Extended QCD phase diagram from the lattice

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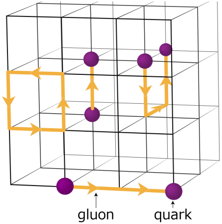
[10.1103/PhysRevD.93.054507, 10.1103/PhysRevD.93.114507]

Monte Carlo methods & cutoff effects

$$\mathcal{Z} = \int \mathcal{D}U \prod_{N_f} \det D(\mu_f, m_f; U) e^{-S_G(\beta;U)}, \qquad \beta = \frac{2N_c}{g^2}$$



http://www.jicfus.jp

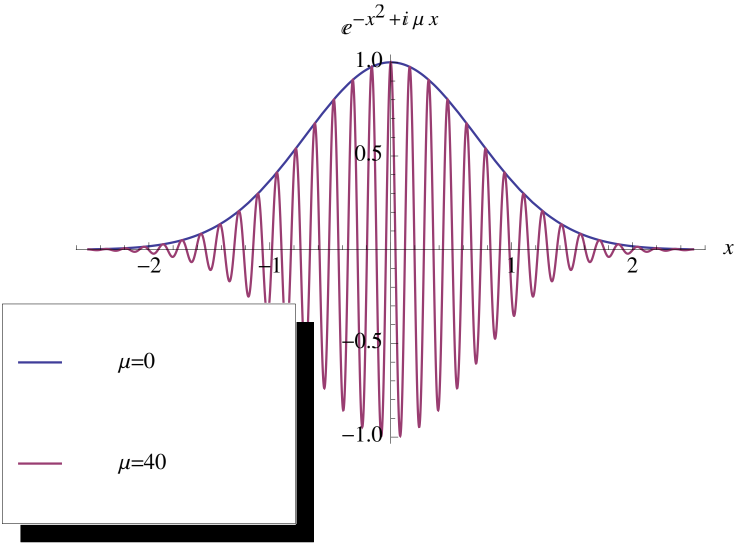
- Importance sampling $\leftrightarrow$ positive Boltzmann weight
- Sign problem for real $\mu \neq 0 \leftrightarrow \det D \in \mathbb{C}$
- Thermodynamical studies with $T = \frac{1}{a(\beta) N_\tau}$
- Thermodynamic and continuum limit at fixed T by $N_\tau, N_\sigma \to \infty$, $a \to 0$

$$S_{lat} = S_{cont} + c_1 a + c_2 a^2 + \dots$$

Non-unique discretization: different lattice actions $\leftrightarrow$ different cutoff effects

- Wilson: LO $\mathcal{O}(a)$
  - local, doublers-free, correct CL
  - no chiral symmetry
- Staggered: LO $\mathcal{O}(a^2)$
  - theoretically not fully understood (rooting)
  - remnants of chiral symmetry

The sign problem in lattice QCD

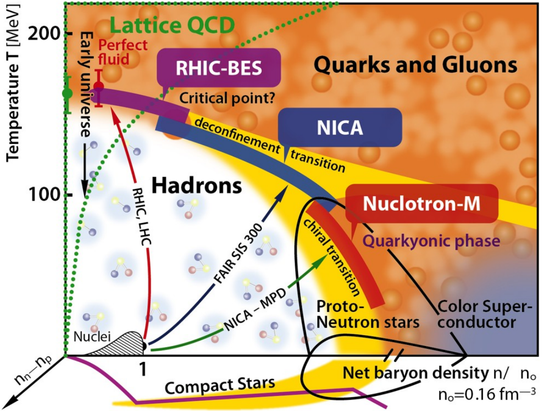


Outline

1. QCD phase diagram at real and imaginary μ
2. Extended QCD Columbia plot $(\mu^2 \neq 0)$
3. The order of the thermal phase transition
4. Extrapolation from imaginary chemical potential
   - Nature of the Roberge-Weiss endpoint at $N_f = 2$
   - Z_2 line in $m_\pi - \left(\frac{\mu}{T}\right)^2$ at $N_f = 2$
5. Extrapolation from non-integer N_f at $\mu = 0$
   - Z_2 line in $m_{Z_2} - (N_f)$
6. Outlook

