Lattice QCD with Optimal Domain-Wall Fermions: Light Meson Spectroscopy

Ting-Wai Chiu（趙挺偉）

Physics Department and
Center for Quantum Science and Engineering (CQSE)
National Taiwan University, Taipei, Taiwan

Collaborators: Tian-Shin Guu (NIU), Tung-Han Hsieh (AS),
Chao-Hsi Huang (NIU), Yao-Yuan Mao (NTU),
Kenji Ogawa (NTU)

June 14, 2010, Lattice 2010

Outlines

- Overview of TWQCD's DWF project
- Optimal Domain-Wall Fermion
- Some Benchmarks for CG with DWF
- Physical Results of Pseudoscalar Meson
- Conclusion and Outlook

An Overview of TWQCD's Unquenched Simulations

- Lattice Size: 16^3 x 32 x 16 (N_s)

- Fermion Action: Optimal Domain-Wall Fermion

  [TWC, PRL, 90, 071601(2003)]

- Gauge Action: (a) Iwasaki (beta=2.20)

  (b) Plaquette (beta=5.90)

- N_f = 2/(2+1) for both (a) Iwasaki (beta=2.20)

  (b) Plaquette (beta=5.90)

- Setting the scale: (i) Sommer parameter, r_0=0.49 [fm]

  (ii) f_π = 131 MeV

An Overview (cont.)

- Lattice Spacings ($N_f = 2$): 0.137(4)[fm], Iwasaki (beta=2.20)
  0.125(3)[fm], Plaq. (beta=5.90)

  1/a = 1.464(34)[GeV], Iwasaki (beta=2.20)
  1.590(38)[GeV], Plaq. (beta=5.90)

- Lattice Volume: > (2 fm)^3

- Pion Masses [MeV] ($N_f = 2$):

  (a) Iwasaki (beta=2.20):

  157(9), 190(10), 219(12), 245(13), 265(15), 285(16), 297(17), 312(18)

  (b) Plaquette (beta=5.90)

  206(10), 252(15), 292(16), 331(15), 360(17), 384(17), 406(18), 428(19)

An Overview (cont.)

- Statistics

(a) Iwasaki (beta=2.20)

For N_f **= 2**, each mass has **5300-5500** accepted traj. After discarding **300** traj. for **thermalization**, measurements are performed every **20** traj., with a total of **250 confs**.

For N_f **= 2+1,** each mass has **2800** accepted traj. After discarding **300** traj. for thermalization, measurements are performed every **10** traj., with a total of **250 confs**.

(b) Plaquette (beta=5.90)

For N_f **= 2**, the statistics are the same as (a).

For N_f **= 2+1**, simulations are still on-going.

The Hardware of TWQCD

- 16 units of Nvidia Tesla S1070 (total 64 GPUs, 64 x 4 GB) connected to 16 servers (total 48 Intel QC Xeon, 16 x 32 GB)
- 32 Nvidia C1060 (total 32 GPUs, 32 x 4 GB), connected to 16 servers (total 16 Intel i7, 32 x 12 GB)
- 122 Nvidia GTX285 (total 122 GPUs, 122 x 2/1 GB), connected to 62 servers (total 62 Intel i7, 62 x 12 GB)
- 6 Nvidia GTX480 (total 6 GPUs, 6 x 1.5 GB), connected to 6 servers (total 6 Intel i7, 6 x 12 GB)
- Hard disk storage > 300 TB, **Lustre** cluster file system
- Peak performance is 220 TFLOPS
- Developed efficient CUDA codes for unquenched LQCD. 232/180/132 **Gflops** for GTX480/GTX285/T10
- Attaining 36 TFLOPS (sustained) for LQCD with Optimal DWF

The GPU Cluster of TWQCD (a snapshot of some nodes)

Salient Features of TWQCD's DWF Simulation

- HMC with Multiple Time Scale Integration and Mass Preconditioning
- Omelyan Integrator for the Molecular Dynamics
- **High Precision of Chiral Symmetry is attained with Optimal DWF**
- Even-Odd Preconditioning for the 4D Wilson-Dirac Quark Matrix
- **Conjugate Gradient with Mixed Precision on GPU**
  (See Y.Y. Mao's talk in Parallel 54, Friday, June 18, 17:00)
- **Topological Sectors are sampled ergodically**
  (See T.H. Hsieh's talk in Parallel 24, Tuesday, June 15, 12:10)
- **A New Algorithm for Simulating One Flavor** [TWQCD: arXiv:0911.5532]
  HMC simulation of 1-flavor is faster than 2-flavors with the same mass

Optimal Domain-Wall Fermion

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

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

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

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

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

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

with boundary conditions

$$P_+ \psi(x,0) = -\frac{m_q}{2m_0} P_+ \psi(x, N_s), \qquad m_q : \text{quark mass}$$

$$P_- \psi(x, N_s + 1) = -\frac{m_q}{2m_0} P_- \psi(x,1)$$

Optimal Domain-Wall Fermion (cont.)

