Lattice QCD with Optimal Domain-Wall Fermion on the 20^3 x 40 Lattice

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- It took 23 years (1974 ~1997) to realize that **Lattice QCD with Exact Chiral Symmetry** is the ideal theoretical framework to study the nonperturbative physics from the first principles of QCD.

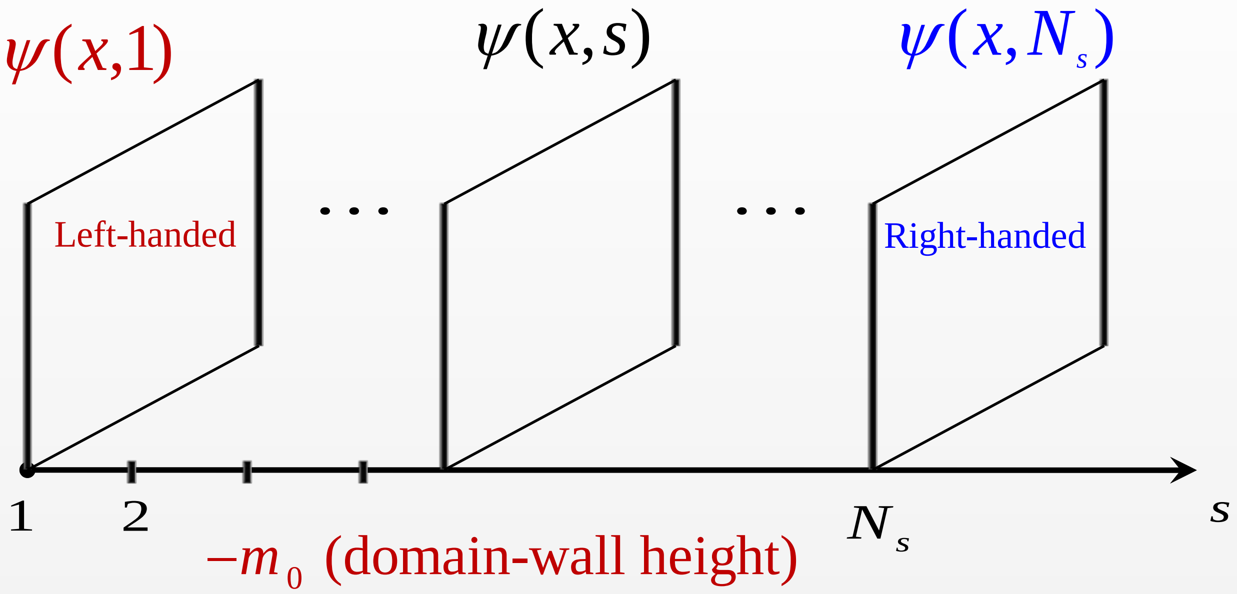
- **It is challenging to perform the HMC simulation** such that the chiral sym. is preserved to very high precision and all topological sectors are sampled ergodically.

- Since 2009, the **TWQCD** collaboration has been using a **GPU cluster** to simulate lattice QCD with **optimal domain-wall quarks**. The chiral sym. is preserved to a good precision with $m_{res} a \approx 0.0004$, and all topological sectors are sampled ergodically.

Outline

- Introduction
- HMC of Lattice QCD with ODWF
- Chiral Symmetry Breaking and Residual Mass
- Pseudoscalar Meson
- Conclusions

Domain-Wall Fermions [Kaplan, 1992]



D_{dwf} is a local op. with the nearest neighbor coupling along $\hat{s}$

$$\int[d\bar{\psi}][d\psi]\exp\left(-\bar{\Psi}D_{\text{dwf}}\Psi\right)=\det D_c \qquad D_c=\frac{1+\gamma_5 S}{1-\gamma_5 S}$$

$$N_s\to\infty,\ \ S\to\frac{H}{\sqrt{H^2}}, \qquad D_c\gamma_5+\gamma_5 D_c=0,\ \text{Exact Chiral Sym.}$$

At finite N_s, S is not equal to the optimal rational approx.

Optimal Rational Approximation for Square Root

For the inverse square root function, the optimal rational approx. was obtained by Zolotarev in 1877.

$$\frac{1}{\sqrt{x}},\ x \in [1,b]$$

$$R_Z^{(n-1,n)}(x) = \frac{2\Lambda}{1+\Lambda}\frac{1}{M}\frac{\prod_{l=1}^{n-1}(1+x/C_{2l})}{\prod_{l=1}^{n}(1+x/C_{2l-1})}$$

$$R_Z^{(n,n)}(x) = \frac{2\lambda}{1+\lambda}\frac{1}{m}\frac{\prod_{l=1}^{n}(1+x/c_{2l})}{\prod_{l=1}^{n}(1+x/c_{2l-1})}$$

where $\lambda, \Lambda, m, M, C_{2l}, C_{2l-1}, c_{2l}, c_{2l-1}$

are expressed in terms of the

Jacobian Elliptic functions.

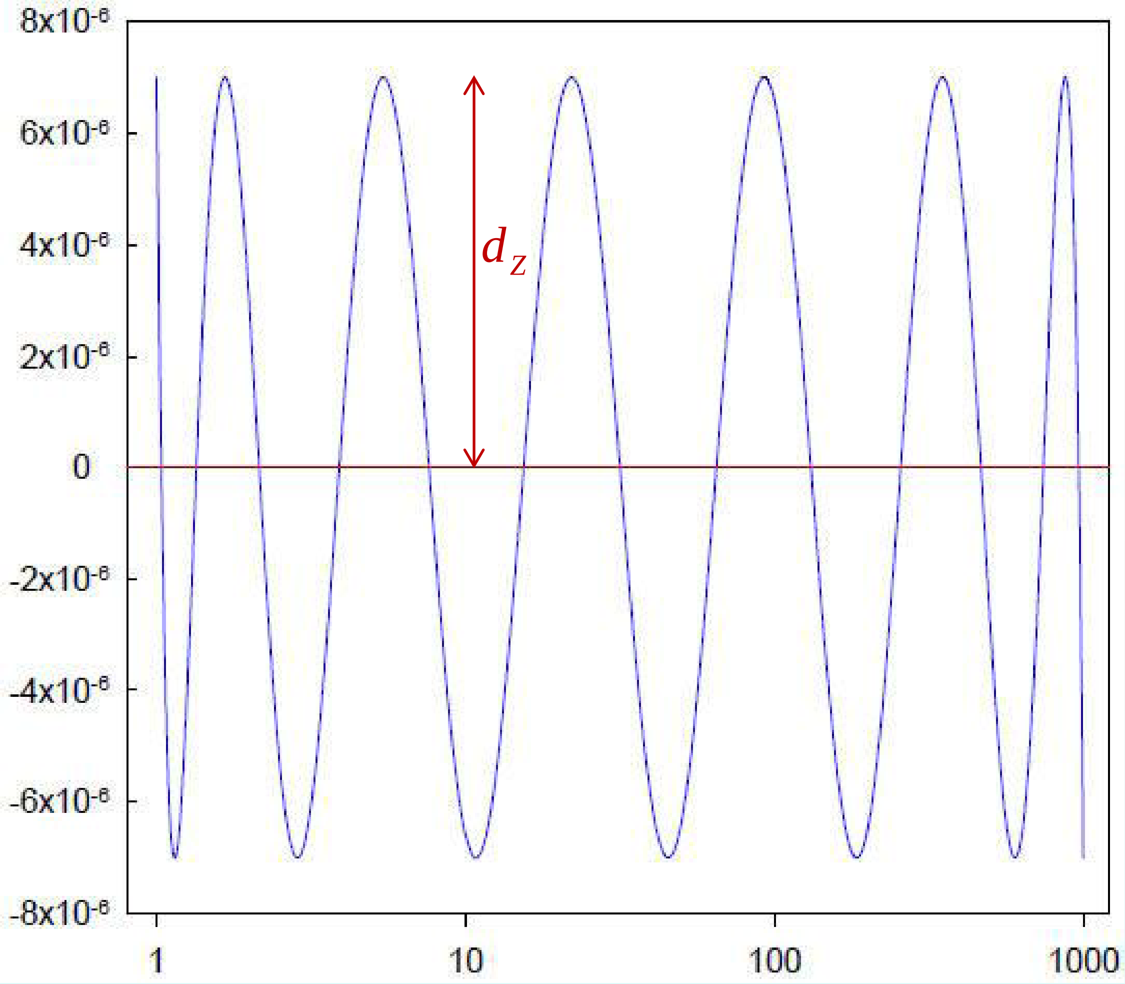
Yegor **I**vanovich **Zolotarev**
(1847 –1878)

