

# Topological Modes in Lattice QCD Evolution

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# Motivation

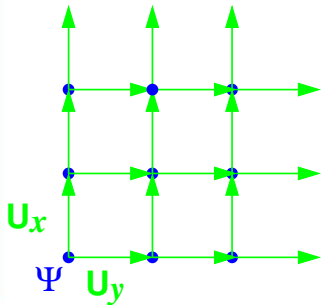
*(Why do you want/need an accurate measurement of Topological index  $Q$  on the lattice?? it is ambiguous anyway..)*

- For any LQCD measurement, it is crucial to have representative samples of QCD vacuum. Distribution of  $Q$  is one of the ways to quantify this.
- As the lattice spacing  $a$  gets smaller, the cost to generate independent samples increase rapidly ( $(\text{cost}) \geq a^{-(10-11)}$ ). One of the major focus in recent LQCD algorithmic study has been elimination of critical slowing down.

# Introduction to lattice QCD

Quantum ChromoDynamics (QCD): Theory of strong interaction which governs interaction between **quarks** and **gluons**.

In contrast to Quantum Electrodynamics (QED), The effective coupling of QCD decreases in high energy, hence is calculable by hand, but not in low energy.  $\rightarrow$  Nonperturbative techniques such as lattice QCD is needed for *ab initio* calculations.  $(\psi(x), A_\mu(x)) \rightarrow (\psi(n), U_\mu(n) = \exp(-iA_\mu))$



$$Z = \int [dU] \det(\not{D} + m) e^{-(S_g)}$$

$$= \int [dU][d\bar{\psi}][d\psi] \exp[-(S_g + S_f)]$$

$$S_f = \bar{\psi}(D^\dagger D)^{-1}\psi, \quad S_{\text{eff}} = S_g + S_f$$

$$S_g = \beta \sum \left[ (U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x)) \right]$$

Current "typical" calculation:  $V = 64^3 \times 128$ ,  $\text{rank}(D) \sim 10^{10}$ , nonzero element per row  $\sim 10^2$

# Different discretizations in Lattice QCD

Basic problem/motivation: Naive discretization

$$(\partial_\mu + iA_\mu)\psi(x) \rightarrow \frac{(U_\mu(x)\psi(x+\mu) - U_\mu^\dagger(x-\mu)\psi(x-\mu))}{2a}$$

turns  $p$  into  $\sin(p)$ .  $2^4 = 16$  particles instead of 1 (doubler).

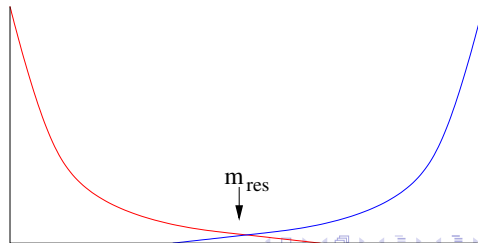
It is impossible to have a chirally invariant, doubler-free, local, translationally invariant, real bilinear fermion action on the lattice (Nielsen-Ninomiya no-go theorem).

Wilson Fermion: Add Laplacian-like term

Additive mass renormalization  $\rightarrow$  fine tuning needed.

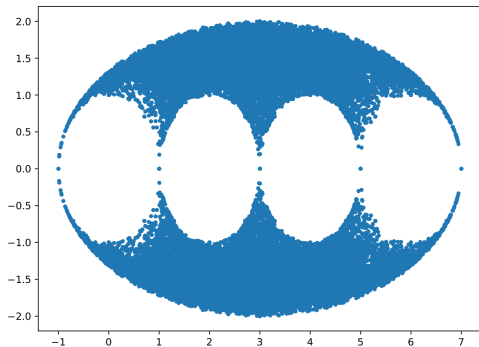
$$-\frac{a}{2}\Delta\psi(x) = -\frac{a}{2}\sum_\mu[\psi(x+a\hat{\mu}) + \psi(x-a\hat{\mu}) - 2\psi(x)]$$

Domain Wall Fermion (DWF) / Mobius/Overlap fermions: Dirac operator in 5D with repeating gauge field in 4D