The weights $\{\omega_s\}$ are fixed such that the effective 4D Dirac operator possesses the optimal chiral symmetry,

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

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

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

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

but with boundary conditions: $P_+\phi(x,0) = -P_+\phi(x,N_s), \quad m_{\text{PV}} = 2m_0$

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

Optimal Domain-Wall Fermion (cont.)

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

The effective 4D Dirac operator

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

(1847 – 1878)

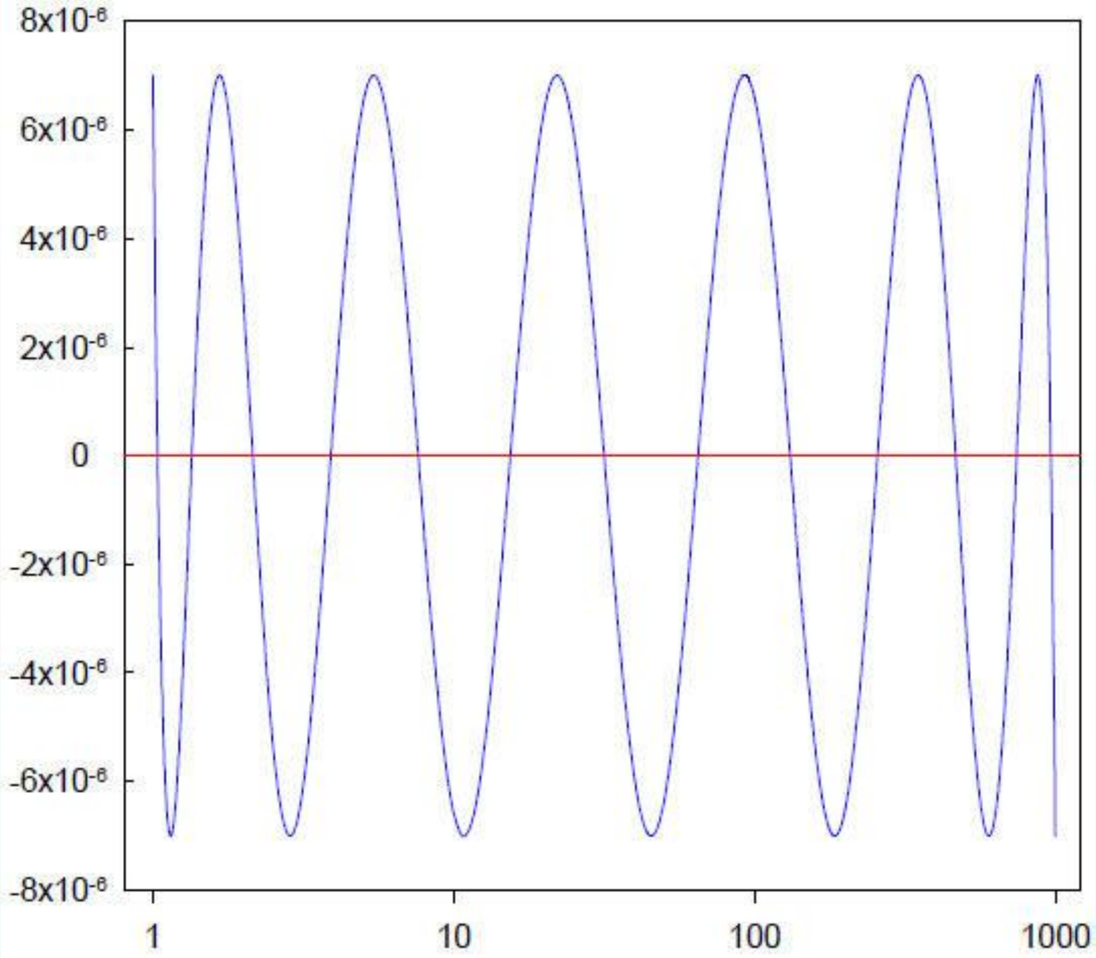
$$S_{opt}\left(H_w\right)=\frac{1-\prod_{s=1}^{N_s}T_s}{1+\prod_{s=1}^{N_s}T_s},\quad T_s=\frac{1-\omega_s H_w}{1+\omega_s H_w}$$

