Topological charge in 2 flavors QCD with optimal domain-wall fermion

Tung-Han Hsieh[1], Ting-Wai Chiu[2], Yao-Yuan Mao[2], Kenji Ogawa[2]

(for TWQCD Collaboration)

[1] Research Center for Applied Sciences, Academia Sinica

[2] Department of physics, National Taiwan University

Introduction

In QCD, the topological susceptibility (χ_t) is the most important quantity to measure the topological charge fluctuation of the QCD vacuum, which plays an important role in breaking the $U_A(1)$ symmetry.

$$\chi_t = \int d^4x \{\rho(x)\rho(0)\} = \frac{\langle Q_t^2 \rangle}{\Omega} \quad (1)$$

$$\rho(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\lambda\sigma}\mathrm{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)], \qquad Q_t = \int d^4x\, \rho(x) \quad (2)$$

(Σ: chiral condensate; Q_t: top. charge; ρ: top. charge density; Ω: lattice volume)

In ChPT, χ_t for $N_f = 2$ at the tree level [Leutwyler & Smilga ('92)] and NLO [Mao & Chiu, PRD ('09)] are:

$$\chi_t/m_u = \Sigma(1 + m_u/m_d)^{-1} \quad (3)$$

$$\chi_t/m_u = \frac{\Sigma}{2}\left[1 + 3\left(\frac{M_\pi^2}{32\pi^2 F_\pi^2}\right)\ln\frac{M_\pi^2}{\mu_{sub}^2} - (2K_6 + 2K_7 + K_8)m_q\right]^{-1} \quad (4)$$

- χ_t is suppressed due to internal quark loops in the chiral limit
- It provides a viable way to extract Σ from χ_t in the chial limit.

Introduction (cont.)

The second normalized cumulant (c_4) is defined as

$$c_4 = -\frac{1}{\Omega}\left[\left\langle Q_t^4\right\rangle - 3\left\langle Q_t^2\right\rangle^2\right] \qquad (5)$$

- The leading anomalous contribution to the $\eta' - \eta'$ scattering amplitude in QCD.
- The dependence of the vacuum energy on the vacuum angle θ.

In ChPT, c_4 for $N_f = 2$ at the tree level is [Mao & Chiu, PRD ('09); Aoki & Fukaya, arXiv:0906.4852]:

$$c_4 = -\Sigma(m_u^{-3} + m_d^{-3})(m_u^{-1} + m_d^{-1})^{-1} \qquad (6)$$

If one can determine Q_t for each gauge configuration, then one can obtain χ_t and c_4 from Eq.(1) and Eq.(5), respectively.

Introduction (cont.)

In this work:

- We determine Q_t and χ_t from gauge confs. of 2 flavors lattice QCD simulation with ODWF.
  [Chiu, PRL (03); hep-lat/0303008]
- Lattice size: $16^3 \times 32 \times 16$, with Wilson gauge action at $\beta = 5.90$.
- Sea quark masses: $m_q a =$ 0.01, 0.02, 0.03, 0.04, 0.05, and 0.08.
- We determine Q_t via the low-mode projection of the lattice Dirac operator, using the Thick-Restart Lanczos algorithm.
  [Wu & Simon, SIAM J. Matrix Anal. Appl. (00)]

Introduction (cont.)

Instead of doing the projection on the 5-D ODWF Dirac operator, we perform the low-mode projection on its effective 4-D operator D (i.e., the overlap Dirac operator with Zolotarev optimal approximation):

$$D = m_0(1+V), \qquad V \equiv \gamma_5 H_w R_Z(H_w) \xrightarrow{N_s\to\infty} \gamma_5 \,\mathrm{sign}(H_w) \tag{7}$$

Then one can solve the eigen-problem of D:

$$D\big|\theta\big\rangle = \lambda(\theta)\big|\theta\big\rangle, \qquad \lambda(\theta) = m_0(1+e^{i\theta}) \tag{8}$$