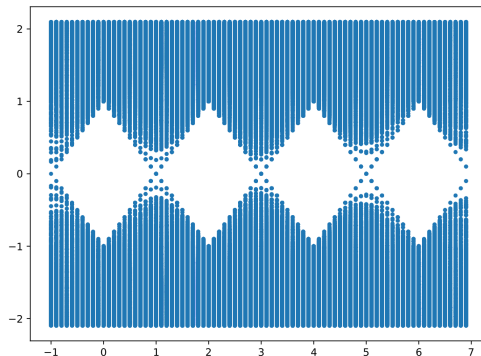


# Spectrum of Free Field $D_w, H_w, D_{ov}$

Wilson-Dirac operator  $D_w(-1)$



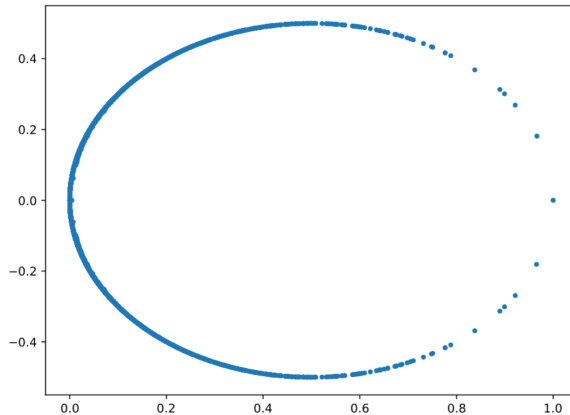
Hermitian Wilson operator  
 $H_w(M_5) = \gamma_5 D_w(-M_5)$  ('spectral flow')



$$D_w(M)_{xx'} = M + 4 - \frac{1}{2} \sum_{\mu} \left[ (1 - \gamma_{\mu}) \mathbf{U}_{\mu}(x) \delta_{x+\mu, x'} + (1 + \gamma_{\mu}) \mathbf{U}_{\mu}^{\dagger}(y) \delta_{x-\mu, y} \right]$$

Positions of 'crossings' where  $H_w(M_5)$  has zero eigenvalue coincides with the real eigenvalues of  $D_w$

# Overlap $D_{ov}$



$$T^{-1} = -[H_M - 1]^{-1}[H_M + 1], H_M = \gamma^5 \frac{(b+c)D_W}{2 + (b-c)D_W}$$

$$\frac{1+m_c}{1-m_c} T^{-Ls} - 1$$

# Topological index measurement on the lattice

Gluonic definition:

5Li (de Forcrand et al, hep-lat/9701012) Discretization of  $\int F\tilde{F}$ . Combination of 5 different size loops to eliminate  $\mathcal{O}(a^2, a^4)$  error. Used in combination with cooling or smearing to control ambiguity from small instantons and produce (near-) integer number for  $Q$ .

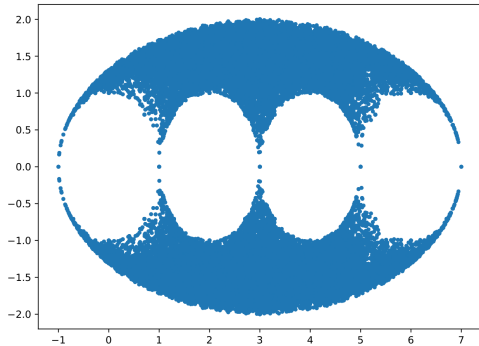
Fermionic Definition:

$Q$  Can be measured by counting the number of pure real modes of non-hermitian Wilson Dirac operator ( $D_w(m)$ ) or the crossings of Hermitian Wilson Dirac Operator ( $H_w(m) = \gamma_5 D_w(m)$ ) between 0 and  $M_5$

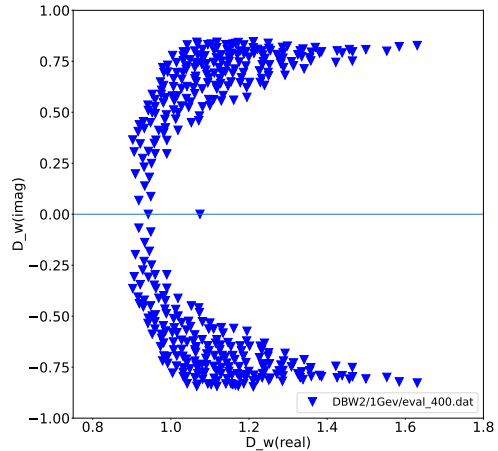
The topological index is the same as the 'net chirality' of exact zero modes of overlap Dirac operator.