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

Zolotarev optimal rational approx. for $\dfrac{1}{\sqrt{H_w^2}}$ (1877)

The salient feature of Optimal Rational Approximation

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



$\log(x)$

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]

Even-Odd Preconditioning of ODWF Matrix

$$[D_{\text{odwf}}]_{x,s;x',s'} = (I + \omega_s D_w)_{x,x'} \delta_{s,s'} - (I - \omega_s D_w)_{x,x'} (P_- \delta_{s',s+1} + P_+ \delta_{s',s-1})$$

$$= \begin{pmatrix} X & D_w^{eo} Y \\ D_w^{oe} Y & X \end{pmatrix}$$

$$Y_{s,s'} = \omega_s (I + L)_{s,s'}$$

$$X_{s,s'} = (4 - m_0) \omega_s (I + L)_{s,s'} + (I - L)_{s,s'}$$

$$L_{s,s'} = P_- \delta_{s',s+1} + P_+ \delta_{s',s-1}$$

with boundary conditions: $P_- L_{N_s,s'} = -\frac{m_q}{2m_0} P_- \delta_{s',1}$

$$P_+ L_{1,s'} = -\frac{m_q}{2m_0} P_+ \delta_{s',N_s}$$

Even-Odd Preconditioning of ODWF Matrix (cont.)

$$\begin{pmatrix} X & D_w^{eo}Y \\ D_w^{oe}Y & X \end{pmatrix} = \begin{pmatrix} I & 0 \\ D_w^{oe}YX^{-1} & I \end{pmatrix} \begin{pmatrix} X & 0 \\ 0 & X - D_w^{oe}YX^{-1}D_w^{eo}Y \end{pmatrix} \begin{pmatrix} I & X^{-1}D_w^{eo}Y \\ 0 & I \end{pmatrix}$$

⇧ Schur complement

$$\det D_{\text{odwf}} \Rightarrow \det(I - D_w^{oe}YX^{-1}D_w^{eo}YX^{-1}) = \det C$$

$$C \equiv I - D_w^{oe}YX^{-1}D_w^{eo}YX^{-1}$$

For 2-flavors QCD, the pseudofermion action is

$$A_{PF} = \phi^\dagger C_{PV}^\dagger (CC^\dagger)^{-1} C_{PV} \phi$$

$$C_{PV} \equiv C(m_q = 2m_0)$$

Comparing Different DWF Fermions

(See Yao-Yuan Mao's talk in Parallel 54, Friday, June 18, 17:00)

- 2-flavors QCD with plaquette gauge action on $16^3 \times 32$ lattice, for one CG (with reliable updates) in HMC, $m_\pi \approx 300\text{MeV}$

	ODWF Ns = 16	Borici Ns = 16	DWF Ns = 16	ODWF Ns = 32	Borici Ns = 32	DWF Ns = 32
GTX 285	173	167	160	---	---	---
GTX 480 *	230	225	217	---	---	---
C1060	131	128	124	154	154	153
C2050 *	148	144	139	170	167	163
GTX 285	320	85	45	---	---	---
GTX 480 *	242	63	33	---	---	---
C1060	421	111	58	1347	518	300
C2050 *	374	99	51	1220	478	281

upper: Gflops / lower: time(s)

Comparing Different DWF fermions (cont.)

- 2-flavors QCD with plaquette gauge action on 16^3 x 32 lattice, for one CG (with reliable updates) in HMC, $m_\pi \approx 300\text{MeV}$

	ODWF Ns = 16	Borici Ns = 16	DWF Ns = 16	ODWF Ns = 32	Borici Ns = 32	DWF Ns = 32
Sign Function Error	$\approx 10^{-7}$	$\approx 10^{-4}$	$\approx 10^{-4}$	$\approx 10^{-10}$	$\approx 10^{-6}$	$\approx 10^{-6}$