Outline

The QCD phase diagram at real μ

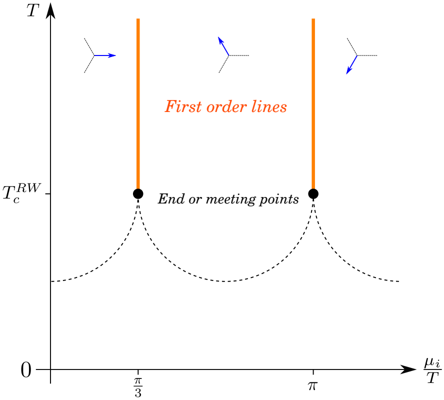


http://nica.jinr.ru/

- PQCD
- Models $\frac{T}{\mu} \ll 1$
- Lattice QCD $\frac{T}{\mu} \gg 1$
- heavy-ion collisions
  - RHIC-BES
  - NICA
  - Nuclotron-M
  - LHC
  - FAIR

- Location and order of thermal phase transitions as a function of μ?
- Existence of a critical endpoint (CEP) at $\mu \neq 0$?

The QCD phase diagram at $\mu = i\mu_i$ the Roberge-Weiss symmetry



Roberge and Weiss (1986),
10.1016/0550-3213(86)90582-1

$$\mathcal{Z}(\mu) = \mathcal{Z}(-\mu)$$

$$\mathcal{Z}\left(\frac{\mu}{T}\right) = \mathcal{Z}\left(\frac{\mu}{T} + i\frac{2\pi N}{N_c}\right)$$

$$\mu_i^c = (2k+1)\frac{\pi T}{N_c}, k \in \mathbb{Z}$$

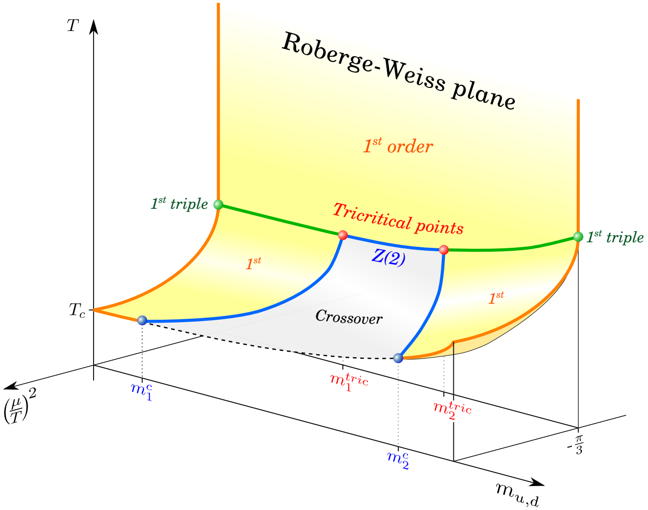
$$|L(\mathbf{n})|e^{-i\varphi} = \frac{1}{3}\mathrm{Tr}_C\left[\prod_{n_0=0}^{N_\tau-1} U_0(n_0, \mathbf{n})\right]$$

$$\langle\varphi\rangle = \frac{2n\pi}{3} \text{ with } n \in \{0,1,2\}$$

$$0 < \mu_i < \frac{\pi}{3}$$

- RW endpoint: true phase transition
- Meeting of RW and chiral/deconfinement phase transitions continued to μ
- Rich phase structure depending on N_f and m_q

$T - \left(\frac{\mu}{T}\right)^2 - m_{u,d}$ PHASE DIAGRAM



- Coarse lattices
- All β critical at μ_i^c
- 1^{st} order regions extend till $\mu = 0$
  - $m_{u,d} \to 0$
  - $m_{u,d} \to \infty$
- 2^{nd} order critical masses m_1^c, m_2^c at $\mu = 0$