Salient Feature of Optimal Rational Approximation

$$1-\sqrt{x}R_Z^{(n,m)}(x)$$

Has $(n+m+2)$ alternate change of sign in $[x_{\min}, x_{\max}]$, and attains its max. and min. (all with equal magnitude)

In the figure, $n = m = 6$ it has 14 alternate change of sign in [1,1000]



$\log(x)$

Optimal Domain-Wall Fermion

[TWC, Phys. Rev. Lett. 90 (2003) 071601]

$$A_{\text{odwf}} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}_{x,s} \left[\left(I + \rho_s D_w \right)_{x,x'} \delta_{s,s'} - \left(I - \sigma_s D_w \right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \psi_{x',s'}$$

$$\equiv \bar{\Psi} D_{\text{odwf}} \Psi$$

$$D_w = \sum_{\mu=1}^{4} \gamma_\mu t_\mu + W - m_0, \qquad m_0 \in (0,2)$$

$$t_\mu(x,x') = \frac{1}{2}\left[U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

$$W(x,x') = \sum_{\mu=1}^{4} \frac{1}{2}\left[2\delta_{x,x'} - U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

with boundary conditions

$$P_+ \psi(x,0) = -r m_q P_+ \psi(x,N_s), \qquad m_q\text{: bare quark mass}$$

$$P_- \psi(x,N_s+1) = -r m_q P_- \psi(x,1), \qquad P_\pm = \frac{1}{2}(1 \pm \gamma_5)$$

Optimal Domain-Wall Fermion (cont.)

The action for Pauli-Villars fields is similar to A_{odwf}

$$A_{PV}=\sum_{s,s'=1}^{N_s}\sum_{x,x'}\bar{\phi}_{x,s}\left[\left(I+\rho_s D_w\right)_{x,x'}\delta_{s,s'}-\left(I-\sigma_s D_w\right)_{x,x'}\left(P_-\delta_{s',s+1}+P_+\delta_{s',s-1}\right)\right]\phi_{x',s'}$$

but with boundary conditions: $P_+\phi(x,0)=-P_+\phi(x,N_s)$,

$$P_-\phi(x,N_s+1)=-P_-\phi(x,1)$$

- In the original formulation of ODWF, $\rho_s=\sigma_s=\omega_s$

$$\omega_s=\frac{1}{\lambda_{\min}}\sqrt{1-\kappa'^2 sn^2(v_s;\kappa')},\quad s=1,\cdots,N_s$$

where $sn(v_s;\kappa')$ is the Jacobian elliptic function with argument v_s and modulus $\kappa'=\sqrt{1-\lambda_{\min}^2/\lambda_{\max}^2}$,
$\lambda_{\min}^2$ and $\lambda_{\max}^2$ are lower and upper bounds of the eigenvalues of H_w^2

Optimal Domain-Wall Fermion (cont.)

$$\int [d\bar{\psi}][d\psi]\left[d\bar{\phi}\right][d\phi]\exp\left(-A_{\text{odwf}} - A_{\text{PV}}\right) = \det D(m_q)$$

The effective 4D Dirac operator

$$D(m_q) = m_q + \left(m_0 - m_q/2\right)\left[1+\gamma_5 S_{opt}\left(H_w\right)\right]$$

$$S_{opt}\left(H_w\right) = \frac{1-\prod_{s=1}^{N_s} T_s}{1+\prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1-\omega_s H_w}{1+\omega_s H_w}$$

$$= \begin{cases} H_w R_Z^{(n-1,n)}\left(H_w^2\right), & N_s = 2n \\ H_w R_Z^{(n,n)}\left(H_w^2\right), & N_s = 2n+1 \end{cases}$$

⇧

Zolotarev optimal rational approximation for $\frac{1}{\sqrt{H_w^2}}$

Optimal Domain-Wall Fermion (cont.)

- For $\rho_s = c\omega_s + d, \ \sigma_s = c\omega_s - d, \quad c, d$ (constants)

The effective 4D Dirac operator becomes

$$D(m_q) = m_q + \left(m_0(1 - dm_0) - \frac{m_q}{2} \right) \left[1 + \gamma_5 S_{opt}(H) \right], \quad H = \frac{cH_w}{1 + d\gamma_5 H_w}$$

$$S_{opt}(H) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H}{1 + \omega_s H}$$

only $d = 0$ is good for the projection of low-modes of $D(0)$

$$= \begin{cases} HR_Z^{(n-1,n)}(H^2), & N_s = 2n \\ HR_Z^{(n,n)}(H^2), & N_s = 2n+1 \end{cases}$$

Optimal Domain-Wall Fermion (cont.)

- For the special case $\rho_s = 1, \ \sigma_s = 0$

It reduces to the conventional DWF which does not have the optimal chiral symmetry.

$$D(m_q) = m_q + \left(\frac{m_0}{2}(2-m_0) - \frac{m_q}{2} \right) \left[1 + \gamma_5 S_{\text{polar}}(H) \right], \quad H = \frac{H_w}{2+\gamma_5 H_w}$$

$$S_{\text{polar}}(H) = \frac{1-T^{N_s}}{1+T^{N_s}}, \qquad T = \frac{1-H}{1+H}$$

$$b_l = \sec^2\left[\frac{\pi}{N_s}\left(l - \frac{1}{2} \right) \right]$$

$$d_l = \tan^2\left[\frac{\pi}{N_s}\left(l - \frac{1}{2} \right) \right]$$

$$= \begin{cases} H\left(\dfrac{2}{N_s} \displaystyle\sum_{l=1}^{n} \dfrac{b_l}{H^2+d_l} \right), & N_s = 2n \\ H\left(\dfrac{1}{N_s} + \dfrac{2}{N_s} \displaystyle\sum_{l=1}^{n} \dfrac{b_l}{H^2+d_l} \right), & N_s = 2n+1 \end{cases}$$

Polar approximation

Features of TWQCD's Simulations

- Use a GPU cluster of 300 GPUs, with sustained 85 Tflops.
- Conjugate Gradient with Mixed Precision.
- Chiral Symmetry is preserved with Optimal DWF.
- Even-Odd Preconditioning for the 4D Wilson-Dirac Matrix.
- HMC with Multiple Time Scale Integration and Mass Preconditioning.
- Omelyan Integrator for the Molecular Dynamics.
- A novel algorithm for the simulation of one flavor.
  (see Yu-Chih Chen's talk in this session)
- Topological Sectors are sampled ergodically.