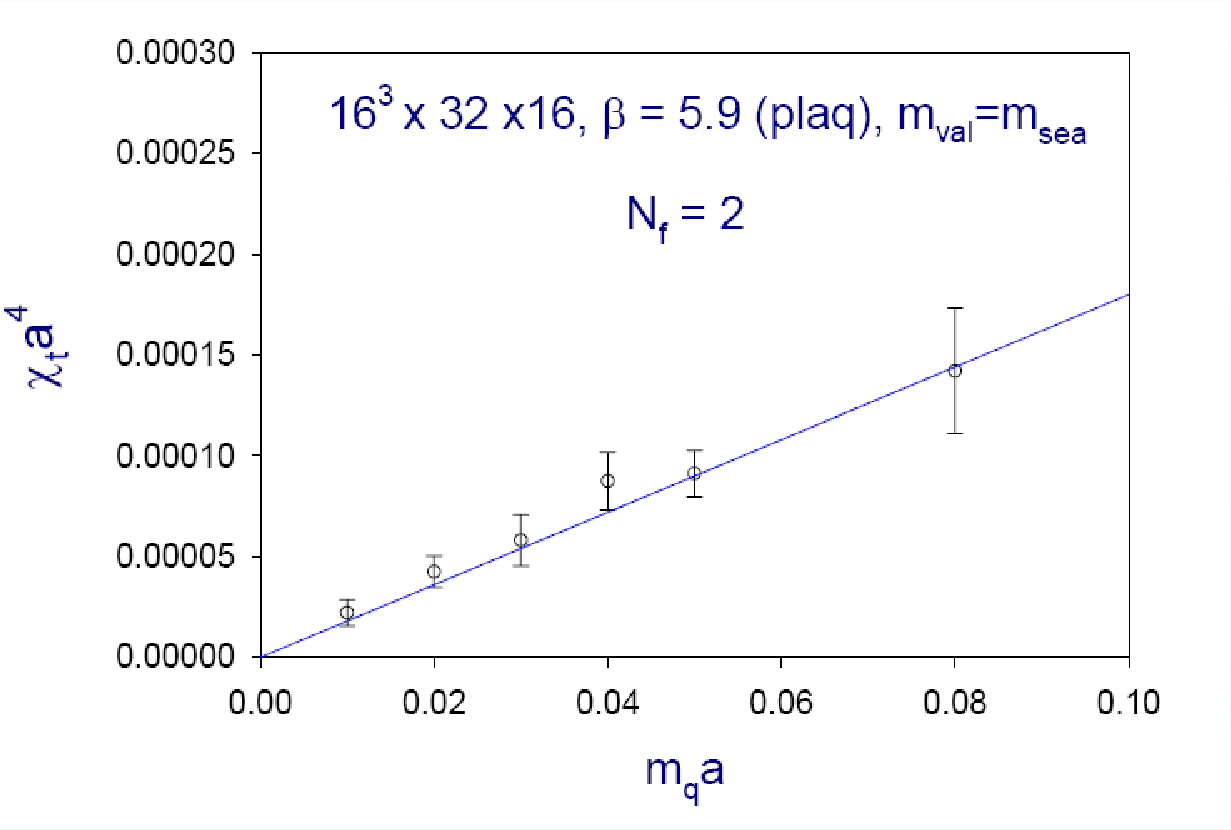
$\Updownarrow$

$$\max_{\forall Y} \left| \frac{Y^\dagger \left\{ 1 - S(H)^2 \right\} Y}{Y^\dagger Y} \right|, \qquad S(H) \approx \frac{H}{\sqrt{H^2}}$$

Topological Susceptibility

(See Tung-Han Hsieh's talk in Parallel 24, on Tuesday, June 15, 12:10)

$$\chi_t = \frac{\langle Q_t^2 \rangle}{V}$$



Fitting to $\chi_t = \Sigma\left(m_u^{-1} + m_d^{-1}\right)^{-1} \Rightarrow \Sigma^{\overline{MS}}(2\ \mathrm{GeV}) = [247(11)(12)\mathrm{MeV}]^3$

(preliminary)