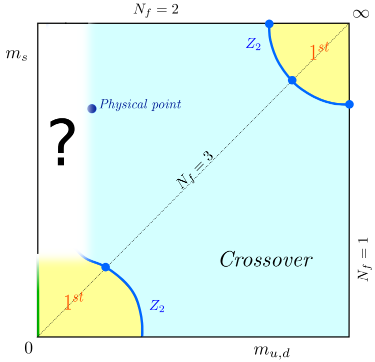
de Forcrand and Philipsen (2002), 10.1016/S0550-3213(02)00626-0,
D'Elia, Lombardo (2003), 10.1103/PhysRevD.67.014505

Outline

2D Columbia plot $m_s - m_{u,d}$ at $\mu = 0$

Dependence of the order of the thermal phase transition on m_q

- Breaking of global $Z(3)$ for $m_{u,d}, m_s \to \infty$
- Restoration of global $SU_L(N_f) \times SU_R(N_f)$ for $m_{u,d}, m_s \to 0$



Current knowledge (no CL)

Order parameters

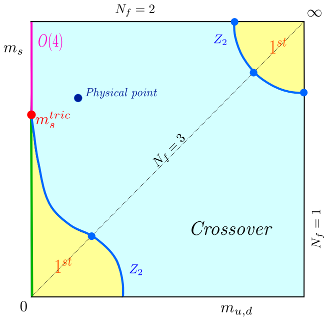
- Polyakov loop for $m_{u,d}, m_s \to \infty$
  $$P = \mathrm{Tr}\, e^{i \int A_t dt}$$
- Chiral condensate for $m_{u,d}, m_s \to 0$
  $$\bar{\psi}\psi = \partial \log \mathcal{Z} / \partial m_{u,d}$$

Svetitsky, Yaffe (1982), 10.1016/0550-3213(82)90172-9
Pisarski, Wilczek (1984), 10.1103/PhysRevD.29.338
Aoki et al. (2006), 10.1038/nature05120
de Forcrand and Philipsen (2007), 10.1088/1126-6708/2007/01/077

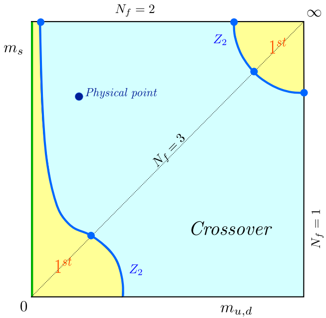
2D Columbia plot $m_s - m_{u,d}$ at $\mu = 0$

At least two possible scenarios on the nature of $N_f = 2$ chiral transition

Second order scenario



First order scenario

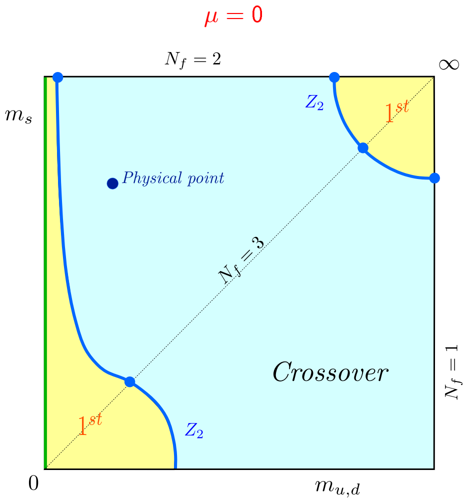


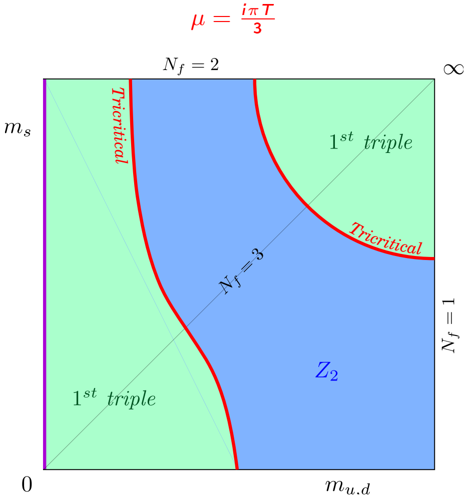
- Direct (expensive) approach: $\mu = 0$ and $m_{u,d} \to 0$
- Indirect (cheaper) approach: $\mu = i\mu_i$, bigger $m_{u,d}$ and scaling laws