Noting that since $[DD^\dagger, \gamma_5] = 0$, one can decompose the eigen problem of $DD^\dagger$ into $+$ and $-$ chiralities. Then one can derive:

$$S_\pm\big|\theta\big\rangle_\pm \equiv P_\pm H_w R_Z(H_w) P_\pm\big|\theta\big\rangle_\pm = \pm\cos\theta\big|\theta\big\rangle_\pm \tag{9}$$

where $\big|\theta\big\rangle = P_+\big|\theta\big\rangle + P_-\big|\theta\big\rangle = \big|\theta\big\rangle_+ + \big|\theta\big\rangle_-$. Thus, one can perform the eigenmode projection on the operator $S_\pm$ instead of Eq.(8). Moreover, $\big|\theta\big\rangle_\pm$ are related to each other:

$$\big|\theta\big\rangle = \frac{1}{i\sin\theta}(V - e^{-i\theta})\big|\theta\big\rangle_+ \qquad \text{for } \theta \neq 0, \pm\pi, \pm 2\pi, \ldots \tag{10}$$

Strategy of projection:

$$D\big|\theta\big\rangle = \lambda(\theta)\big|\theta\big\rangle, \qquad \lambda(\theta) = m_0(1 + e^{i\theta})$$

- Project the smallest eigenmodes of $S_+\big|\theta\big\rangle_+ = \cos\theta\big|\theta\big\rangle_+$. If D has zero modes in positive chirality, the smallest eigenvalues will have values $\simeq -1$.
- If D has zero modes in positive chirality, use Eq.(10) to compute the whole eigenvectors of D.
- If D does not have zero modes in positive chirality, then they may appear in negative chirality:
  - Project the largest eigenmodes of $S_-\big|\theta\big\rangle_- = -\cos\theta\big|\theta\big\rangle_-$. If there are zero modes in negative chirality, the largest eigenvalues will have values $\simeq +1$.
  - Form the whole eigenvectors of D from $\big|\theta\big\rangle_+$ and $\big|\theta\big\rangle_-$.

Low-mode projection

To project the low-lying eigenmodes of a large sparse matrix:

$$Ax = x\lambda \tag{11}$$

one construct an orthonormal basis from the Krylov subspace, starting from the initial vector r_0:

$$\mathcal{K}(A, r_0) = \left\langle r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0 \right\rangle \tag{12}$$

This basis, the linear combination of $\{A^i r_0, i = 0, 1, \ldots m-1\}$, are the Ritz vectors (the approximated eigenvectors) of A.

The Lanczos algorithm is the standard procedure to perform orthonormalization on the subspace $\mathcal{K}(A, r_0)$, dedicated for $A^\dagger = A$.

Basic Lanczos algorithm

Basic Lanczos iteration:

Input: r_0, $\beta_0 = ||r_0||$, $q_0 = 0$
For: i = 1, 2, . . .

- $q_i = r_{i-1}/\beta_{i-1}$
- $p = Aq_i$
- $\alpha_i = q_i^H p$
- $r_i = p - \alpha_i q_i - \beta_{i-1} q_{i-1}$
- $\beta_i = ||r_i||$

In this iteration, we are constructing:

$$AQ_m = Q_m T_m + \beta_m q_{m+1} e_m^T$$

$$Q_m = [q_1, q_2, \ldots, q_m]$$

$$T_m = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \cdots & \cdots \\ \beta_1 & \alpha_2 & \beta_2 & 0 & \cdots \\ 0 & \beta_2 & \alpha_3 & \beta_3 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

with q_1, q_2, . . . , q_m form a (orthonormal) complete set of a m dimensional subspace.

