Determination of chiral condensate from low-lying eigenmodes of Mobius domain-wall Dirac operator

based on arXiv:1607.01099 [hep-lat]

JLQCD collaboration: Guido Cossu (Edinburgh),
Hidenori Fukaya (Osaka), Shoji Hashimoto,
Takashi Kaneko, Jun Noaki (KEK)

@ Lattice 2016, University of Southampton

July 25, 2016

計算基礎科学連携拠点
Joint Institute for
JICFuS Computational Fundamental Science

国立大学法人
総合研究大学院大学
The Graduate University for Advanced Studies [SOKENDAI]

JLQCD collaboration

- Members
  - KEK: Y. Aoki, B. Colquhoun, B. Fahy, S. Hashimoto, T. Kaneko, H. Matsufuru, K. Nakayama, M. Tomii
  - Osaka: H. Fukaya, T. Onogi
  - Kyoto: S. Aoki
  - Edinburgh: G. Cossu
  - RIKEN: N. Yamanaka
  - Wuhan: A. Tomiya

- Machines @ KEK
  - Hitachi SR16000 M1
  - IBM Blue Gene /Q

Chiral condensate

- VEV of scalar density operator : $\langle \bar{q}q \rangle$
  - Characterizes the QCD vacuum after the spontaneous chiral symmetry breaking.

- Eigenvalue density of the Dirac operator

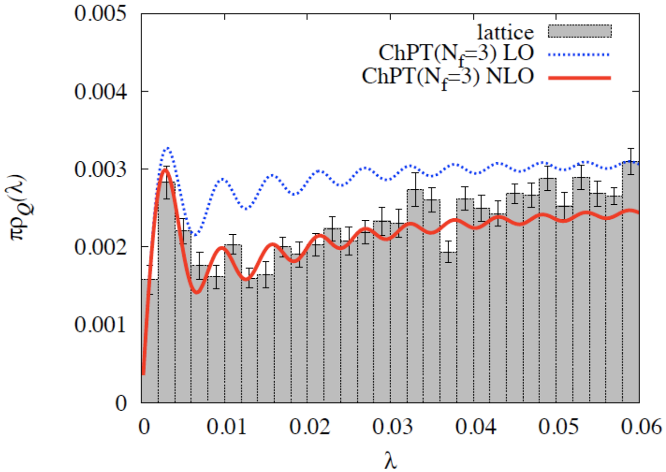
$$\rho(\lambda) = \frac{1}{V}\left\langle \sum_i \delta(\lambda - \lambda_i) \right\rangle$$

  - Related to the chiral condensate in the thermodynamical limit (Banks-Casher relation):

$$\rho(\lambda) = \frac{1}{\pi}\mathrm{Re}\langle \bar{q}q \rangle_{m_v = i\lambda} \quad \Rightarrow \quad \rho(0) = \frac{\Sigma}{\pi}$$

QCD Dirac spectrum

- Our previous work with overlap fermion



JLQCD, PRL101, 122002 (2010)

- 2 and 2+1 flavors
- p and ε regimes (various quark masses)
- 16^3x48 and 24^3x48
- various topological charges

  – Damgaard-Fukaya (2009): NLO ChPT in p- and ε-regime
  – Limitation due to computational cost: finite lattice spacing, finite volume

New data set of JLQCD

- With Mobius domain-wall fermion (2012~)
  - 2+1 flavor (uds)
  - Mobius domain-wall fermion [with stout link]
  - residual mass < O(1 MeV)
  - lattice spacing : 1/a = 2.4, 3.6, 4.5 GeV
  - volume : L = 2.7 fm（32^3, 48^3, 64^3 lattices）
  - quark mass : m_π = 230, 300, 400, 500 MeV
  - statistics : 10,000 MD time each

β = 4.17, 1/a ~ 2.4 GeV, 32^3x64 (x12)

m_{ud}	m_π [MeV]	MD time
m_s = 0.030		
0.007	310	10,000
0.012	410	10,000
0.019	510	10,000
m_s = 0.040		
0.0035	230	10,000
0.0035 (48^3x96)	230	10,000
0.007	320	10,000
0.012	410	10,000
0.019	510	10,000

β = 4.35, 1/a ~ 3.6 GeV, 48^3x96 (x8)

m_{ud}	m_π [MeV]	MD time
m_s = 0.018		
0.0042	300	10,000
0.0080	410	10,000
0.0120	500	10,000
m_s = 0.025		
0.0042	300	10,000
0.080	410	10,000
0.0120	510	10,000

β = 4.47, 1/a ~ 4.6 GeV, 64^3x128 (x8)

0.0030	~ 300	10,000

Calculation of eigenvalue distribution

- Explicit calculation of individual ev
  - (with Lanczos or related)
  - Number of ev's to be calculated increases as V.
  - Computational cost increases as $O(V^2)$.

- Stochastic counting
  - Stochastic estimate of ev's in a given interval.
  - Some (controlled) approximation is involved.
  - Computational cost scales $O(V)$.

Previous work

Giusti, Luscher, JHEP 0903, 013 (2009).

- Well established method to count the ev's below some threshold.

$$\mathbb{P}_M \simeq h(\mathbb{X})^4, \qquad \mathbb{X} = 1 - \frac{2M_*^2}{D_m{}^\dagger D_m + M_*^2},$$

- h(X) : Step function approximated by Chebyshev polynomial, n~32.
- M_* needs to be fixed.
- Cost: 2n x N_{iter} ~ O(5000) $D^\dagger D$ multiplication

Chebyshev filtering

Di Napoli, Polizzi, Saad, arXiv:1308.4275 [cs.NA].
See also, Fodor, Holland, Kuti, Mondal, Nogradi, Wong, arXiv:1605.08091 [hep-lat].

- Stochastic counting of ev's of an Hermitian matrix *A*
  - Number of ev's in a range $[a,b]$:

$$n[a,b] = \frac{1}{N_v} \sum_{k=1}^{N_v} \xi_k^\dagger h(A) \xi_k$$

  - ξ_k : N_v (normalized) Gaussian noise vector
  - $h(A)$: filtering function approximated by a Chebyshev polynomial.

$$h(x) = \begin{cases} 1 & \text{for } x \in [a,b] \\ 0 & \text{otherwise} \end{cases} \qquad \cong \sum_{j=0}^{p} g_j^p \gamma_j \, T_j(x)$$

Chebyshev filtering

- Chebyshev approximation

$$h(x) = \begin{cases} 1 & \text{for } x \in [a,b] \\ 0 & \text{otherwise} \end{cases} \qquad \cong \sum_{j=0}^{p} g_j^p \gamma_j \, T_j(x)$$

  - Coefficients are uniquely determined for a given $[a,b]$ within [-1,+1].
  - Larger the *p*, the approximation is better.
  - Unwanted oscillations suppressed by the Jackson term g_j^p , also given once $[a,b]$ is fixed.