Svetitsky, Yaffe (1982), 10.1016/0550-3213(82)90172-9
Pisarski, Wilczek (1984), 10.1103/PhysRevD.29.338
Aoki et al. (2006), 10.1038/nature05120
de Forcrand and Philipsen (2007), 10.1088/1126-6708/2007/01/077

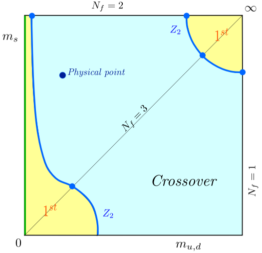
2D Columbia plot $m_s - m_{u,d}$ at $\mu = \frac{i\pi T}{3}$

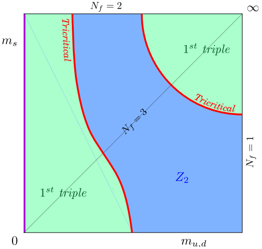
Assuming the "first order scenario" is realized

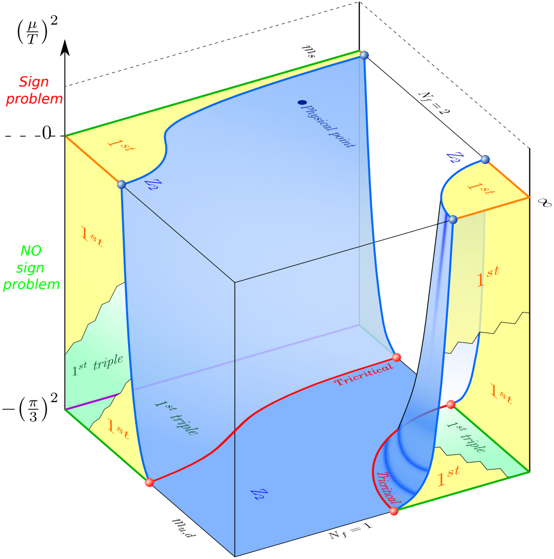




3D Columbia plot $\left(\frac{\mu}{T}\right)^2 - m_s - m_{u,d}$

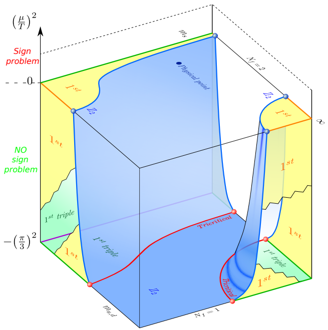






courtesy of A. Sciarra arXiv:1610.09979

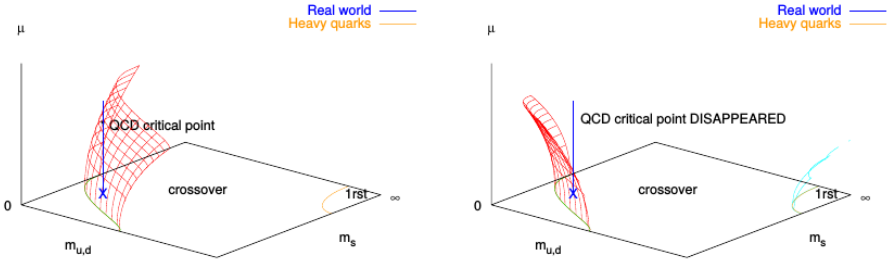
$\left(\frac{\mu}{T}\right)^2 - m_{u,d}$ Columbia plot



courtesy of A. Sciarra arXiv:1610.09979

- From m_1^{tric} in RW plane $\mu = i\mu_i = \frac{i\pi T}{3}$
- Send $\mu_i \to 0$ mapping $\mu_i^{Z_2}(m_{u,d})$ ($3D$ Ising)
- Expected tricritical scaling $m_{u,d}^{2/5} = C\left[\left(\frac{\mu}{T}\right)^2 - \left(\frac{\mu}{T}\right)^2_{tric}\right]$

