First Study of Nf=2+1+1 Lattice QCD with Physical Domain-Wall Quarks

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Outline

- Current status of lattice QCD at the physical point
- Simulate LQCD with physical (u,d,s,c) DW quarks
- Computational platform - Nvidia DGX-1
- Lattice setup and simulation parameters
- Topological susceptibility
- Hadron mass spectrum
- Conclusion and outlook

Current Status of lattice QCD at the physical point

The holy grail of lattice QCD is to simulate QCD with (u,d,s,c,b) quarks at their physical masses, with sufficiently large volume and fine lattice spacing, then to extract physics from these gauge ensembles.

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Collaboration	Lattice Fermion	u/d	u/d, s	u/d, s, c	u, d, s, c	u/d, s, c, b
MILC	highly improved staggered fermion		X	X		
PACS	Improved Wilson fermion		X			
tmQCD	twisted mass Wilson fermion	X	X	X		
RBC/UKQCD	DWF (Shamir, Möbius)		X			
TWQCD	optimal DWF			X		

Lattice Fermions

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- It took 24 years (1974 ~1998) 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 Monte Carlo simulation** such that the chiral symmetry is preserved to very high precision and all topological sectors are sampled ergodically, and all quarks at their physical masses.
- The computational requirement for **Lattice QCD with overlap/DW quarks** is ~**10-100 times** more than their counterparts with traditional lattice fermions (e.g., Wilson, staggered, and their variants).

Lattice Setup and Simulation Parameters

- Quarks: optimal DWF [TWC, PRL 2003] with $N_s = 16$, $\lambda_{max} / \lambda_{min} = 6.20 / 0.05$.
  Gluons: plaquette gauge action at $\beta = 6 / g^2 = 6.20$.
- Lattice size: $64^3 \times 64$, $a \approx 0.062$ fm, $M_\pi L \approx 3$, $L \approx 4$ fm.
- For the one-flavor, use the Exact One-Flavor pseudofermion Action (EOFA)
  [Y.C. Chen & TWC, Phys. Lett. B738 (2014) 55; TWC, Phys. Lett. B744 (2015) 95]
- For the 2-flavor, use the two-flavor algorithm for DWF.
  [TWC, T.H. Hsieh, Y.Y. Mao, Phys. Lett. B702 (2012) 131]
- HMC with Multiple Time Scale Integration and Mass Preconditioning.
- Omelyan Integrator for the Molecular Dynamics.
- Conjugate Gradient with Mixed Precision.
- Thermalization: one unit of DGX-1 ($\approx$ 8 months), TWC, arXiv: 1811.08095
  Production runs: 4 DGX-1 ($\approx$ 2 months) $\rightarrow$ 25 DGX-1 ($\approx$ 2 months).
  Generated $\approx$ 1250 trajectories $\rightarrow$ $\approx$ 250 configurations.

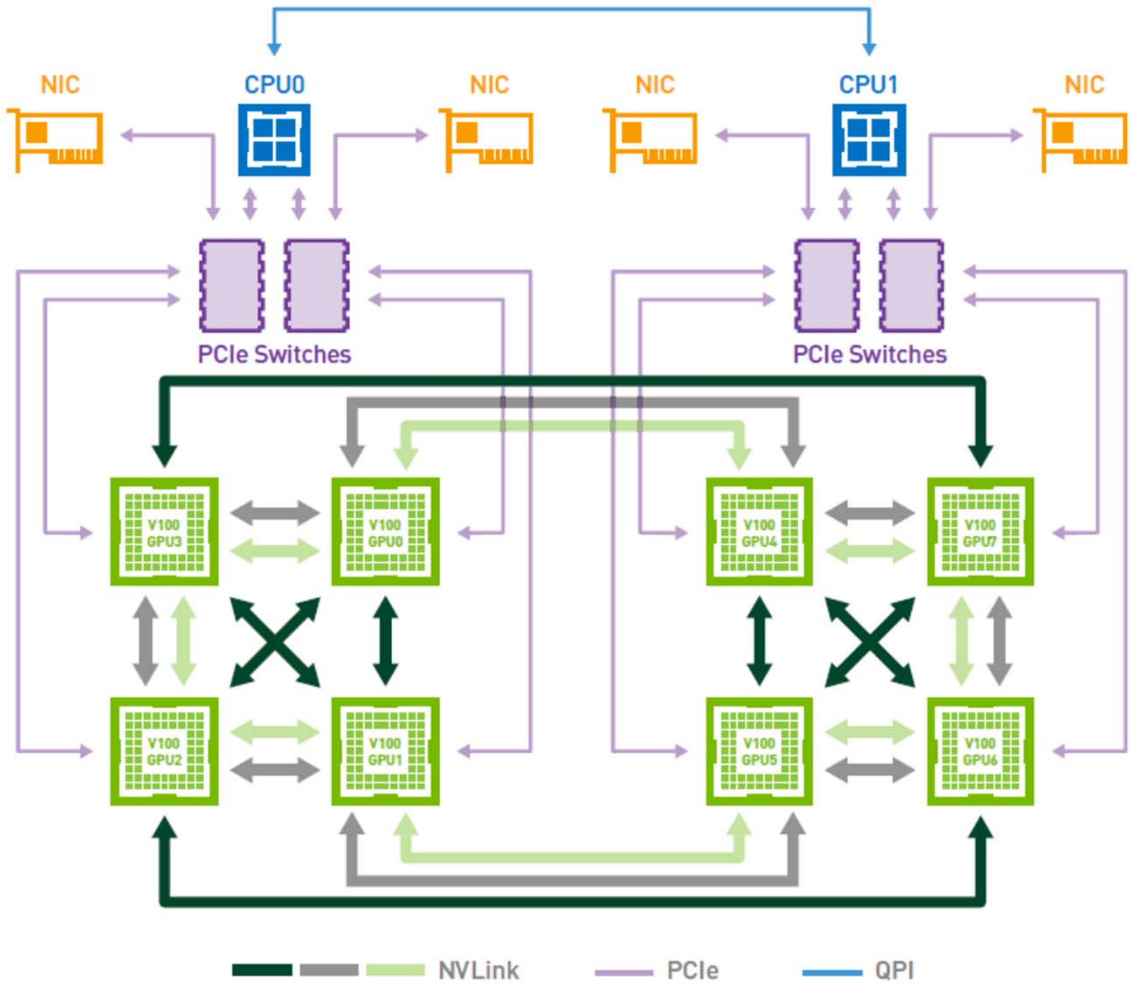
Nvidia DGX-1 (on the table top)