Even-Odd Preconditioning of ODWF

$$\mathcal{D}(m_q) = S_1^{-1} \begin{pmatrix} 1 & M_5 D_w^{\mathrm{EO}} \\ M_5 D_w^{\mathrm{OE}} & 1 \end{pmatrix} S_2^{-1}$$

Schur decomposition ↓

$$\mathcal{D}(m_q) = S_1^{-1} \begin{pmatrix} 1 & 0 \\ M_5 D_w^{\mathrm{OE}} & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & C \end{pmatrix} \begin{pmatrix} 1 & M_5 D_w^{\mathrm{EO}} \\ 0 & 1 \end{pmatrix} S_2^{-1}$$

$$C \equiv 1 - M_5 D_w^{\mathrm{OE}} M_5 D_w^{\mathrm{EO}}$$

For 2-flavors QCD, the pseudofermion action is

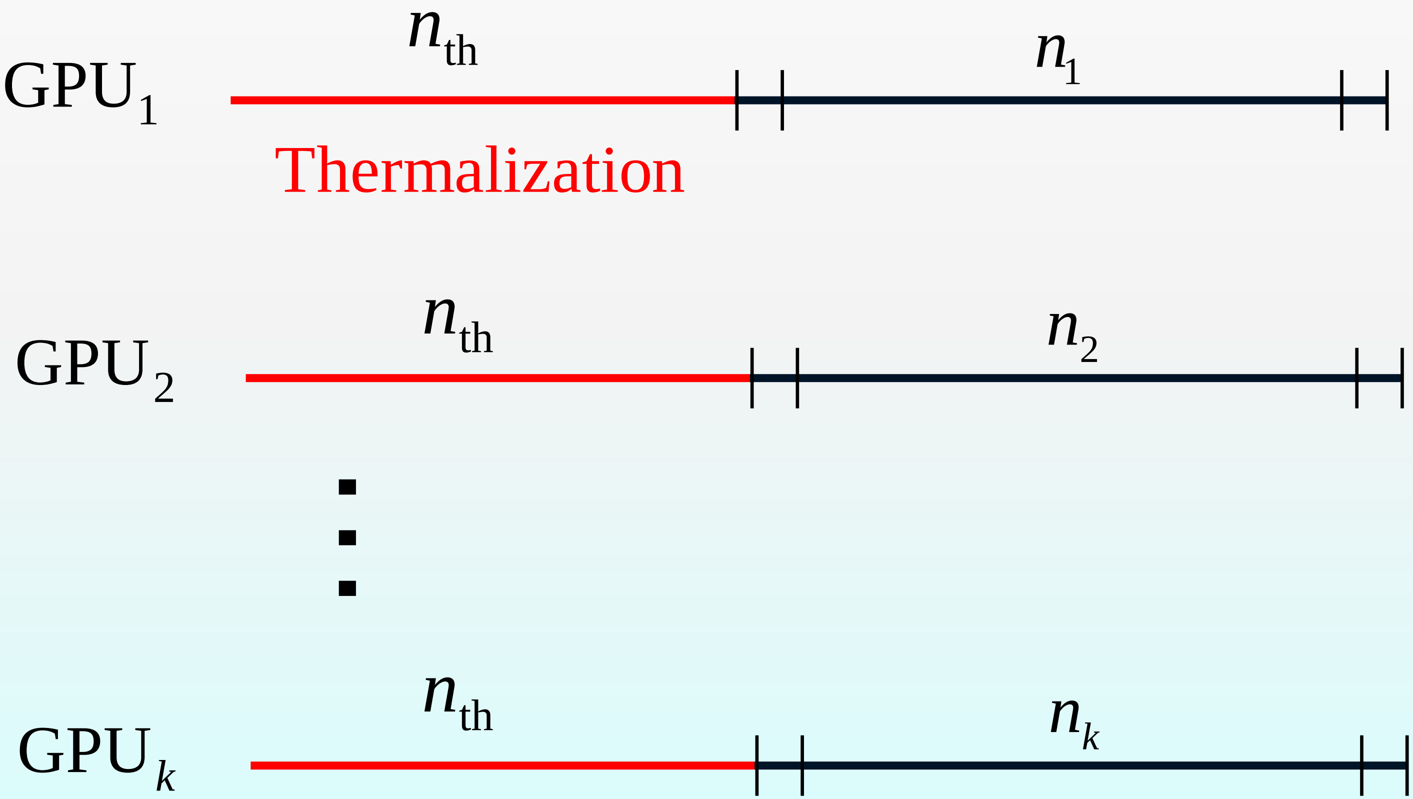
$$A_{PF} = \phi^\dagger C_{PV}^\dagger (CC^\dagger)^{-1} C_{PV} \phi \qquad C_{PV} \equiv C(m_q = 2m_0)$$

Lattice Setup for 2-flavor QCD with ODWF

- Lattice Sizes: 16^3 x 32 x 16, 20^3 x 40 x 16
- Quark Action: Optimal Domain-Wall Fermion (ODWF)
- Gluon Action: Plaquette (beta = 5.95)
- Lattice Spacing: a ~ 0.1 [fm], 1/a ~1.9 [GeV]
- Spatial Volume: ~$(1.7\text{ fm})^3$, ~$(2.1\text{ fm})^3$
- 8/6 sea quark masses, with pion masses 230 – 560/490 MeV.
- Each mass has **~5500** traj. After discarding initial **300-500** traj. for **thermalization**, measurements are performed every **10** traj., **~500 confs** for each sea quark mass
- For each conf, **zero modes** and 80/180 **conjugate pairs of low-lying eigenmodes** of the overlap operator are projected. (see Tung-Han Hsieh's talk in this session)

