

QCD phase transition from Lattice

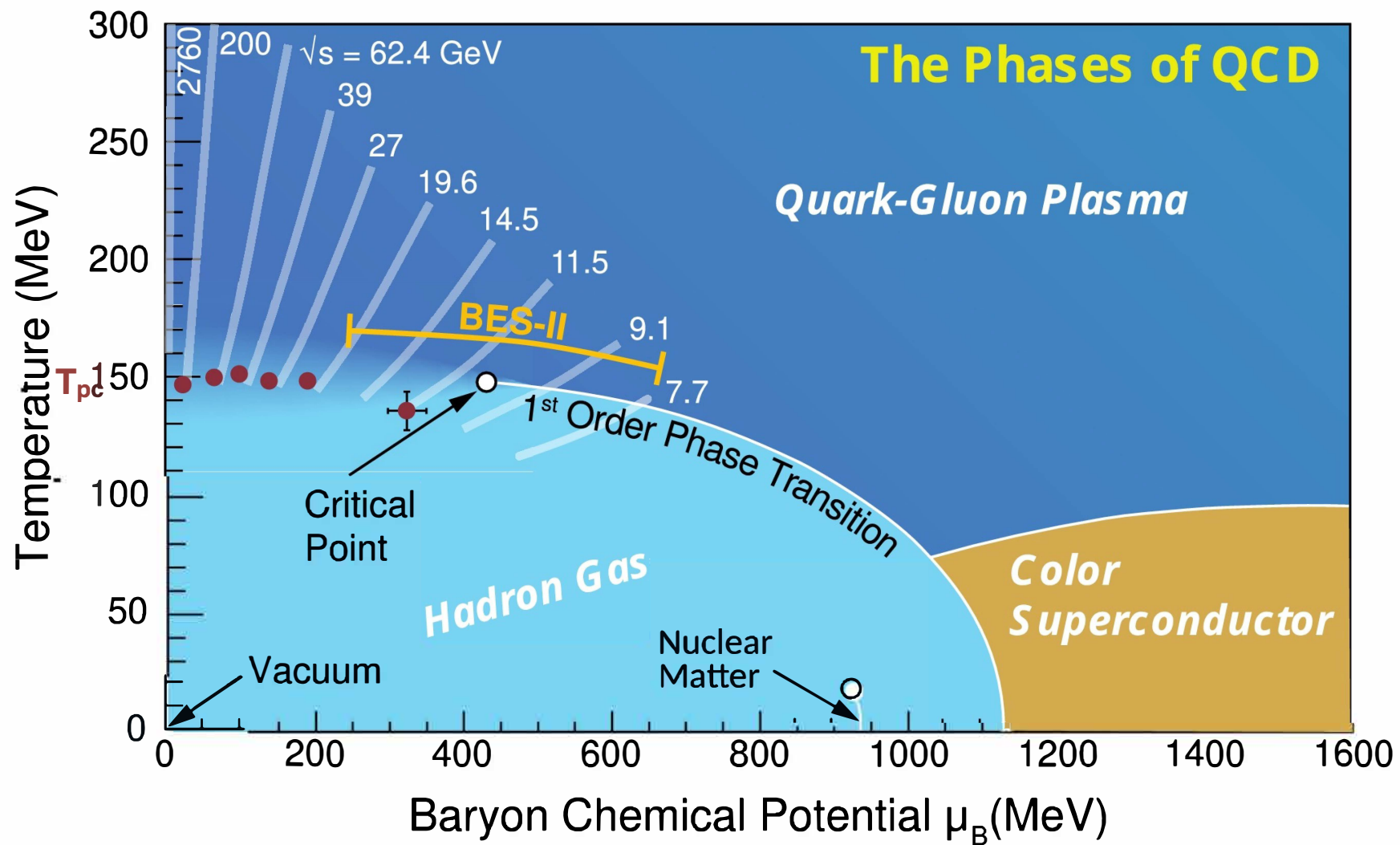
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The 15th workshop on QCD Phase Transition and Relativistic Heavy-Ion Physics,
Zhuhai, Dec.15-19, 2023



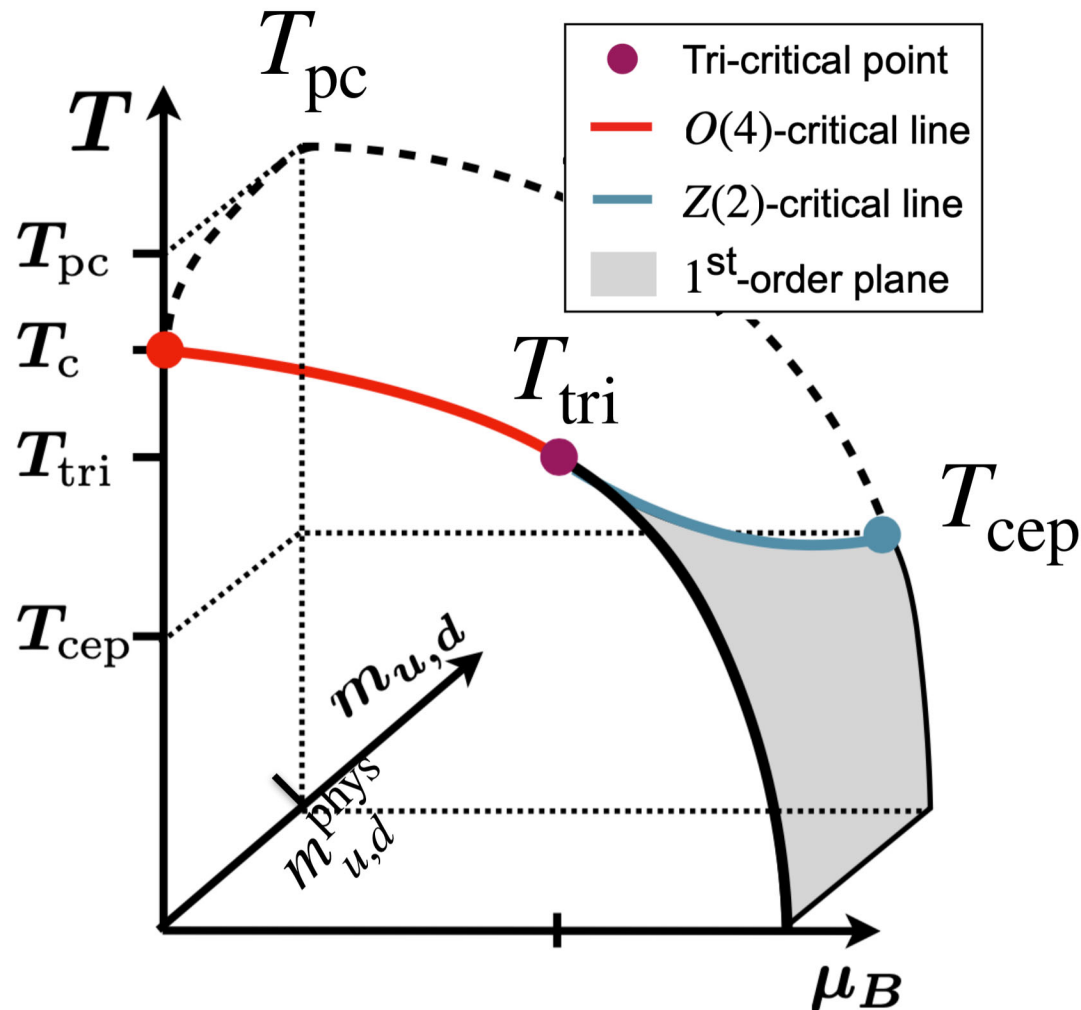
Conjectured QCD phase diagram



X. An et al., Nucl.Phys.A 1017 (2022), 122343

QCD phase diagram in 3D

The nature of QCD chiral phase transition in massless limit constrains the QCD phase diagram



F. Karsch. arXiv: 1905.03936

- Random Matrix Model & NJL suggests:

$$T_{tri} - T_{cep}(m) \propto m^{2/5}$$

Y. Hatta, T. Ikeda, PRD 67 (2023) 014028
M. A. Halasz et al, PRD 58 (1998) 096007

- $T_c(\mu_B)$ decreases as μ_B from LQCD

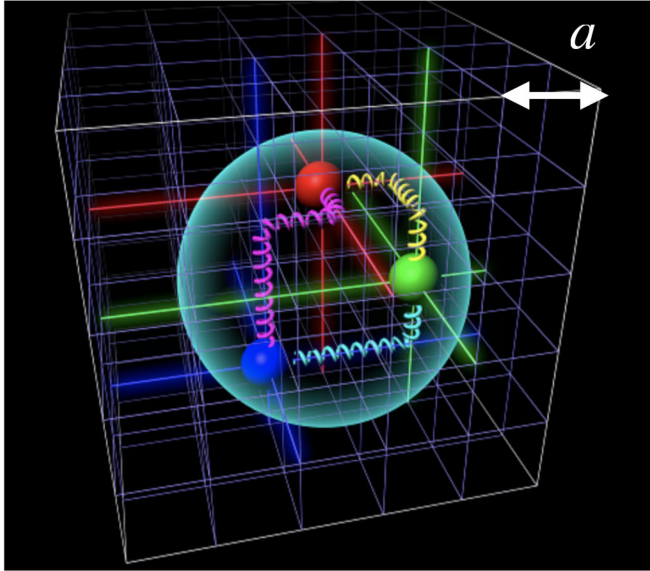
O. Kaczmarek et al., PRD83 (2011) 014504
P. Hegde & H.-T. Ding PoS LATTICE2015 (2016) 141



$$T_{cep} < T_{tri} < T_c$$

Determination of chiral phase transition temperature T_c sets a bound on T_{cep}

Lattice QCD (K. G. Wilson 1974)



- Euclidean space-time: $N_\sigma^3 \times N_\tau$
- quark field $\psi(x)$, $\bar{\psi}(x)$ on lattice sites
- gluon field $U_\mu(x)$ on lattice links
- Temperature $T = 1/(N_\tau a)$

$$\mathcal{L}_E = \frac{1}{4} F_a^{\mu\nu} F_{\mu\nu}^a + \bar{\psi}(\gamma^\mu D_\mu^E + m)\psi$$

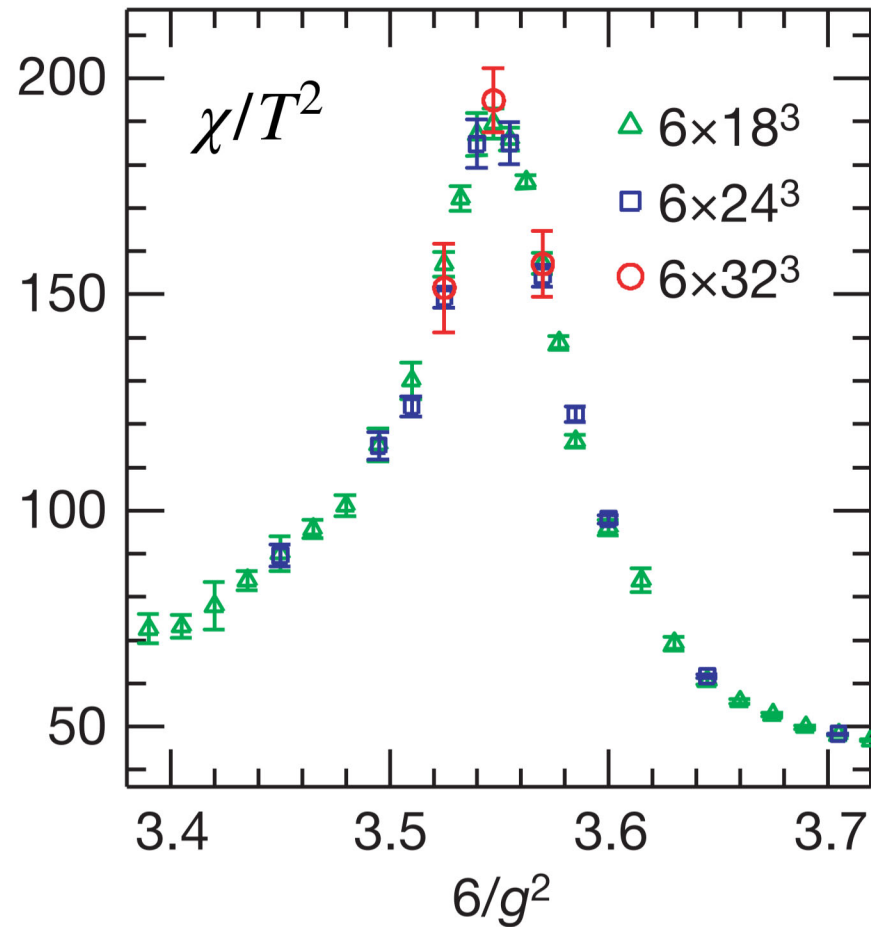
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{O}(U, \psi, \bar{\psi}) e^{-\int d^4x \mathcal{L}_E}$$

$$S_{latt} = \int d^4x \mathcal{L}_E = S_g + S_f \quad Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{latt}} = \int \mathcal{D}U e^{-S_g} \det M_f$$

