Exploring the QCD phase diagram with three flavors of Möbius domain wall fermions

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Outline

- Background & Motivation
- Previous lattice studies
- Lattice setup
- Results
- Summary & Outlook
The nature of QCD phase transition at $\mu_B = 0$

Order of phase transition depends on $m_l$, $m_s$ & $N_f$

- $\epsilon$ expansion: $1^{\text{st}}$ order phase transition in the chiral limit for $N_f = 3$
  [Pisarski, Wilczek PRD 84]

- RG flows of all couplings up to $\phi^6$ in 3d Ginzburg-Landau potential for $N_f = 3$ in the chiral limit: a possible $2^{\text{nd}}$ order phase transition
  [G. Fejos, PRD 22]

This work:
→ Explore $N_f = 3$ chiral region using first-principle lattice QCD
## Previous Nf=3 lattice QCD studies

<table>
<thead>
<tr>
<th>Action</th>
<th>$N_t$</th>
<th>$m_\pi Z_2$ [MeV]</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Staggered, standard</td>
<td>4</td>
<td>290</td>
<td>Karsch et al. (2001)</td>
</tr>
<tr>
<td>Staggered, standard</td>
<td>6</td>
<td>150</td>
<td>de Forcrand et al. (2007)</td>
</tr>
<tr>
<td>Staggered, HISQ</td>
<td>6</td>
<td>$\lesssim 50$</td>
<td>Bazavov et al. (2017)</td>
</tr>
<tr>
<td>Staggered, stout</td>
<td>4-6</td>
<td>0?</td>
<td>Varnhost (2014)</td>
</tr>
<tr>
<td>Staggered, HISQ</td>
<td>8</td>
<td>$\lesssim 80$</td>
<td>Dini et al. (2022)</td>
</tr>
<tr>
<td>Wilson, standard</td>
<td>4</td>
<td>$\lesssim 670$</td>
<td>Iwasaki et al. (1996)</td>
</tr>
<tr>
<td>Wilson-Clover</td>
<td>6-10</td>
<td>$\lesssim 170$</td>
<td>Jin et al. (2017)</td>
</tr>
<tr>
<td>Wilson-Clover</td>
<td>6-12</td>
<td>$\lesssim 110$</td>
<td>Kuramashi et al. (2020)</td>
</tr>
</tbody>
</table>

Evidence for continuum chiral limit to feature 2nd order PT with staggered fermion [Cuteri et al.(2021)]

$1^{\text{st}}$ order region shrinks as $a \to 0$ or even disappear with both staggered and Wilson fermions

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**Our aim is to investigate Nf = 3 QCD phase structure with Mobius Domain Wall Fermion**

Why MDWF

- Exact chiral symmetry at finite $a$ for infinite Ls
- Reduced $\chi_{SB}$ parameterized by residual mass when Ls is finite
Lattice Setup

$N_f=3$ Mobius Domain Wall Fermion

Tree-level Symanzik improved gauge action and stout smearing at $\beta = 4.0$ ($a=0.1361(20)$ fm)

Using Wilson flow $t_0$ to set the scale and matching with $N_f=2+1$ physical point

$\sqrt{\frac{t_0}{\text{phys}}} = 0.1465(21)(13)$ fm

[S.Borsanyi et al., JHEP 2012]

$\star$ $T = 0$:  

$N_s=24$, $N_t=48$, $L_s=16$: $0.02 \leq am_q \leq 0.045$, $am_{\text{res}}$ (estimated) $\approx 0.006$

$\star$ $T > 0$:

$N_t=12$ ($T=120.8(1.8)$ MeV), $L_s=16$: $N_s=36$, $-0.005 \leq am_q \leq 0.001$

$N_s=24$, $-0.006 \leq am_q \leq 0.1$

$L_s=32$: $N_s=24$, $-0.001 \leq am_q \leq 0.003$

Measured: residual mass, chiral condensate, chiral susceptibility & Binder cumulant

Codes: Grid & Hardons

Resources: Supercomputer Fugaku & Wisteria/BDEC-01 Oddysey at Univ. Tokyo
Residual chiral symmetry breaking

- For finite \( L_s \) chiral symmetry is broken, its leading contribution is equivalent to an additive renormalization to the input quark mass \( m_q \), which knows as \( m_{\text{res}} \), so the total quark mass becomes \( m_q + m_{\text{res}} \).