Simulation Scheme (I) $16^3 \times 32 \times 16$

$n_{\text{th}} > 300$ $k \simeq 30-32$



GPU_1 n_{th} n_1

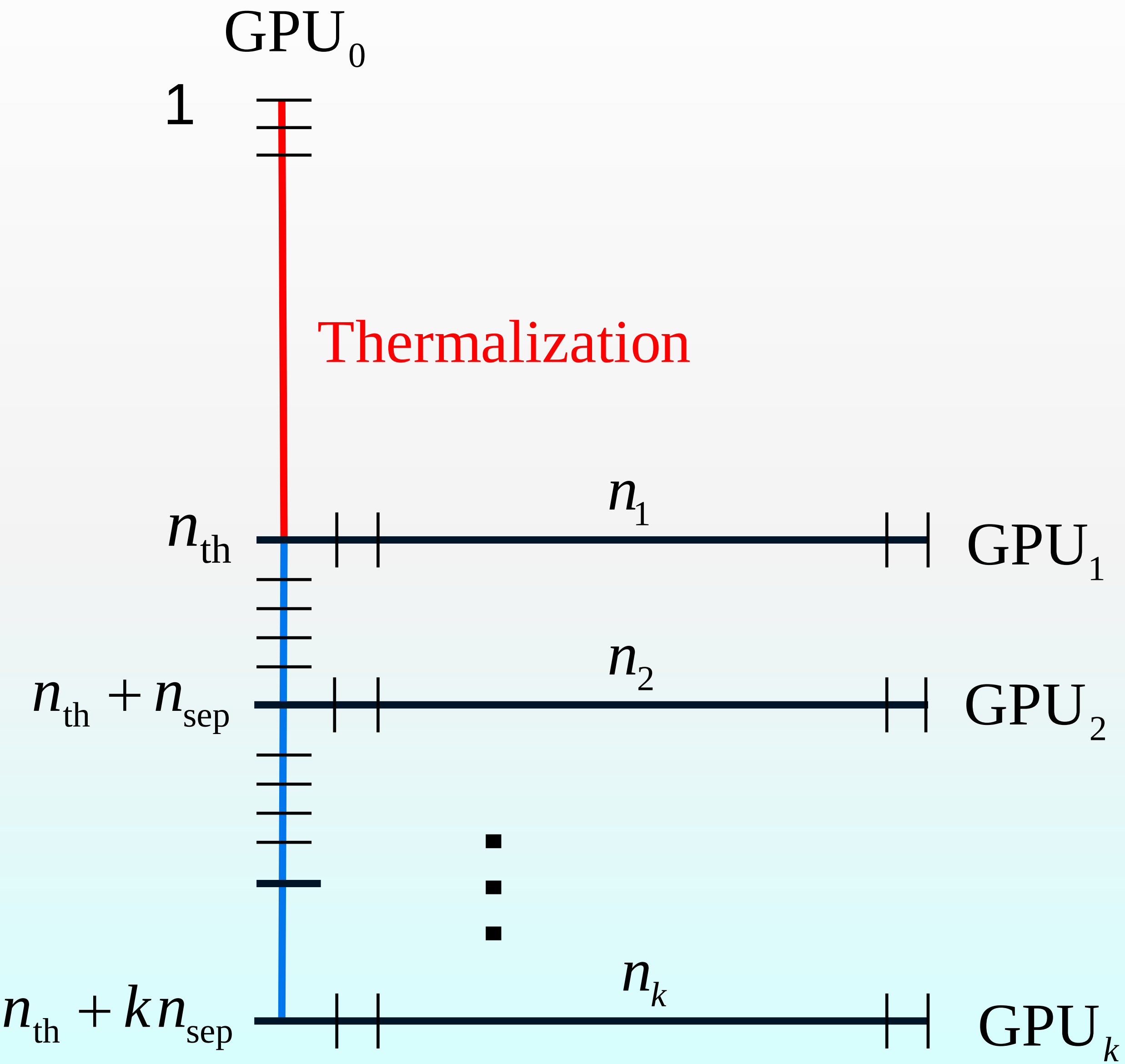
Thermalization

GPU_2 n_{th} n_2

⋮

GPU_k n_{th} n_k

Simulation Scheme (II) $20^3 \times 40 \times 16$