Towards real-μ Columbia plot



- Analytical continuation on constraint that no non-analyticity is met
- Existence of 2^{nd} order CEP depending on the bending of the Z_2 surfaces continued from μ_i

Outline

Establishing the order of the transition

- Analysis of the order parameter $\langle \mathcal{O} \rangle$ distribution and its moments

$$B_n(\langle \mathcal{O} \rangle, \beta, m_q, \mu, V) \equiv B_n(\beta, m_q, \mu, N_\sigma) = \frac{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^n \rangle}{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle^{n/2}}$$

$$\mathcal{O} = L_{\text{Im}},\ \bar{\psi}\psi$$

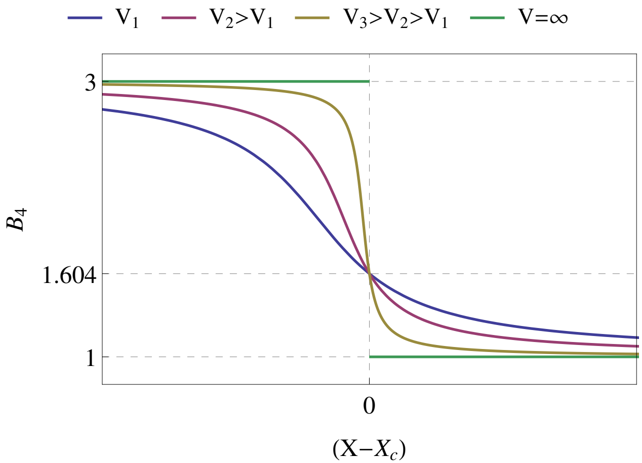
- $\forall m_q$ identify β_c by $\begin{cases} \text{the condition } B_3(\beta, m_q, \mu, N_\sigma) = 0\ \forall N_\sigma; \\ \text{the crossing of } B_4(\beta, m_q, \mu, N_\sigma) \text{ for different } N_\sigma. \end{cases}$

- $B_4(\beta_{(c)}, m_q, \mu, N_\sigma)$ gives the order of the transition as function of β, m_q or μ

$$B_4(\beta_{(c)}, m_q, \mu, N_\sigma) = \left. \frac{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^4 \rangle}{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle^2} \right|_{\beta_c} \underset{V \to \infty}{\sim} \begin{cases} 1, & 1^{st} \text{order;} \\ 1.604, & 2^{nd} \text{order} Z_2; \\ 3, & \text{crossover.} \end{cases}$$

Finite Size Scaling (FSS) analysis

Critical exponent ν by either fit or quantitative collapse



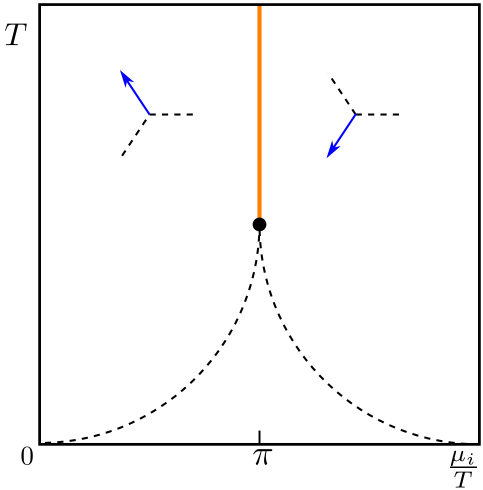
$$B_4(X, N_\sigma) = B_4(X_c, \infty) + a_1\, x + a_2\, x^2 + \mathcal{O}(x^3)$$