Di Napoli, Polizzi, Saad, arXiv:1308.4275 [cs.NA].

Chebyshev filtering

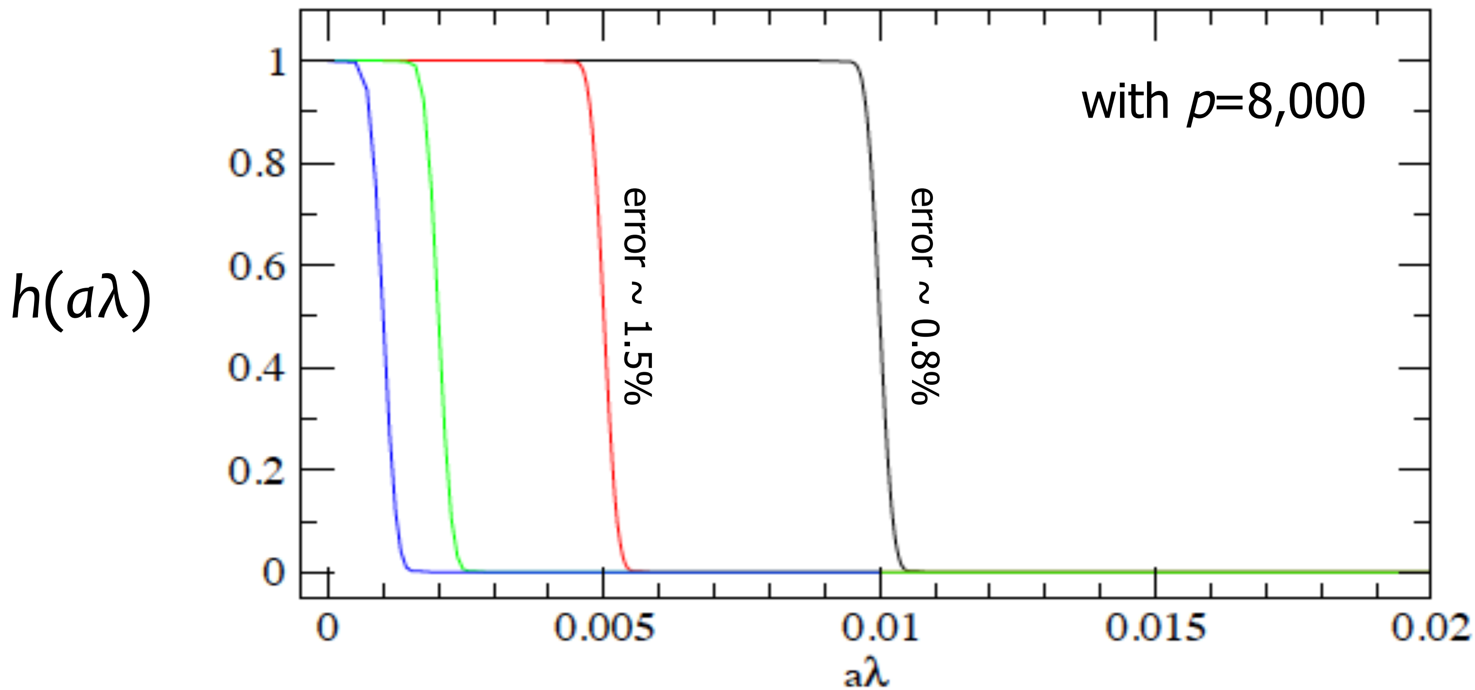
- Chebyshev polynomial
  - constructed using the recursion relation:

$$T_0(x) = 1, \quad T_1(x) = x,$$
$$T_j(x) = 2x\, T_{j-1}(x) - T_{j-2}(x)$$

- Error due to truncation
  - depends on the width of $[a,b]$, compared to the entire ev range [-1,+1].
  - For the domain-wall operator $D^{\dagger}D$, the ev's are in [0,1]. So, stretched to [-1,+1].

Step function approximation

for the lowest bin



- Typical example: 0.8% (1.5%) when p=8,000 and δ=0.01 (0.005).
- The error scales as ~ $0.06/p\delta$.

Recipe

As easy as

1. Generate Gaussian random noise vector ξ_k and recursively calculate $T_j(A)\,\xi_k$
2. Calculate an inner-product $\xi_k^\dagger\, T_j(A)\,\xi_k$ and store.
3. … then, the remaining analysis is off-line.

- Ensemble average

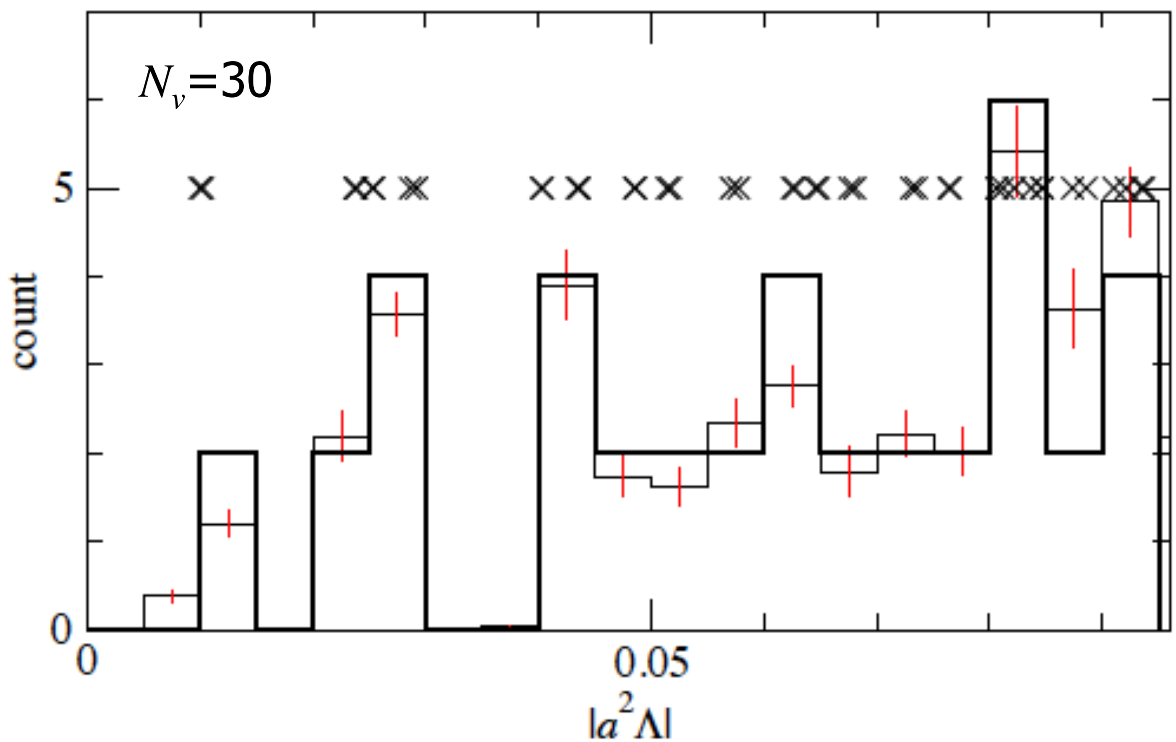
$$\overline{n}[a,b] = \frac{1}{N_v}\sum_{k=1}^{N_v}\left[\sum_{j=0}^{p} g_j^p \gamma_j \left\langle \xi_k^\dagger T_j(A)\xi_k \right\rangle\right]$$