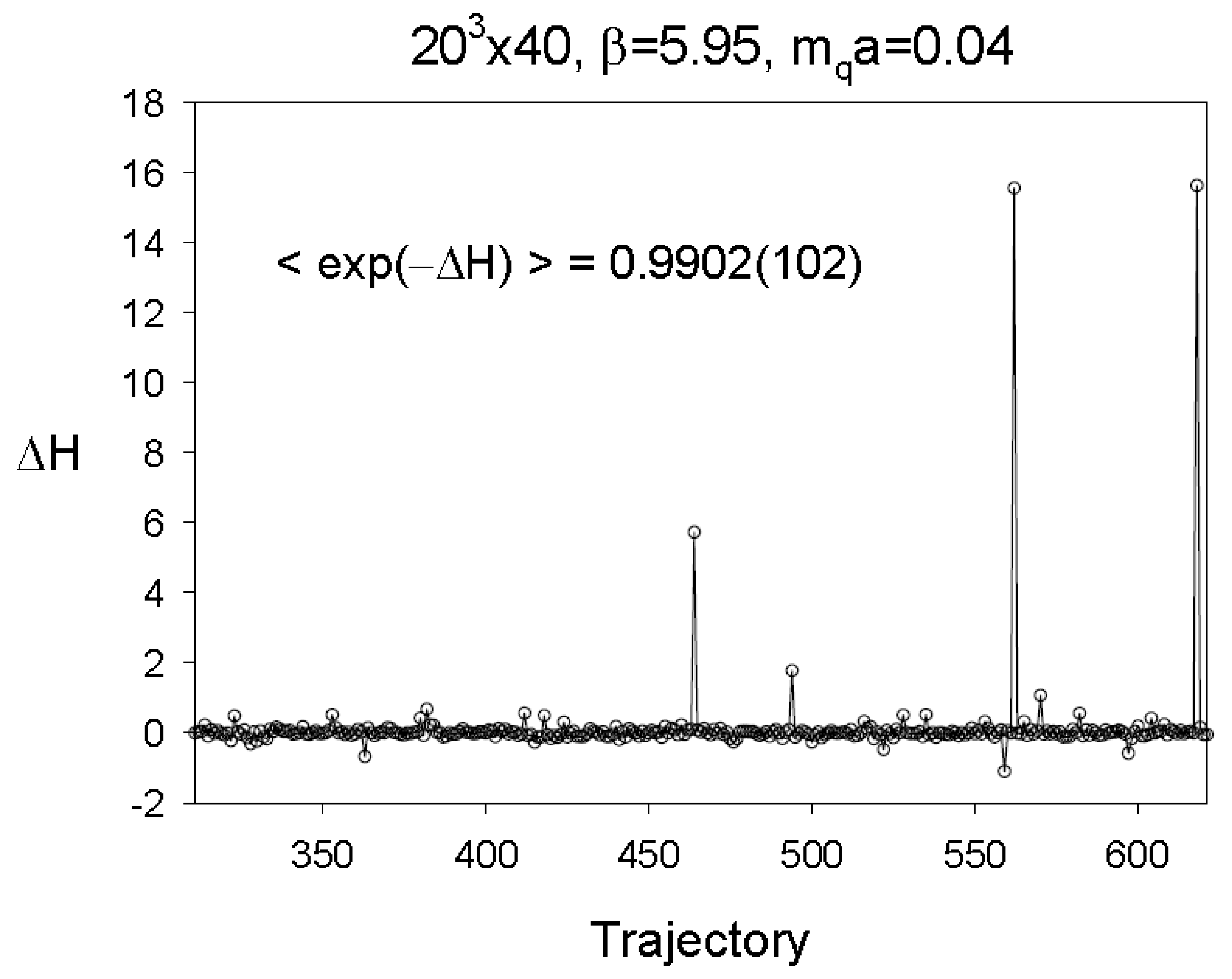


$n_{\mathrm{th}} > 300$

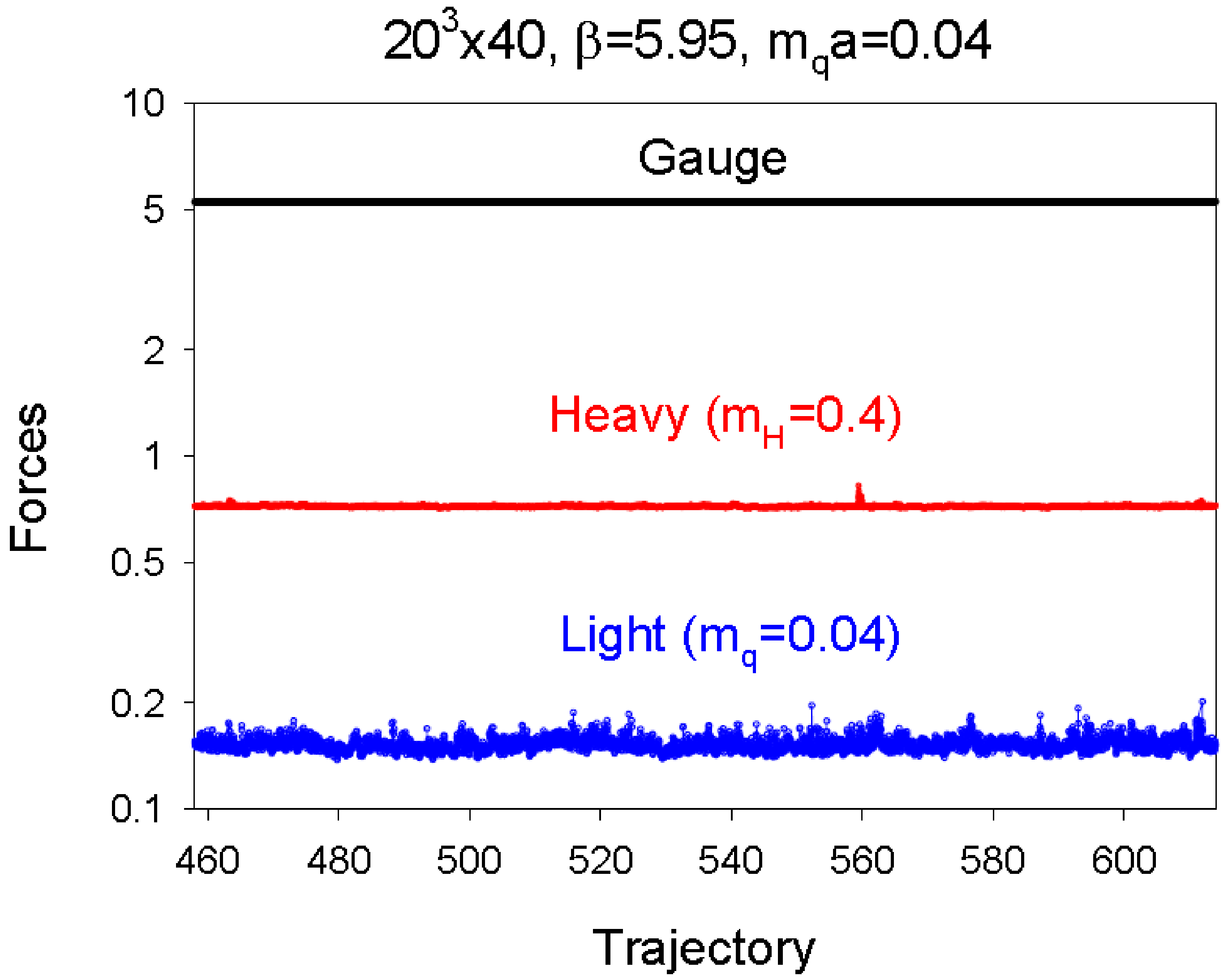
$n_{\mathrm{sep}} \simeq 2-5$

$k \simeq 16-20$

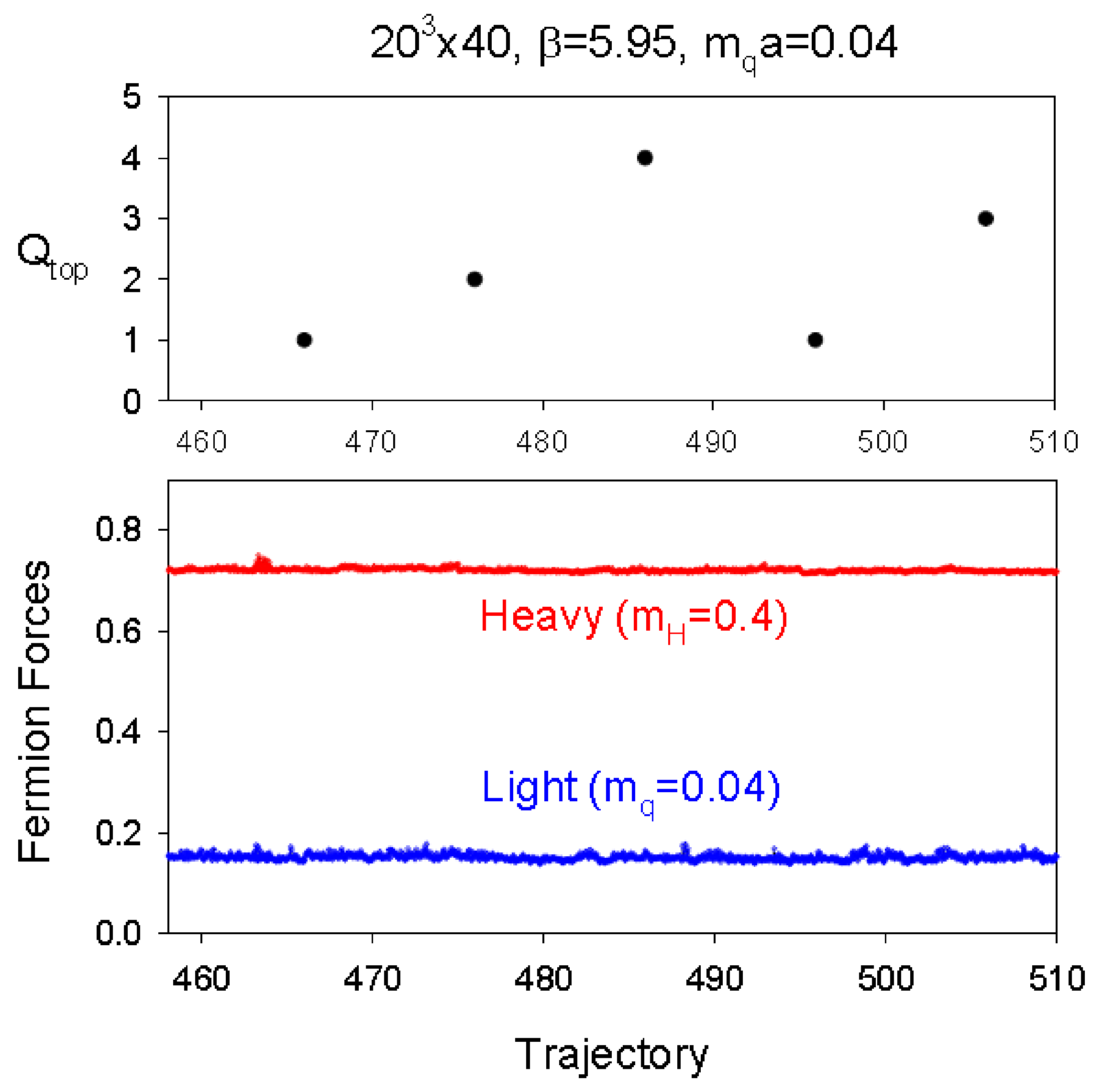
HMC in a single GPU



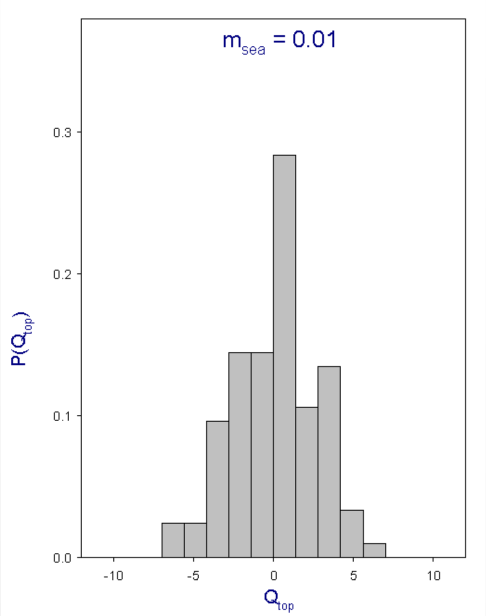
HMC in a single GPU (cont)

