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U.S. DEPARTMENT of ENERGY

Topological Modes in Lattice QCD Evolution

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May 8, 2026

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 ((cost)$\geq a^{-(10-11)}$). One of the major focus in recent LQCD algorithmic study has been elimination of critical slowing down.

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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 combintion 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 'physcial' or 'doubler' modes.

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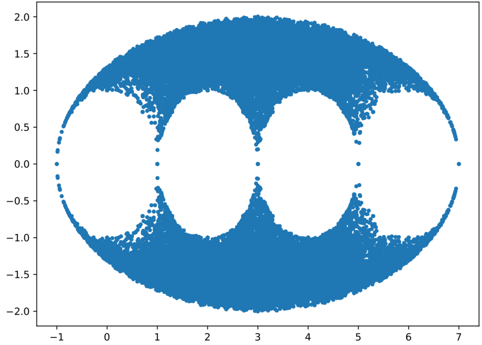
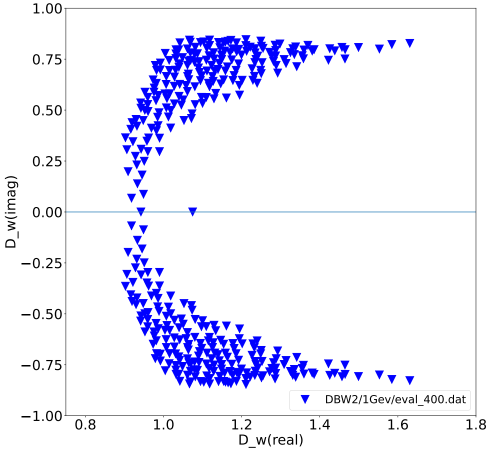
Spectrum of D_w

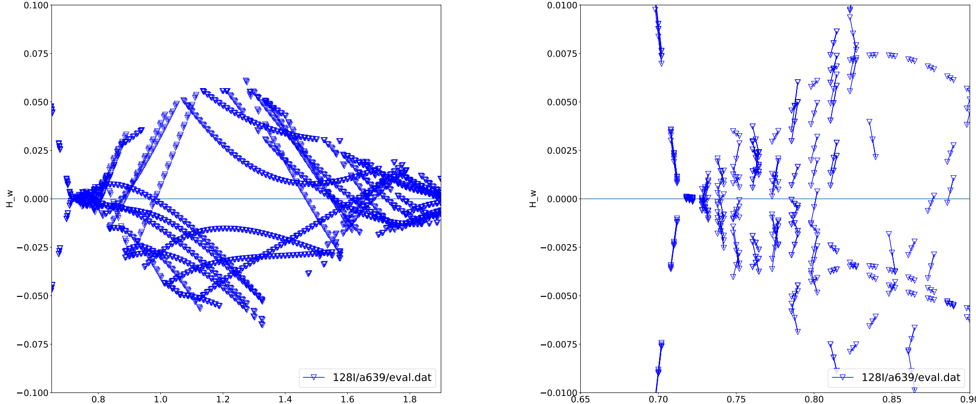


$D_w(-1)$, Free field



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

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.

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Non-hermitian solver to locate real eigenvalues of D_w may be better.

Krylov–Schur Algorithm

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

$$AV_m = V_m H_m + f_m e_m^T \tag{1}$$

  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 $v_1 \to P(A)v1$. 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 eigenpairs

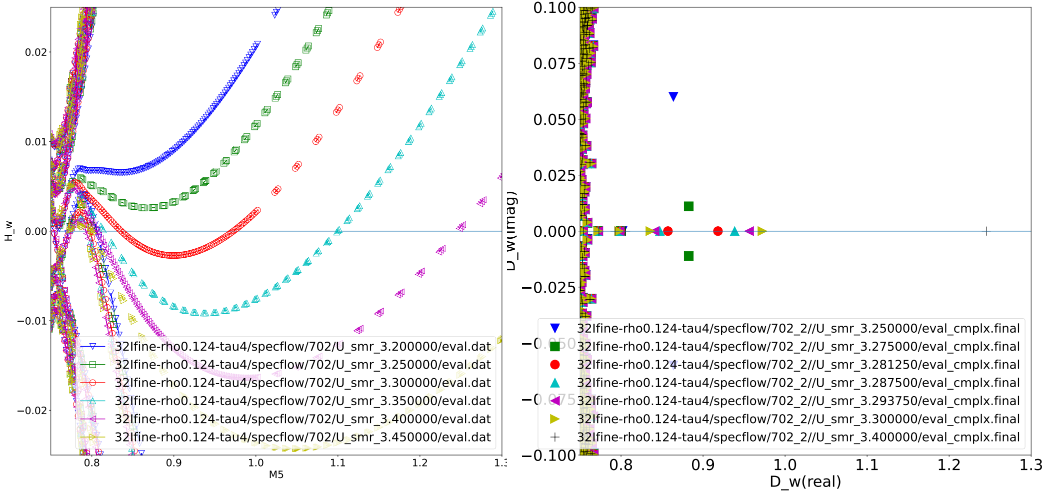
Harmonic Krylov–Schur

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

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

  - 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.