$$x \equiv (X - X_c) N_\sigma^{1/\nu}, \qquad X = \beta,\ m,\ \frac{\mu_i}{T}$$

Outline

Roberge-Weiss transition in $N_f = 2$ QCD

(Unimproved) Wilson fermions on $N_\tau = 4, 6$ [10.1103/PhysRevD.93.054507]



$$\frac{\mu_i}{T} = \pi \pm 2\pi k, \; k \in \mathbb{Z}$$

$$T = \frac{1}{a(\beta)\, N_\tau} \rightarrow a\mu_i = \frac{\pi}{N_\tau}$$

$$\mathcal{O} = L_{\mathrm{Im}}$$

$$\kappa = \frac{1}{2(am+4)}$$

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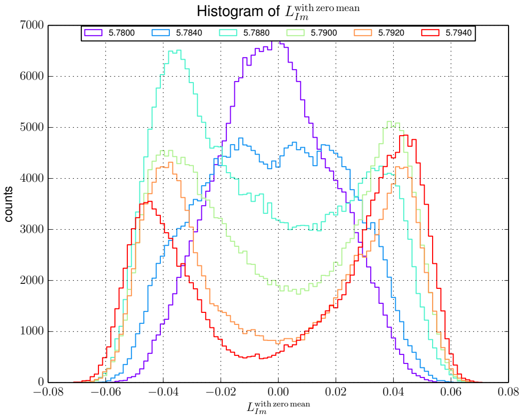

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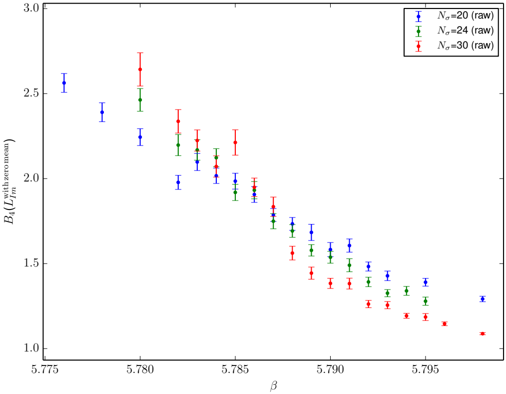

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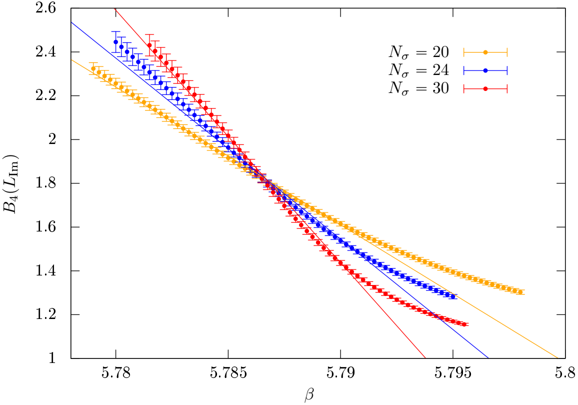

$$\frac{\mu_i}{T} = \pi \pm 2\pi k,\ \ k \in \mathbb{Z}$$

$$T = \frac{1}{a(\beta)\, N_\tau} \to a\mu_i = \frac{\pi}{N_\tau}$$

$$\mathcal{O} = L_{\rm Im}$$

$$\kappa = \frac{1}{2(am+4)}$$

fit reweighted data by $B_4(\beta, N_\sigma) = B_4(\beta_c, \infty) + a_1\,(\beta - \beta_c) N_\sigma^{1/\nu} + \ldots\ .$