- S_f : staggered, Wilson, Domain Wall fermions (chiral fermion) ...
- Evaluate path integrals by Monte Carlo with dimensions $> 10^7$, $\times L_s$ for DWF
- Physics is recovered in the continuum limit $a \rightarrow 0$ (increase N_τ at fixed T)

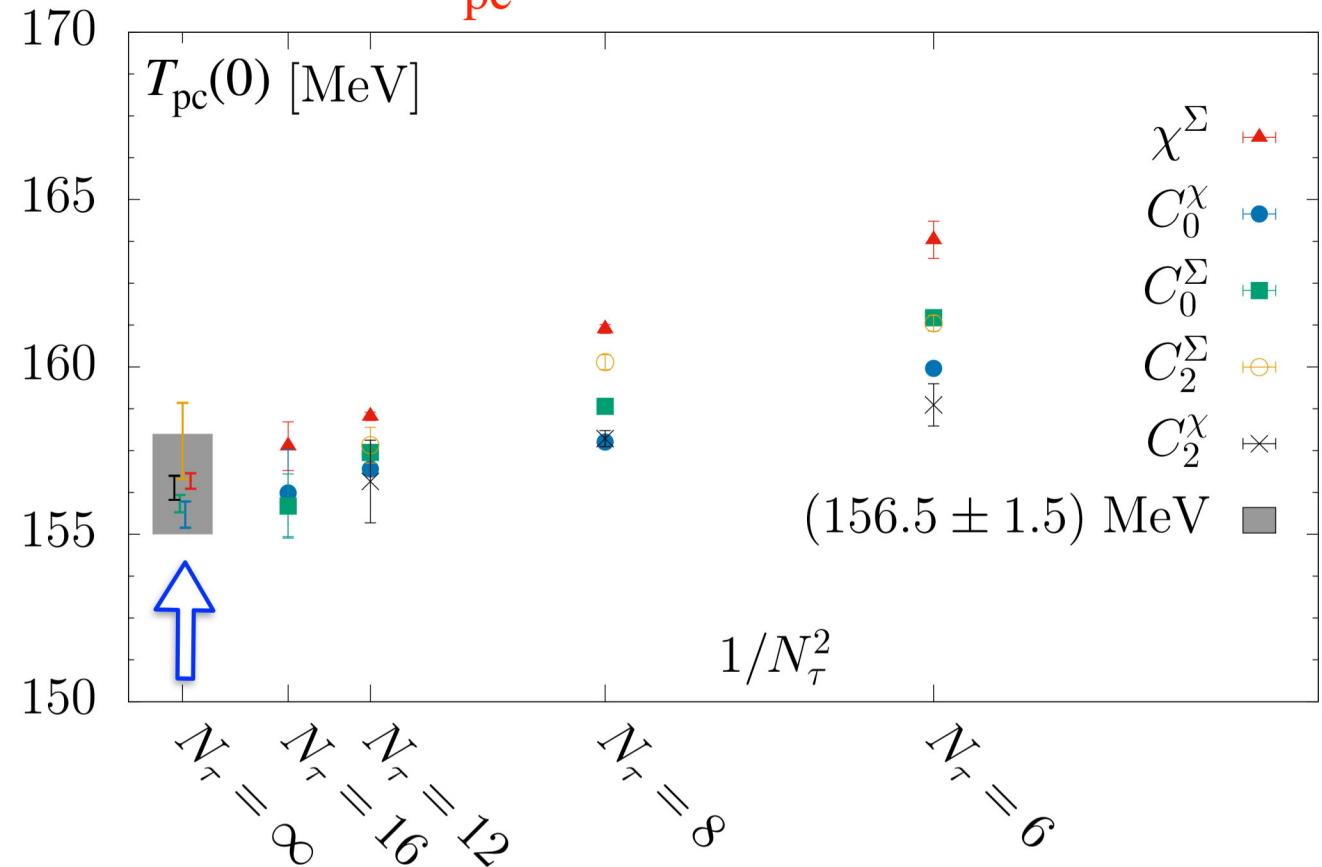
QCD transition in Nature at $\mu_B = 0$

Crossover (non-singular)



Y.Aoki et al., Nature 443 (2006) 675-678

$$T_{pc} = 156.5 \pm 1.5 \text{ MeV}$$

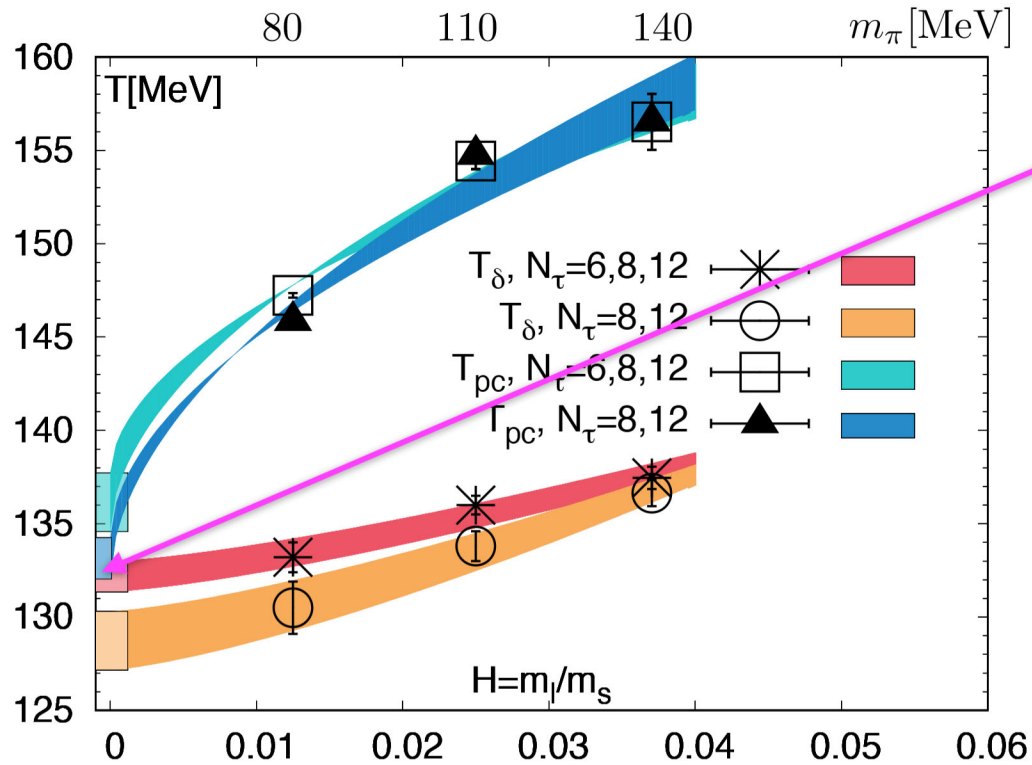


Continuum limit

A. Bazavov, H.-T. Ding et al. [HotQCD], PLB 795 (2019) 15
See also S. Borsanyi et al., PRL 125 (2020) 5, 052001

QCD chiral phase transition temperature T_c

$$\mu_B = 0$$



H.-T. Ding et al. [HotQCD], PRL 123 (2019) 062002

$$O(4) \text{ scaling for chiral extrapolation: } T_{pc}(H) = T_c \left(1 + \frac{z_p}{z_0} H^{\frac{1}{\beta\delta}}\right)$$

$$m_u = m_d = 0, m_s^{phys}: T_c = 132^{+3}_{-6} \text{ MeV}$$

Consistent results from twisted mass Wilson fermion: $T_c = 134^{+6}_{-4} \text{ MeV}$
 A. Y. Kotov et al., PLB 823 (2021) 136749

T_c puts an upper limit on T_{cep} : $T_{cep} < 132 \text{ MeV}$

Key question: Nature of chiral phase transition for two massless quarks: 2nd order, O(4)?

Depends on the magnitude of $U_A(1)$ symmetry breaking near T_c

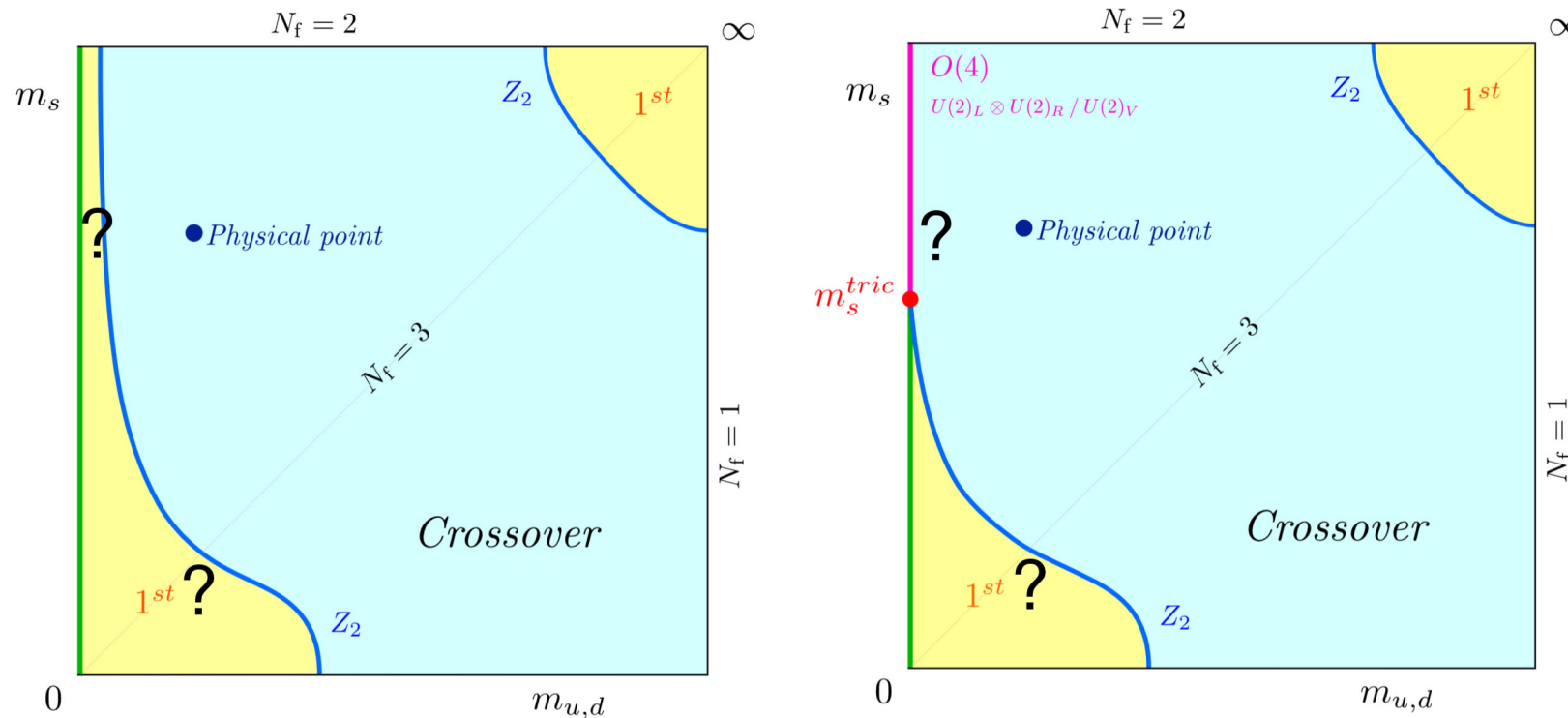
Critical behavior of QCD at $\mu_B = 0$

Axial anomaly plays a key role

Ginzburg-Landau-Wilson approach

Pisarski, Wilczek PRD 29 (1984) 338

Columbia plot



(a) First-order scenario for $N_f = 2, m_{u,d} = 0$.

(b) Second-order scenario for $N_f = 2, m_{u,d} = 0$.