For the TWQCD code, it attains $\approx$ 12 Tflops/s (sustained),

and generates $\approx$ 1 trajectory/day with $P_{accept} \approx 70\%$

Nvidia DGX-1(8 V100+NVLink)

Figure taken from the White Paper
NVIDIA DGX-1 With Tesla V100 System Architecture



NVLink 2.0, data rate ~ 300 GB/s

Lattice spacing and Quark masses

- The inverse lattice spacing ($a^{-1} \simeq 3.187 \pm 0.017$ GeV) is determined by the Wilson flow, using $\sqrt{t_0} = 0.1416(8)$ fm obtained by the MILC collaboration for $N_f = 2+1+1$.
- The masses of s and c quarks are fixed by the masses of $\phi(1020)$ and $J/\psi(3097)$ respectively, while the mass of u/d quarks by $M_\pi(140)$.
- Quark masses: $m_{u/d}a = 0.00125,\ m_s a = 0.04,\ m_c a = 0.55$
- Point-to-point quark propagators with $m_{valence} = m_{sea}$

Basic Questions about the Simulation

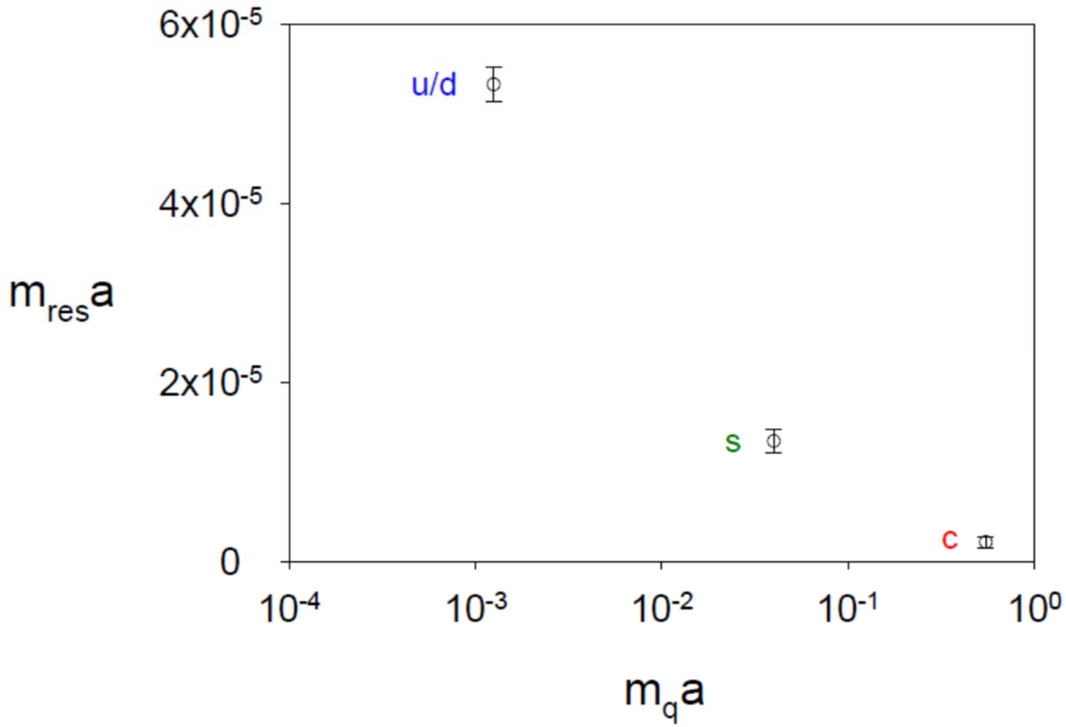
- What is chiral symmetry breaking due to finite Ns ?
  What are the residual masses for (u/d, s, c) quarks ?

- Does the simulation suffer from the topology freezing ?
  Does it sample all topological sectors ergodically ?