Ferrenberg, Swendsen (1989), 10.1103/PhysRevLett.61.2635

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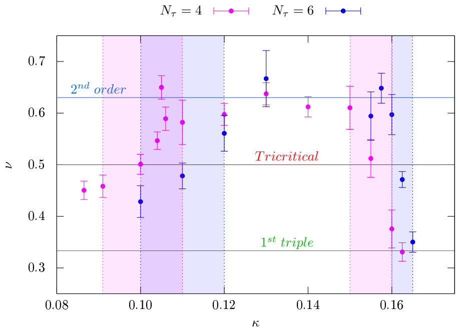

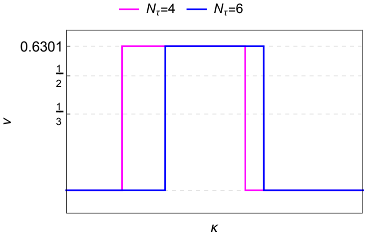

$$\kappa_{\text{heavy}}^{\text{tricr.}} = 0.10(1), \qquad \kappa_{\text{light}}^{\text{tricr.}} = 0.155(5)$$

$$\kappa_{\text{heavy}}^{\text{tricr.}} = 0.11(1), \qquad \kappa_{\text{light}}^{\text{tricr.}} = 0.1625(25)$$

Roberge-Weiss transition in $N_f = 2$ QCD

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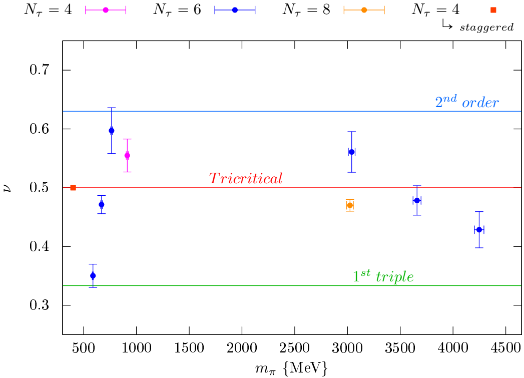
Pinke, Philipsen (2014), 10.1103/PhysRevD.89.094504, F.C. et al (2015), 10.1103/PhysRevD.93.054507

Bonati et al. (2011), 10.1103/PhysRevD.83.054505



$$m_\pi^{\text{tricr. heavy}} = 3659^{+589}_{-619}\ \text{MeV}, \qquad m_\pi^{\text{tricr. light}} = 669^{+95}_{-81}\ \text{MeV}$$

$$0.12\ \text{fm} \lesssim a \lesssim 0.18\ \text{fm}$$

Roberge-Weiss transition in $N_f = 2$ QCD

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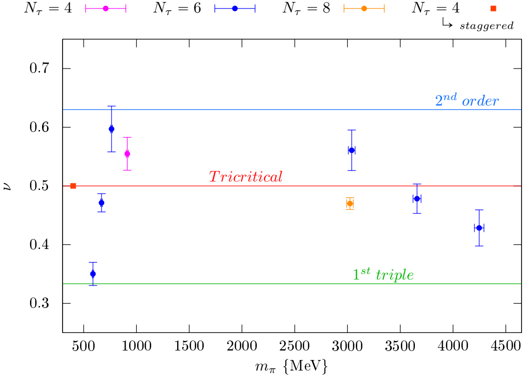
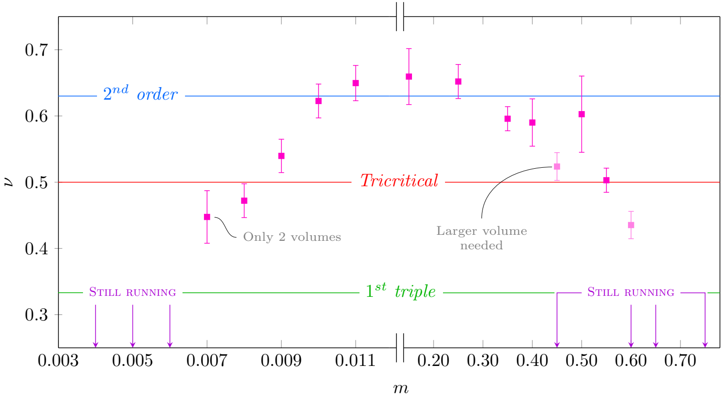