- Measure the ratio of midpoint correlator to the pion correlator evaluated at large distance

\[
m_{\text{res}} = R(t) = \frac{\left\langle \sum_{x} J_{5q}^d(\overrightarrow{x}, t) \pi^d(0, 0) \right\rangle}{\left\langle \sum_{x} J_{5}^d(\overrightarrow{x}, t) \pi(0, 0) \right\rangle}
\]

Intercept zero within error at \( m_q = -m_{\text{res}} \).

- \( \langle \bar{\psi} \psi \rangle |_{\text{DWF}} \sim C \frac{m_q + x m_{\text{res}}}{a^2} + \langle \bar{\psi} \psi \rangle |_{\text{cont.}} + \ldots \), \( x \) is not known, expected \( x = \mathcal{O}(1) \)

Additive divergence remains if one extrapolates to \( m = m_q + m_{\text{res}} = 0 \):

\[
\lim_{m \to 0} \lim_{V \to 0} \langle \bar{\psi} \psi \rangle |_{\text{DWF}} \sim \langle \bar{\psi} \psi \rangle |_{\text{cont.}} + C(x - 1) \frac{m_{\text{res}}}{a^2} + \ldots
\]

[S. Sharpe, arXiv:0706.0218]
Chiral condensate at $T \sim 121$ MeV

Order parameter for $\chi_{SB}$: $$\langle \bar{\psi} \psi \rangle = \frac{N_f}{N_s^3 N_t} \text{Tr} \langle M^{-1} \rangle$$

Quark mass renormalization in $\overline{\text{MS}}$ scheme: $$m^{\overline{\text{MS}}}(2 \text{ GeV}) = Z_m^{\overline{\text{MS}}}(2 \text{ GeV}) \cdot a^{-1} \cdot am$$

Multiplicative renormalization: $$\langle \bar{\psi} \psi \rangle^{\overline{\text{MS}}}(2 \text{ GeV}) = \frac{a^{-3} \cdot a^3 \langle \bar{\psi} \psi \rangle}{Z_m^{\overline{\text{MS}}}(2 \text{ GeV})}$$

Remove additive divergence $C \frac{m_q + x m_{\text{res}}}{a^2}$ by $\langle \bar{\psi} \psi \rangle^{T>0} - \langle \bar{\psi} \psi \rangle^{T=0}$
Chiral condensate at $T \sim 121$ MeV

Additively and multiplicatively renormalized order parameter

$$\left[ \langle \bar{\psi} \psi \rangle^{T \geq 0} - \langle \bar{\psi} \psi \rangle^{T=0} \right]_{\text{MS}}^{\text{MS}} (\mu = 2 \text{ GeV}) [\text{GeV}^3]$$

Finite size dependence is visible around $(m_q + m_{\text{res}})_{\text{MS}} \sim 4 - 9$ MeV
Chiral susceptibility at $T \sim 121$ MeV

$$\chi_\sigma = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial m^2} = \chi_\text{disc} + \chi_\text{con}, \quad \chi_\text{disc} = \frac{N_f^2}{N_s^3 N_t} \left[ \langle (\text{Tr} M^{-1})^2 \rangle - \langle \text{Tr} M^{-1} \rangle^2 \right], \quad \chi_\text{con} = -\frac{N_f}{N_s^3 N_t} \langle \text{Tr} M^{-2} \rangle$$

Renormalize susceptibility to $\overline{\text{MS}}(\mu = 2 \text{ GeV})$ with $(Z_m^{\overline{\text{MS}}})^{-2}$ to remove the multiplicative divergence

The change in peak height & position for $\chi_\text{disc}$ and $\chi_\sigma$ is not as large as anticipated from the first order transition (see next slide)

$\rightarrow$ Consistent with the crossover rather than true phase transition

For crossover transition, the peak height of susceptibility would be volume independent for large volumes, currently $48^3 \times 12$ simulation is underway

The transition mass point determined from $\chi_\text{disc}$ and $\chi_\sigma$ is around 3.6 MeV & 2.5 MeV in the $\overline{\text{MS}}$ scheme at a scale of $\mu = 2$ GeV, they coincide in the chiral phase transition temperature
Finite size scaling: susceptibility $\chi_\sigma$ at $T \sim 121$ MeV