Chiral Symmetry Breaking due to finite Ns

Residual Mass

- Quark masses: $m_{u/d}a = 0.00125,\ m_s a = 0.04,\ m_c a = 0.55$



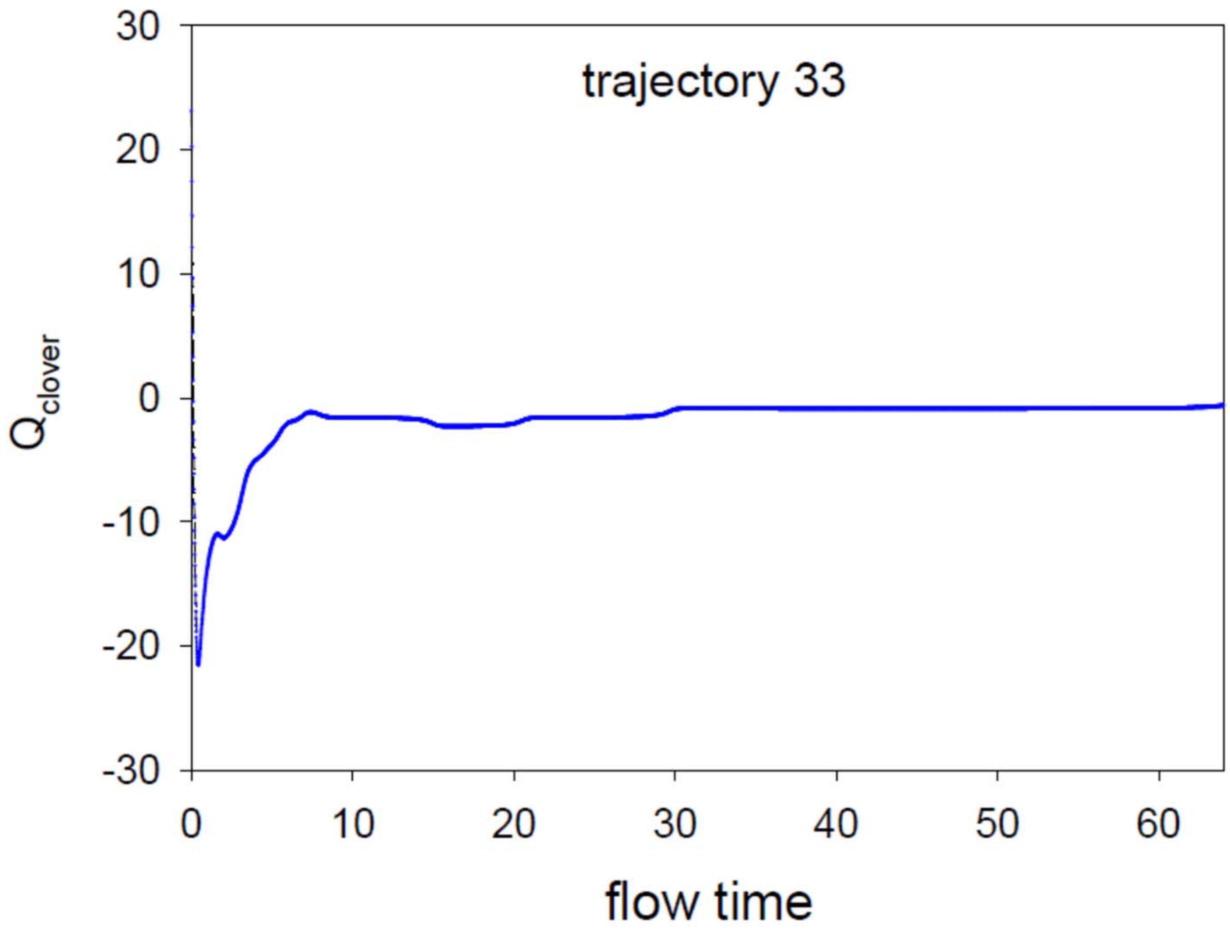
- Residual mass: $m_{res}a = 5.33(20)\times 10^{-5},\ 1.34(13)\times 10^{-5},\ 0.22(7)\times 10^{-5}$

