Charm in Lattice QCD with Domain-Wall Fermion

Ting-Wai Chiu (趙挺偉)
National Taiwan University
(for the TWQCD Collaboration)

Collaborators:
W.P. Chen, Y.C. Chen, H.Y. Chou, T.S. Guu, T.H. Hsieh

Lattice 2014, New York, USA
June 23-28, 2014

Outline

- Introduction
- Charm quark in LQCD with DWF
- Gauge ensembles
- Lowest lying mass spectra of $c\bar{c},\ c\bar{s},\ c\bar{d}\,(c\bar{u})$
- Leptonic decay constants, f_D , f_{Ds}
- Concluding Remarks

Introduction

- In QCD, both light and heavy quarks are Dirac fermions with different bare quark masses. Thus it seems unnatural to treat them differently (with different actions) in any theoretical studies involving both heavy and light quarks.
- Theoretically, LQCD with exact chiral symmetry (domain-wall/overlap fermion) is the ideal theoretical framework to tackle any nonperturbative physics involving quarks, no matter whether they are heavy or light, valence or sea, all with the same action.

Domain-Wall Fermion [Kaplan, 1992]

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

$$\equiv \bar{\Psi} D_{\mathrm{dwf}} \Psi$$

$$\rho_s = c\omega_s + d$$
$$\sigma_s = c\omega_s - d$$
$$c, d \ \text{(constants)}$$

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

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

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

with boundary conditions

$$P_+ \psi(x,0) = -r m_q P_+ \psi(x, N_s), \quad m_q\text{: bare mass}, \quad r = 1/[2m_0(1 - dm_0)]$$

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

Domain-Wall Fermion (cont.)

The action for Pauli-Villars fields is

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

with boundary conditions:

$$P_+ \phi(x,0) = -P_+ \phi(x, N_s),$$

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

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

The effective 4D Dirac operator

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

$$\lim_{N_s \to \infty} S(H) = \frac{H}{\sqrt{H^2}}$$

Domain-Wall Fermion (cont.)

- Conventional DWF with Shamir kernel

$$\left[c = d = 1/2,\ \omega_s = 1 \Rightarrow \rho_s = c\omega_s + d = 1,\ \sigma_s = c\omega_s - d = 0\right]$$

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

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

$$\boxed{\begin{aligned} b_l &= \sec^2\left[\frac{\pi}{N_s}\left(l - \frac{1}{2}\right)\right] \\ d_l &= \tan^2\left[\frac{\pi}{N_s}\left(l - \frac{1}{2}\right)\right] \end{aligned}}$$

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

polar approximation of $\dfrac{1}{\sqrt{H^2}}$

Domain-Wall Fermion (cont.)

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

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

where $sn\left(v_s;\kappa'\right)$ is the Jacobian elliptic function with argument v_s

and modulus $\kappa' = \sqrt{1-\lambda_{\min}^2/\lambda_{\max}^2}$, and $\lambda_{\min}^2$ and $\lambda_{\max}^2$ are

lower and upper "bounds" of the eigenvalues of H^2

Then the effective 4D Dirac operator becomes

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

Domain-Wall Fermion (cont.)

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

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

Zolotarev optimal rational approximation of $\frac{1}{\sqrt{H^2}}$

Chiral Sym Breaking due to Finite Ns

[Y.C. Chen, TWC, Phys. Rev. D 86, 094508 (2012)]

It can be measured by the residual mass

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

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

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

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

Chiral Sym Breaking due to Finite Ns (cont)