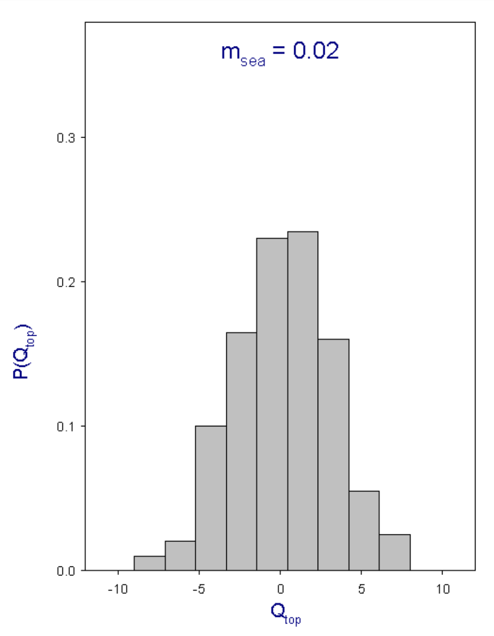


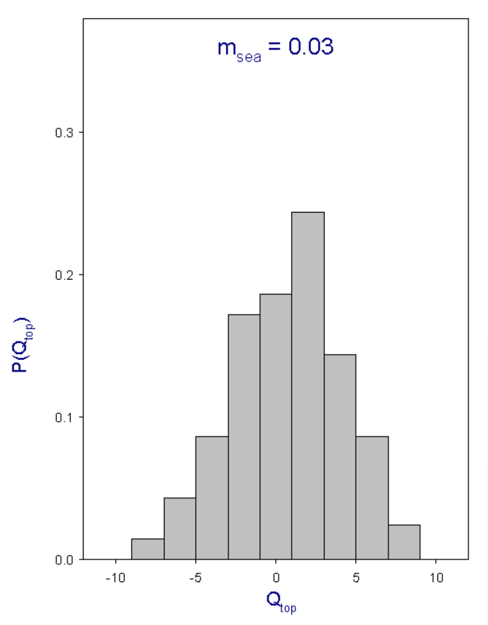
HMC in a single GPU (cont)

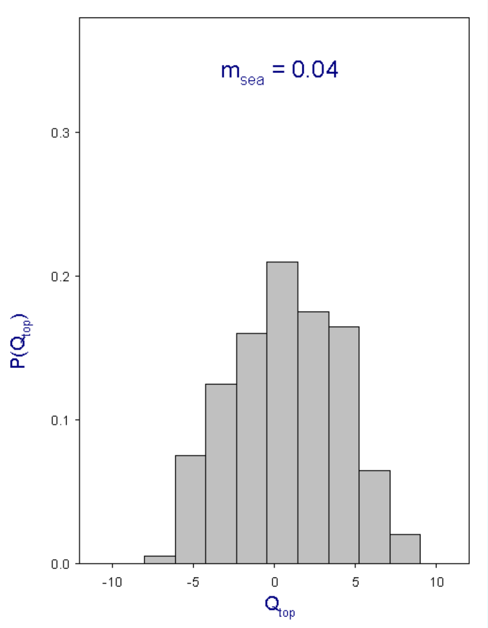


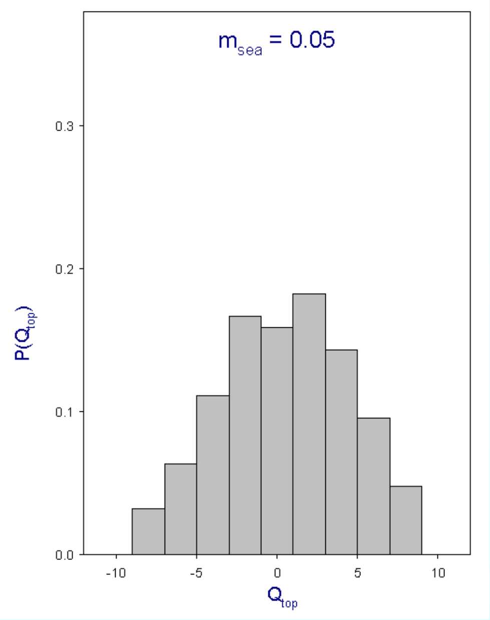
Topological Charge











only ~200 confs of each sea-quark mass are measured.

Chiral Sym Breaking due to Finite Ns

[Y.C. Chen, TWC, arXiv:1205.6151]

It can be measured by the residual mass

$$m_{res}(y) = \left\langle \frac{\sum_x \langle J_5(x,n)\overline{q}(y)\gamma_5 q(y)\rangle}{\sum_x \langle \overline{q}(x)\gamma_5 q(x)\overline{q}(y)\gamma_5 q(y)\rangle} \right\rangle_{\{U\}}, \quad n = \frac{N_s}{2}$$

$$= \left\langle \frac{\mathrm{Re}\,\mathrm{tr}\left(D_c + m_q\right)^{-1}_{y,y}}{\mathrm{tr}\left[\left(D_c^\dagger + m_q\right)\left(D_c + m_q\right)\right]^{-1}_{y,y}} \right\rangle_{\{U\}} - m_q$$

$$J_5(x,n) \equiv \overline{\psi}_{n+1}(x)P_+\psi_n(x) - \overline{\psi}_n(x)P_-\psi_{n+1}(x)$$

$\left(D_c + m_q\right)^{-1}$ valence quark propagator with $m_q = m_{sea}$

Chiral Sym Breaking due to Finite Ns (cont)

[Y.C. Chen, TWC, arXiv:1205.6151]