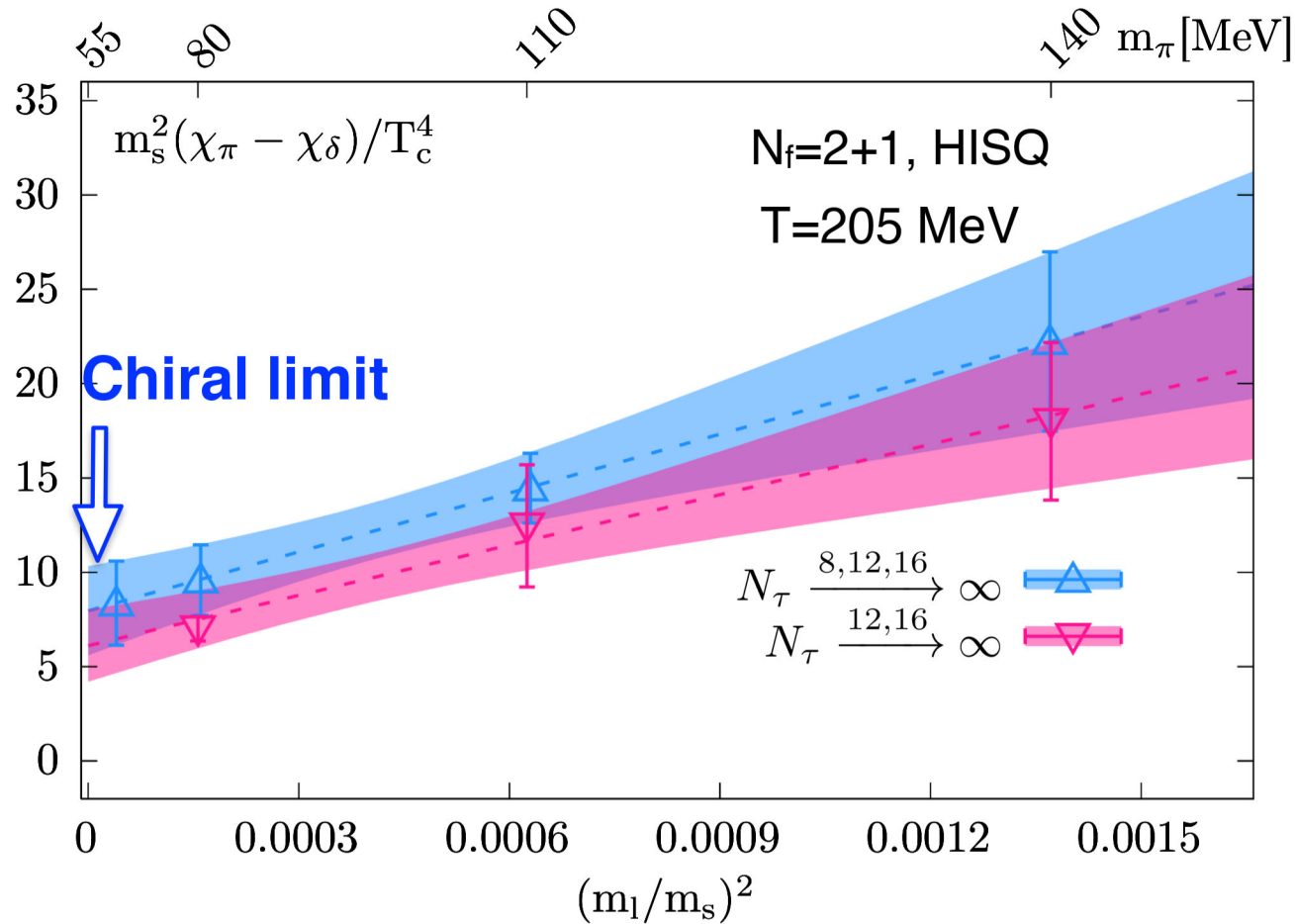
Axial anomaly in $m_u = m_d = 0$ at T_c :

- manifested \rightarrow 2nd order $O(4)$
- not \rightarrow 1st order
or 2nd order $U(2)_L \otimes U(2)_R / U(2)_V$

Pisarski, Wilczek PRD 29 (1984) 338; Butti et. al., JHEP 08 (2003) 029; F. Cuteri et. al., JHEP 11 (2021) 141

Axial anomaly at 1.6 T_c

Continuum & chiral extrapolation of U_A(1) measure



- Difference of integrated correlators

$$\chi_\pi - \chi_\delta = \int d^4x [\langle \pi(x)\pi(0) \rangle - \langle \delta(x)\delta(0) \rangle]$$

- Eigenvalue decomposition:

$$\chi_\pi - \chi_\delta = \int_0^\infty d\lambda \frac{8m_l^2 \rho}{(\lambda^2 + m_l^2)^2}$$

- ✓ Axial anomaly remains manifested at 1.6T_c
- ✓ 2nd order chiral phase transition belongs to 3d O(4) universality class

Novel method to probe the quark mass dependence of ρ

Eigenvalue spectrum for (2+1)-flavor QCD:

$$\rho(\lambda, m_l) = \frac{T}{V Z[U]} \int D[U] e^{-S_G[U]} \det[\not{D}[U] + m_s] \times (\det[\not{D}[U] + m_l])^2 \rho_U(\lambda)$$

Eigenvalue spectrum for a given configuration: $\rho_U(\lambda) = \sum_j \delta(\lambda - \lambda_j)$

Partition function: $Z[U] = \int D[U] e^{-S_G[U]} \det[\not{D}[U] + m_s] \times (\det[\not{D}[U] + m_l])^2$

$$\det[\not{D}[U] + m_l] = \prod_j (+i\lambda_j + m_l)(-i\lambda_j + m_l) = \exp\left(\int_0^\infty d\lambda \rho_U(\lambda) \text{In}[\lambda^2 + m_l^2]\right)$$

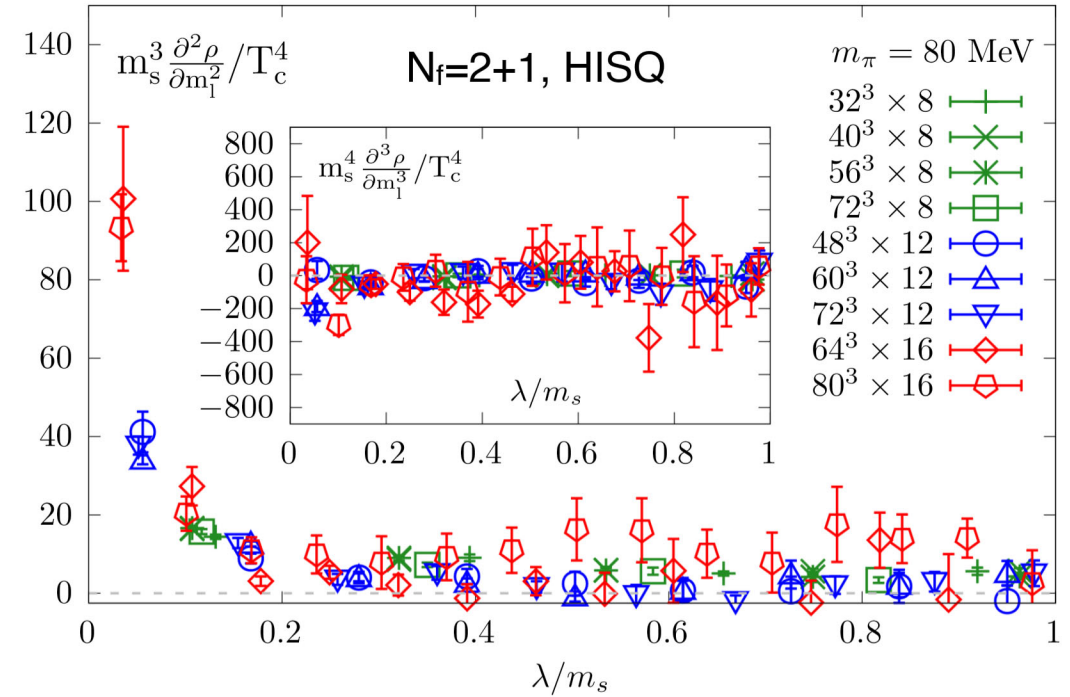
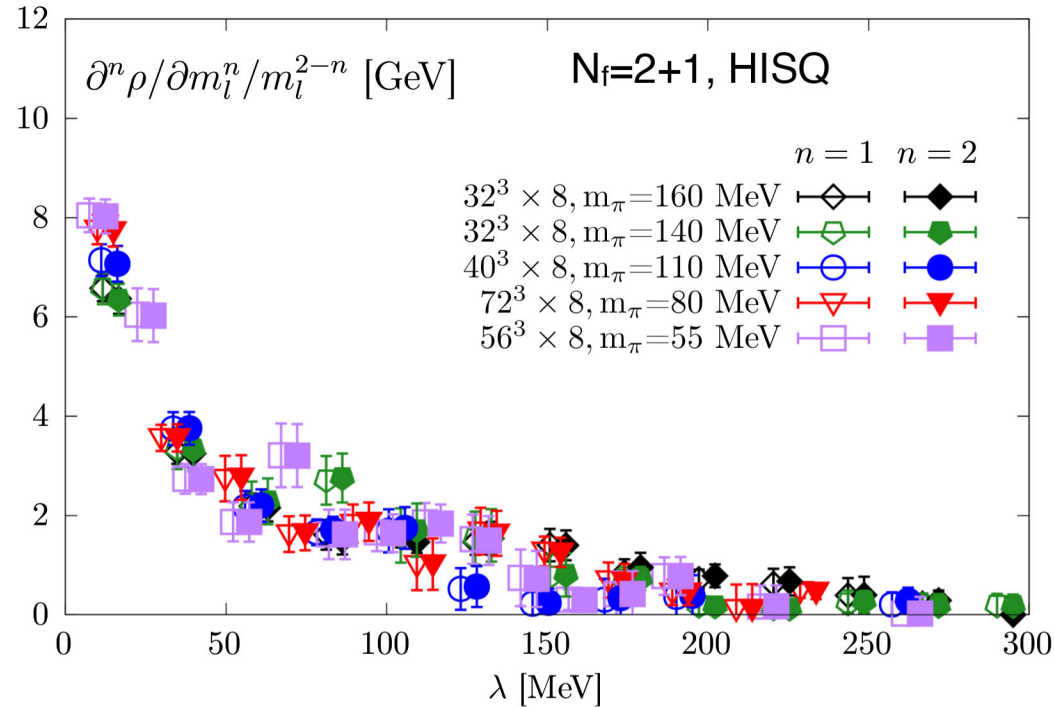


$$\frac{V}{T} \frac{\partial \rho}{\partial m_l} = \int_0^\infty d\lambda_2 \frac{4m_l C_2}{\lambda_2^2 + m_l^2}$$

$$C_2(\lambda, \lambda_2) = \langle \rho_U(\lambda) \rho_U(\lambda_2) \rangle - \langle \rho_U(\lambda) \rangle \langle \rho_U(\lambda_2) \rangle$$

Microscopic origin of the axial anomaly: weakly interacting instanton

$T = 1.6T_c = 205 \text{ MeV}$



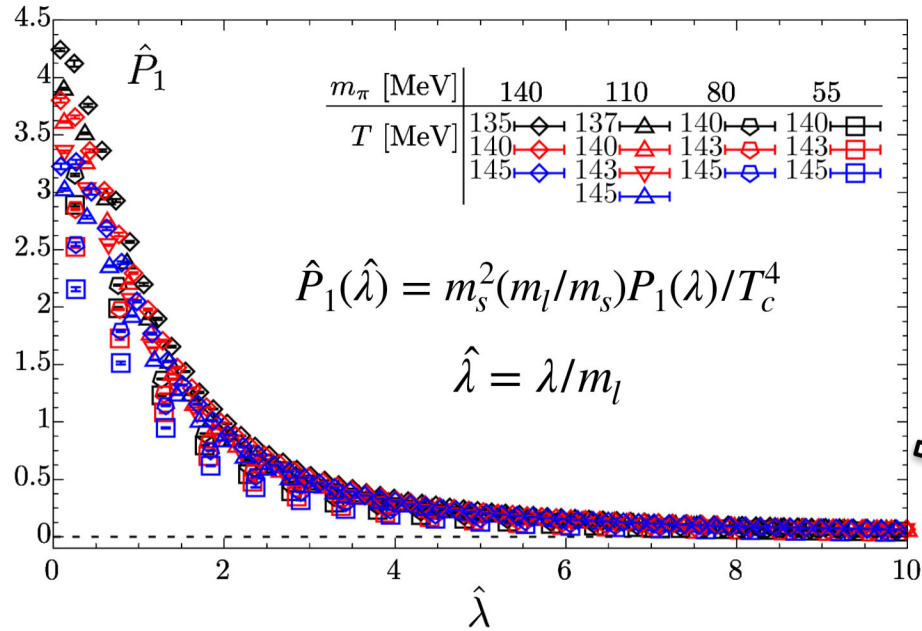
$$m_l^{-1} (\partial \rho / \partial m_l) \approx \partial^2 \rho / \partial m_l^2$$

$$\partial^3 \rho / \partial m_l^3 \approx 0$$

$$\rho(\lambda \rightarrow 0, m_l \rightarrow 0) \propto m_l^2 \delta(\lambda)$$

Consistent with the dilute instanton gas approximation

Microscopic encoding of Macroscopic criticality

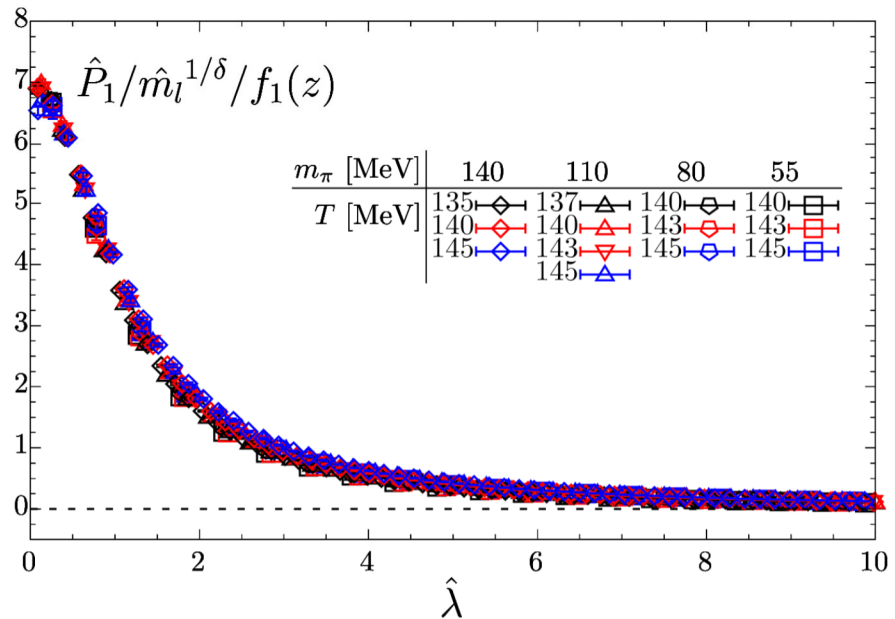


At small m_l and close to T_c

Universal $O(N)$ scaling functions

$$\frac{T}{V} \langle \bar{\psi} \psi(m_l) \rangle = \frac{T}{V} \int_0^\infty d\lambda \frac{4m_l \langle \rho_U(\lambda) \rangle}{\lambda^2 + m_l^2} = \int_0^\infty d\lambda P_1(\lambda) \sim m_l^{1/\delta} f_1(z)$$