  - Range $[a,b]$ may be specified later. The entire distribution is obtained at once.

Numerical test

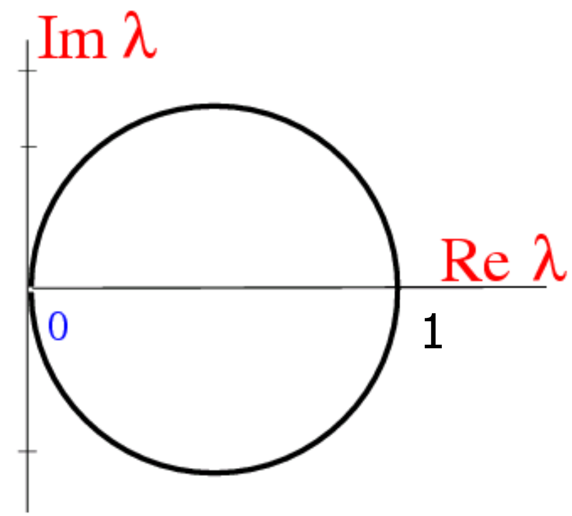
Direct comparison on a config with known ev's:

finite temp lattice, 32^3x12

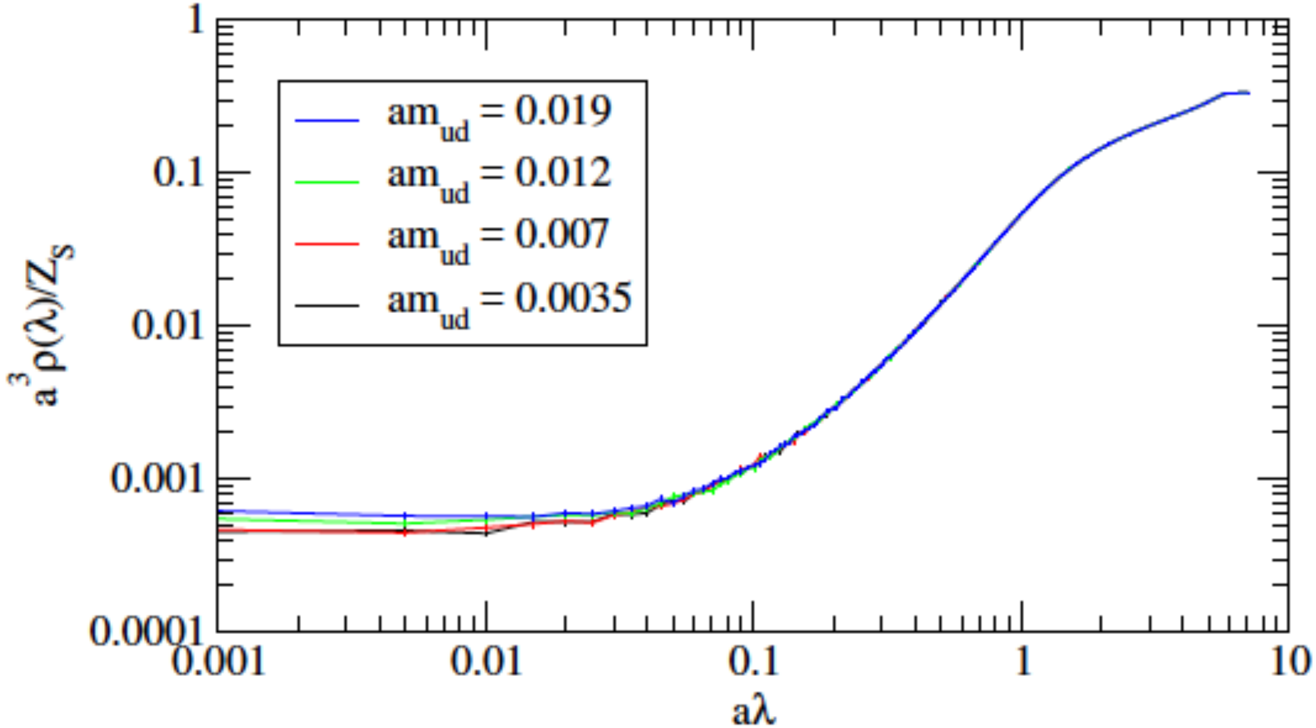


Domain-wall operator

- 5D → effective 4D operator
  $$D^{(4)} = \left[P^{-1} (D^{(5)}(m=1))^{-1} D^{(5)}(m) P \right]_{11}$$
  - Approximately satisfies the Ginsparg-Wilson relation
    $$D\gamma_5 + \gamma_5 D = 2aD\gamma_5 D$$
  - costly, because of PV inverse.
  - ev's on a complex circle.
  - ev's of $D^\dagger D$ are in [0,1].
  - then, project on the imaginary axis.

