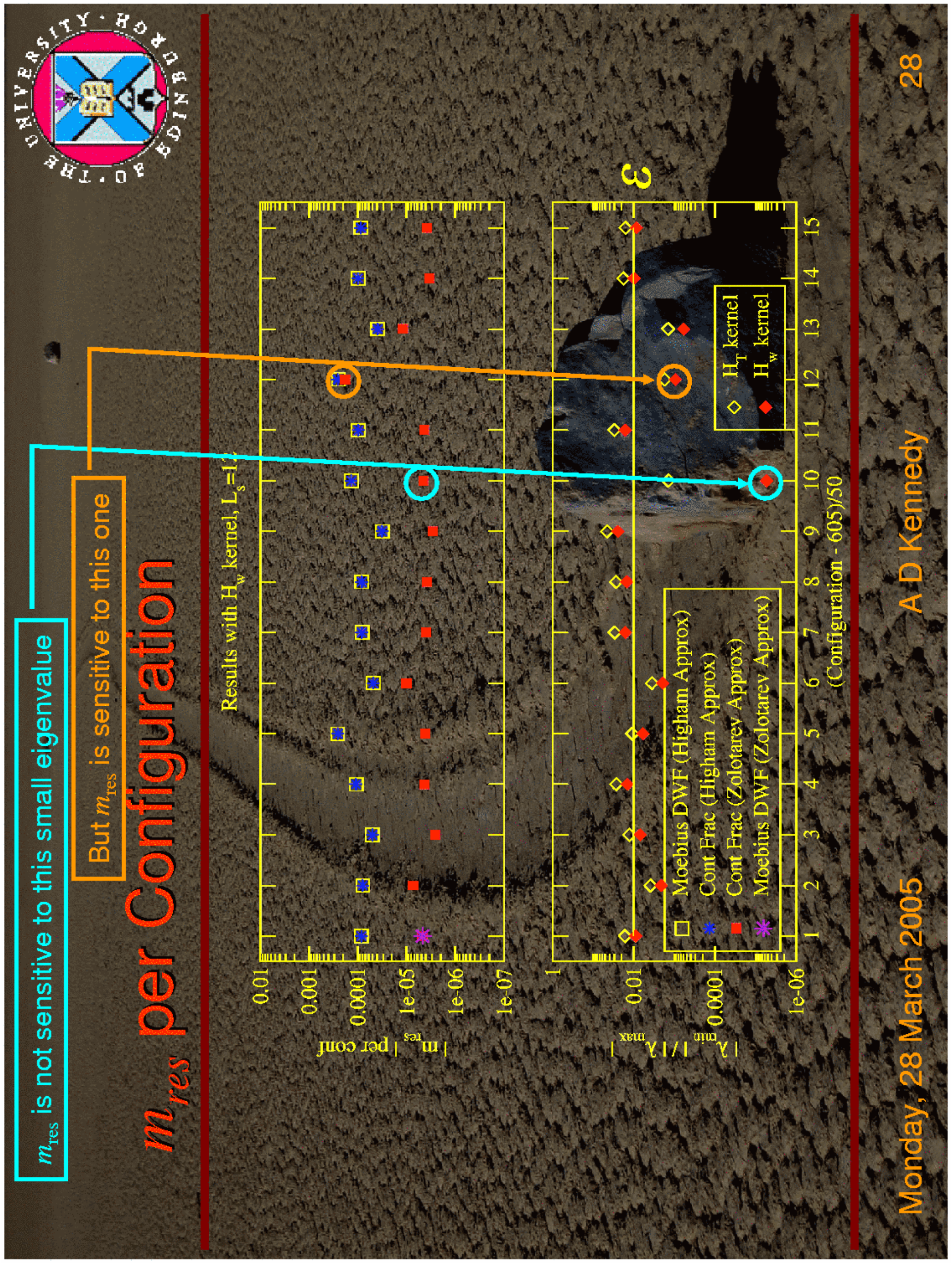
m_{res} per Configuration
m_{res} is not sensitive to this small eigenvalue
But m_{res} is sensitive to this one
Results with H_w kernel, L_s=12
| m_res | per conf
| λ_min | / | λ_max |
(Configuration - 605)/50
ε
H_T kernel
H_w kernel
Moebius DWF (Higham Approx)
Cont Frac (Higham Approx)
Cont Frac (Zolotarev Approx)
Moebius DWF (Zolotarev Approx)
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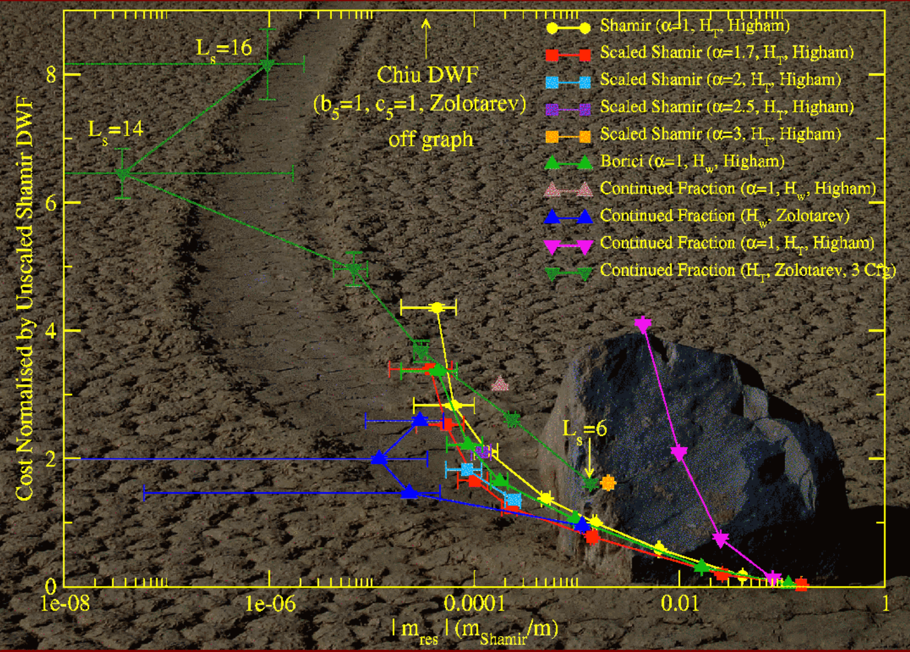
Cost versus m_{res}



Conclusions

- Good
  - Zolotarev Continued Fraction
  - Rescaled Shamir DWF via Möbius (tanh)
- Poor
  - Standard Shamir DWF
  - Zolotarev DWF (Chiu)
- Still to do…
  - Projection of small eigenvalues
  - HMC
    - 5 dimensional versus 4 dimensional dynamics
    - Hasenbusch acceleration
      - 5 dimensional multishift?
      - Possible advantage of 4 dimensional nested Krylov solvers
    - Tunnelling between different topological sectors
      - Algorithmic or physical problem (at $\mu=0$)
      - Reflection/refraction
      - Use Золотарев approximation which is infinite at origin?