For lattice QCD with ODWF, it can be shown that

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

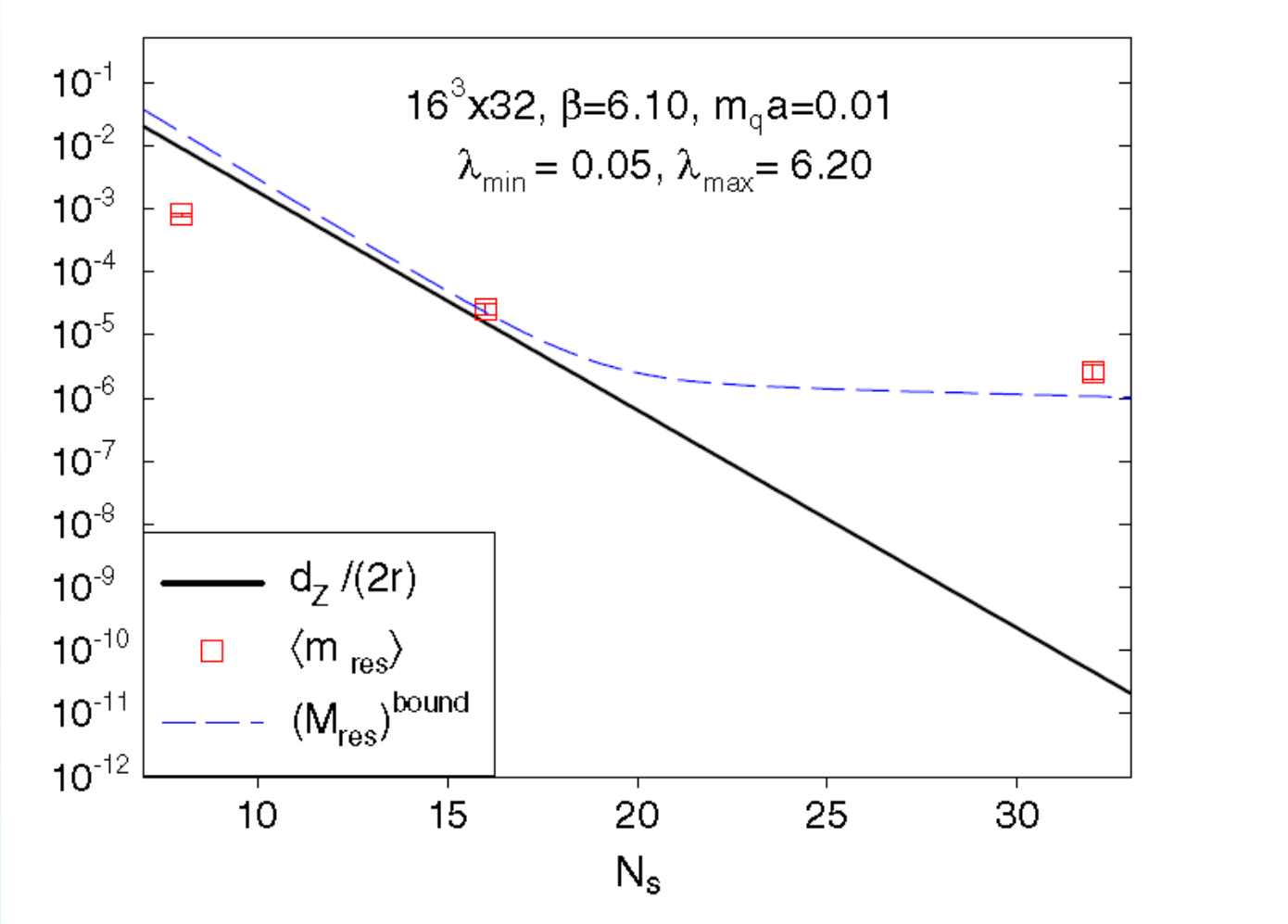
For ODWF, $d_Z \ll 1$ in most cases, and it gives

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

If there are some eigenvalues of H^2 smaller than $\lambda^2_{\rm min}$

$$M_{\rm res} \le \left[\frac{d_Z + (d_a - d_Z)Q_a}{2r}\right]\left[\frac{2(1+m)}{2-(3-m)d_a}\right]$$
$$\equiv F(N_s, m, N_a/N, h_1),$$

Chiral Sym Breaking due to Finite Ns (cont)



Charm quark in LQCD with DWF

The quark mass in DWF enters through the boundary conditions

$P_+\psi(x,0) = -rm_q P_+\psi(x,N_s)$, m_q: bare mass, $r = 1/[2m_0(1-dm_0)]$

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

The upper bound of m_q is $m_{PV} = 1/r = 2m_0(1-dm_0)$, $0 < m_0 < 2$

If one sets $m_q = m_{PV}$, the theory goes to the quenched limit with $\det(D) = 1$.

To minimize the cutoff effects, it is necessary to choose d and m_0 such that $m_c \ll m_{PV}$.

Also, it requires $m_c a \ll 1$ to minimize the discretization error.