Pseudoscalar Meson

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

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

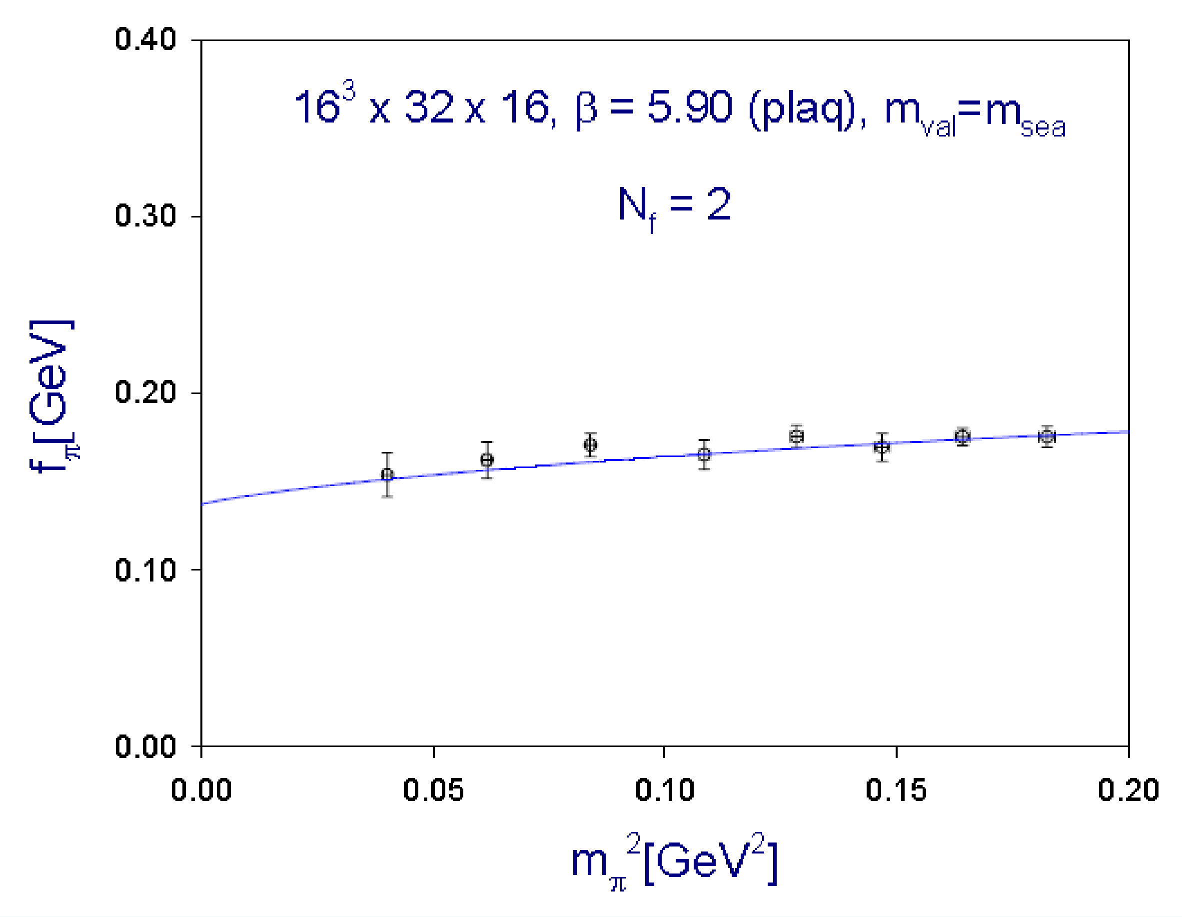
$$= \mathrm{Tr}\left\{\left[(D_c+m_u)^{-1}(0,x)\right]^\dagger (D_c+m_d)^{-1}(x,0)\right\}$$