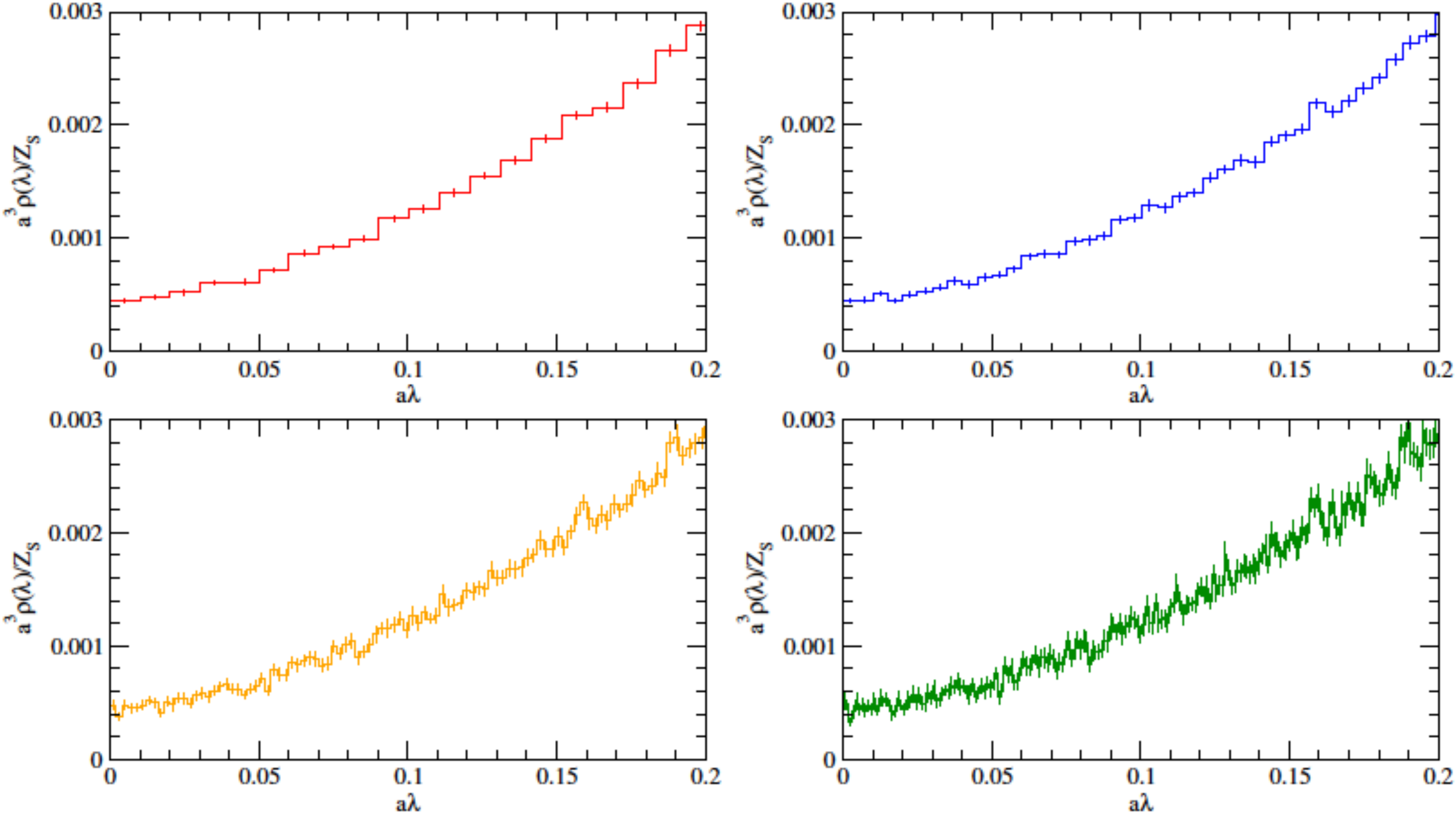


Entire spectrum



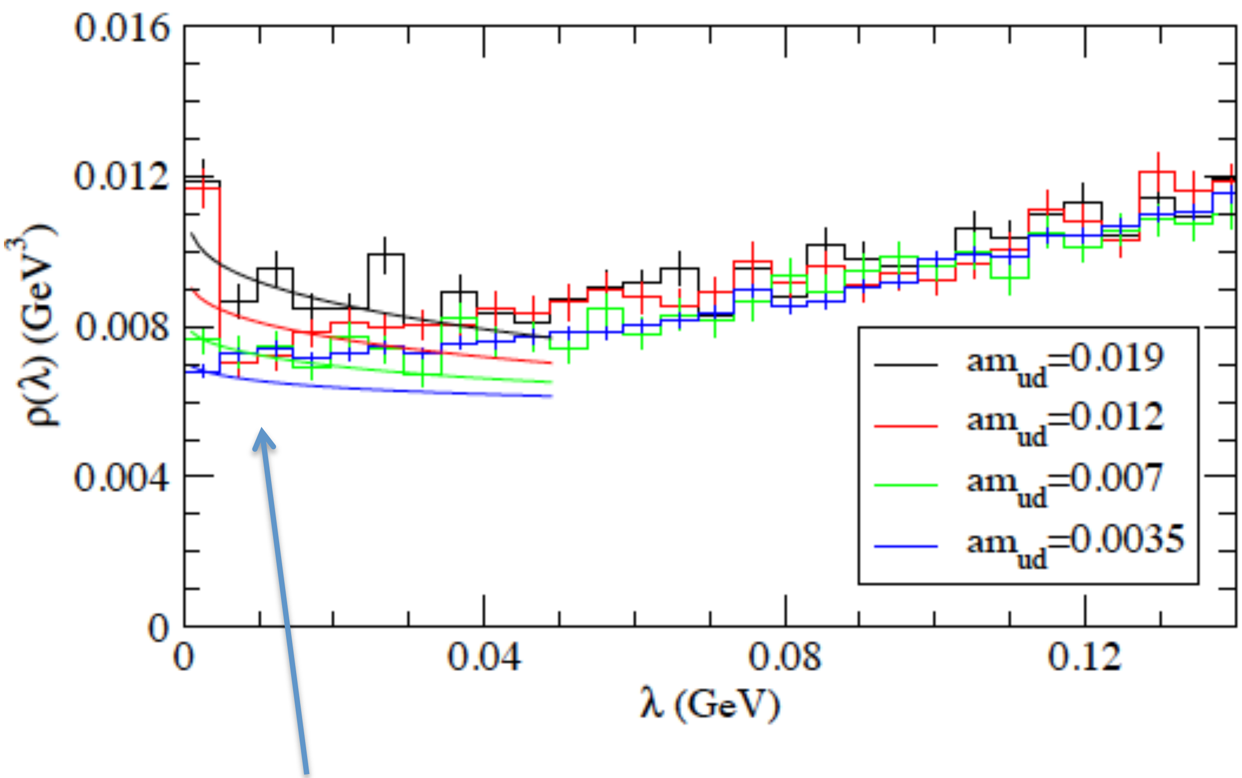
β=4.17
($1/a$ ~ 2.4 GeV)
32^3x64
50 conf each

calculated at once, from a set of inner-products.



different bin sizes from the same set of inner-products.