Charm quark in LQCD with DWF (cont)

Conventional DWF: $d = 1/2,\ m_{PV} = m_0(2 - m_0),\ \max(m_{PV}) = 1/a$

RBC/UKQCD: $m_0 = 1.8,\ m_{PV} = m_0(2 - m_0) = 0.36$

$$m_c a \ll 0.36 \ \Rightarrow\ a^{-1} \gg 2.78 m_c \approx 3.3 \text{ GeV}$$

(stronger than the constraint $m_c a < 1$)

For DWF with $d = 0,\ m_{PV} = 2m_0$

TWQCD: $m_0 = 1.3,\ m_{PV} = 2m_0 = 2.6$

$$m_c a \ll 2.6 \ \Rightarrow\ a^{-1} \gg 0.38 m_c \approx 0.46 \text{ GeV}$$

(weaker than the constraint $m_c a < 1$)

For $\beta = 6.10,\ a^{-1} \approx 3 \text{ GeV},\ m_c a \approx 0.5,$ the discretization error is small.

Recent TWQCD simulations of Nf=2 QCD

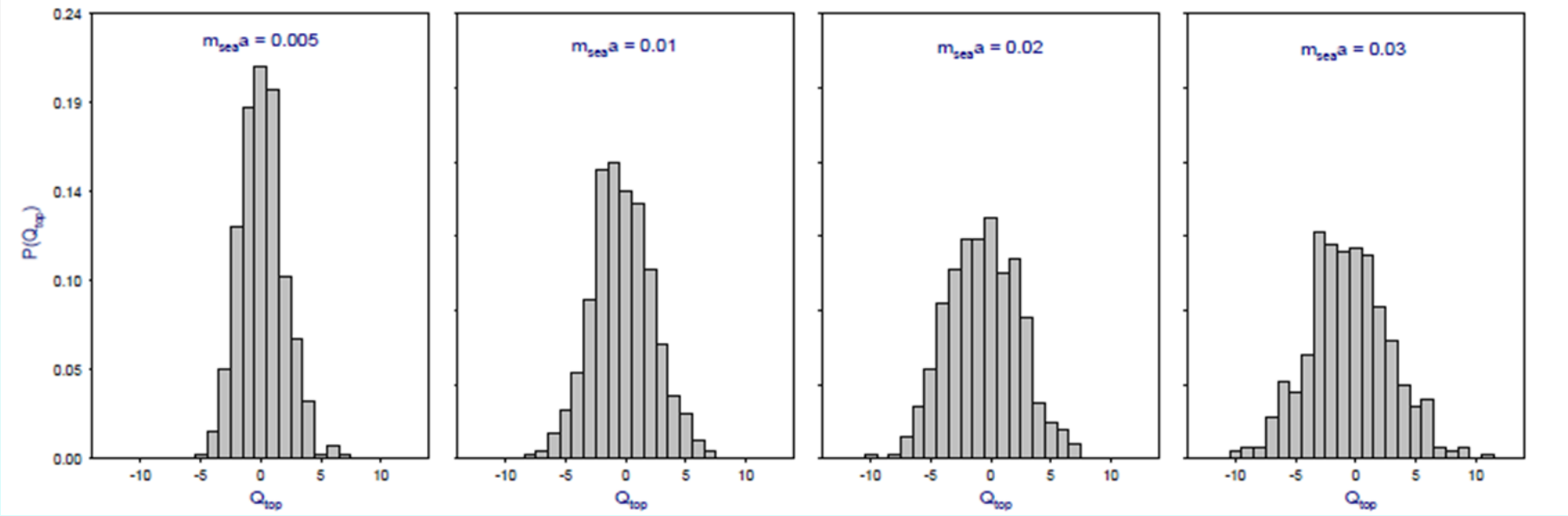
- Lattice size: $24^3 \times 48$
- Quark action: optimal domain-wall fermion

$$(\text{with } c = 1,\ d = 0,\ N_s = 16,\ \lambda_{\min} = 0.05,\ \lambda_{\max} = 6.2)$$

- Gluon action: Wilson plaquette action at beta = 6.10
- 4 sea-quark Masses, with pion masses ~ 260, 350, 470, 560 [MeV].
- Lattice spacing: a ~ 0.065 [fm], 1/a ~ 3.2, 3.1, 3.0, 3.0 [GeV]
- Spatial volume: ~$(1.6\ \text{fm})^3$
- Residual mass < 0.17 MeV
- For each sea-quark mass, after thermalization, ~**5000** trajectories are generated, measurements are performed every **10** trajectory, with a total of ~**500 confs**.