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



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

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

Click to Play

Click to Play

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

Click to Play

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

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

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

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

Click to Play

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

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

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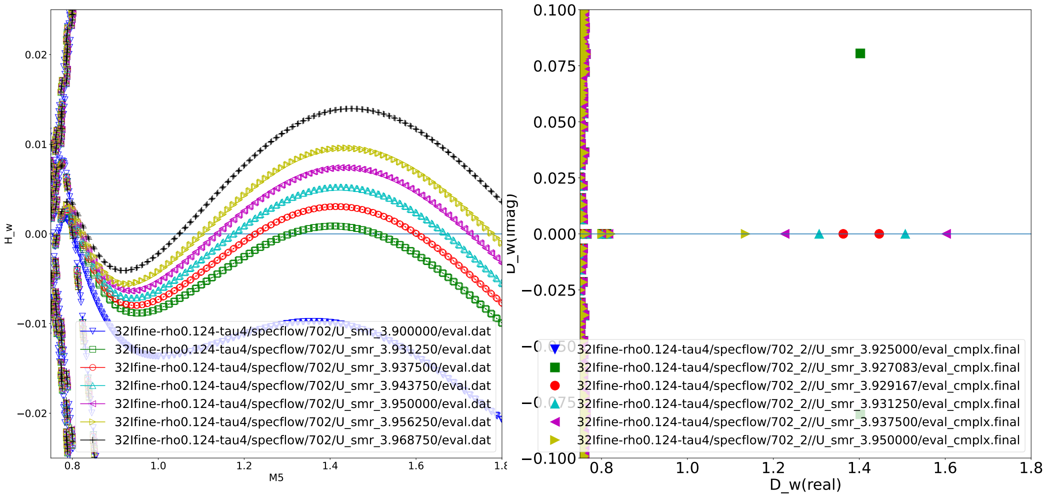

H_w
M5
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.900000/eval.dat
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.931250/eval.dat
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.937500/eval.dat
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.943750/eval.dat
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.950000/eval.dat
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.956250/eval.dat
32Ifine-rho0.124-tau4/specflow/702/U_smr_3.968750/eval.dat
D_w(imag)
D_w(real)
32Ifine-rho0.124-tau4/specflow/702_2//U_smr_3.925000/eval_cmplx.final
32Ifine-rho0.124-tau4/specflow/702_2//U_smr_3.927083/eval_cmplx.final
32Ifine-rho0.124-tau4/specflow/702_2//U_smr_3.929167/eval_cmplx.final
32Ifine-rho0.124-tau4/specflow/702_2//U_smr_3.931250/eval_cmplx.final
32Ifine-rho0.124-tau4/specflow/702_2//U_smr_3.937500/eval_cmplx.final
32Ifine-rho0.124-tau4/specflow/702_2//U_smr_3.950000/eval_cmplx.final

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

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

Click to Play

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

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

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

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

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

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

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Observation

- QCD vacuum often has multiple near (anti-)instantions 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 nuianced picture of the difficulties in changing topology: Extended topological modes (low λ_{real}) are persistent, while the pair created modes have significant probability to revert instead of 'grow' and solidifiy.
- 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?

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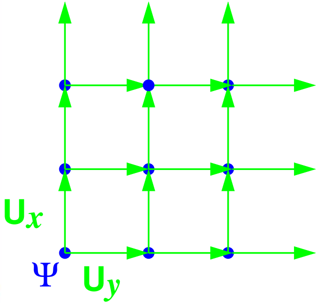
Introduction to lattice QCD

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. $(\psi(x), A_\mu(x)) \rightarrow (\psi(n), U_\mu(n) = \exp(-iA_\mu))$



$$
\begin{aligned}
Z &= \int [dU] \det(\not{D} + m) e^{-(S_g)} \\
&= \int [dU][d\bar{\psi}][d\psi] \ \exp[-(S_g + S_f)] \\
S_f &= \bar{\psi}(D^\dagger D)^{-1}\psi, \qquad S_{eff} = S_g + S_f \\
S_g &= \beta \sum \left[(U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x) \right]
\end{aligned}
$$

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

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