Ambiguity eliminated? No - Location of crossings w.r.t  $m$  can change which mode(s) becomes 'physical' or 'doubler' modes.

# Spectrum of $D_w$

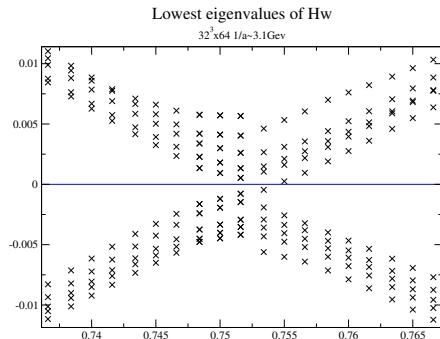
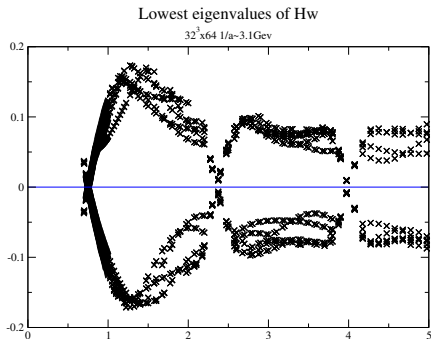


$D_w(-1)$ , Free field



$8^4 a^{-1} \sim 1\text{Gev}$  pure gauge(DBW2), 400 modes

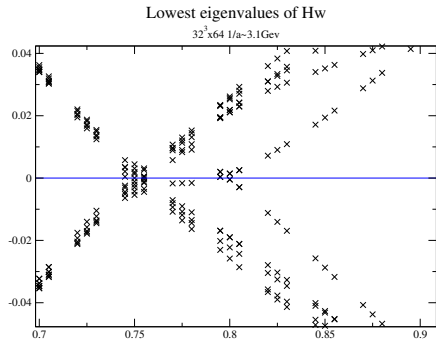
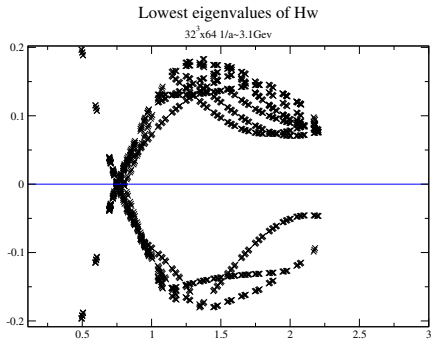
# Spectral flow of $2+1f$ $1/a \sim 3.1\text{Gev}$ configuration ( $Q=1$ )



$Q=1$ , also from Gluonic measurement

For an eigenvector  $|\lambda\rangle$  of  $H_w(-M_5)$ ,  $\frac{d\lambda}{dM_5} = -\langle\lambda|\gamma_5|\lambda\rangle$ .

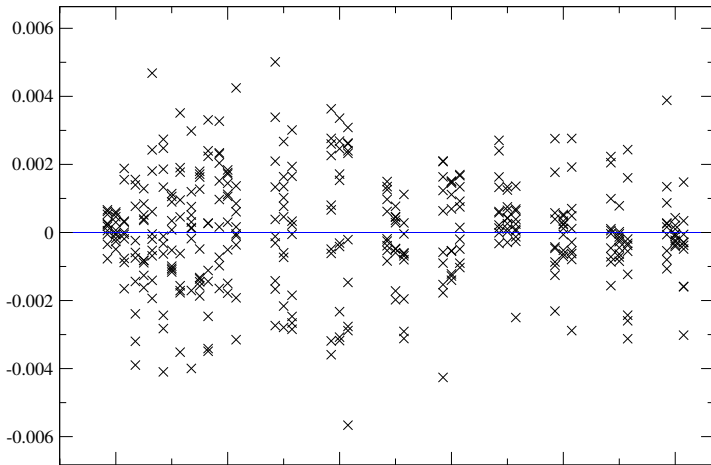
# Spectral flow of $2+1f$ $1/a \sim 3.1\text{GeV}$ configuration