Recent TWQCD simulations of Nf=2 QCD (cont)

- Multiple-time scale integration and mass preconditioning.
- Even-Odd Preconditioning for the 4D Wilson-Dirac Matrix.
- Omelyan Integrator for the Molecular Dynamics.
- Conjugate gradient with mixed precision.
- Use a GPU cluster of 300 GPUs, with sustained 100 Tflops
- Topological sectors are sampled ergodically.



Recent TWQCD simulations of Nf=2 QCD (cont)

- **Pion mass and decay constant** are in good agreement with the sea-quark mass dependence predicted by NLO ChPT, and gives a determination of the chiral condensate, the pion decay constant, m_{ud}, $\bar{l}_3$, $\bar{l}_4$.

  (see Tung-Han Hsieh's talk on Wednesday, Chiral Symmetry, 5D, 10:20)

Determination of lattice spacing

Use Wilson flow with the condition $t^2 \langle E(t) \rangle \big|_{t=t_0} = 0.3$

to obtain $\sqrt{t_0}/a$ for each ensemble.

To determine the input parameter t_0, we use our gauge ensembles

at $\beta = 5.95$ on the $16^3 \times 32$ lattice [TWC, Hsieh, Mao, PLB, 2012].

Table 1
The parameters of A, B, and σ obtained by fitting our data of heavy quark potential $V(R)$ to Eq. (2), together with the χ^2/dof of the fit. The lattice spacing in the last column is obtained by (4).

$m_q a$	A	B	σ	χ^2/dof	a [fm]
0.01	0.7777(57)	−0.3814(70)	0.0577(10)	0.0329	0.1045(13)
0.02	0.7827(46)	−0.3818(41)	0.0584(9)	0.0275	0.1051(10)
0.03	0.7792(54)	−0.3789(62)	0.0595(9)	0.0368	0.1060(12)
0.04	0.7916(71)	−0.3995(78)	0.0598(13)	0.0440	0.1071(16)
0.05	0.7797(73)	−0.3798(72)	0.0615(13)	0.0456	0.1078(16)
0.06	0.7762(50)	−0.3785(44)	0.0628(11)	0.0458	0.1089(11)
0.07	0.7783(47)	−0.3855(53)	0.0633(8)	0.0255	0.1097(10)
0.08	0.7719(69)	−0.3744(64)	0.0649(12)	0.0569	0.1105(14)

$$V(R) = A + \frac{B}{R} + \sigma R$$

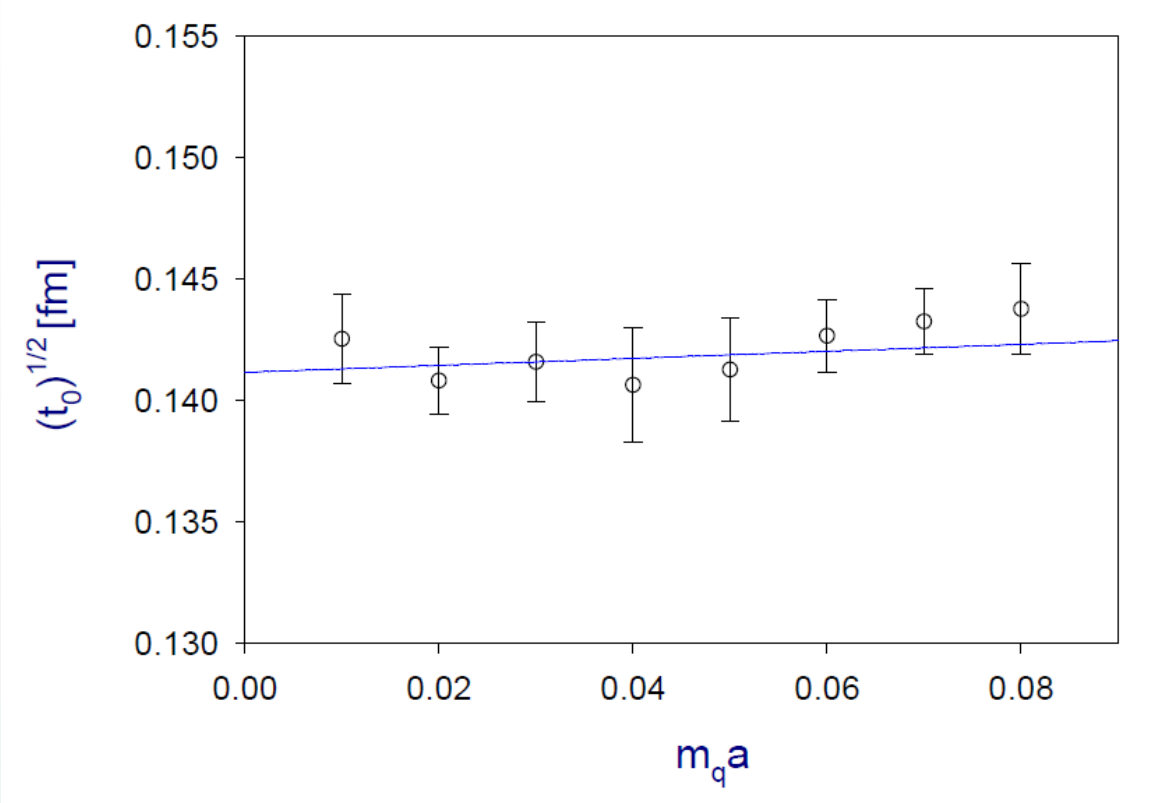
$$F(r) \equiv \frac{d}{dr} V(r) = -\frac{B}{r^2} + \sigma$$