$\approx$ 0.15 MeV, $\approx$ 0.04 MeV, $\approx$ 0.01 MeV

u/d s c

Topological Charge versus the Wilson Flow Time

The flow equation is integrated from $t = 0 \to 64$ with $\Delta t = 0.01$



Topological Ergodicity

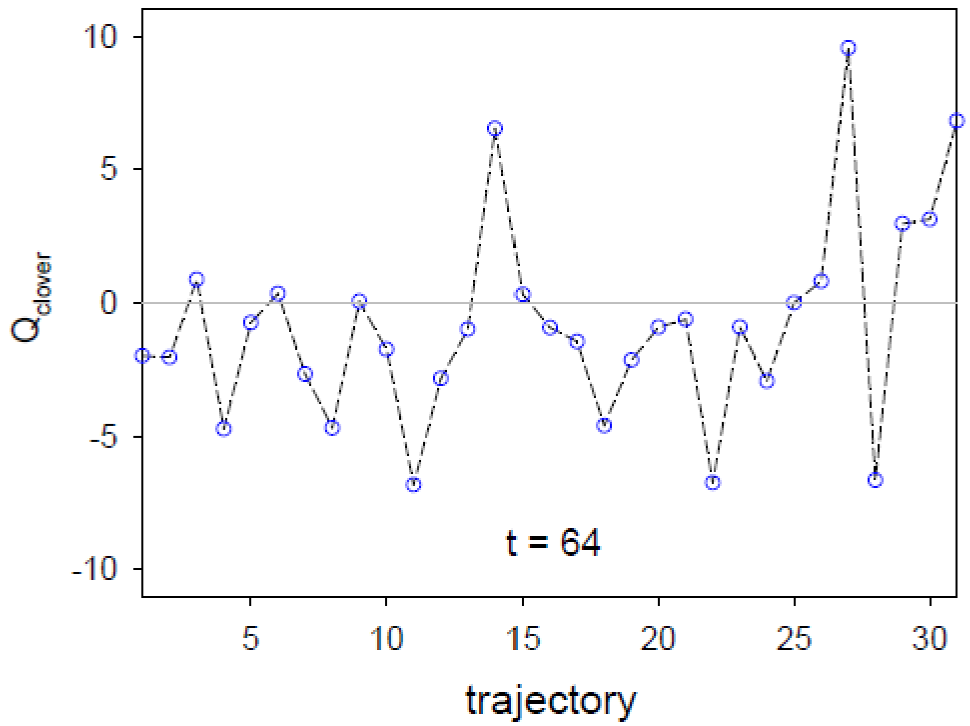


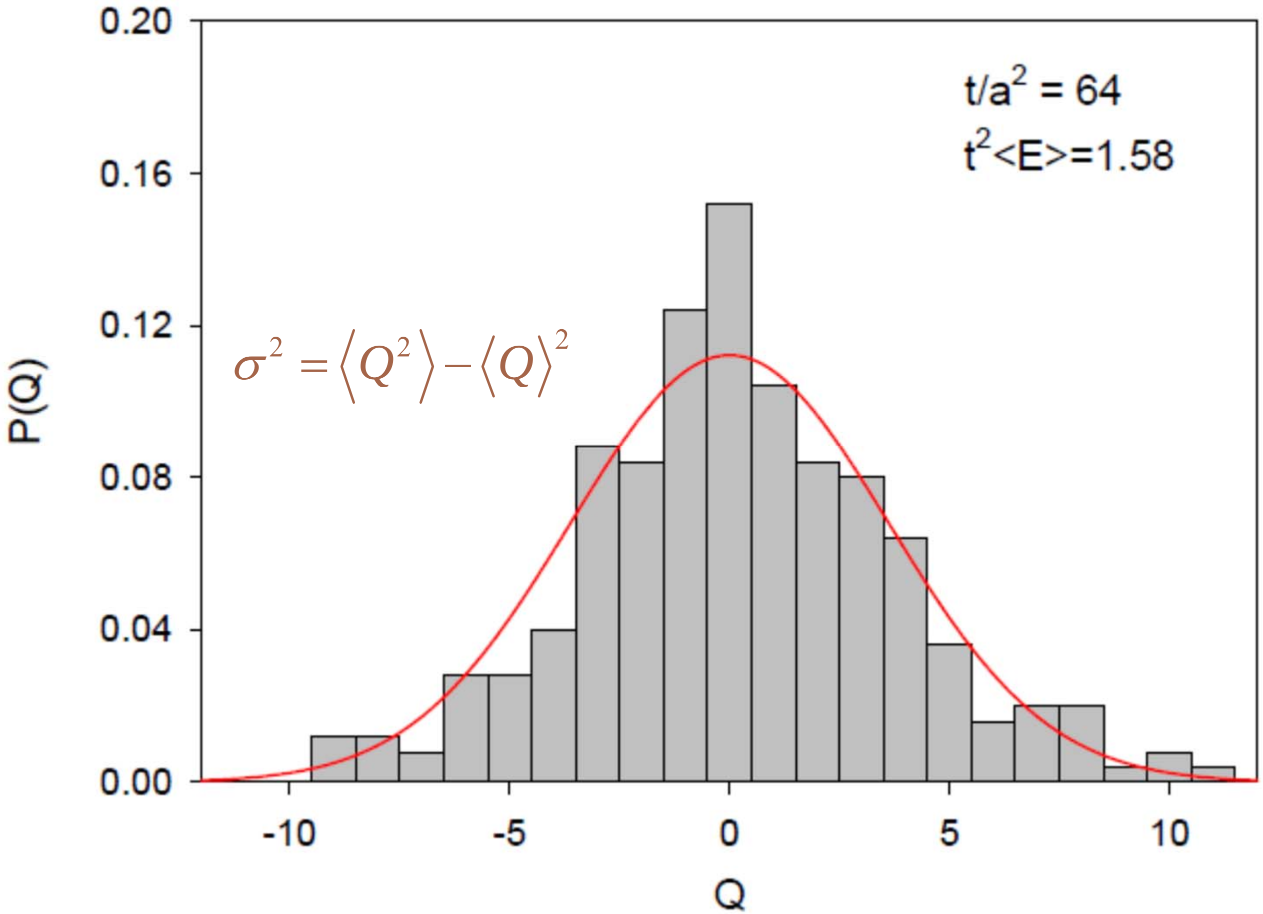
Figure 3: The evolution of the topological charge of 31 successive HMC trajectories.

[TWC, arXiv:1811.08095, PoS LATTICE2018 (2018) 040]

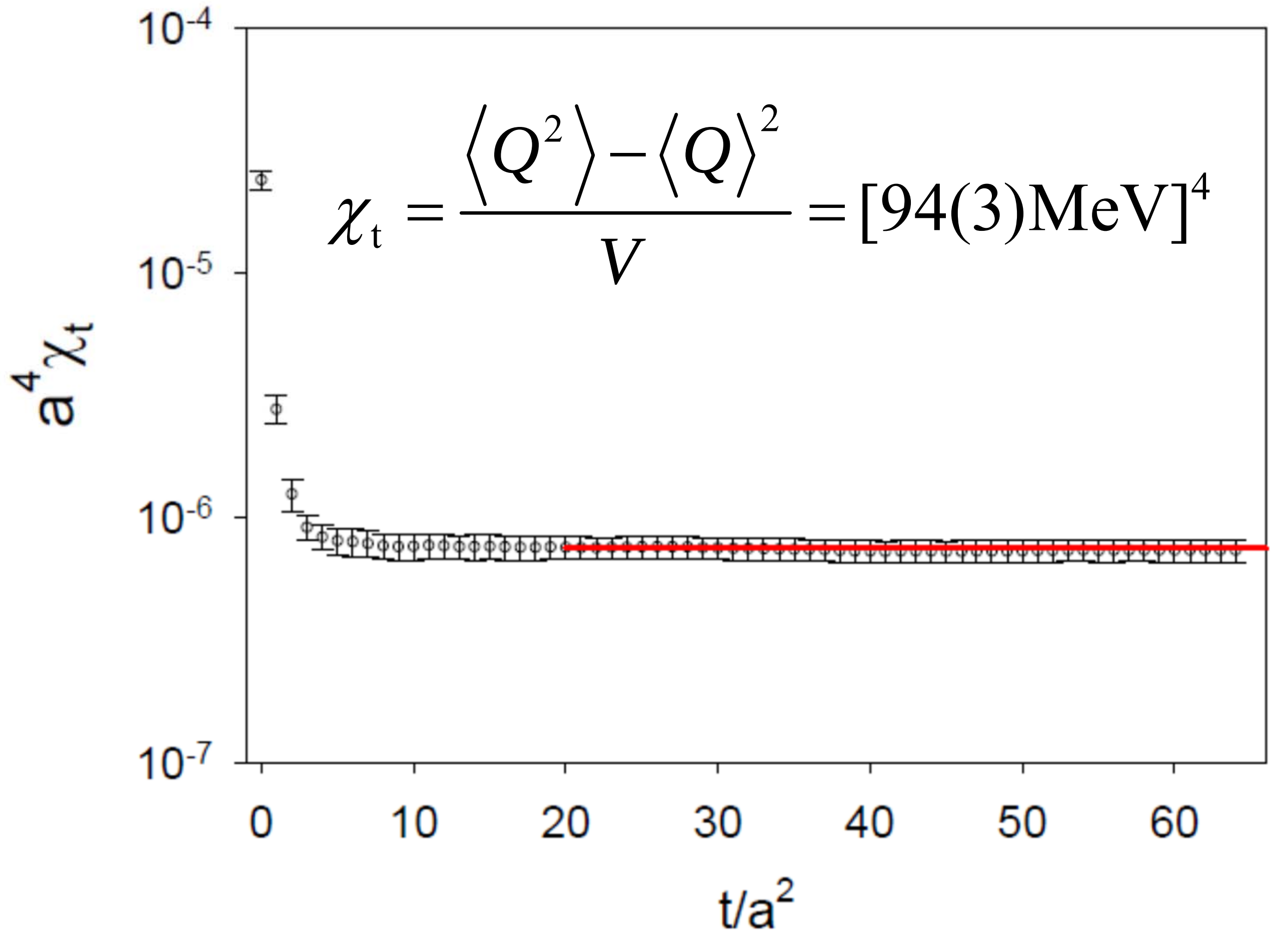
This confirms that the HMC does not suffer from the topology freezing.