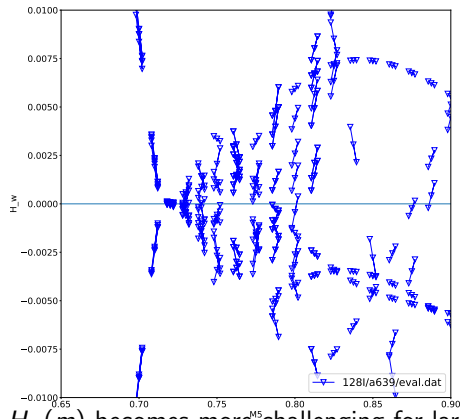
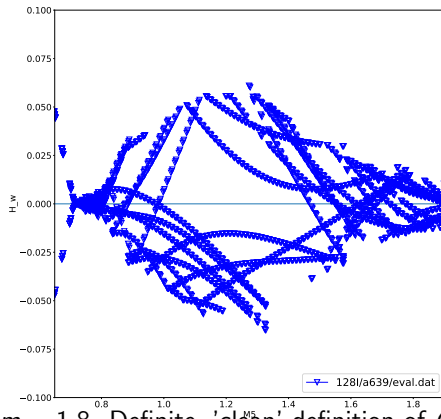
# Spectral flow of $2+1f$ $1/a \sim 1.7\text{Gev}$ configuration(48l)

Lowest eigenvalues of Hermitian Wilson operator

$48^3 \times 96$   $1/a \sim 1.7\text{Gev}$



# Spectral flow $128^3 \times 288(a^{-1} \sim 3.6\text{Gev})$ ensemble



$m = 1.8$ . Definite, 'clean' definition of  $Q$  using  $H_w(m)$  becomes more challenging for larger ensembles.

# Krylov–Schur Algorithm

- Eigenvalue problem: find  $(\lambda, v)$  such that  $Av = \lambda v$
- Build a **Krylov subspace**  $\mathcal{K}_m(A, v_1) = \text{span}\{v_1, Av_1, \dots, A^{m-1}v_1\}$
- Arnoldi relation after  $m$  steps:

$$AV_m = V_m H_m + f_m e_m^T \quad (1)$$

$V_m$ : orthonormal basis,  $H_m$ : upper Hessenberg,  $f_m$ : residual vector

- IRAM (Implicitly Restarted Arnoldi Method) restarts by applying implicit QR shifts to  $H_m$ , to effectively  $v_1 \rightarrow P(A)v_1$ . but deflation is fragile and implementation is complex
- **Krylov–Schur** (Stewart 2001): restart using the *Schur decomposition* of  $H_m$ 
  - Compute  $H_m = QSQ^T$  (Schur form, eigenvalues on diagonal of  $S$ )
  - Retain  $k$  wanted Schur vectors; deflate the rest
  - Relation truncates *cleanly*:  $A\tilde{V}_k = \tilde{V}_k S_{11} + \tilde{f}_k e_k^T$
  - Restart by extending  $\tilde{V}_k$  back to dimension  $m$
- Advantages over IRAM: simpler deflation, numerically stable, easy locking of converged

# Harmonic Krylov–Schur

- Target eigenvalues *near a shift*  $\sigma$  (interior spectrum, e.g. smallest modes of  $A^\dagger A$ )
- **Harmonic Ritz values:** approximate eigenvalues of  $A$  from the subspace, but weighted toward  $\sigma$ 
  - Seek  $\tilde{\lambda}$  satisfying the *harmonic* Galerkin condition:

$$(A - \sigma I)^{-1} V_m \tilde{y} = \tilde{\theta} V_m \tilde{y}, \quad \tilde{\theta} = \frac{1}{\tilde{\lambda} - \sigma} \quad (2)$$