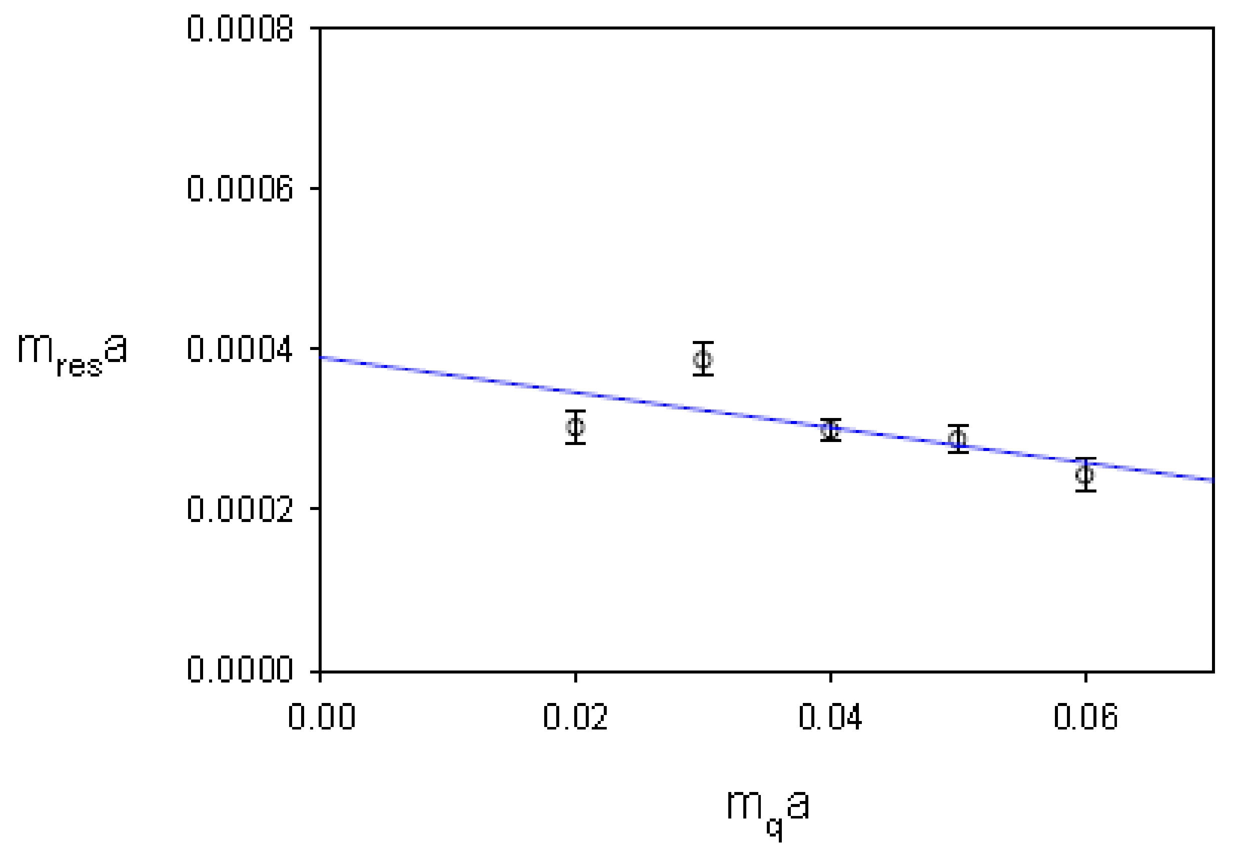
For lattice QCD with ODWF, it can be shown that

$$M_{res} \le \frac{d_Z}{2r}\left\{(1-m)^2 + 2(1-m)\left[m + \frac{(1+m)d_Z}{2-(3-m)d_Z}\right] + (1+m)\left[\frac{2m+(1-m)^2 d_Z}{2-(3-m)d_Z}\right]\right\}$$

For ODWF, $d_Z \ll 1$ in most cases, and it gives

$$M_{res} \le \frac{d_Z}{2r}\left(1 + r m_q\right) \simeq \frac{d_Z}{2r}$$

Chiral Symmetry Breaking due to Finite Ns (cont)



In the chiral limit: $m_{res}a = 0.00039(6)$

Pseudoscalar Meson

$$\langle 0|\pi^-(\vec{x},t)\pi^+(\vec{0},0)|0\rangle = -\langle 0|\left(\bar{u}\gamma_5 d\right)(\vec{x},t)\left(\bar{d}\gamma_5 u\right)(\vec{0},0)|0\rangle$$

$$= \mathrm{tr}\left[\left(D_c+m_u\right)^{-1}_{0,x}\gamma_5\left(D_c+m_d\right)^{-1}_{x,0}\gamma_5\right]$$

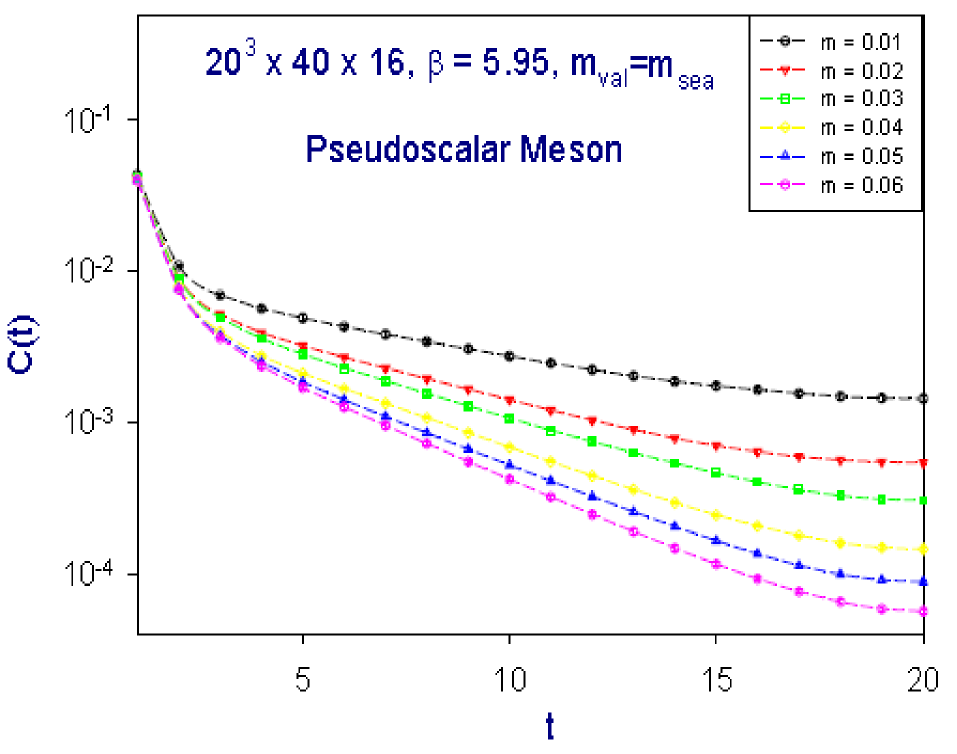
Fitting $C_\pi(t)=\sum_{\vec{x}}\langle 0|\pi^-(\vec{x},t)\pi^+(\vec{0},0)|0\rangle$ to

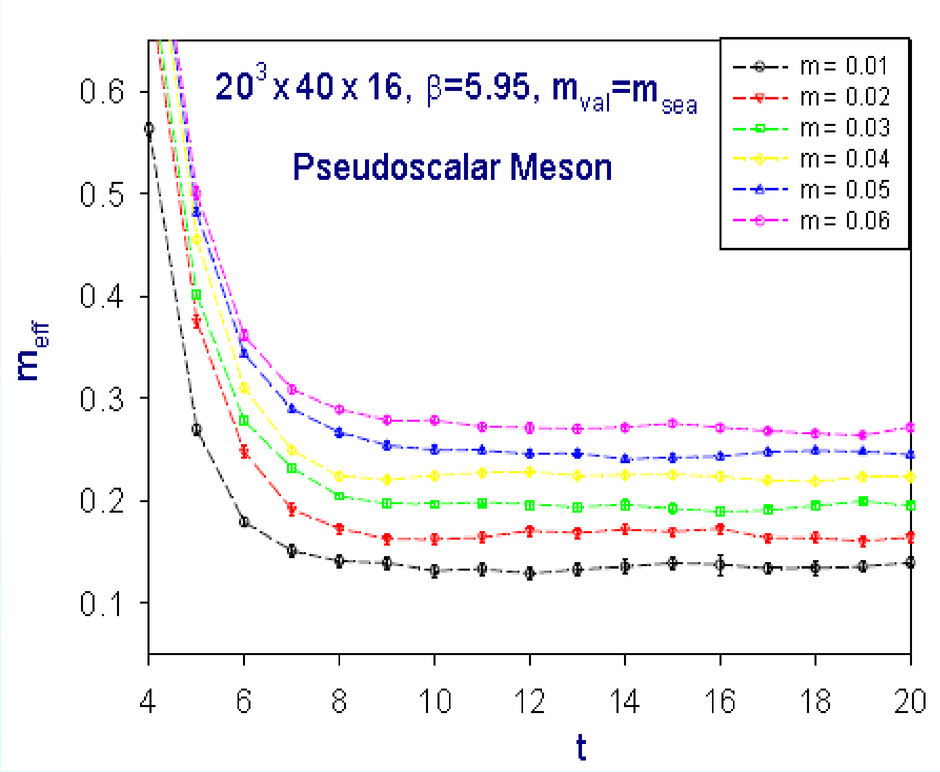
$$\frac{\left|\langle\pi^+(\vec{p}=0)|\pi^-(\vec{0},0)|0\rangle\right|^2}{2M_\pi}\left(e^{-M_\pi t}+e^{-M_\pi(T-t)}\right)+\underset{\searrow\, 0}{\text{excited states}}$$