Histogram of Topological Charge

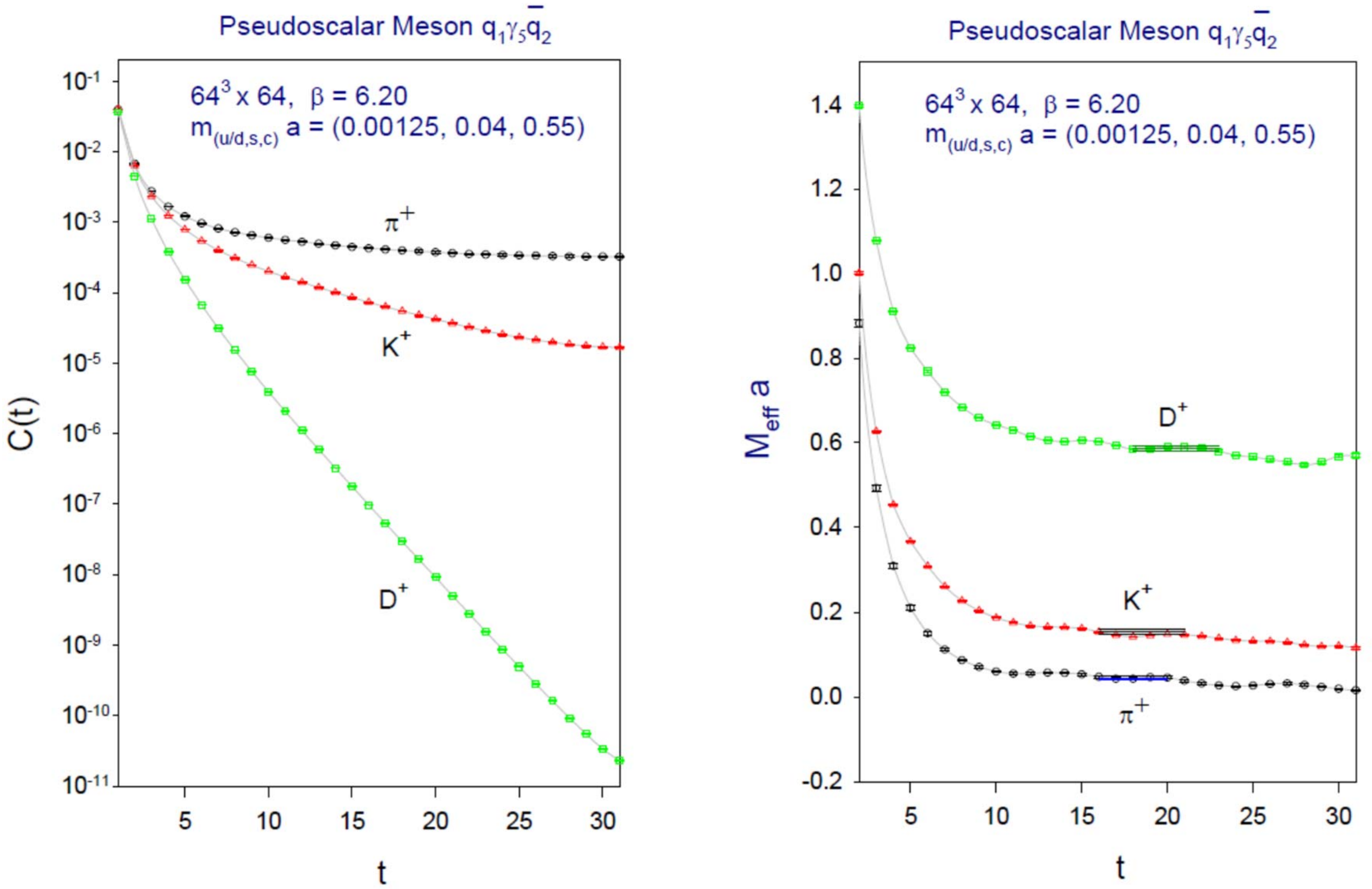
For 254 confs, each gives $Q = \left[Q_{\text{clover}} + \frac{1}{2} \right]$



Topological Susceptibility



Masses of lowest-lying pseudoscalar mesons



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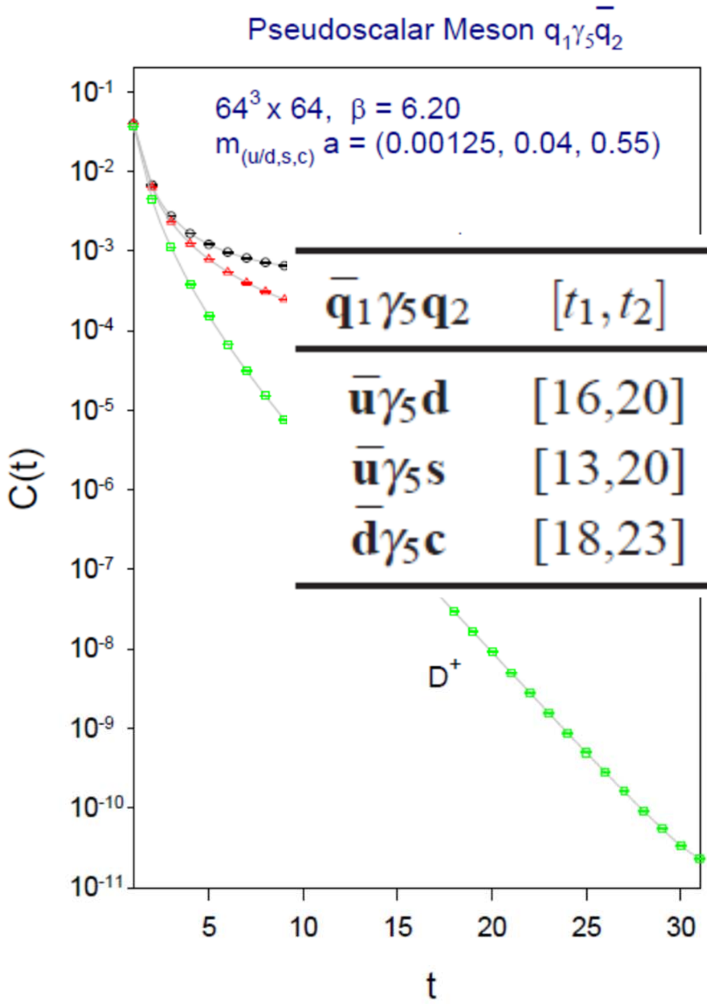