- Equivalent to a small generalized eigenproblem on  $H_m$  — *no inversion of  $A$  required*
- Replace standard Ritz pairs with harmonic Ritz pairs in the Krylov–Schur restart
  - Sort Schur values by  $|\tilde{\lambda} - \sigma|$  (smallest first)
- In lattice QCD: used to compute low modes of the Dirac operator  $D^\dagger D$  near zero
  - Shift  $\sigma \approx 0$  selects near-zero modes
  - For topological modes, selects modes with smallest imaginary parts. Use shift to find interior points near  $M_5$ .

# Block (Harmonic) Krylov–Schur

- **Block extension:** use  $N_{\text{block}}$  starting vectors; block Arnoldi relation

$$AV = VH + FB^\dagger, \quad V^\dagger V = I, \quad V^\dagger F = 0 \quad (3)$$

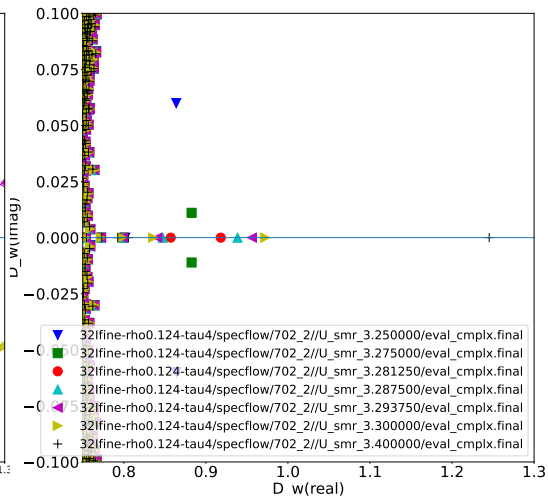
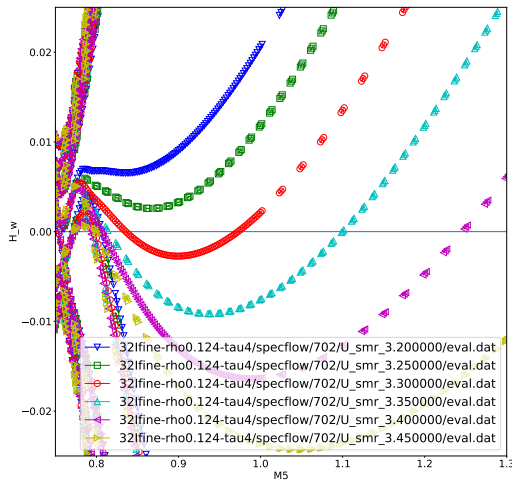
$V \in \mathbb{C}^{n \times N_m}$ ,  $H \in \mathbb{C}^{N_m \times N_m}$  block upper-Hessenberg,  $F, B \in \mathbb{C}^{n \times N_{\text{block}}}$

- **Two variants** (Grid/KS):

- HarmonicBlockKrylovSchur: Schur-decompose  $H - \sigma I$ , sort by  $|\lambda - \sigma|$  — exact restart, but selects standard Ritz values (spurious “ghost” values for interior/indefinite spectrum)
- TrueHarmonicBlockKrylovSchur: solve generalized eigenproblem  $\hat{H}g = (\theta - \sigma)g$ ,  
 $\hat{H} = H_\sigma + H_\sigma^{-\dagger} B B^\dagger$  for *true harmonic* Ritz pairs; avoids ghost values

- **Exact thick restart:** residual of every harmonic pair lies in the fixed  $N_{\text{block}}$ -dim space of  $W = F - V H_\sigma^{-\dagger} B \Rightarrow$  block Arnoldi relation preserved to machine precision after restart
- On  $8^4$  Wilson test: true-harmonic variant  $\sim 10\%$  faster, converged more eigenpairs, recovered an eigenvalue the base solver missed (spurious Ritz selection)