Strong quark mass and temperature dependence



Universal Scaling behavior in eigenvalue spectrum around T_c

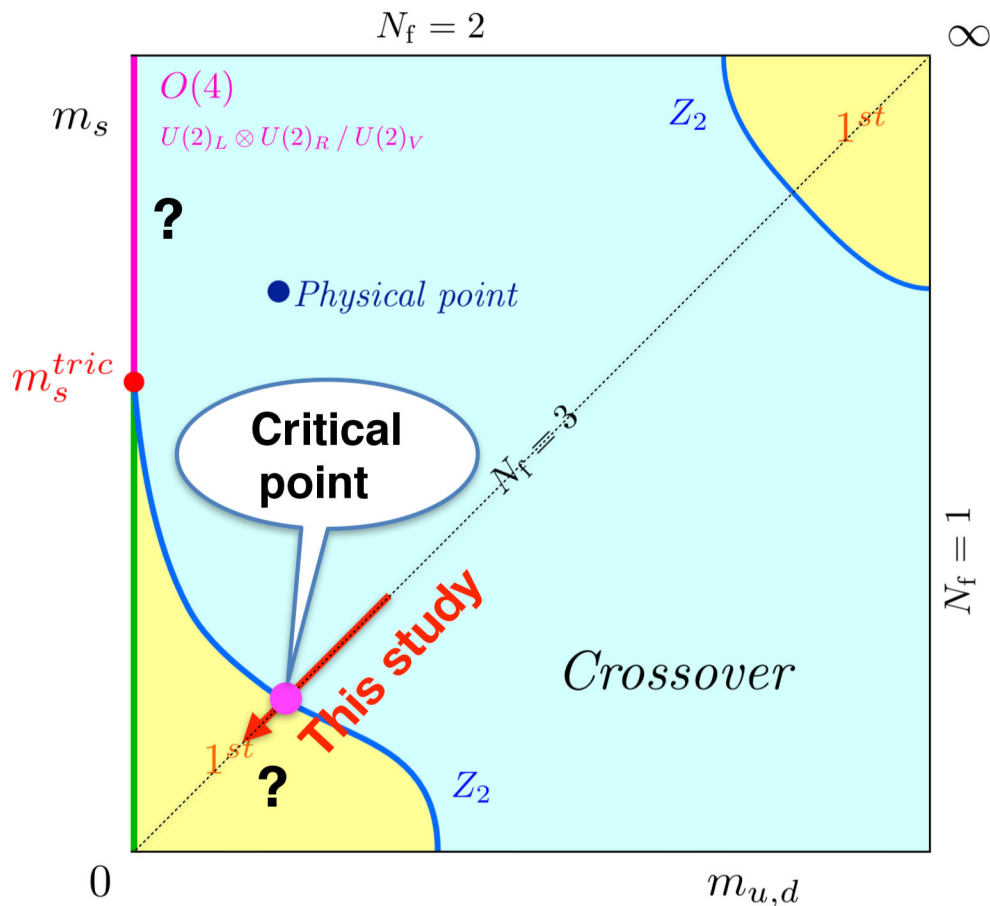
$3d$ $O(2)$ universality class for staggered fermion at $a \neq 0$

See talk by Wei-Ping Huang (黄玮平)

12/17, 3:00—3:20 PM

QCD phase structure in quark mass plane at $\mu_B = 0$

Columbia plot



Pisarski, Wilczek PRD 29 (1984) 338

Sigma model predication:

$$N_f = 3$$

Wilczek, Pisarski (1984)

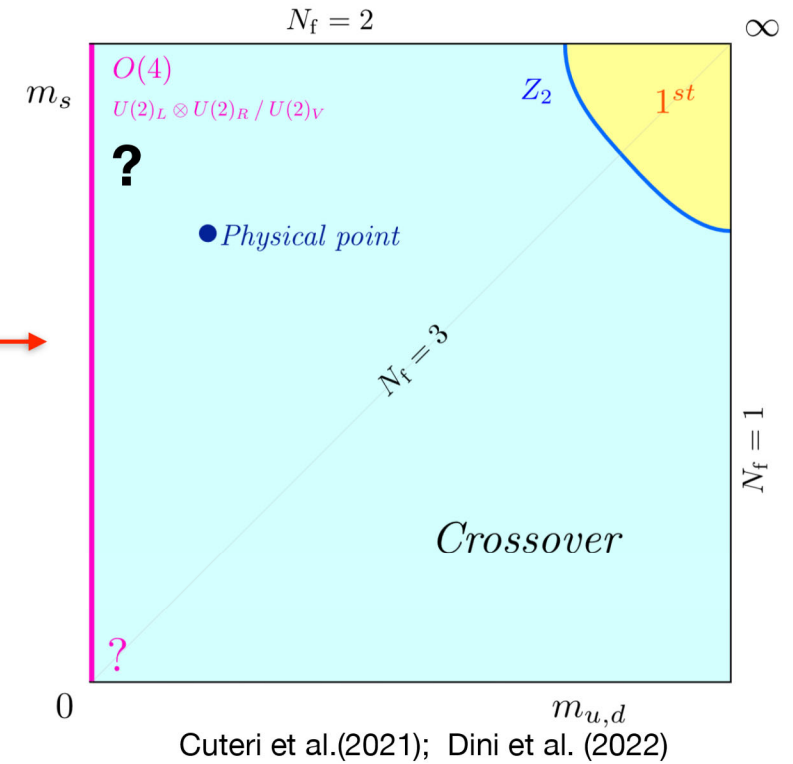
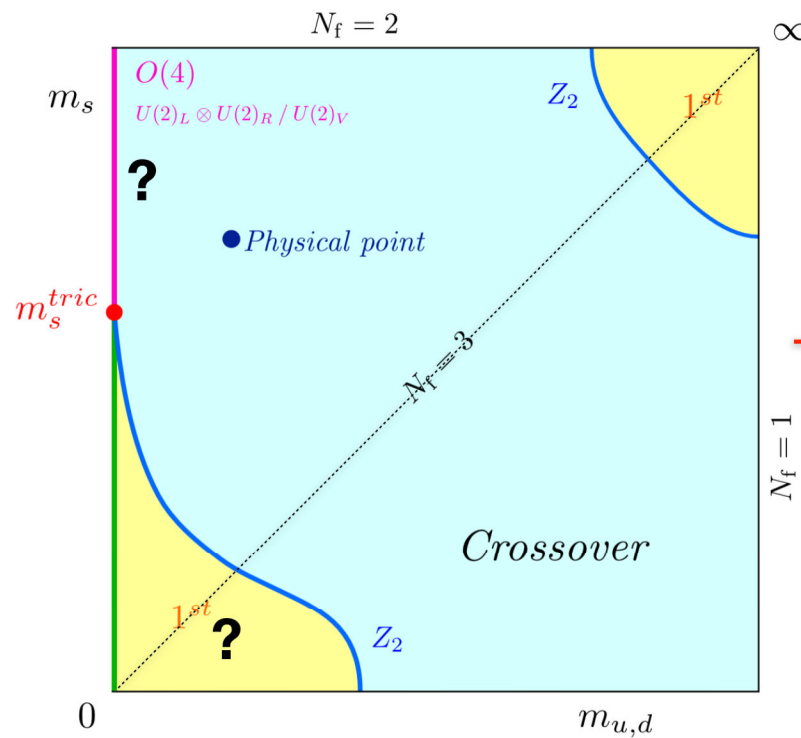
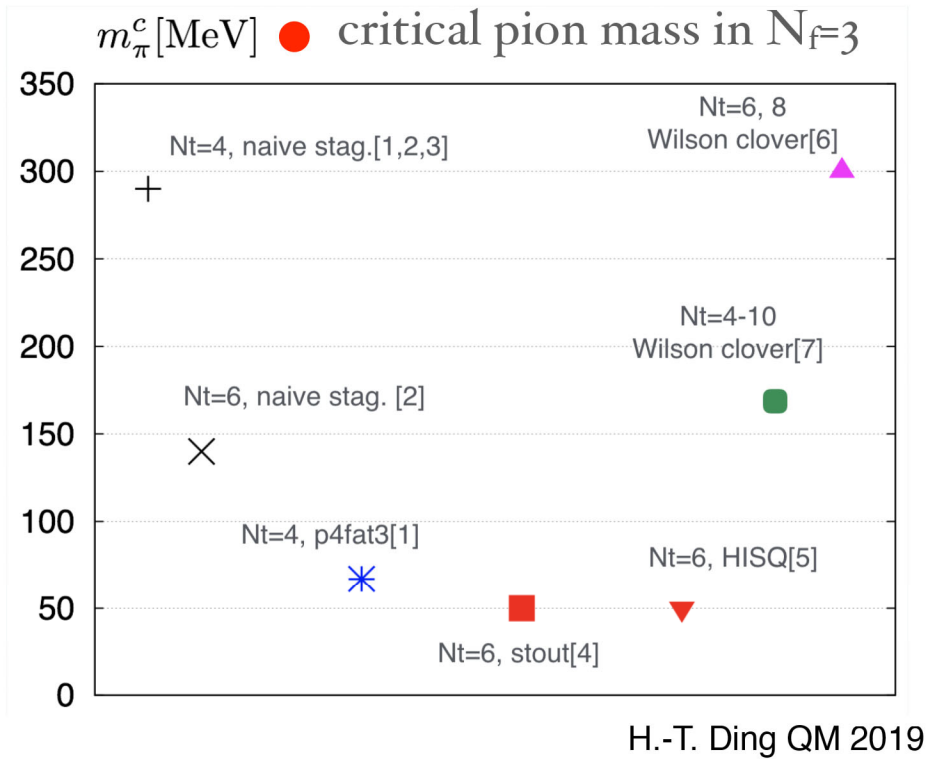
- 1st order PT in the chiral limit
- at critical end point: 2nd order PT with $Z(2)$ universality class

Need to be checked by lattice QCD

Critical point on the $N_f = 3$ chiral region:

- Location? (existence?)
- Universality class?