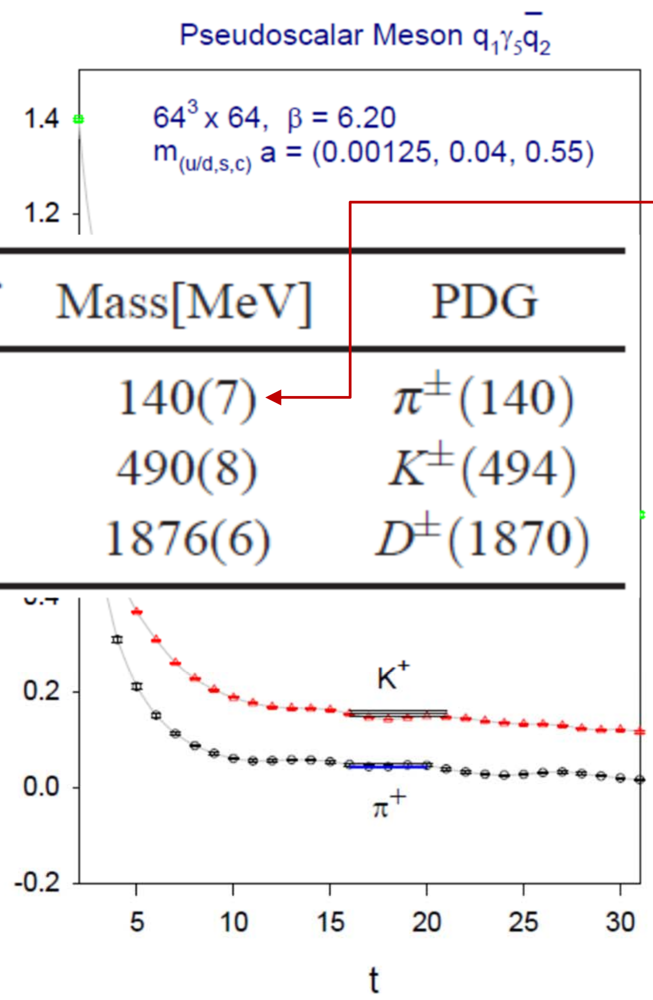

$\bar{q}_1\gamma_5 q_2$	$[t_1, t_2]$	χ^2/dof	Mass[MeV]	PDG
$\bar{u}\gamma_5 d$	[16,20]	0.03	140(7)	$\pi^{\pm}(140)$
$\bar{u}\gamma_5 s$	[13,20]	0.05	490(8)	$K^{\pm}(494)$
$\bar{d}\gamma_5 c$	[18,23]	0.20	1876(6)	$D^{\pm}(1870)$

Mass spectrum of lowest-lying charmonium

$\bar{c}\Gamma c$

Preliminary

Γ	J^{PC}	$[t_1, t_2]$	χ^2/dof	Mass[MeV]	PDG
$\mathbb{1}$	0^{++}	[10,20]	0.82	3411(18)	$\chi_{c0}(3415)$
γ_5	0^{-+}	[10,16]	0.73	2978(5)	$\eta_c(2983)$
γ_i	1^{--}	[24,30]	0.78	3100(4) ← Input	$J/\psi(3097)$
$\gamma_5\gamma_i$	1^{++}	[14,22]	1.18	3514(22)	$\chi_{c1}(3510)$
$\epsilon_{ijk}\gamma_j\gamma_k$	1^{+-}	[16,25]	0.96	3529(9)	$h_c(3525)$

Mass spectrum of lowest-lying $\bar{c}\Gamma s$ mesons

Preliminary

Γ	J^P	$[t_1, t_2]$	χ^2/dof	Mass[MeV]	PDG
$\mathbb{1}$	0^+	[10,15]	0.55	2303(12)	$D_{s0}^*(2317)$
γ_5	0^-	[9,21]	0.66	1963(9)	$D_s(1968)$
γ_i	1^-	[12,20]	0.18	2106(12)	$D_s^*(2112)$
$\gamma_5\gamma_i$	1^+	[11,17]	1.19	2445(14)	$D_{s1}(2460)$
$\epsilon_{ijk}\gamma_j\gamma_k$	1^+	[9,14]	0.98	2521(14)	$D_{s1}(2536)$

Mass spectrum of baryons with c and s quarks

Preliminary

Baryon	J^P	$[t_1, t_2]$	χ^2/dof	Mass(MeV)	PDG
Ω	$3/2^+$	[10, 17]	0.47	1657(28)	1672
Ω	$3/2^-$	[9, 17]	0.68	2254(33)	2250
Ω_c	$1/2^+$	[10,22]	0.84	2697(16)	2695
Ω_c	$1/2^-$	[18,23]	0.58	3007(24)	
Ω_c	$3/2^+$	[11,17]	0.29	2761(31)	2766
Ω_c	$3/2^-$	[9,16]	0.84	3194(30)	
Ω_{cc}	$1/2^+$	[17,21]	0.94	3752(19)	
Ω_{cc}	$1/2^-$	[10,20]	0.30	4185(31)	
Ω_{cc}	$3/2^+$	[19,22]	0.40	3737(15)	
Ω_{cc}	$3/2^-$	[13,22]	1.11	4198(23)	
Ω_{ccc}	$3/2^+$	[16,23]	0.89	4873(14)	
Ω_{ccc}	$3/2^-$	[17,25]	0.43	5301(40)	