$$F(r_0) r_0^2 = 1.65$$

$$r_0 = 0.49 \text{ fm}$$

$$a = r_0 \sqrt{\frac{\sigma}{1.65 + B}}$$

Determination of lattice spacing (cont)



$$\sqrt{t_0} = 0.1407(9)(6)\ \mathrm{fm}$$

the systematic error is estimated by varying the number of sea-quark masses and the difference between the linear fit and the constant fit.

Time-Correlation functions

Compute $$C_\Gamma(t)=\left\langle \sum_{\vec{x}} \mathrm{tr}\{\Gamma(D_c+m_Q)^{-1}_{x,0}\Gamma(D_c+m_q)^{-1}_{0,x}\}\right\rangle$$

for scalar (S), pseudoscalar (P), vector (V), axial-vector (A), and tensor (T) mesons with Dirac matrix $\Gamma = \{\mathbb{1}, \gamma_5, \gamma_i, \gamma_5\gamma_i, \gamma_5\gamma_4\gamma_i\}$

For vector mesons

$$C_V(t) = \left\langle \frac{1}{3}\sum_{i=1}^{3}\sum_{\vec{x}} \mathrm{tr}\{\gamma_i(D_c+m_Q)^{-1}_{x,0}\gamma_i(D_c+m_q)^{-1}_{0,x}\}\right\rangle$$

and similarly for the axial-vector and tensor mesons.

$C_\Gamma(t)$ is measured for $(m_q, m_Q) = \{\ (m_{sea}, m_{sea}),\ (m_{sea}, m_s),\ (m_{sea}, m_c),$
$(m_s, m_s),\ (m_s, m_c),\ (m_c, m_c)\ \}$

Determination of the bare quark masses of s, c

$\phi(1020) \to m_s$ $\qquad$ $J/\psi(3097) \to m_c$

$$C_V(t) = \left\langle \frac{1}{3}\sum_{\mu=1}^{3}\sum_{\vec{x}} \mathrm{tr}\{\gamma_\mu (D_c + m_Q)^{-1}_{x,0}\gamma_\mu (D_c + m_q)^{-1}_{0,x}\} \right\rangle_U$$

fitting to $\frac{z^2}{2Ma}[e^{-Mat} + e^{-Ma(T-t)}]$ to extract M

$m_{sea}a$	$m_s a$	M_ϕ[MeV]	$[t_1, t_2]$	χ^2/dof	$m_c a$	$M_{J/\psi}$[MeV]	$[t_1, t_2]$	χ^2/dof
0.005	0.04	1018(4)	[14,20]	0.76	0.53	3102(11)	[16,22]	0.17
0.01	0.04	1020(8)	[11,23]	0.11	0.55	3104(15)	[17,23]	0.58
0.02	0.04	1020(8)	[16,23]	0.20	0.55	3099(13)	[16,24]	0.22
0.03	0.04	1025(9)	[13,24]	1.16	0.56	3097(11)	[13,24]	0.81