Previous $N_f = 3$ lattice studies



We propose to use chiral fermion (Mobius domain wall fermion)

- 1st order region shrinks as $a \rightarrow 0$ or even disappear?
with both staggered & Wilson fermions
- For fixed a : apparent contradictions between staggered and Wilson fermion actions

➡ Strong cutoff and discretization effects

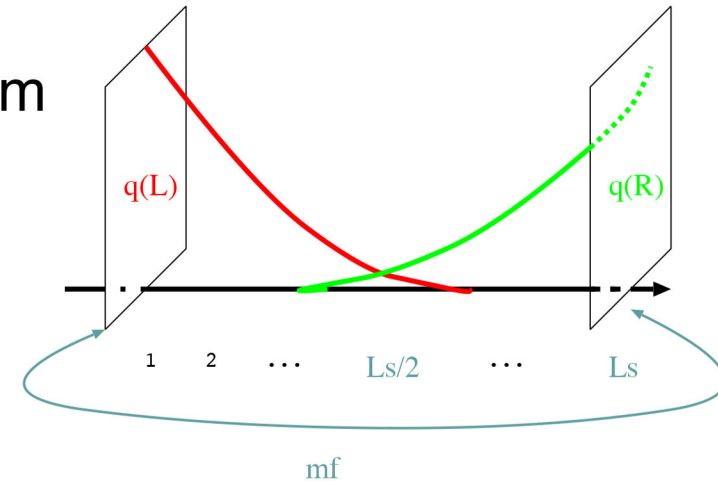
[1] F.Karsch et al. (2004) [2] P.de Forcrand et al. (2007) [3] D.smith et al. (2011) [4] Endrodi et al (2007) [5] Bazavov et al. (2017) [6] Nakamura et al. (2015) [7] Jin et al. (2017)

Domain wall fermion (Kaplan 92)

Define 4d quark fields on the wall, couple the two walls with a mass term

- Advantages of Domain Wall Fermions

- **Exact chiral and $U_A(1)$ symmetries** at finite a for infinite L_s
- For finite L_s , **reduced χ_{SB} parameterized by residual mass**, leading to additive renormalization of the mass: $m_q \rightarrow m_q + m_{\text{res}}$



- Drawback: Numerical cost is high

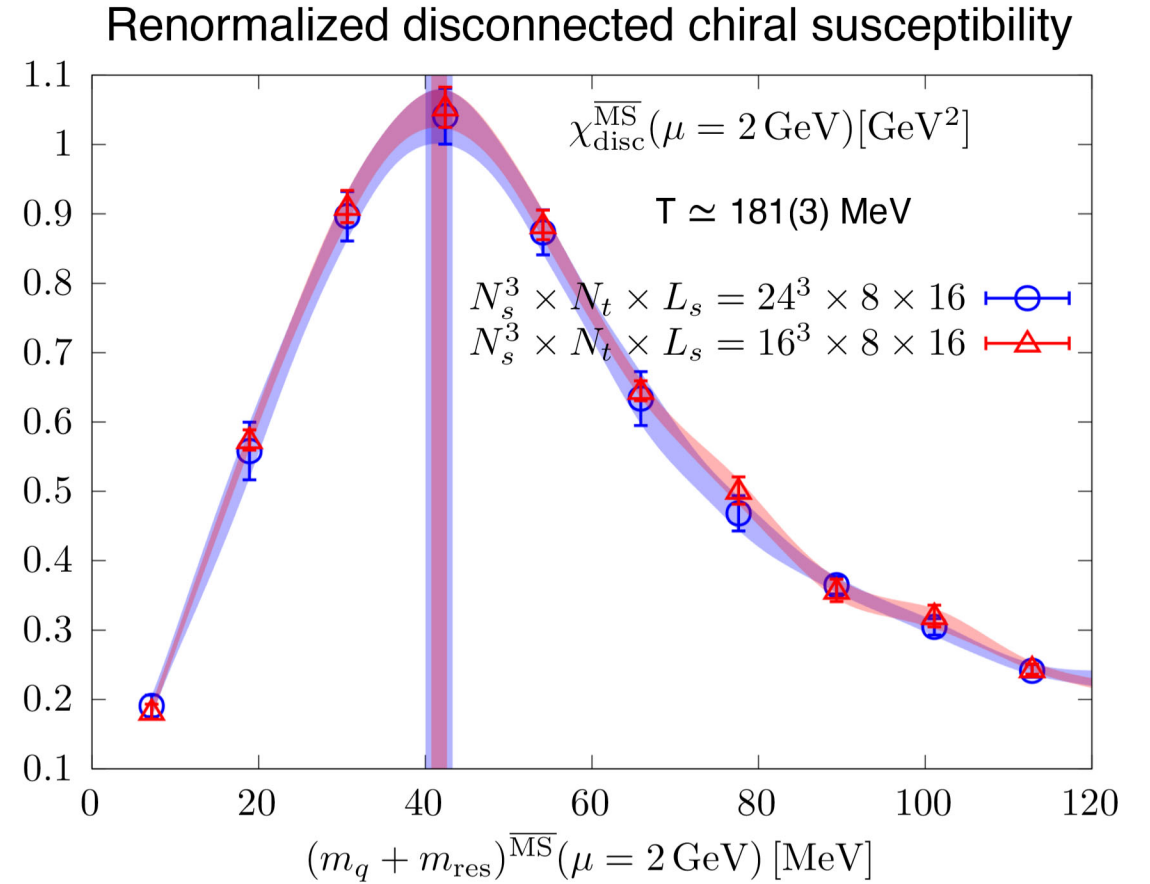
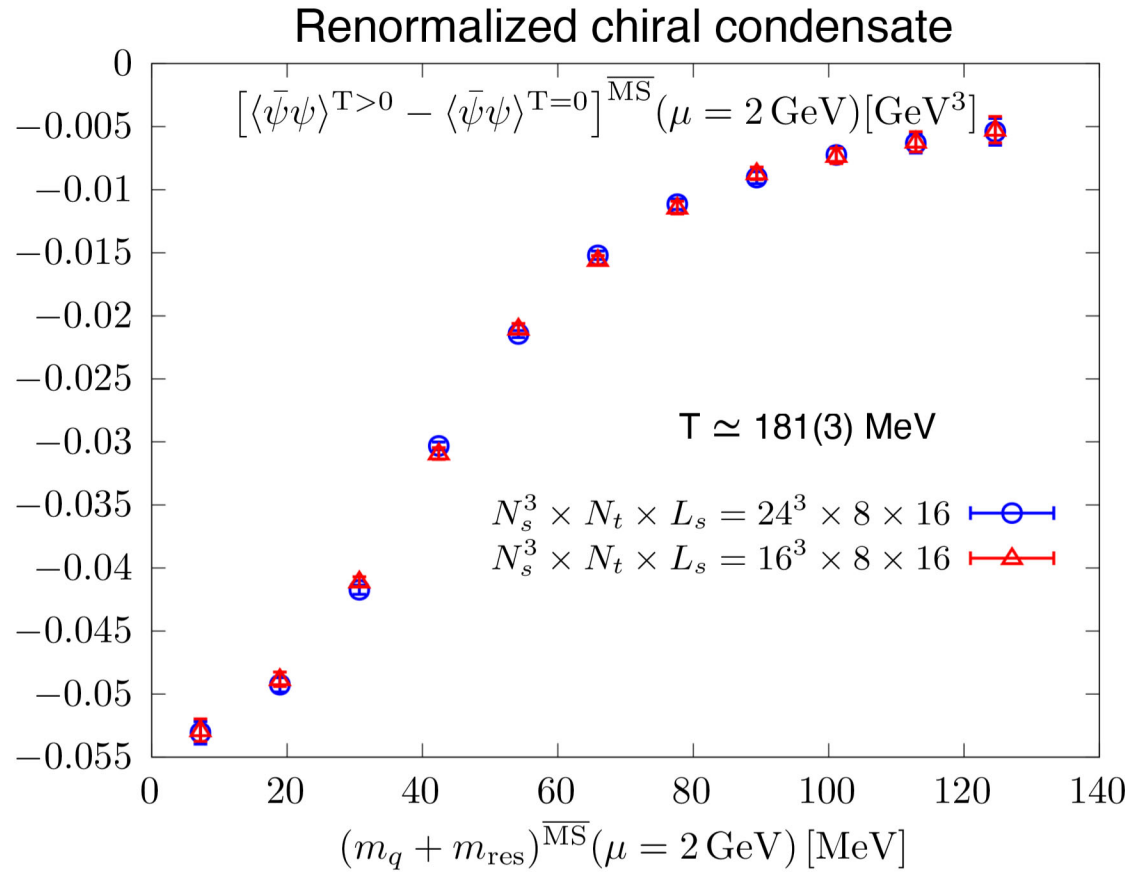
- Calculations not possible without state of the art HPC

- Algorithm: **Mobius**
- Machines: **Supercomputer Fugaku**



$N_f=3$ QCD phase structure with chiral fermions at $T \sim 181(3)$ MeV

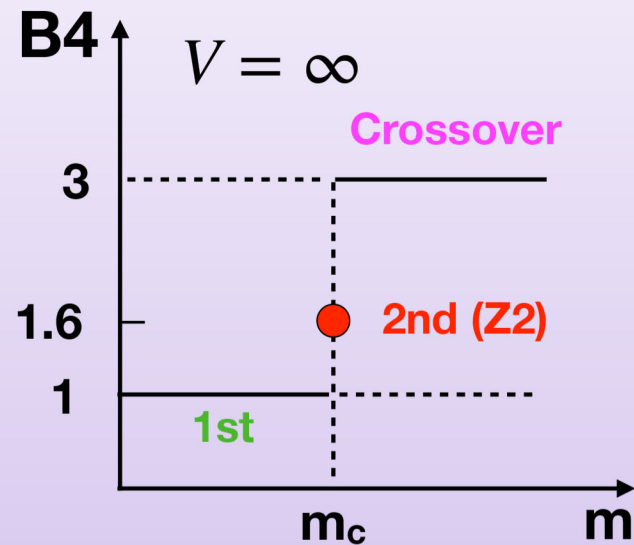
✓ Rapid transition near $m \simeq 41.7(1.6)$ MeV is a crossover for $T \simeq 181(3)$ MeV



Y. Zhang*, et al., PoS LATTICE2022 (2023) 197

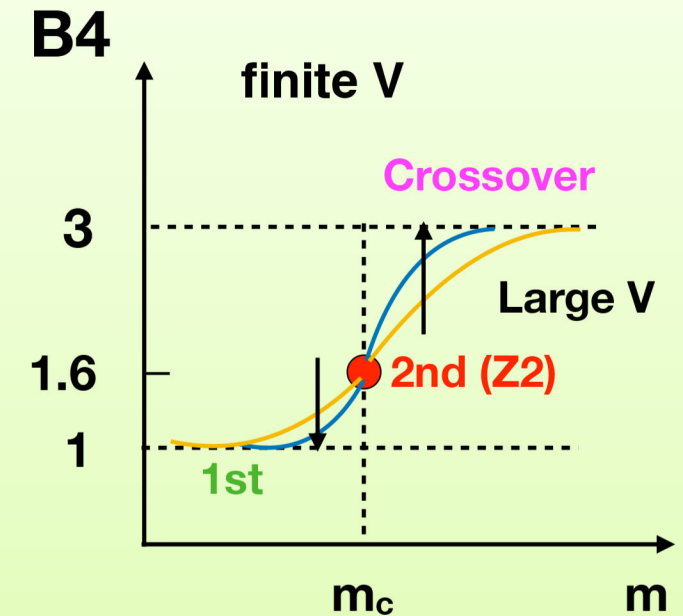
Methodology to determine the order of transition

Binder Cumulant: $B_4(\bar{\psi}\psi) = \frac{\langle(\delta\bar{\psi}\psi)^4\rangle}{\langle(\delta\bar{\psi}\psi)^2\rangle^2}$, $\delta\bar{\psi}\psi = \bar{\psi}\psi - \langle\bar{\psi}\psi\rangle$



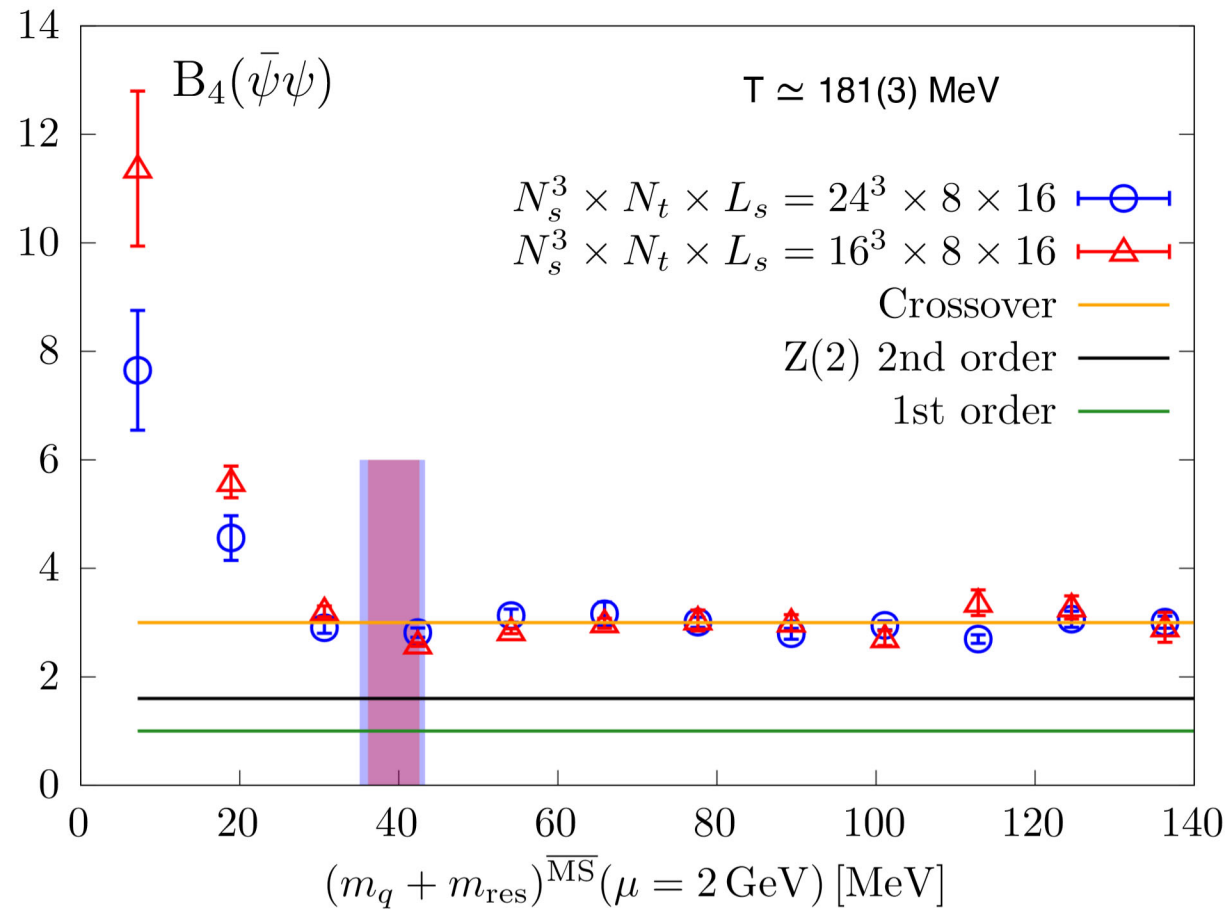
The distribution of $\bar{\psi}\psi$ approaches these functions in $V \rightarrow \infty$ on crossover and first order line at transition point

$$B_4 = \begin{cases} 3 & \text{Gauss distribution} \\ 1 & \text{two delta functions} \end{cases}$$