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Ω_c(3000) -- LHCb (March 2017)

predicted by TWQCD
arXiv:1701.02581

Conclusion and Outlook

- It is feasible to simulate lattice QCD with physical (u, d, s, c) optimal DW quarks, with good chiral symmetry, and sampling all topological sectors ergodically.
- The exact pseudofermion action for one-flavor DWF plays the crucial role in the simulation, not only to save the memory such that the HMC (on $64^4 \times 16$ lattice) can fit into the 128 GB device memory of DGX-1, but also to enhance the HMC efficiency significantly.
- Having gauge ensembeles with physical (u, d, s, c) quarks, we are in a good position to extract the hardon mass spectra, decay constants, ..., as well as to understand some subtle nonperturbative physics, e.g, GIM mechanism, $\Delta I = 1/2$ rule, ...

Acknowledgement

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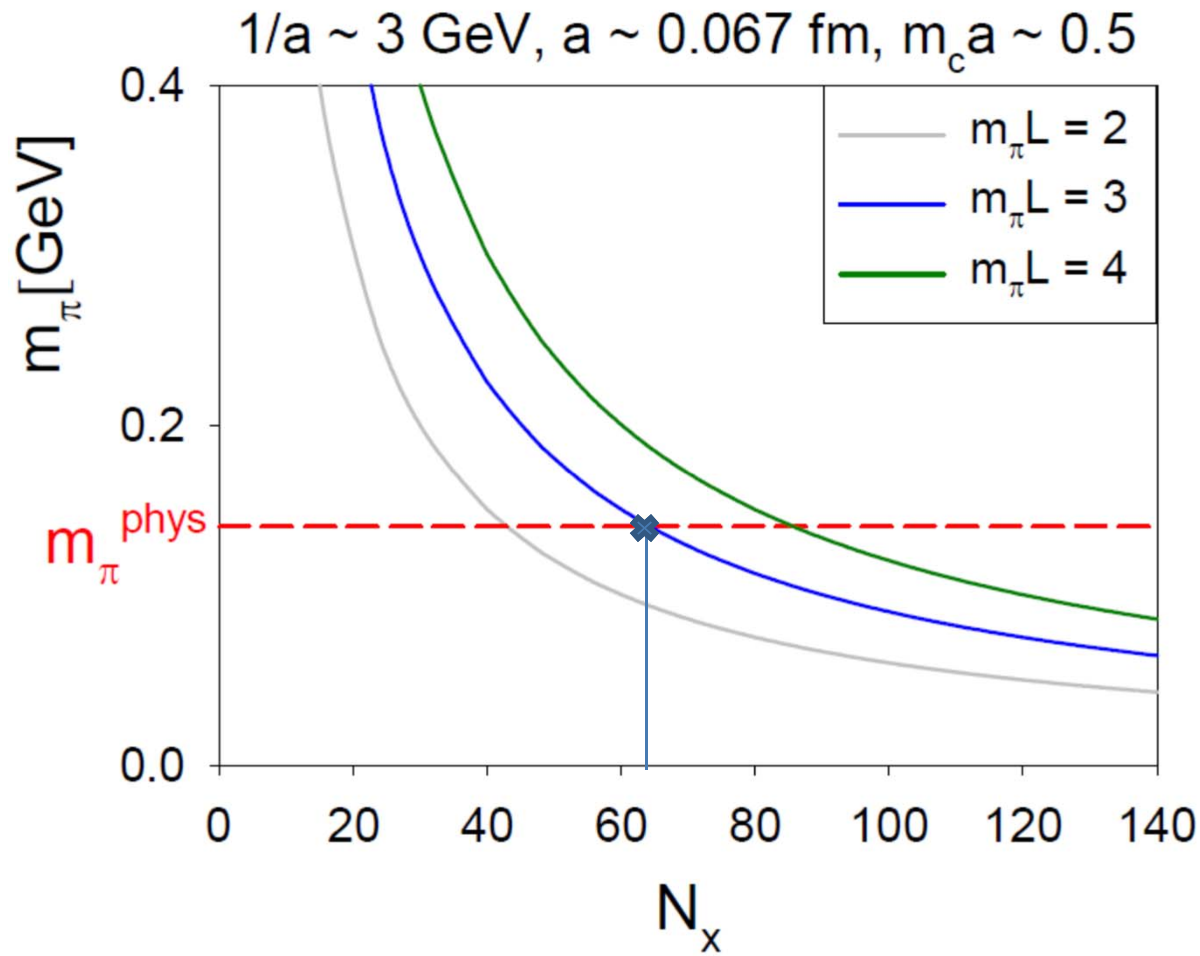
National Taiwan Normal University

National Taiwan University

Backup Slides

Design lattice QCD with physical (u,d,s,c) quarks



For the $L^3 \times T = 64^3 \times 128$ lattice, $M_\pi L \approx 3$, $M_\pi \approx 140$ MeV, $L \approx 4$ fm

Domain-Wall Fermion

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

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

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

$$\rho_s = c\omega_s + d$$

$$\sigma_s = c\omega_s - d$$

c, d (constants)

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

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

with boundary conditions

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

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

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:

$$P_+ \phi\left(x, 0\right) = -P_+ \phi\left(x, N_s\right),$$
$$P_- \phi\left(x, N_s + 1\right) = -P_- \phi\left(x, 1\right)$$

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

The effective 4D Dirac operator

$$m_{PV} = 2m_0(1 - dm_0)$$

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

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

Variants of Domain-Wall Fermion

Sharmir DWF: $c = d = \frac{1}{2}, \ \omega_s = 1, \ \ H = H_w(2 + \gamma_5 H_w)^{-1}, \ \ S(H) = \text{polar approx. of } \frac{H}{\sqrt{H^2}}$

Möbius DWF: $d = \frac{1}{2}, \ \omega_s = 1, \ \ H = 2cH_w(2 + \gamma_5 H_w)^{-1}, \ \ S(H) = \text{polar approx. of } \frac{H}{\sqrt{H^2}}$

Borici DWF: $c = 1, \ d = 0, \ \omega_s = 1, \ \ H = H_w, \ \ S(H) = \text{polar approx. of } \frac{H_w}{\sqrt{H_w^2}}$

Optimal DWF: $c = 1, \ d = 0, \ H = H_w,$ [TWC, Phys. Rev. Lett. 90 (2003) 071601]

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

$$S(H) = \text{Zolotarev optimal rational approximation of } \frac{H_w}{\sqrt{H_w^2}}$$

ODWF can keep the residual mass very small, for both light and heavy quarks.