to extract M_π and $F_\pi = \dfrac{(m_u+m_d)}{\sqrt{2M_\pi^2}}\left|\langle\pi^+(\vec{p}=0)|\pi^-(\vec{0},0)|0\rangle\right|$

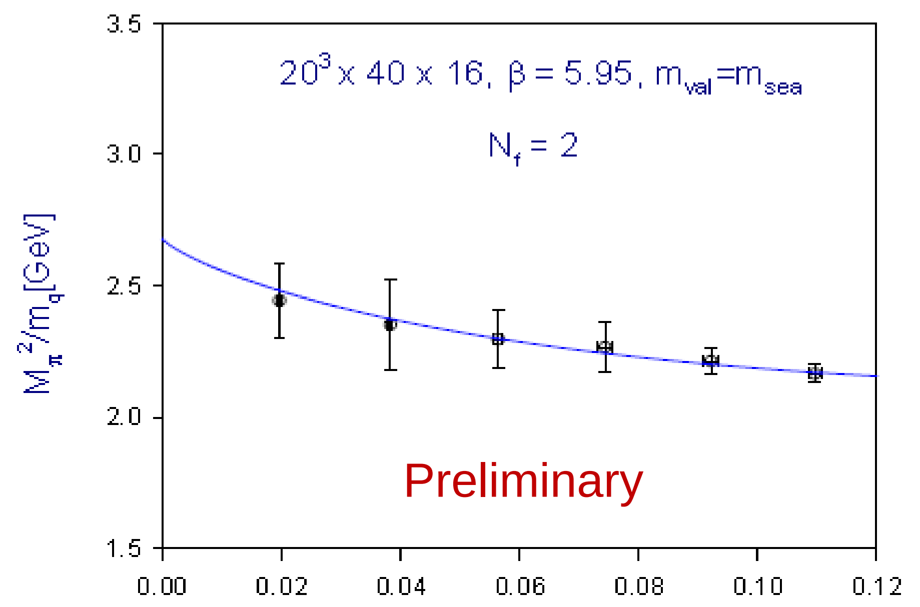
Pseudoscalar Meson: C(t) and Effective Mass

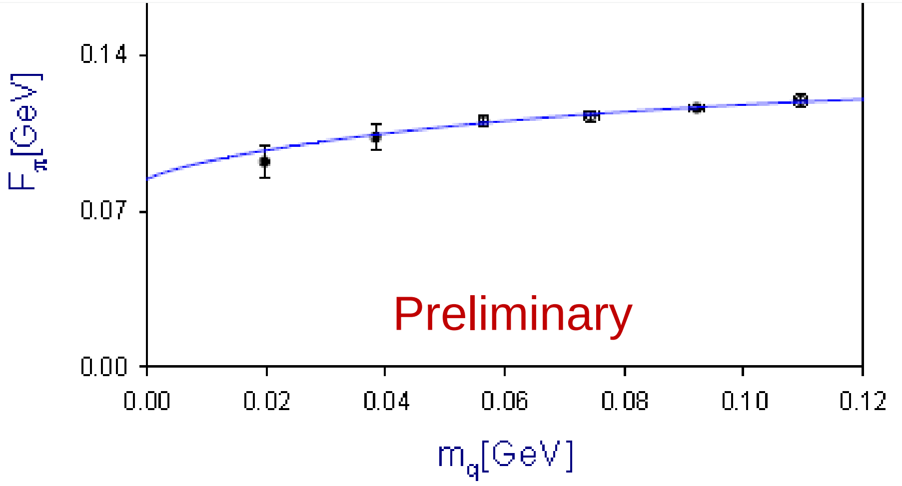
$$M_{\text{eff}}(t) = \cosh^{-1}\left[\frac{C(t+1)+C(t-1)}{2C(t)}\right]$$





Fitting to NLO ChPT





$$M_\pi \simeq 230 - 490 \text{ MeV}$$

NLO ChPT
(Gasser & Leutwyler, 1985)

$$\frac{M_\pi^2}{m_q} = 2B\left(1 + \frac{Bm_q}{(4\pi F)^2}\ln\frac{2Bm_q}{\Lambda_3^2}\right),$$

$$B \equiv \frac{\Sigma}{F^2}$$

$$F_\pi = F\left(1 - \frac{2Bm_q}{(4\pi F)^2}\ln\frac{2Bm_q}{\Lambda_4^2}\right)$$

$$\bar{l}_3 \equiv \ln\frac{\Lambda_3^2}{m_{\pi^\pm}^2}, \quad \bar{l}_4 \equiv \ln\frac{\Lambda_4^2}{m_{\pi^\pm}^2},$$

$$m_{\pi^\pm} = 0.14 \text{ GeV}$$

Fitting to NLO ChPT (cont)

Simultaneous fit of 6 pairs of (M_π, F_π) to NLO ChPT, with correlation between M_π and F_π at the same m_q, we obtain

$$F = 0.085(2) \text{ GeV}$$

$$\Sigma^{\overline{\text{MS}}}(2 \text{ GeV}) = \left[230(3)\,\text{MeV}\right]^3$$

$$\bar{l}_3 = 4.186(68)$$

$$\bar{l}_4 = 4.315(79)$$

Preliminary

Conclusions

- ODWF provides a viable framework for the simulation of QCD, which not only preserves the chiral symmetry to a good precision, but also samples all topological sectors ergodically.

- For 2-flavors QCD

  (a) 16^3 x 32: two ensembles, β = 5.90, and β = 5.95.
  For each ensemble, 8 sea quark masses,
  each of ~5000 trajectories after thermalization.

  (b) 20^3 x 40: one ensemble, β = 5.95, with 6 sea-quark masses, each of ~5000 trajs. after thermalization.

- A novel algorithm for the simulation of one flavor.
  [see Yu-Chih Chen's talk in this session]

Conclusions (cont)

- Pion mass and decay constant are in good agreement with the sea-quark mass dependence predicted by NLO ChPT. [arXiv:1109.3675]

- The topological susceptibility is in good agreement with sea-quark mass dependence predicted by NLO ChPT [arXiv:1105.4414, and Tung-Han's talk in this session]

- These demonstrate that the nonperturbative chiral dynamics of the sea quarks are well under control in the HMC simulations with ODWF.