Basic Lanczos algorithm

Then the Ritz pairs $(\hat{\lambda}_i, \hat{x}_i)$ can be abtained from

$$\hat{T}_m = U_m^\dagger T_m U_m, \qquad X_m = Q_m U_m$$

where $\hat{T}_m$ is diagonal with eigenvalues $\hat{\lambda}_i$, U_m is unitary, and X_m has columns $\hat{x}_i$. When $m \to \infty$, $(\hat{\lambda}_i, \hat{x}_i) \to (\lambda_i, x_i)$

However, the basic Lanczos algorithm suffers the following problems:

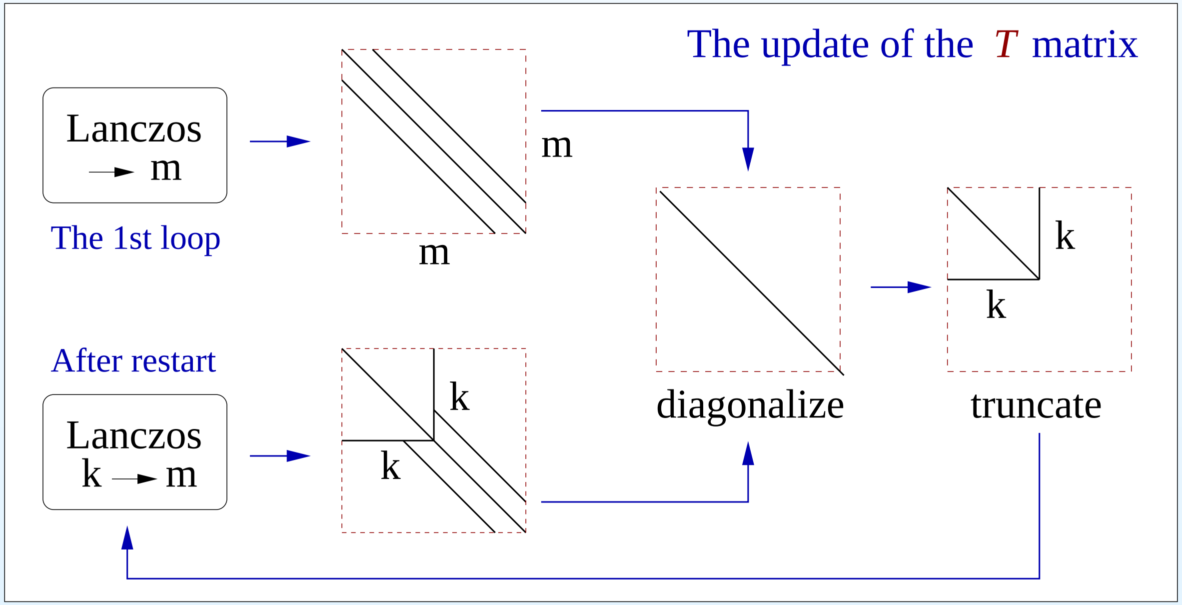
1. Some Ritz values may repeatedly appear when m goes larger.
   - q_i loses orthogonality rapidly in the finite precision arithmatics.
   - Re-orthogonal q_i during the iteration.
2. It requires a lot of columns q_i in order to project several Ritz pairs.
   - Restart the Lanczos process in a fixed m dimensional subspace.

Thick-Restart Lanczos algorithm

Suppose that we try to project k' eigenpairs of A within the m dimensional Krylov subspace:

$$AQ_m = Q_m T_m + \beta_m q_{m+1} e_m^T \qquad (13)$$

Then we *truncate* the dimenstion of the subspace to k and restart the Lanczos iteration ($k, k' < m$):



The schematic diagram for the Thick-Restart Lanczos process.
The non-zero values of the T matrix are illustrated as black lines.

Thick-Restart Lanczos algorithm

1. Given a starting vector r_0, perform the Lanczos process to construct Eq.(13). The Gram-Schmidt procedure is performed to ensure the orthogonalization of q_i.
2. Diagonalize T_m: $T_m = U_m^\dagger \hat{T}_m U_m$.
3. Pick the first k columns of U, and let $\hat{Q}_k = Q_m U_k$:

   $$A\hat{Q}_k = \hat{Q}_k \hat{T}_k + \beta_m \hat{q}_{k+1} s^\dagger, \qquad \hat{q}_{k+1} = q_{m+1}, \quad s = U_m^\dagger e_m$$

   i.e., truncate the dimension of subspace from m to k.
4. Restart the Lanczos process, with the next basis constructed by:

   $$\hat{\beta}_{k+1}\hat{q}_{k+2} = \hat{r}_{k+1} = (I - \hat{Q}_{k+1}\hat{Q}_{k+1}^\dagger)A\hat{q}_{k+1} \tag{14}$$

   Then extend the Krylov subspace from dimension $k+1$ to m via the Lanczos process.