2+1+1 = 2+2+1

For domain-wall fermions

$$\frac{\det D(m_{u/d})}{\det D(m_{PV})}\frac{\det D(m_{u/d})}{\det D(m_{PV})}\frac{\det D(m_s)}{\det D(m_{PV})}\frac{\det D(m_c)}{\det D(m_{PV})}$$

$$=\left(\frac{\det D(m_{u/d})}{\det D(m_{PV})}\right)^2\left(\frac{\det D(m_c)}{\det D(m_{PV})}\right)^2\frac{\det D(m_s)}{\det D(m_c)}$$

2-flavor 2-flavor 1-flavor

- For the one-flavor, use the exact pseudofermion action for one-flavor DWF [Y.C. Chen & TWC, Phys. Lett. B738 (2014) 55; TWC, Phys. Lett. B744 (2015) 95]
- For the 2-flavor part, use the two-flavors algorithm for DWF [TWC, T.H. Hsieh, Y.Y. Mao, Phys. Lett. B702 (2012) 131]

Exact One-Flavor Pseudofermion Action (EOFA)

[Y.C. Chen & TWC, Phys. Lett. B738 (2014) 55; TWC, Phys. Lett. B744 (2015) 95]

The exact pseudofermion action for one-flavor DWF can be written as

$$S_{pf} = \begin{pmatrix} 0 & \phi_1{}^{\dagger} \end{pmatrix} \left[I - k v_-{}^T \omega^{-1/2} \frac{1}{H(m)} \omega^{-1/2} v_- \right] \begin{pmatrix} 0 \\ \phi_1 \end{pmatrix}$$

$$+ \begin{pmatrix} \phi_2{}^{\dagger} & 0 \end{pmatrix} \left[I + k v_+{}^T \omega^{-1/2} \frac{1}{H(1) - \Delta_+(m) P_+} \omega^{-1/2} v_+ \right] \begin{pmatrix} \phi_2 \\ 0 \end{pmatrix}$$

with a positive-definite and Hermitian Dirac operator.

Here $H(m) = \gamma_5 R_5 D(m)$, $R_5 = \delta_{s', N_s+1-s}$

$$\Delta_{\pm}(m) = k \omega^{-1/2} v_{\pm} v_{\pm}{}^T \omega^{-1/2}$$

$$k = \frac{c}{1 - c\lambda} \frac{1 - m}{1 + m(1 - 2c\lambda)}$$

Salient Features of EOFA

- The operator in the pseudofermion action of the one-flavor DWF is exact, Hermitian, and positive-definite, without taking square root.
- It can be used for all variants of DWF, and for any approximations (polar or Zolotarev) of the sign function.
- The memory consumption of EOFA is much smaller than that of RHMC. This feature is crucial for using GPUs to simulate QCD.
- The efficiency of HMC with EOFA is more than 3 times faster than that using RHMC.

2-flavors algorithm for DWF

By even-odd preconditioning

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

Schur decomposition

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

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

Since $\det \mathcal{D} = \det S_1^{-1} \cdot \det C \cdot \det S_2^{-1}$
and S_1 and S_2 do not depend on the gauge field,
we can just use C in the Monte Carlo simulation.

For 2-flavors QCD, the pseudofermion action can be written as

$$S_{pf}^{2\mathrm{F}} = \phi^\dagger C_{PV}^\dagger (CC^\dagger)^{-1} C_{PV} \phi, \quad C_{PV} = C(m_{PV}), \quad m_{PV} = 2m_0(1 - dm_0)$$

2-flavors algorithm for DWF (cont)

$$L(m) = P_+ L_+(m) + P_- L_-(m) = \begin{pmatrix} L_+(m) & 0 \\ 0 & L_-(m) \end{pmatrix}_{Dirac}$$

$$L_+(m)_{s,s'} = \begin{cases} \delta_{s',s-1} \ , 1 < s \le N_s \\ -m\delta_{s',N_s} \ , s = 1, \end{cases} \quad m = r m_q \ , \ r = 1/[2m_0(1 - d m_0)]$$

$$L_-(m) = L_+(m)^T$$

$L_\pm(m)$ are matrices in the fifth dimension, with dependence on quark mass.

$$M_5 = \left\{ \left(4 - m_0\right) + \omega^{-1/2} [c\left(1 - L\right)\left(1 + L\right)^{-1} + d\omega^{-1}]^{-1} \omega^{-1/2} \right\}^{-1}$$

How much does it take to simulate lattice QCD with physical (u,d,s,c) DW quarks ?

- To satisfy $M_\pi L \approx 3,\ L \simeq 4$ fm, $M_\pi \approx 140$ MeV, $a^{-1} \approx 3$ GeV, $m_c a \approx 0.5$, the lattice size must be at least $64^3 \times 64$.
- For DW quarks with $N_s = 16$, the 5D lattice is $64^3 \times 64 \times 16$, and the HMC (using EOFA) requires a memory space $\geq$ 128 GB.
- For DWF with good chiral symmetry ($m_{res} a < 5 \times 10^{-5}$), it requires >10 Tflops/s (sustained) to generate > 1 trajectory/day with $P_{\text{accept}} \approx 70\%$
- So far, only Nvidia DGX-1, DGX-2, ... (or compatible systems with NVLink) can meet the requirements: device memory >128 GB, and with sustained speed > 10 Tflops/s.