Finite size scaling function for the susceptibility at critical point:

$$\chi_\sigma^{\text{max}}(N_s) \sim \begin{cases} N_s^3, & \text{first order phase transition} \\ N_s^{1.966}, & \text{Z(2) second order phase transition} \end{cases}$$

finite-size scaled susceptibility

The peak height of chiral susceptibility does not scale like a first order and Z(2) second order phase transition
The histogram of chiral condensate at $T\sim 121$ MeV

The normalized histogram at transition mass point determined from $\chi_{\text{disc}}$ and $\chi_{\sigma}$ behaves like a Gaussian distribution. No evidence that a double peak structure would appear as volume increases.
Binder cumulant of chiral condensate at $T \sim 121$ MeV

$$B_4(\bar{\psi}\psi) = \frac{\langle (\delta\bar{\psi}\psi)^4 \rangle}{\langle (\delta\bar{\psi}\psi)^2 \rangle^2}, \quad \delta\bar{\psi}\psi = \bar{\psi}\psi - \langle \bar{\psi}\psi \rangle$$
Residual mass and Chiral condensate at varying $L_s$

- $am_{\text{res}}$ computed at fixed $\beta = 4.0$ for both zero & finite $T$ are consistent
- Adjust input quark mass for $L_s=32$ so that $a(m_q + m_{\text{res}})$ is similar with $L_s=16$
- $am_{\text{res}}$ reduced almost half for $L_s=32$, $1/L_s$ dependence dominates the contribution

\[ am_{\text{res}}(0) \text{ from linear fit with zero T data} \]

\[ \lim_{(m_q + m_{\text{res}}) \to 0} \lim_{V \to 0} \langle \bar{\psi} \psi \rangle |_{DWF} \sim \langle \bar{\psi} \psi \rangle |_{\text{cont.}} + C \frac{(x-1)m_{\text{res}}}{a^2} \]

The result has contamination due to the lack of exact chiral symmetry after taking chiral limit

- Residual chiral symmetry breaking effect is smaller for $L_s=32$

[S. Sharpe, arXiv: 0706.0218]
For two lattices with the approximate same total quark mass, we observe the consistent results in the susceptibility, the transition mass point is similar

⇒ The choice of our negative input quark mass for $L_s=16$ is safe

- Susceptibility seems to be function of total light quark mass $m_q + m_{\text{res}}$
Summary and outlook

- $(m_q + m_{\text{res}})^{\text{MS}}_{pc} \sim 42 \text{ MeV}, T \sim 181 \text{ MeV} (N_t = 8, \text{MDWF})$
  $\Leftrightarrow m_{\pi}^{\text{pc}} \sim 480 \text{ MeV}, \text{no phase transition}$
  
  [Y. Zhang lattice 2022]

- $(m_q + m_{\text{res}})^{\text{MS}}_{pc} \sim 3.6 \text{ MeV}, T \sim 121 \text{ MeV} (N_t = 12, \text{MDWF})$
  $\Leftrightarrow m_{\pi}^{\text{pc}} \sim 141 \text{ MeV}, \text{no phase transition}$

- $T \sim 104 \text{ MeV} (N_t = 14, \text{MDWF}), \text{lighter quark mass simulation is underway}$
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• Codes
  • HMC
    • Grid (implementation for A64FX: thanks to the Regensburg group)
  • Measurements
    • Bridge++
    • Hadrons / Grid

• Computers
  • Supercomputer Fugaku provided by the RIKEN Center for Computational Science through HPCI project #hp210032 and Usability Research ra000001.
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  • Ito supercomputer at Kyushu University through HPCI project #hp190124 and hp200050
  • Hokusai BigWaterfall at RIKEN

• Grants
  • JSPS Kakenhi (20H01907)
Backup slide
\[ B_4(\langle \bar{\psi} \psi \rangle) = \frac{\langle (\delta \bar{\psi} \psi)^4 \rangle}{(\langle (\delta \bar{\psi} \psi)^2 \rangle)^2} \]

\[ N_s^3 \times N_t \times L_s = 24^3 \times 12 \times 32 \]

\[ N_s^3 \times N_t \times L_s = 24^3 \times 12 \times 16 \]

Crossover

\[ Z(2) \] 2nd order

1st order

\[ (m_q + m_{res})_{\text{MS}}(\mu = 2 \text{ GeV}) \text{ [MeV]} \]