Low-lying spectrum



β=4.17
(1/a ~ 2.4 GeV)
32^3x64
50 conf each

Sea quark mass dependence due to the fermion determinants.

Chiral fit

NLO χPT formula by Damgaard-Fukaya (2009)

$$\rho(\lambda) = \frac{\Sigma}{\pi}\left[1 - \frac{1}{F^2}\left(\sum_i \mathrm{Re}\Delta(0, M_{vi}^2) - \mathrm{Re}G(0, M_{vv}^2, M_{vv}^2) - 16L_6\sum_i M_{ii}^2\right)\right]_{m_v = i\lambda}$$

$$M_{ij} = (m_i + m_j)\Sigma/F^2$$

F fixed with 90 MeV. Minor effect to control the curvature.

$$\Delta(0, M^2) = \frac{M^2}{16\pi^2}\ln\frac{M^2}{\mu_{sub}^2} + \cancel{g_1(M^2)}$$

finite volume (negligible)

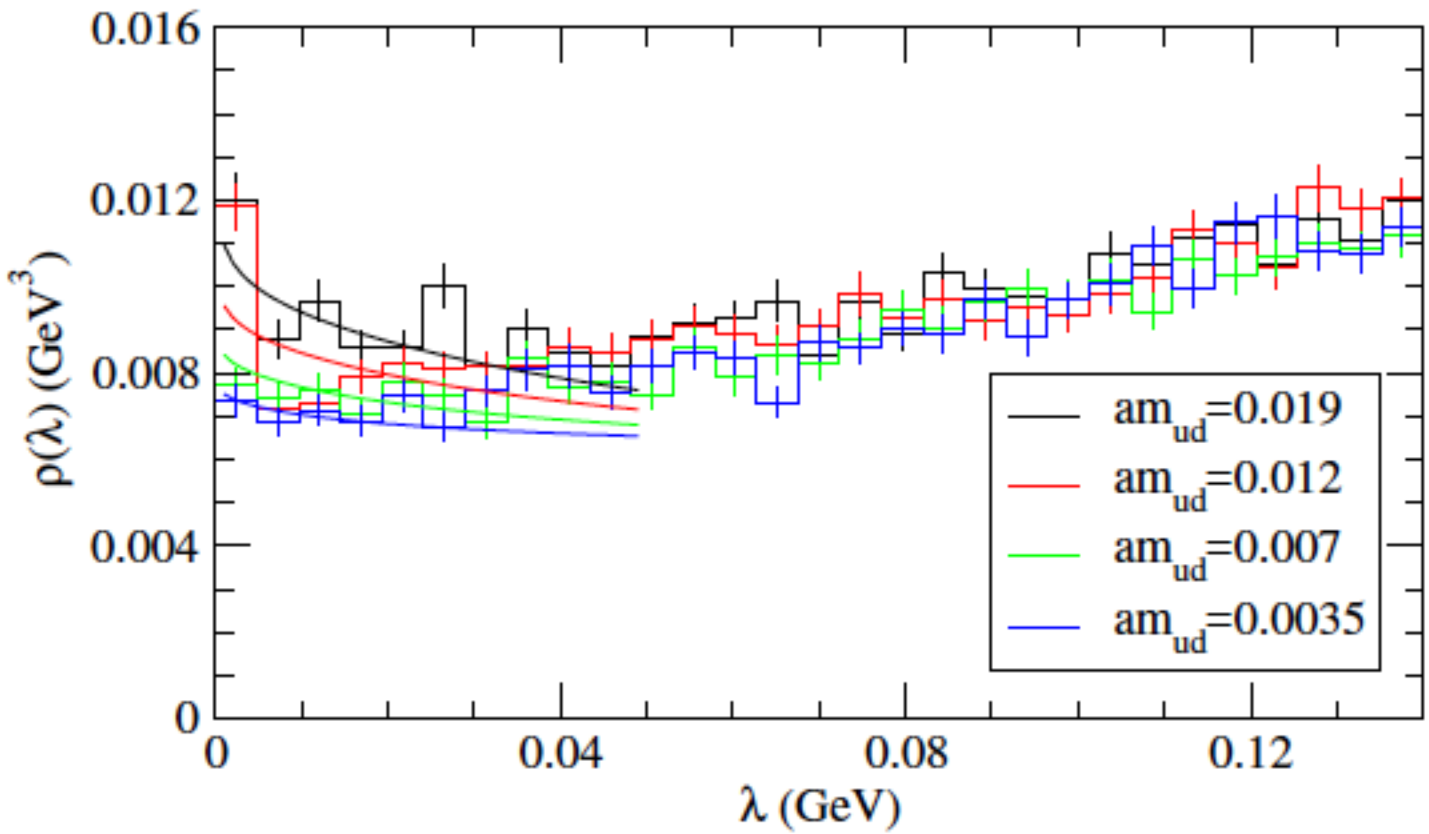
$$G(0, M^2, M^2) = \frac{1}{2}\left[\Delta(0, M^2) + (M^2 - M_\pi^2)\partial_{M^2}\Delta(0, M^2)\right]$$

Terms accounting for a and m_s dependence

$$\left(1 + c_a a^2\right)\left(1 + c_s\left(M_{\eta_{ss}}^2 - M_{\eta_{ss}}^{(\mathrm{phys})2}\right)\right) \times \rho(\lambda)$$

Fit result (1)