Lowest-lying mass spectra of $c\bar{c}$

For the gauge ensemble with sea-quark mass $m_{sea}a = 0.01$

Γ	J^{PC}	$n^{2S+1}L_J$	$[t_1, t_2]$	χ^2/dof	Mass[MeV]	PDG [MeV]
$\mathbb{1}$	0^{++}	1^3P_0	[12,22]	0.30	3392(25)(22)	$\chi_{c0}(1P)$[3414.75(31)]
γ_5	0^{-+}	1^1S_0	[11,24]	0.82	2982(10)(4)	$\eta_c(1S)$[2983.7(7)]
γ_i	1^{--}	1^3S_1	[17,23]	0.58	3104(15)(5)	$J/\psi(1S)$[3096.916(11)]
$\gamma_5\gamma_i$	1^{++}	1^3P_1	[15,20]	0.12	3513(22)(5)	$\chi_{c1}(1P)$[3510.66(7)]
$\gamma_i\gamma_j$	1^{+-}	1^1P_1	[15,20]	0.18	3529(28)(7)	$h_c(1P)$[3525.38(11)]

Lowest-lying mass spectra of $c\bar{s}$

For the gauge ensemble with sea-quark mass $m_{sea}a = 0.01$

Γ	J^P	$[t_1, t_2]$	χ^2/dof	Mass[MeV]	PDG [MeV]
$\mathbb{1}$	0^+	[13,24]	0.28	2311(18)(7)	$D_{s0}^*(2317)^\pm$ [2317.8(6)]
γ_5	0^-	[13,24]	0.54	1968(9)(8)	$D_s^\pm$ [1968.50(32)]
γ_i	1^-	[15,23]	0.31	2112(11)(4)	D_s^*[2112.3(5)]
$\gamma_5\gamma_i$	1^+	[17,24]	0.34	2466(26)(10)	$D_{s1}(2460)^\pm$ [2459.6(6)]
$\gamma_i\gamma_j$	1^+	[14,19]	0.14	2538(27)(8)	$D_{s1}(2536)^\pm$ [2535.12(13)]