Adaptive Thick-Restart Lanczos algorithm

The performance of *TRLan* depends on the setting of k for a given eigen-problem and the dimension m of the Krylov subpace. It is instructive to search for the optimal value of k such that the following object function $f(k)$ is maximized, in order to attain the maximum performance: [Yamazaki, Bai, Simon, Wang, Wu, *Tech. Rep. LBNL-1059E (08)*]

$$f(k) = \frac{\text{The reduction factor } d_j \text{ of the residule of } j\text{th Ritz pair}}{\#\text{ of FPO}} \quad (15)$$

Suppose that for the j-th (non-converged) Ritz pair, its residules at $(l-1)$-th and l-th restarts are related by the reduction factor d_j:

$$\beta_j^{(l)} = \beta_j^{(l-1)}/d_j, \qquad d_j \simeq \mathcal{C}_{m-k}(1+2\gamma_e), \qquad \gamma_e = \frac{\hat{\lambda}_{k+1}^{(l)} - \hat{\lambda}_j^{(l)}}{\hat{\lambda}_m^{(l)} - \hat{\lambda}_{k+1}^{(l)}} \quad (16)$$

where $\mathcal{C}_n(z)$ is the Chebyshev polynomial of degree n.

Adaptive Thick-Restart Lanczos algorithm

For the # of FPO in each restart, we only count the dominated parts:

- Reorthogonalization: $q_j \leftarrow (I - Q_{j-1}Q_{j-1}^H)q_j$, $j = k+1, \ldots, m$.
- Update of Ritz vectors: $\hat{Q}_k = Q_m U_k$.

Salient features of Adaptive *TRLan* algorithm:

- The dimension of the subspace m is kept finite.
- The reorthogonalization of subspace Q_k is imposed in order to prevent obtaining specious Ritz values.
- The info. of the wanted eigenmodes (within dimension k) in the previous loop is fully used to improve the Ritz pairs after restart.
- The dimension of the truncated subspace k is dynamically adjusted for each restart, in order to attain the max. performance.
- It is numerically more reliable, and easier to implement, comparing to the other Restart schemes.

Benchmark

For one of the gauge confs. simulated at $16^3 \times 32 \times 16$, $\beta = 5.9$, $m_q a = 0.01$, which possess top. charge $Q_t = 3$, we perform the benchmark on low-mode projections for H_w and S_+, respectively.

(Intel Xeon E5530 @ 2.4GHz, 8 cores, 24GB memory)

- H_w: $k' = 240$, $m = 340$

method	# of restarts	# of Av	time(s)	speed up
ARPACK	388	35390	136460	1.00
TRLan	999	100140	572951	0.24
ν-TRLan	383	59145	78058	1.75

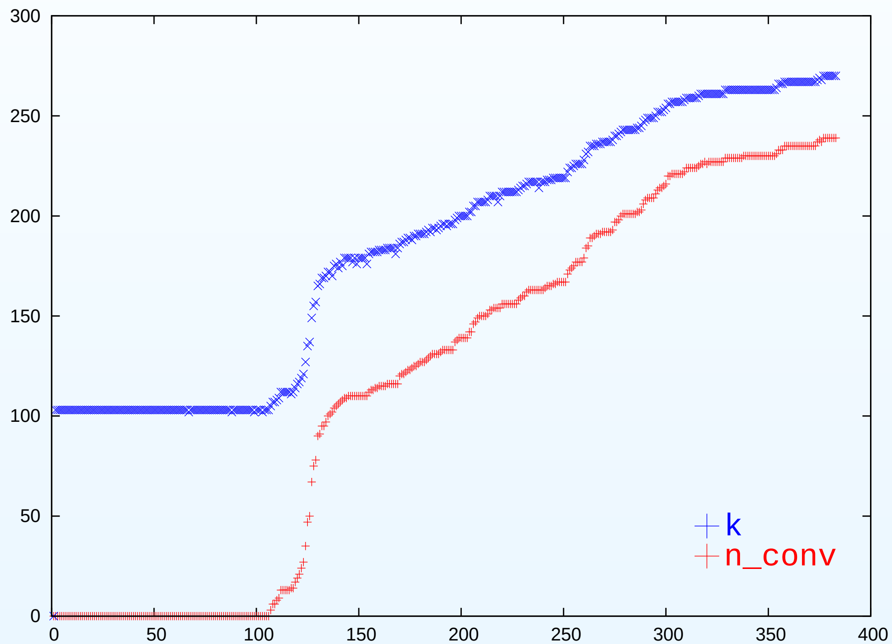
- S_+: $k' = 100$, $m = 200$, $n_p = 240$