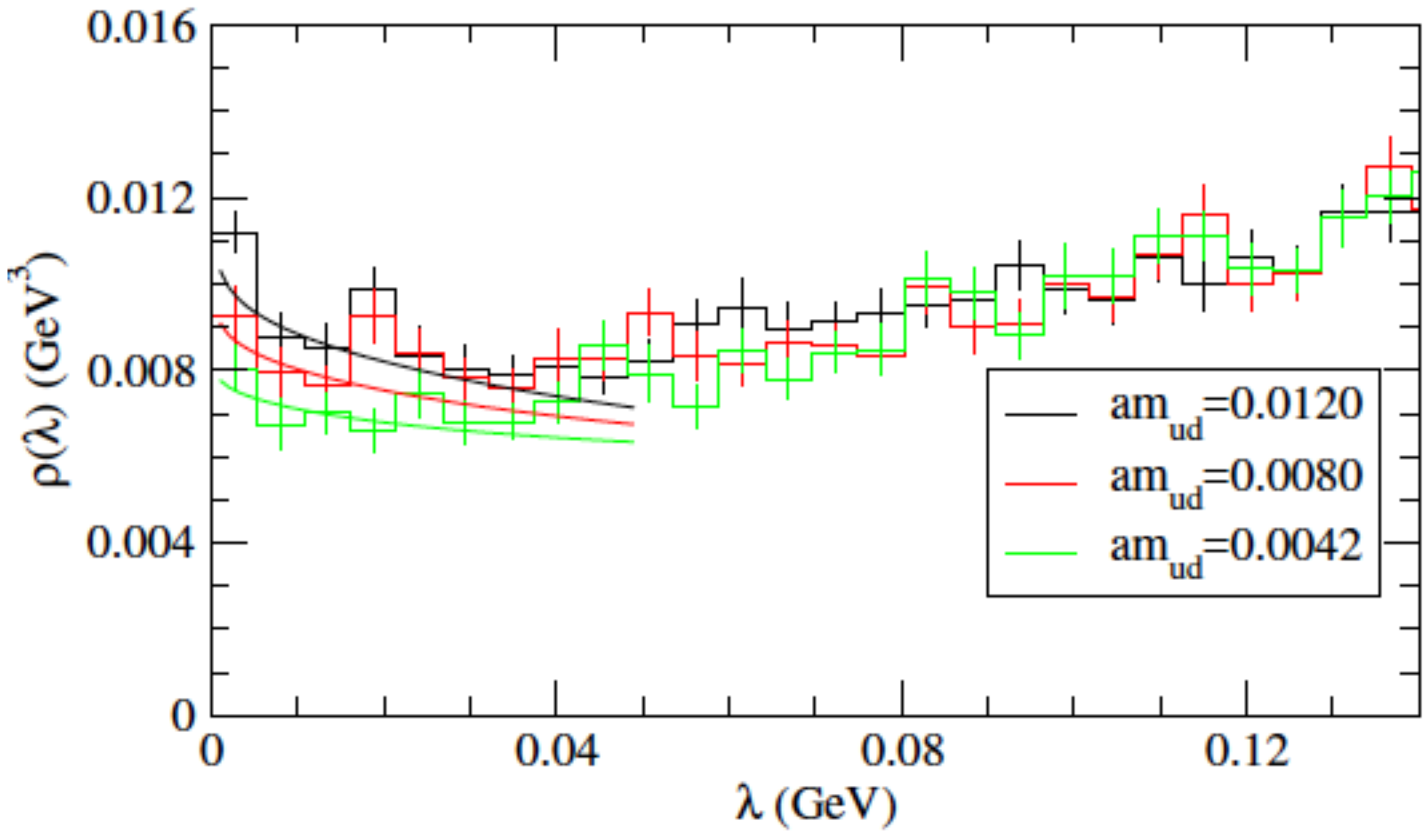
a^{-1} = 2.45 GeV



Lowest 3 bins (< 15 MeV) are averaged before fitting.
Effect of residual mass (~ 1 MeV) is minor.

Fit result (2)