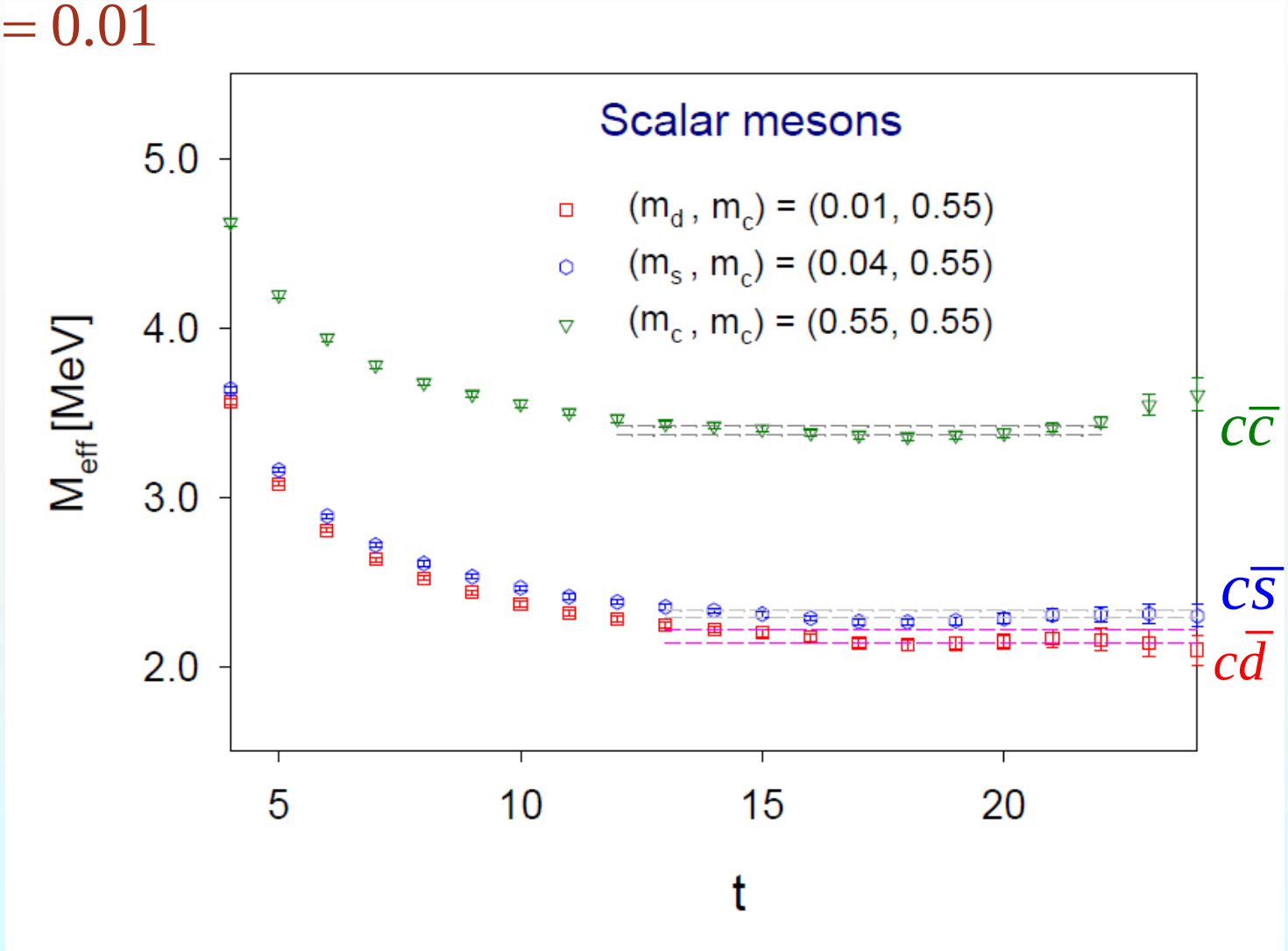
Lowest-lying mass spectra of $c\bar{d}$

For the gauge ensemble with sea-quark mass $m_{sea}a = 0.01$

Γ	J^P	$[t_1, t_2]$	χ^2/dof	Mass[MeV]	PDG [MeV]
$\mathbb{1}$	0^+	[13,24]	0.32	2180(28)(25)	$D_0^*(2410)[2318(29)]$
γ_5	0^-	[16,24]	0.26	1870(10)(8)	$D^{\pm}[1869.62(15)]$
γ_i	1^-	[17,22]	0.23	2018(14)(10)	$D^*(2010)^{\pm}[2010.29(13)]$
$\gamma_5\gamma_i$	1^+	[15,20]	0.22	2421(20)(4)	$D_1(2420)^0$ [2421.4(6)]

Mass Spectra of Charmed Scalar Mesons

$m_{sea}a = 0.01$



Leptonic Decay Constants

In the Standard Model (SM), the quark and antiquark of a charged pseudoscalar meson P (with quark content $Q\bar{q}$) can decay into a charged lepton and its associated neutrino through a virtual W boson. This is the purely leptonic decay of the charged pseudoscalar

$$\langle 0|\bar{q}\gamma_\mu\gamma_5 Q(0)|P(\vec{q})\rangle = i f_P q_\mu$$

In lattice QCD with exact chiral symmetry

$$\partial_\mu\left(\bar{q}\gamma_\mu\gamma_5 Q\right) = (m_q + m_Q)\bar{q}\gamma_5 Q \quad \Longrightarrow \quad f_P = (m_q + m_Q)\frac{|\langle 0|\bar{q}\gamma_5 Q|P(\vec{0})\rangle|}{M_P^2}$$