# $32^4$ (2+1)-flavor evolution (MD traj. length=4)



MD=3.25,  $\lambda = (0.753448884, 0)$

MD=3.25,  $\lambda = (0.771929604, 0)$

MD=3.25,  $\lambda = (0.863874691, 0.0599750107)$  MD=3.25,  $\lambda = (0.863874691, -0.0599750107)$

MD=3.281250,  $\lambda = (0.857186762, 0)$

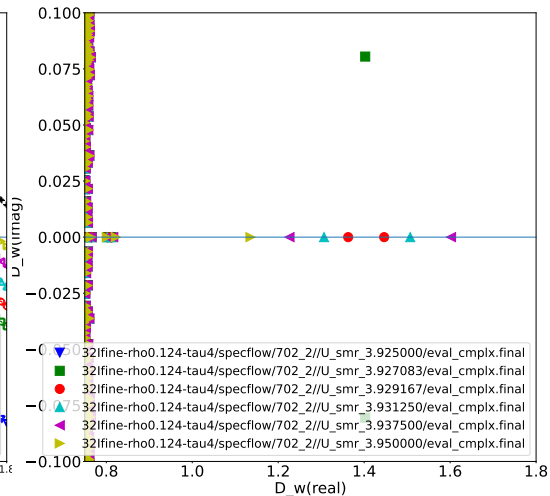
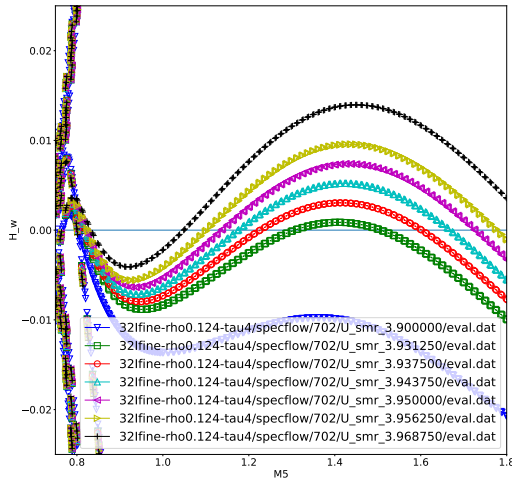
MD=3.281250,  $\lambda = (0.918185199, 0)$

MD=3.4,  $\lambda = (0.805605983, 0)$

MD=3.4,  $\lambda = (1.24529773, 0)$

MD=3.5,  $\lambda = (0.797462892, 0)$

MD=3.6,  $\lambda = (0.782388907, 0)$



MD=3.927083,  $\lambda$   
(1.40246012, 0.0804984524)

=MD=3.927083,  $\lambda$  =  
(1.40246012, -0.0804984524)

MD=3.937500,  $\lambda = (1.22624494, 0)$

MD=3.937500,  $\lambda = (1.60209226, 0)$

MD=3.937500,  $\lambda = (1.22624494, 0)$

MD=3.4,  $\lambda = (1.24529773, 0)$

# Observation

- QCD vacuum often has multiple near (anti-)instantons which generates near zero modes, and mixes heavily with exact zero modes
- Isolated (in eigenvalue space) modes are spatially better localized, consistent with 'dislocation' picture, where small (anti) instantons changes  $Q$ .
- Real eigenmodes of  $D_w$  or zero eigenmodes of  $H_w$  can be useful in tracking and improving topology evolution during ensemble generation.
- Study of topological modes during evolution reveals a more nuanced picture of the difficulties in changing topology: Extended topological modes (low  $\lambda_{real}$ ) are persistent, while the pair created modes have significant probability to revert instead of 'grow' and solidify.
- While we see the topological modes correlate well with fermion 'force term', gauge force term is orders or magnitude larger: is there small, but more persistent force pushing back on the topological modes? Can we identify these modes?

MD=3.931250,  $\lambda = (1.50713179, 0)$

MD=3.931250,  $\lambda = (1.3066435, 0)$

MD=3.931250,  $\lambda = (0.813718746, 0)$

Click to Play

Click to Play

Click to Play

Traj 703, MD=0.025000,  $\lambda = (1.01713555, 0)$  MD=3.4,  $\lambda = (1.17337705, 0)$