method	# of restarts	# of Av	time(s)	speed up
ARPACK	13	1050	112632	1.00
TRLan	12	1300	105790	1.06
ν-TRLan	11	1030	90496	1.24

k': # of required eigenmodes; m: dim. of subspace; n_p: # of eigenmodes of H_w for preconditioning

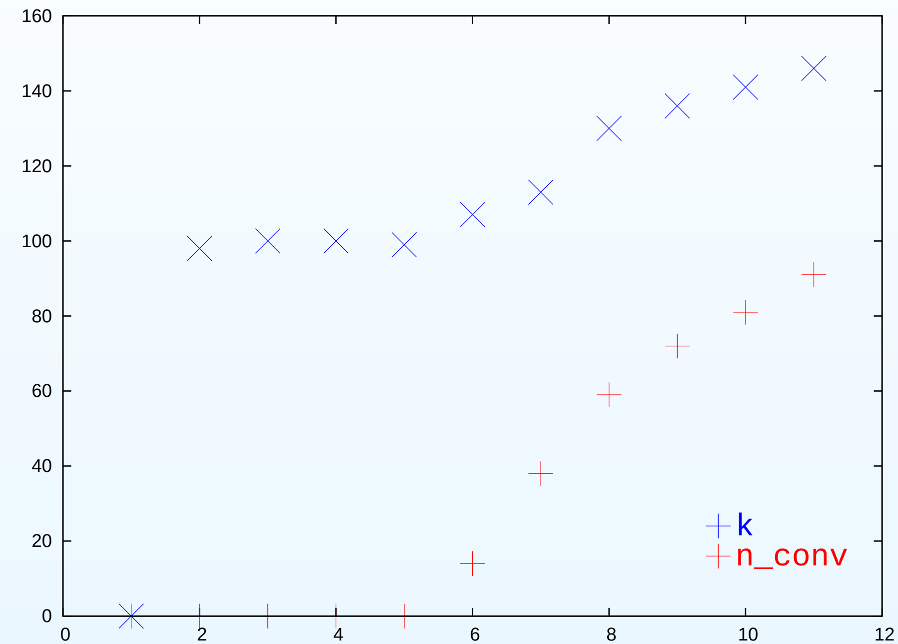
Benchmark

ν-TRLan: k v.s. n_{conv} for H_w projection



# of restarts

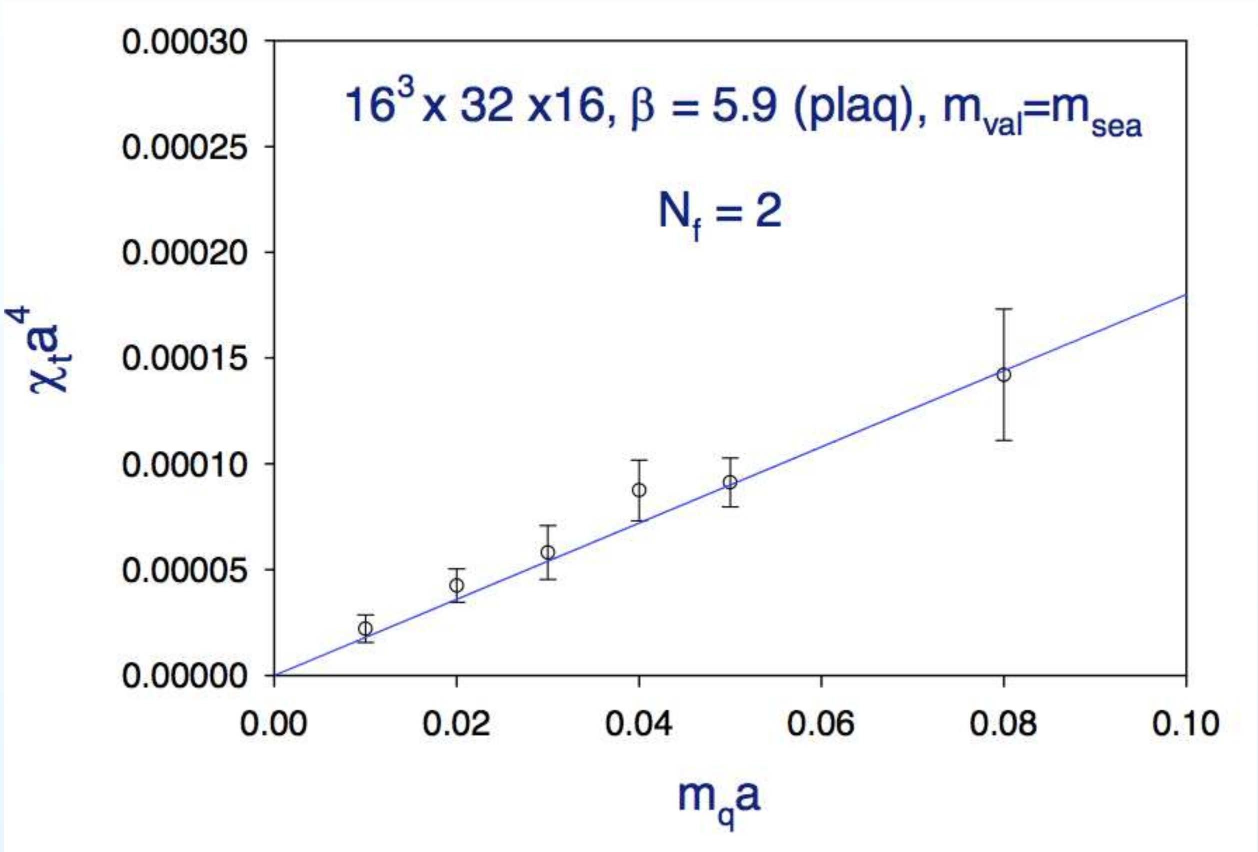
ν-TRLan: k v.s. n_{conv} for S_+ projection



# of restarts

Adaptive Thick-Restart Lanczos: The change of k with respect to the number of converged eigenmodes (n_{conv}), for the projection of H_w and S_+, respectively.

Topological susceptibility



(preliminary)

- Fitting our data of χ_t to Eq.(3), we get $a^3\Sigma = 0.0031(4)$.
- Using $a^{-1} = 1590(20)$ MeV, $Z_m = 0.85(1)(2)$, we transcribe Σ to:

$$\Sigma^{\overline{\rm MS}}(2\ {\rm GeV}) = [247(11)(12)\ {\rm MeV}]^3 \tag{17}$$

Concluding Remarks

- We determine Q_t and χ_t from gauge confs. of 2 flavors lattice QCD simulation with ODWF, on the lattice $16^3 \times 32 \times 16$ with Wilson gauge action at $\beta = 5.90$.
- We use Adaptive Thick-Restart Lanczos algorithm to do the low-mode projection on H_w and $S_\pm$ operators, which can attain 1.7 - 2.0 (for H_w) and 1.2 - 1.4 (for $S_\pm$) times faster than ARPACK.
- Our preliminary result of χ_t agrees with the sea-quark mass dependence predicted by the chiral perturbation theory, from which we can extract the chiral condensate.
- Our statistics is still too small to determine c_4 unambigously.
- We plan to port the ν-*TRLan* code to the GPU.