- Discontinuity of B_4 at critical end point is smeared on finite V
- B_4 has a crossing from different V at CEP

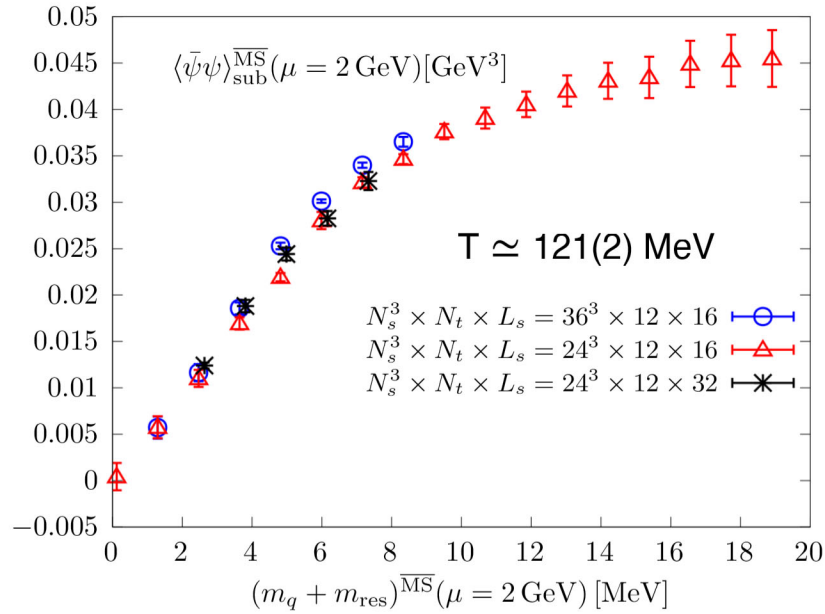
Binder cumulant at $T \sim 181(3)$ MeV



Y. Zhang*, et al., PoS LATTICE2022 (2023) 197

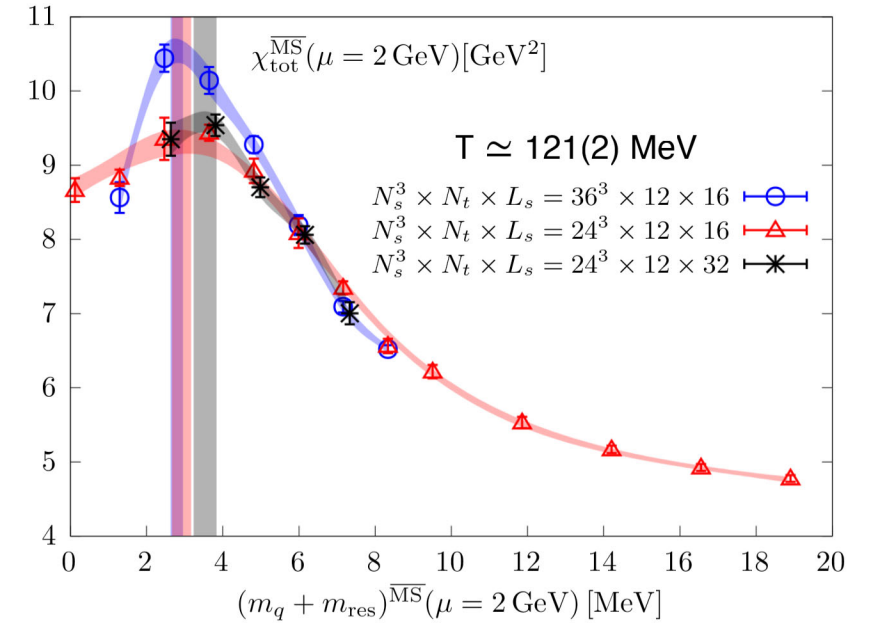
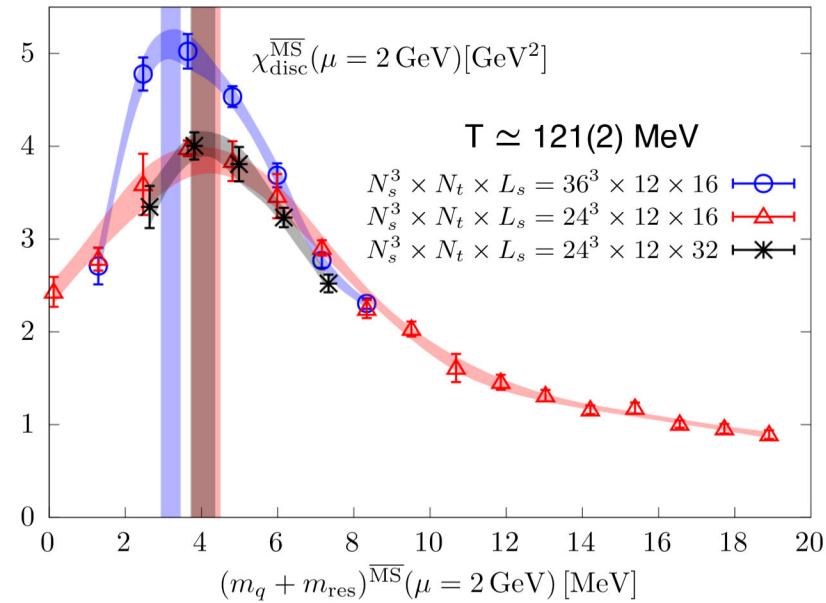
Binder cumulant indicate a crossover at transition mass range for $T \sim 181(3)$ MeV

$N_f=3$ QCD phase structure with chiral fermions at $T \sim 121(2)$ MeV



$$m_{\text{res}}^{\overline{\text{MS}}}(2 \text{ GeV}) \simeq 7.2(1) \text{ MeV for } L_s=16$$

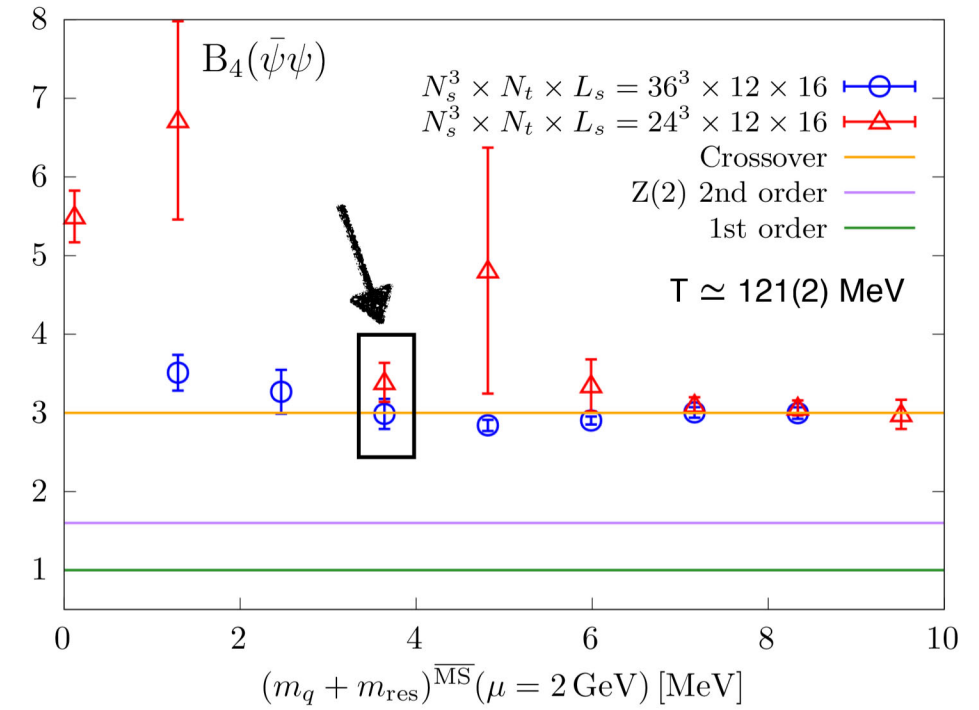
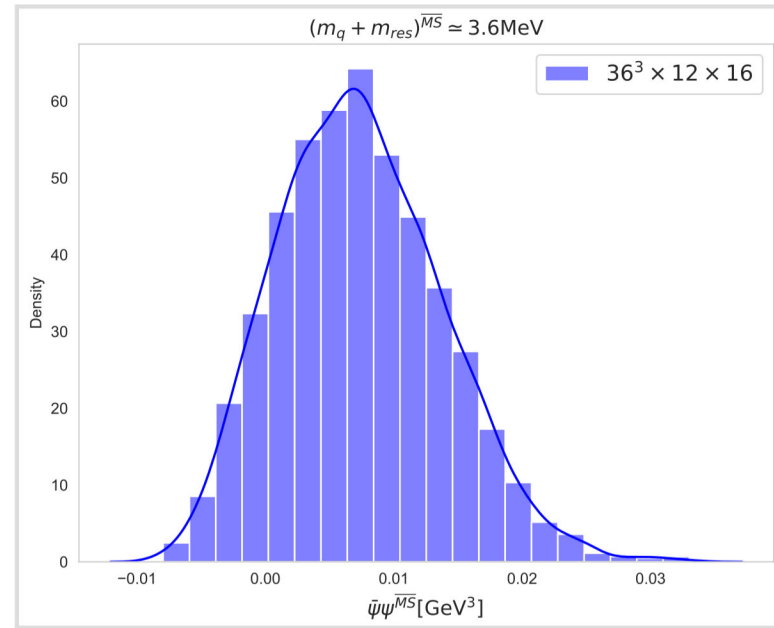
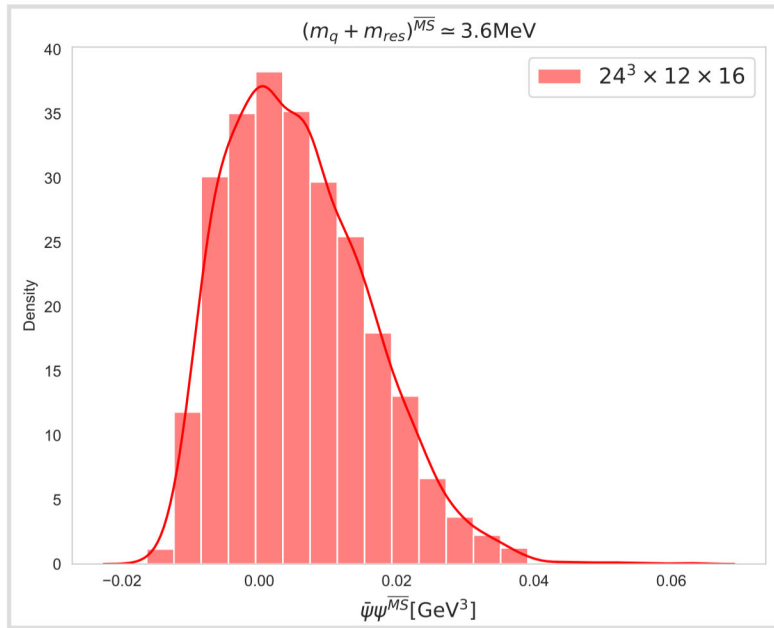
$$m_{\text{res}}^{\overline{\text{MS}}}(2 \text{ GeV}) \simeq 3.81(4) \text{ MeV for } L_s=32$$