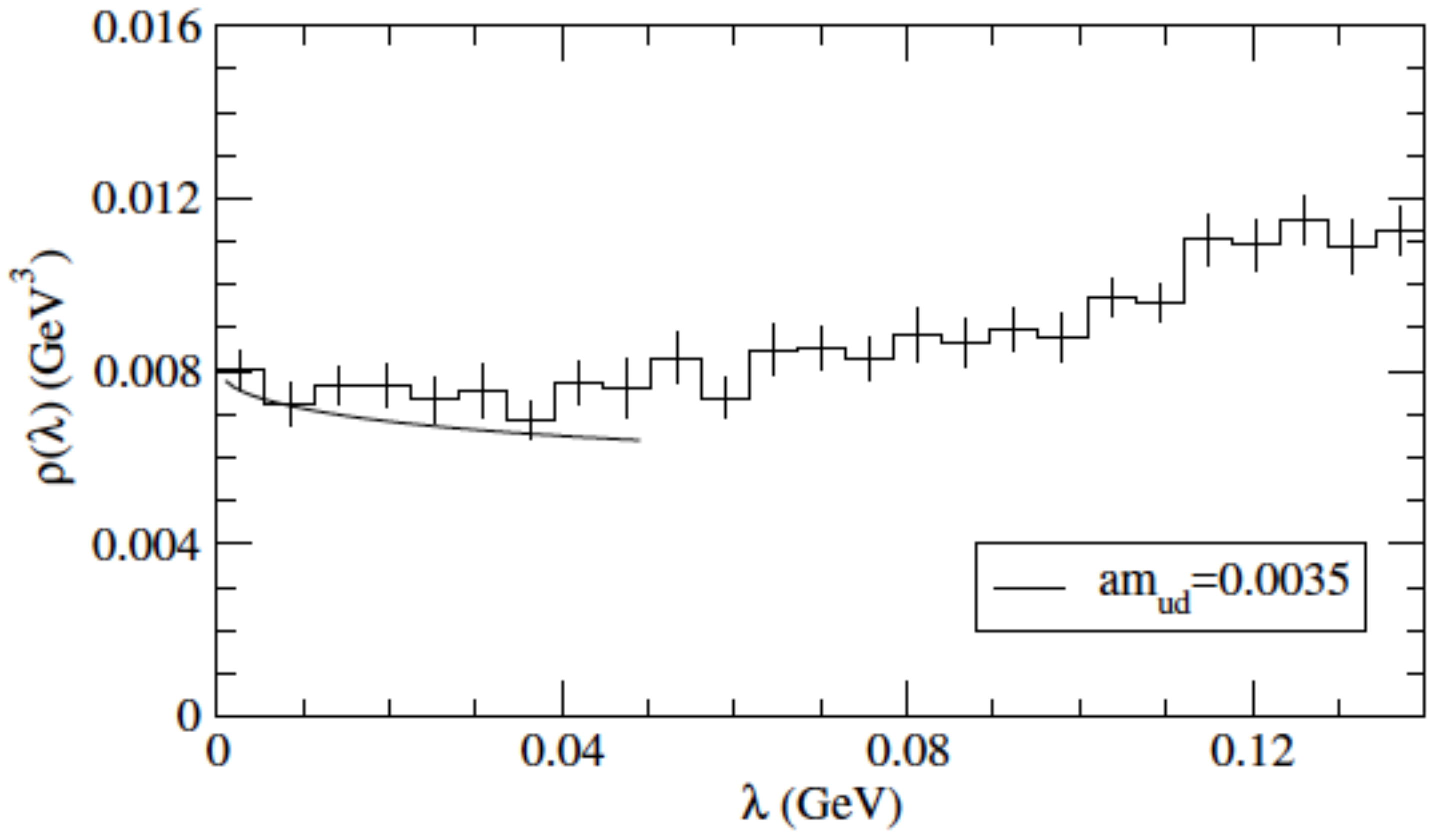
a^{-1} = 3.61 GeV



Discretization effect insignificant.

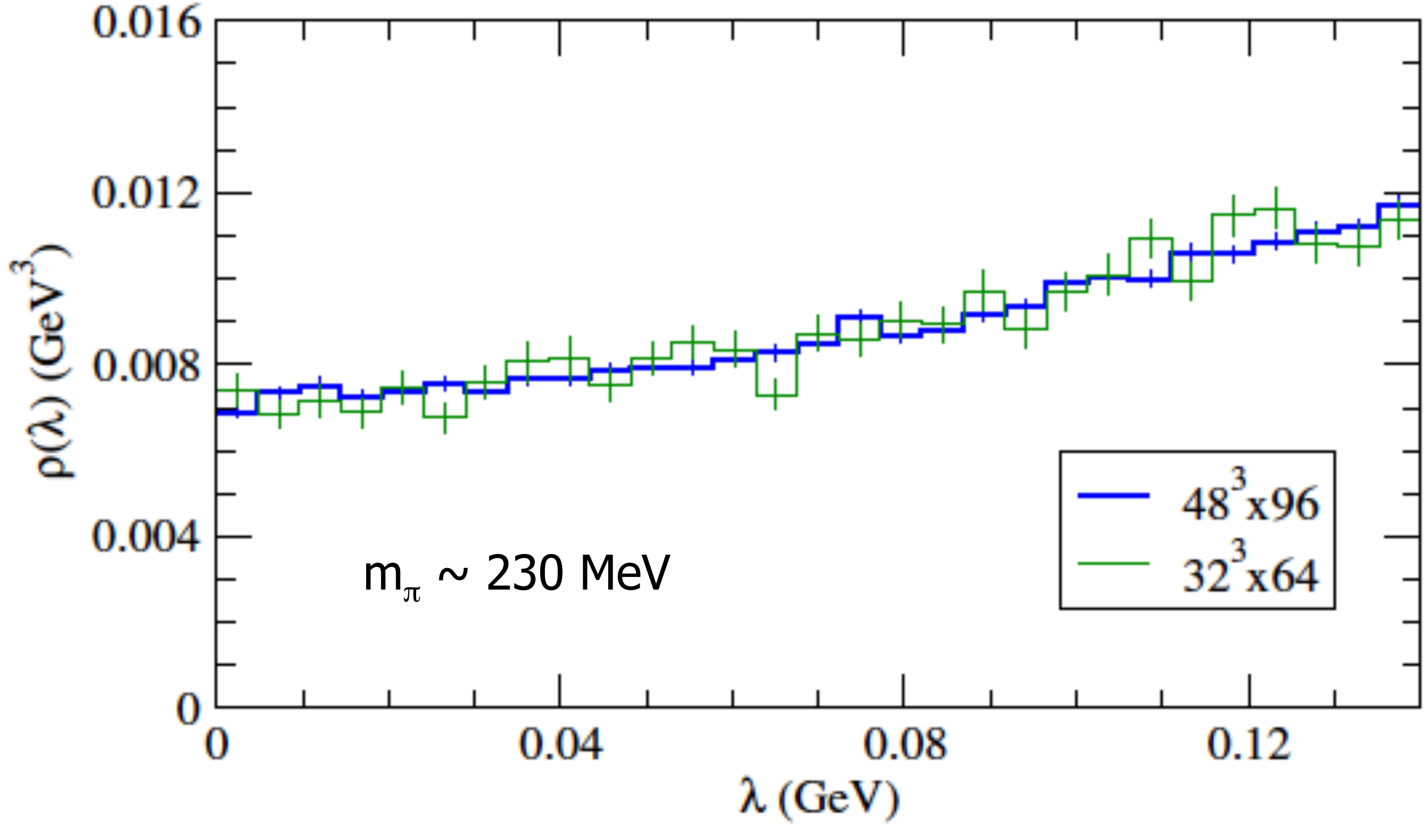
Fit result (3)

a^{-1} = 4.50 GeV



Discretization effect insignificant.