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

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

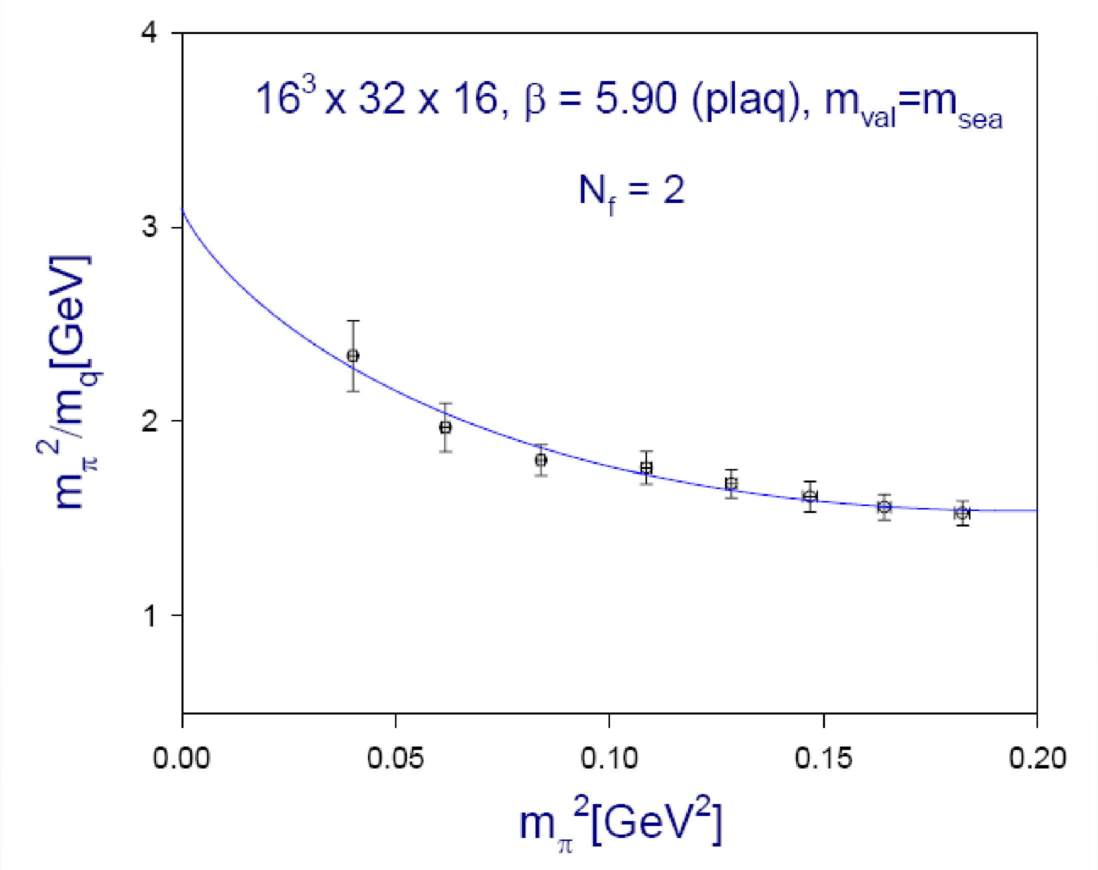
to extract m_π and $f_\pi=\frac{(m_u+m_d)}{m_\pi^2}\left|\langle\pi^+(\vec{k})|\pi^-(0,0)|0\rangle\right|$

Physical Results of Pseudoscalar Meson



NLO ChPT $\quad f_\pi = f\left(1 - x\ln x\right) + c_4 x, \quad x = \frac{4Bm_q}{(4\pi f)^2} \rightarrow \xi = \frac{m_\pi^2}{8\pi^2 f_\pi^2}$

Physical Results of Pseudoscalar Meson (cont.)



NLO ChPT $\quad \dfrac{m_\pi^2}{m_q} = 2B\left(1+\dfrac{1}{2}x\ln x\right)+c_3 x, \quad x = \dfrac{4Bm_q}{(4\pi f)^2} \to \xi = \dfrac{m_\pi^2}{8\pi^2 f_\pi^2}$

Physical Results of Pseudoscalar Meson (cont.)

$$f = 0.1221(42)\ \text{GeV}$$

$$B = 1.5488(812)\ \text{GeV}$$

$$Z_m^{\overline{\text{MS}}}(2\ \text{GeV}) = 0.76(1)(2)$$ [NPR, RI/MOM]

$$\Sigma = \frac{Bf^2}{2} \Rightarrow \Sigma^{\overline{\text{MS}}}(2\ \text{GeV}) = \left[248(7)(2)\text{MeV}\right]^3$$

At $m_q = 0.0061(5)\ \text{GeV},\ m_\pi = 0.135\ \text{GeV}$,

$$f_\pi = 131.4(3.5)\ \text{MeV}$$

$$m_{ud}^{\overline{\text{MS}}}(2\ \text{GeV}) = 4.6(0.5)(0.1)\text{MeV}$$

Conclusion and Outlook

- Optimal Domain-Wall Fermion provides a viable framework to simulate unquenched QCD with exact chiral symmetry.

- First physical results of pseudoscalar meson for 2-flavors QCD are in good agreement with NLO ChPT, and provide a determination of the following physical quantities:

$$\Sigma^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = \left[248(7)(2)\mathrm{MeV}\right]^3$$

$$f_\pi = 131.4(3.5)\ \mathrm{MeV}$$

$$m_{ud}^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = 4.6(0.5)(0.1)\mathrm{MeV}$$

Conclusion and Outlook (cont.)

- Our novel one-flavor algorithm provides an efficient way to simulate (2+1)-flavors, (2+1+1)-flavors, (1+1+1+1)-flavors QCD with exact chiral symmetry, as well as for any vector gauge theory with an arbitrary number of flavors.
- Simulations of (2+1)-flavors QCD are on-going, which will be completed soon, and the new confs will provide new physical results.
- All-to-all quark propagators will be computed for physical quantities involving disconnected diagrams, with LMP and LMA.