- ☑ The change in peak height & position for χ_{disc} and χ_{tot} is not as large as anticipated from the true phase transition
 → **Consistent with the crossover rather than true phase transition**
- ☑ The transition mass point determined from χ_{disc} and χ_{tot} is around 3.6 MeV & 2.5 MeV, they coincide in the chiral T_c

The histogram of chiral condensate near transition point and B_4

Transition mass point is determined from the peak of chiral susceptibility

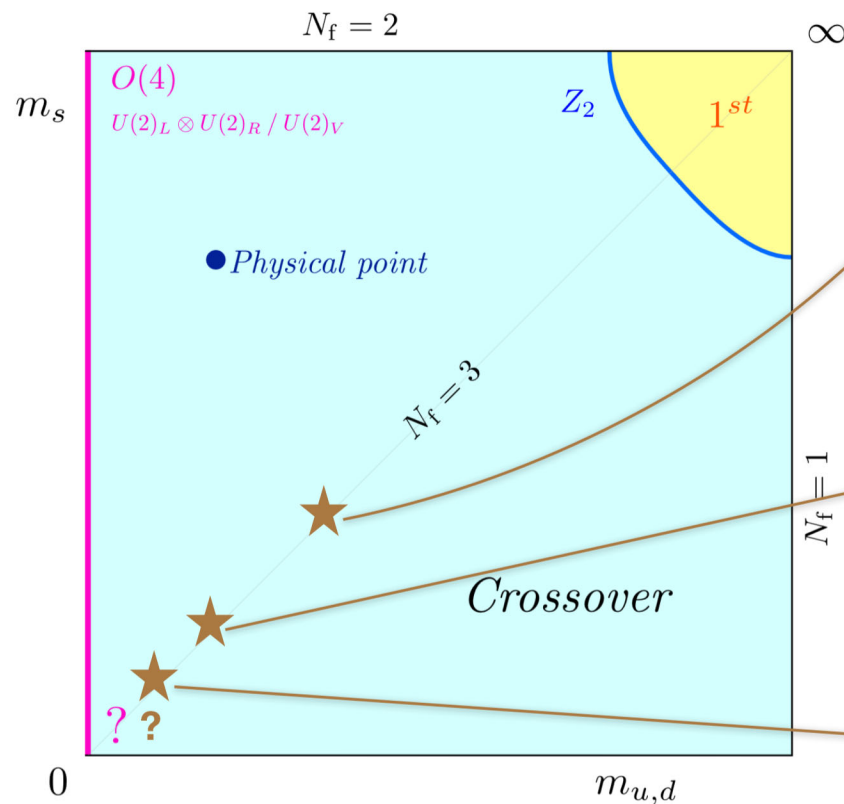


YZ*, et al., Manuscript in preparation

- ☑ Behaves like a Gaussian distribution, no evidence of a double peak structure would appear as $V \uparrow$
- ☑ B_4 suggests a crossover transition at $m \simeq 3.6 \text{ MeV}$ for $T \sim 121(2) \text{ MeV}$

Summary for $N_f=3$ study with chiral fermion(MDWF)

No evidence of a first order phase transition in our explored quark mass region
If a first order region exist, the critical mass should be less than 3.6 MeV



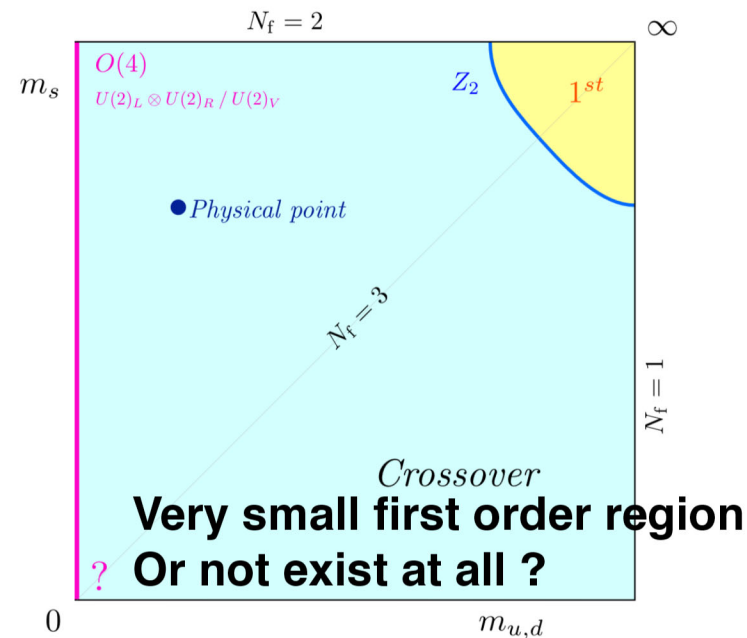
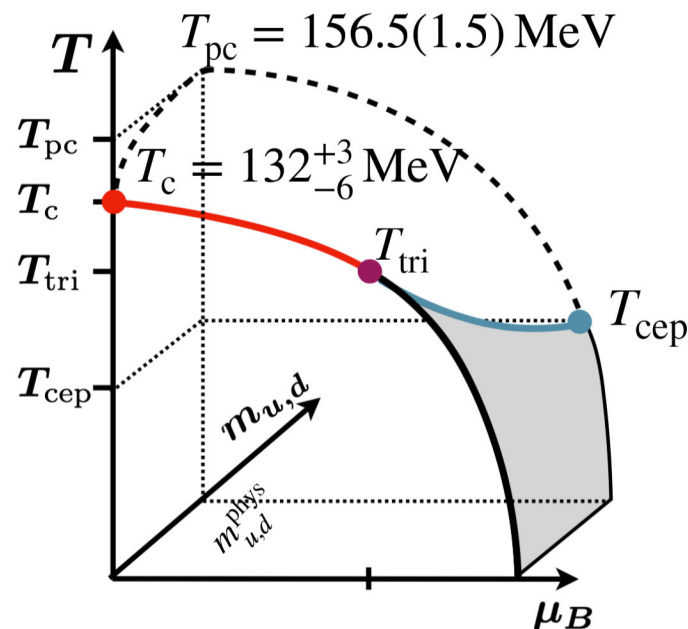
• $T \sim 181 \text{ MeV} (N_t = 8), (m_q + m_{\text{res}})_{pc}^{\overline{\text{MS}}} \sim 42 \text{ MeV}$
 $\Leftrightarrow m_{\pi}^{pc} \sim 476 \text{ MeV}$, crossover transition
 YZ*, et al., PoS LATTICE2022 (2023) 197

• $T \sim 121 \text{ MeV} (N_t = 12), (m_q + m_{\text{res}})_{pc}^{\overline{\text{MS}}} \sim 3.6 \text{ MeV}$
 $\Leftrightarrow m_{\pi}^{pc} \sim 141 \text{ MeV}$, crossover transition
 YZ*, et al., Manuscript in preparation

• $T \sim 104 \text{ MeV} (N_t = 14)$, lighter quark mass simulation is underway

Summary

- Axial anomaly remains manifested, the microscopic origin is driven by weakly interacting instantons
 - ⇓
- 2nd order O(4) chiral phase transition
 - ⇓
- $T_{\text{cep}} < T_c \simeq 132 \text{ MeV}$
- Microscopic encoding of Macroscopic Universality: Scaling properties of $\rho(\lambda, m)$ near T_c
- No evidence of a 1st order transition in $N_f = 3$ chiral region for $m_q > m_{u,d}^{\text{phys}}$



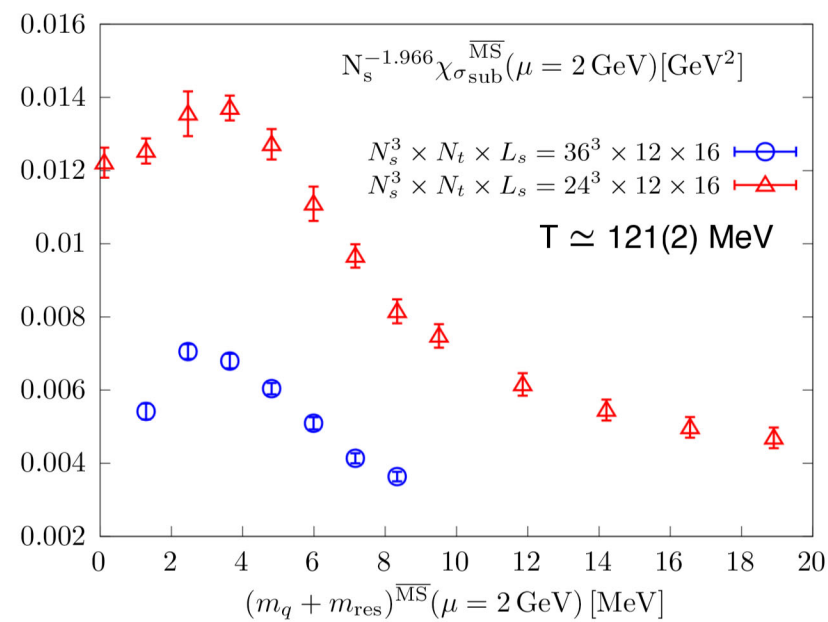
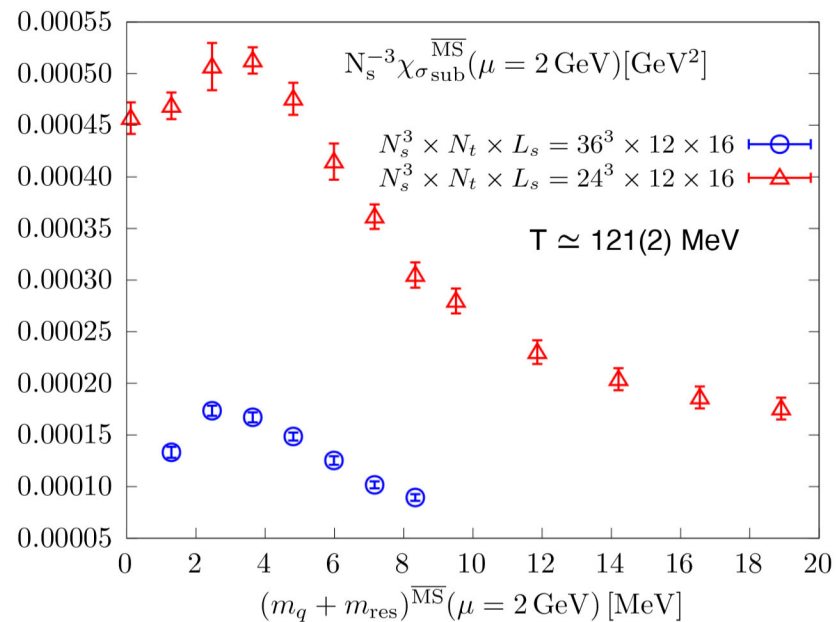
Backup slide

Finite size scaling: susceptibility at $T \sim 121(2)$ MeV

Chiral susceptibility is the order parameter distinguishing the phases: $\chi_\sigma(N_s, N_t) = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial m_q^2} = \frac{\partial \langle \bar{\psi} \psi \rangle}{\partial m_q}$