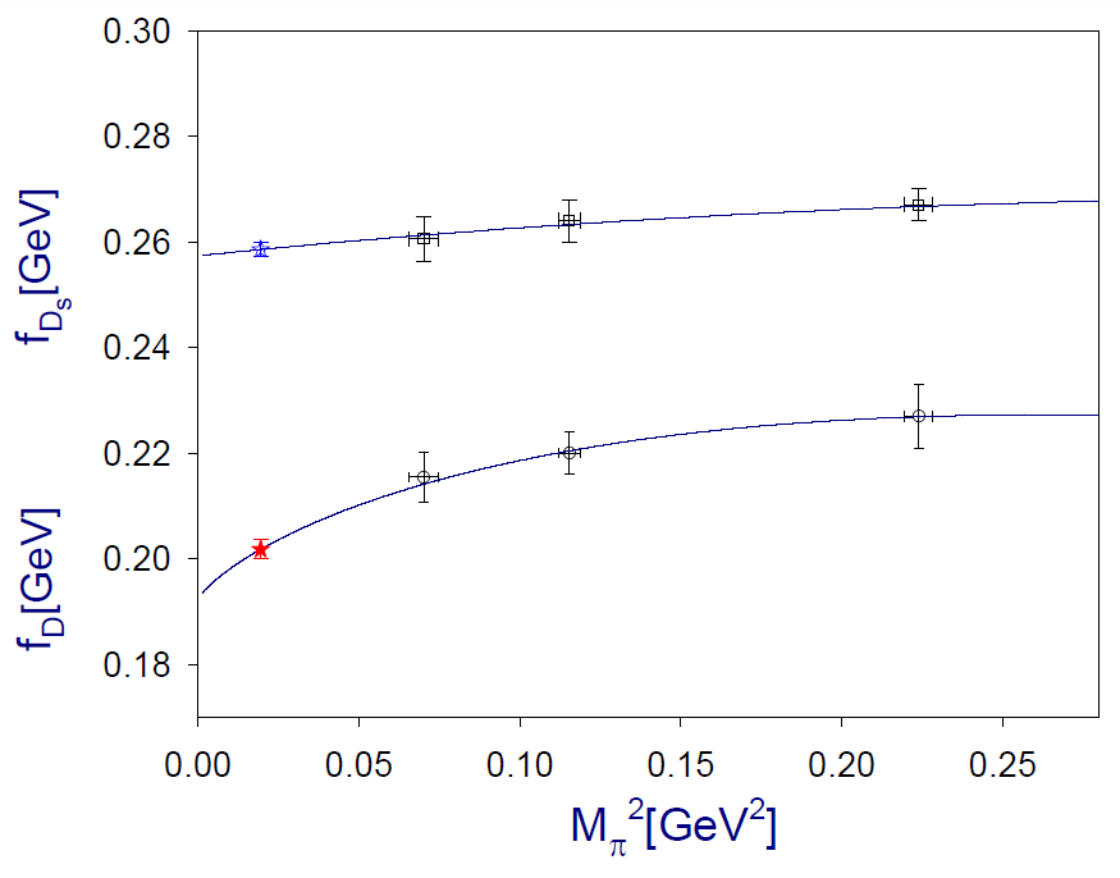
pseudoscalar mass M_P and the decay amplitude $z \equiv |\langle 0|\bar{q}\gamma_5 Q|P(\vec{0})\rangle|$ can be obtained by fitting the pseudoscalar time-correlation function $C_P(t)$ to

$$\frac{z^2}{2M_P}[e^{-M_P t} + e^{-M_P(T-t)}]$$

To determine f_P precisely is crucial for the determination of the CKM matrix element $|V_{Qq}|$.

Leptonic Decay Constants f_D , f_{Ds}

Chen et al. (TWQCD), arXiv: 1404.3648



Use heavy meson ChPT (Sharpe, Zhang, 1996) to extrapolate to the physical point $M_\pi = 140$ MeV.

Leptonic Decay Constants f_D , f_{Ds} (cont)

Chen et al. (TWQCD), arXiv: 1404.3648

At the physical $M_\pi = 140$ MeV

$$f_D = 202 \pm 3 \pm 4 \text{ MeV}$$

$$f_{D_s} = 260 \pm 2 \pm 1 \text{ MeV}$$

$$\frac{f_{D_s}}{f_D} = 1.287 \pm 0.034$$

in good agreement with the experimental values (PDG 2013)

$$f_D = 204.6 \pm 5.0 \text{ MeV}$$

$$f_{D_s} = 257.5 \pm 4.6 \text{ MeV}$$

$$f_{D_s}/f_D = 1.258 \pm 0.038$$

Concluding Remarks

- LQCD with optimal DWF provides an ideal framework for studying physical observables involving light and heavy quarks, for the sea and the valence quarks.

- Dynamical simulation preserves the chiral symmetry to a good precision, and samples all topological sectors ergodically.

- For 2-flavors gauge ensembles on $24^3 \times 48$ at $\beta = 6.1$, pion mass and decay constant are in good agreement with the sea-quark mass dependence predicted by NLO ChPT, and gives a determination of the chiral condensate, the pion decay constant, m_{ud}, $\bar{l}_3$, $\bar{l}_4$.

  (see Tung-Han Hsieh's talk on Wednesday, Chiral Symmetry, 5D, 10:20)

Concluding Remarks (cont)

- Lowest-lying mass spectra of $c\bar{c}$, $c\bar{s}$, $c\bar{d}$ are in good agreement with the experimental values, except for the scalar meson of $c\bar{d}$

- Leptonic decay constants f_D and f_{Ds} are in good agreement with the experimental values.

- This gives confidence to proceed to further studies with this set of ensembles, on the charmed baryons, light meson spectra, and matrix elements, etc.