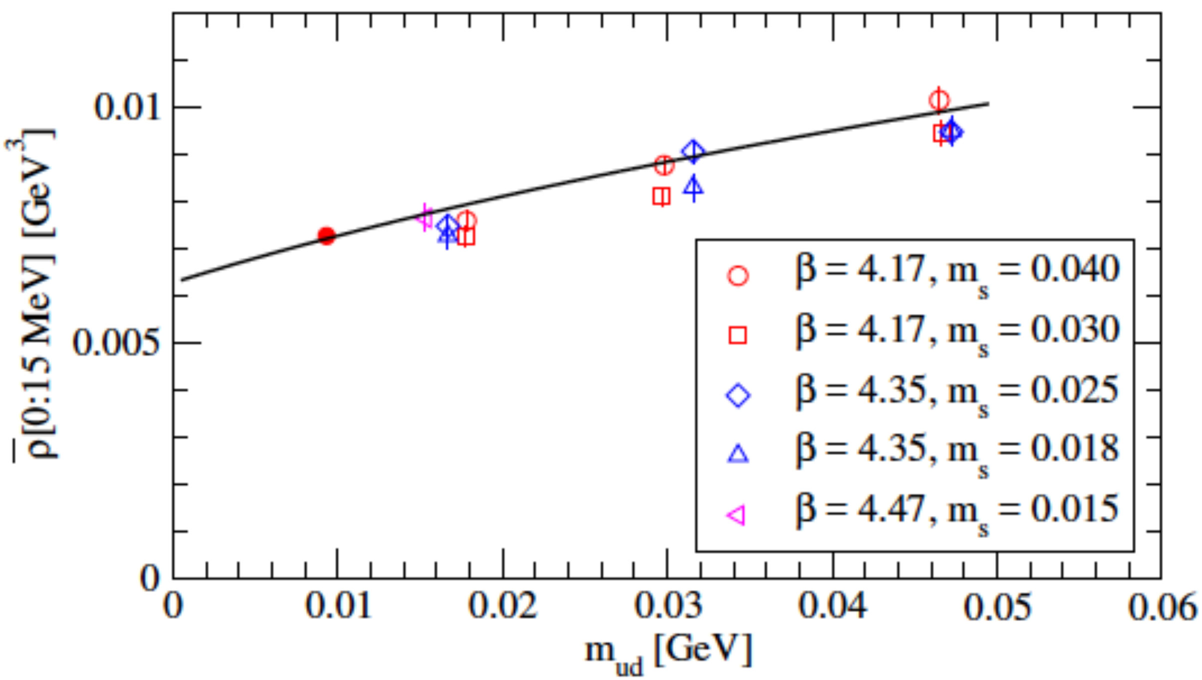
Finite volume effect



m_π ~ 230 MeV

Finite volume effect invisible.

Chiral condensate

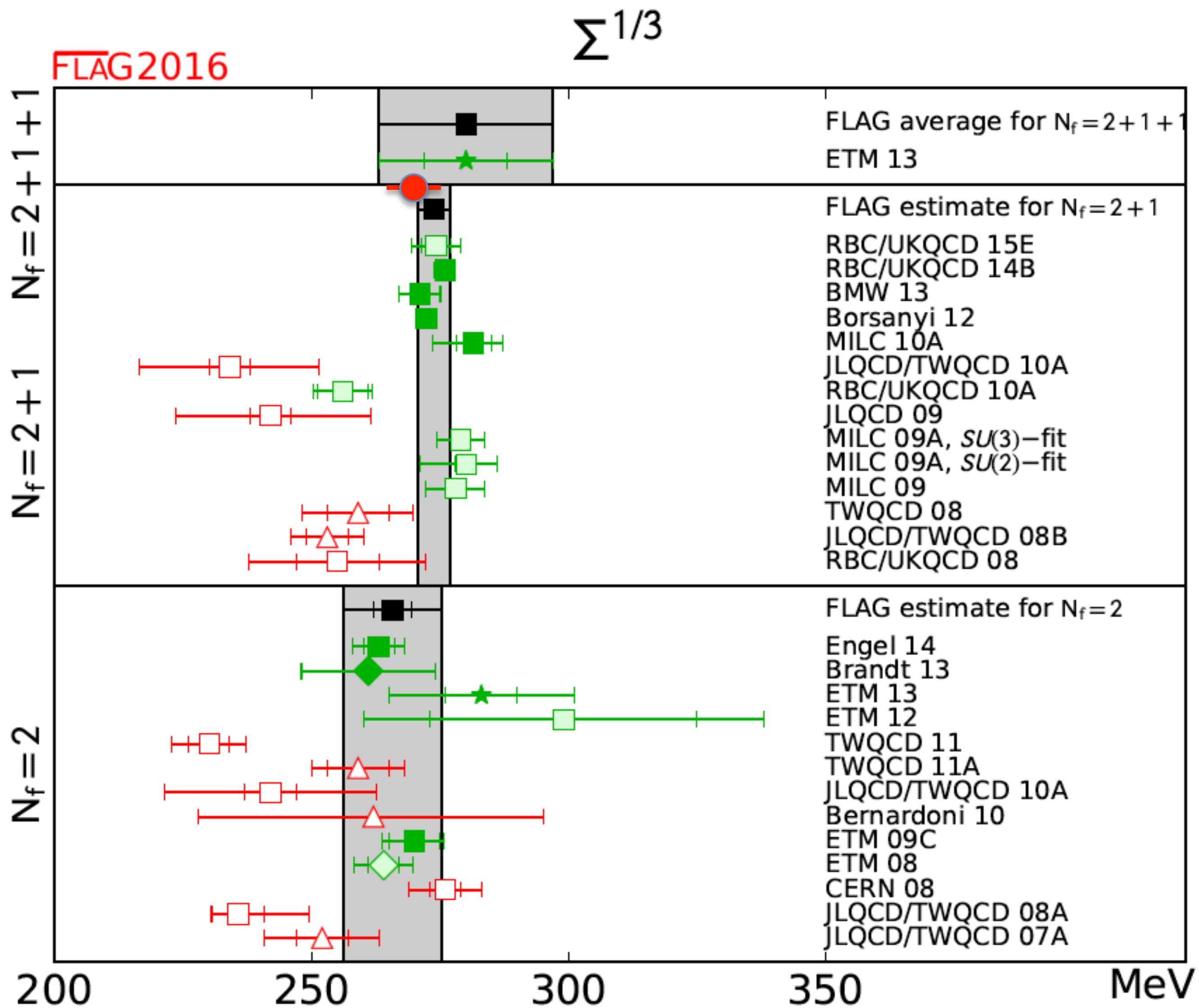


$$\Sigma^{MS}(2\ \mathrm{GeV}) = [\ 270.0 \pm 1.3 \pm 1.3 \pm 4.6\ \mathrm{MeV}\ ]^3$$

$$L_6 = 0.00016(6)$$

(stat)(renorm)(scale)

$$c_a = 0.00(15)\ \mathrm{GeV}^2,\ c_s = 0.50(30)\ \mathrm{GeV}^{-2}$$



$\Sigma^{1/3}$ (2 GeV) = 270.0 ± 4.9 MeV [JLQCD]

$\Sigma^{1/3}$ (2 GeV) = 274 ± 3 MeV [FLAG average 2016]

Summary

- Stochastic estimate of the ev count
  - Simple and flexible
- Precise calculation of $\rho(\lambda)$ with domain-wall fermions
  - Well controlled effect of residual mass.
  - Reproduce the spectrum predicted by χPT.
  - Continuum extrapolation essentially flat.
  - Among the most precise determination of Σ.