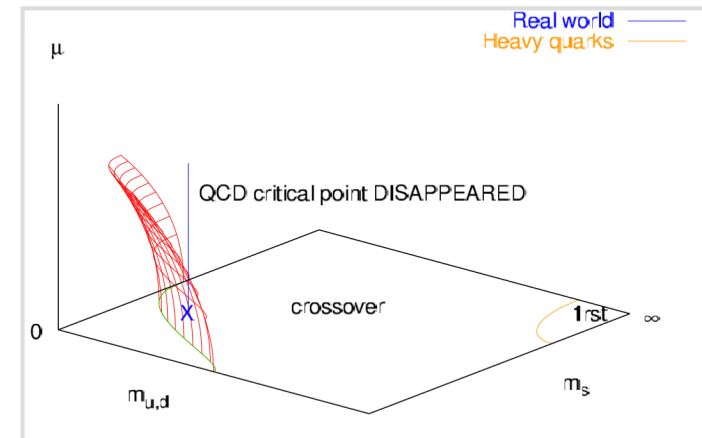
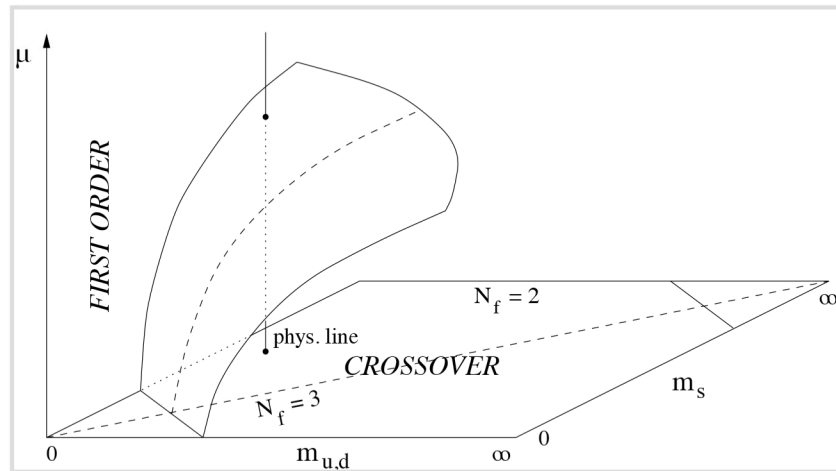
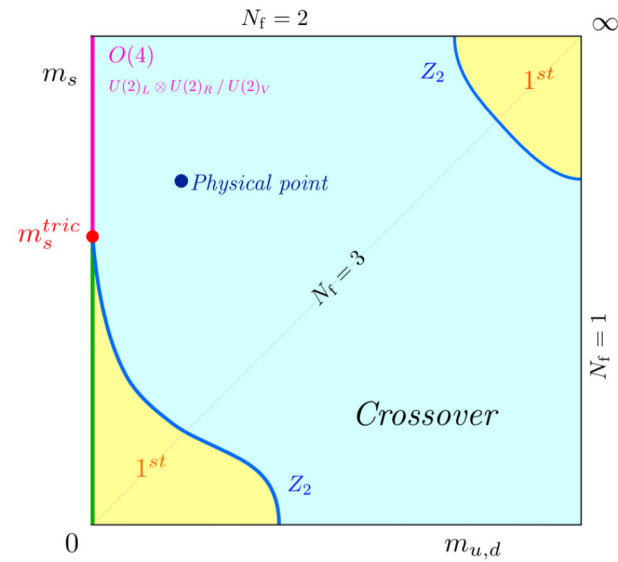
$\left\{ \begin{array}{l} \text{Crossover:} \\ \text{1st order PT:} \\ \text{Z(2) 2nd order PT:} \end{array} \right. \quad \begin{array}{l} \chi_\sigma^{\max}(N_s, N_t) \text{ independent of } V \\ \chi_\sigma^{\max}(N_s, N_t) \propto V \\ \text{a singular behavior should be observed in } \chi_\sigma^{\max}(N_s, N_t) \text{ with } V \\ ((N_s^3 \times N_t)^\alpha, \alpha = 1.966 \text{ is the critical exponent}) \end{array}$

finite-size scaled renormalized chiral susceptibility



☑ The peak height of chiral susceptibility does not scale like a first order or Z(2) second order phase transition

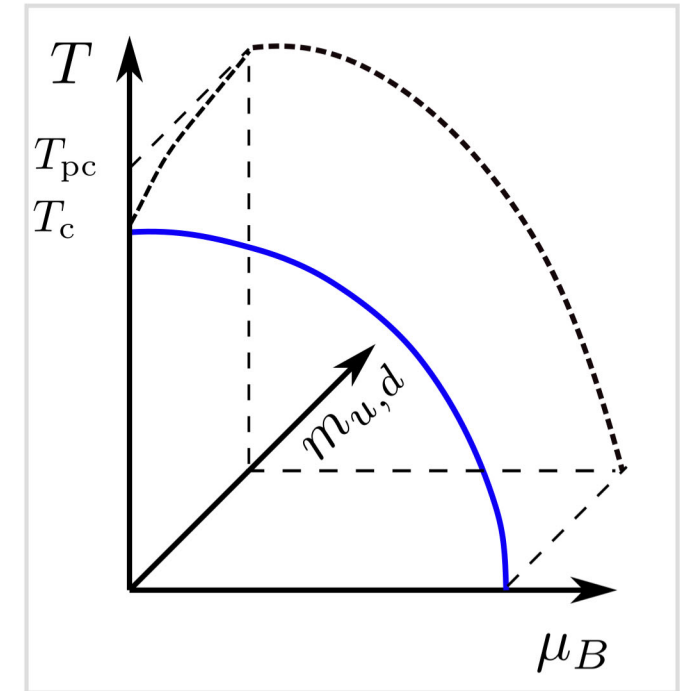
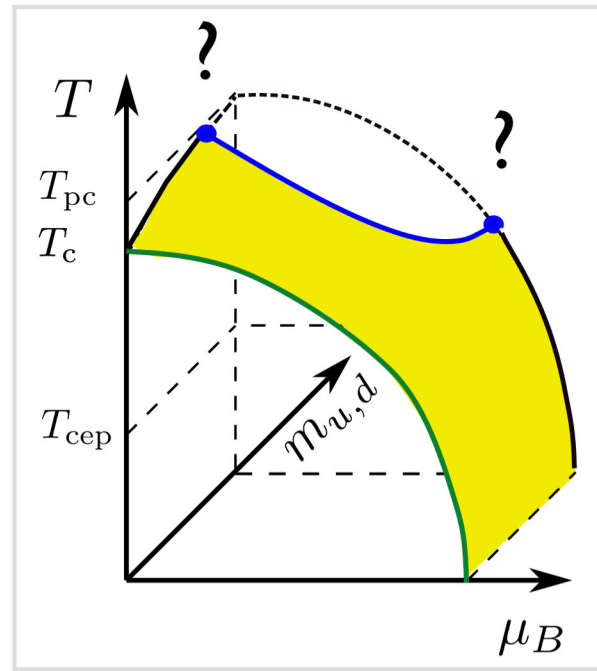
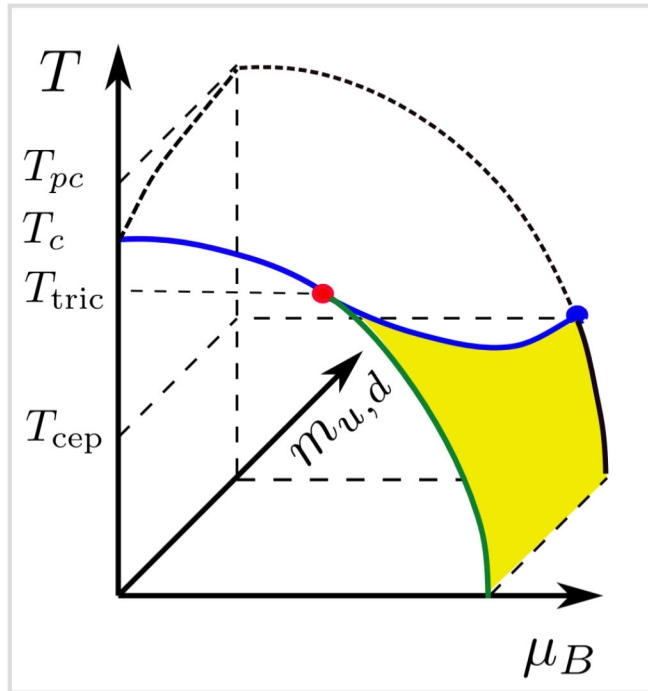
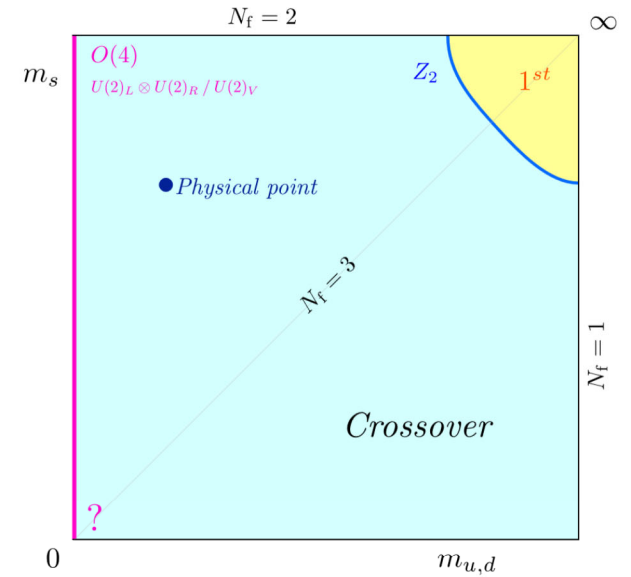
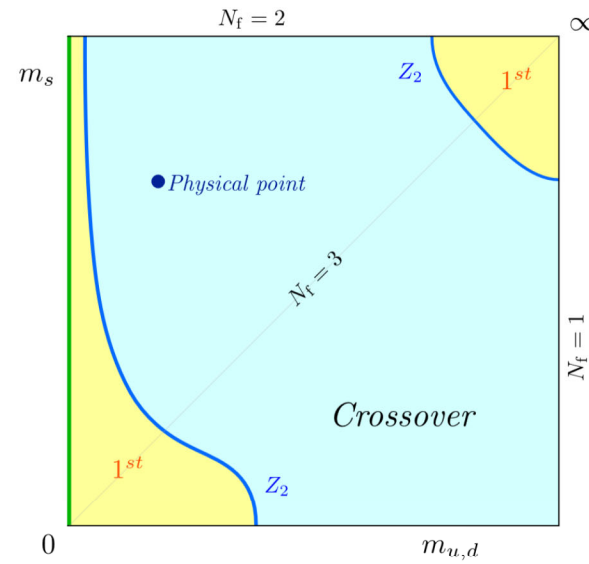
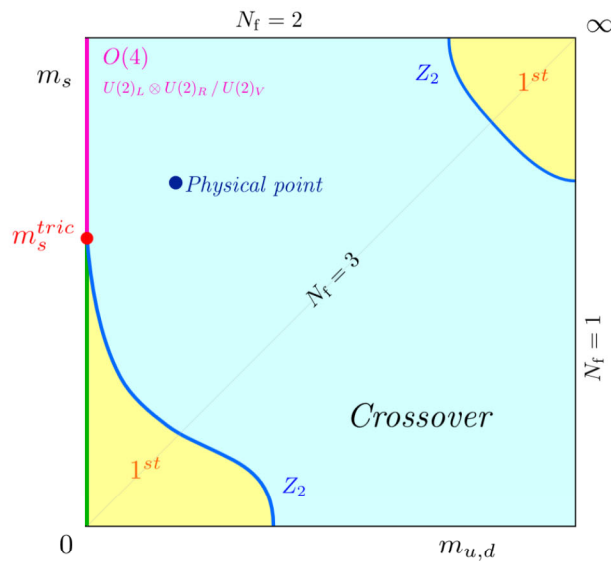
Possible QCD phase diagram at physical point



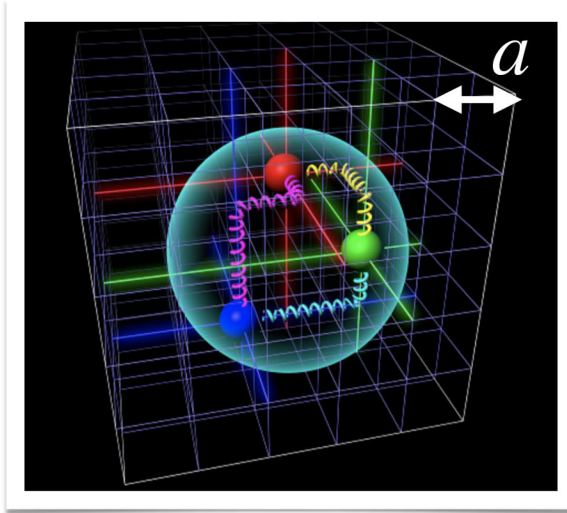
F. Karsch et al., '03, X.-Y. Jin et al., '15, H.-T. Ding talk@FuDan '17

de Forcrand & Philipsen, '07

Possible QCD phase diagram at physical point



Lattice QCD (K. G. Wilson 1974)



- Euclidean space-time: $N_\sigma^3 \times N_\tau$
- quark field $\psi(x), \bar{\psi}(x)$ on lattice sites
- gluon field $U_\mu(x)$ on lattice links
- Temperature $T = 1/(N_\tau a)$

Different fermion actions should give the same physical results in the continuum limit $a \rightarrow 0$

$$\mathcal{L}_E = \frac{1}{4} F_a^{\mu\nu} F_{\mu\nu}^a + \bar{\psi}(\gamma^\mu D_\mu^E + m)\psi$$

$$Z = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{latt}} = \int \mathcal{D}U e^{-S_g} \det M_f$$

Evaluate path integrals by Monte Carlo with dimensions $> 10^7$

Naive discretization \rightarrow **Fermion doubling problem**

No-go theorem: doublers appear unless chiral symmetry is broken

• Staggered fermion

- 16 doublers = 4 spinors x 4 flavors (“taste”), keep 1 spinor component
- taste-breaking effect $O(a^2)$, various improved action to reduce it (HISQ....)
- Numerical cost is low

• Wilson fermion

- No doublers but chiral symmetry is broken explicitly
- Numerical cost is moderate

• Domain wall fermion

- No doublers, 5 dim. formulation, chiral symmetry breaking exponentially suppressed: $m_{res} \rightarrow 0$ as $L_s \rightarrow \infty$ (small $O(a^2)$ discretization effect)
- Numerical cost is high: $\propto L_s$ for DWF

And

Domain wall fermions

Substantial cost reductions

Mobius formulation:

- . generalize Shamir formulation with overall scaling factor
- . improve sign function approximation
- . achieve target m_{res} at further reduced L_s