- Tension between results for different discretizations (Wilson, staggered)
- Need larger N_τ to attain continuum limit

Roberge-Weiss transition in $N_f = 2$ QCD

(Unimproved) Staggered fermions on $N_\tau = 6$ [Philipsen and Sciarra arXiv:1610.09979]

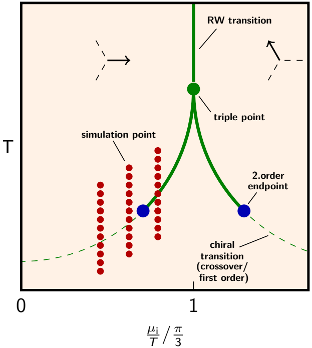


- Simulations ongoing
- Waiting for pion mass measurement
- Shift wrt $N_\tau = 4$ (d'Elia, Sanfilippo (2009), 10.1103/PhysRevD.80.111501 Bonati et al. (2011), 10.1103/PhysRevD.83.054505)

Z_2 CRITICAL LINE IN $m_\pi - \left(\frac{\mu}{T}\right)^2$ IN $N_f = 2$ QCD

(Unimproved) Wilson fermions on $N_\tau = 4$ [10.1103/PhysRevD.93.114507]

- Starting point m_1^{tric} at $N_\tau = 4$ (Pinke, Philipsen (2014), 10.1103/PhysRevD.89.094504)



$$\mathcal{O} = \bar{\psi}\psi = N_f \,\mathrm{Tr}\, D^{-1}$$

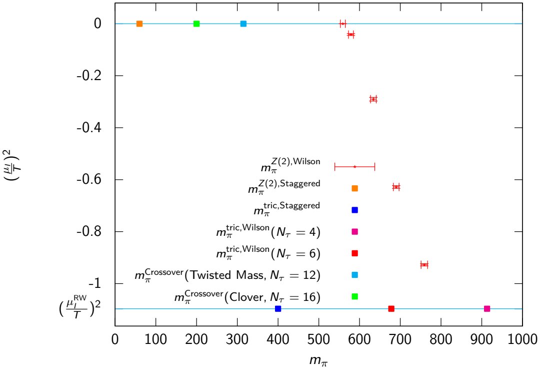
$$T = \frac{1}{a(\beta)\, N_\tau} \rightarrow a\mu_i = \frac{\pi}{3N_\tau}$$

$$\kappa = \frac{1}{2(am+4)}$$

$$\text{fixed } \kappa \longleftrightarrow B_4\left(\frac{\mu_i}{T}, N_\sigma\right) = B_4\left(\frac{\mu_i^c}{T}, \infty\right) + a_1 \left[\left(\frac{\mu_i}{T}\right)^2 - \left(\frac{\mu_i^c}{T}\right)^2\right] N_\sigma^{1/\nu} + \dots$$

$$\text{fixed } \mu = 0 \longleftrightarrow B_4(\kappa, N_\sigma) = B_4(\kappa, \infty) + b_1 \left[\frac{1}{\kappa} - \frac{1}{\kappa_c}\right] N_\sigma^{1/\nu} + \dots$$

Different discretizations compared



$a \gtrsim 0.25$ fm

$\kappa_c(\mu = 0) = 0.1815(1)$

$m_\pi^c(\mu = 0) \approx 560$ MeV

- Wilson $\mathcal{O}(a)$ improved results from Burger et al. (2013), 10.1103/PhysRevD.87.074508 (Twisted Mass) and Brandt et al. (2014), arXiv:1310.8326 (clover)
- No need for extrapolation using tricritical scaling law
- Only qualitative agreement between different discretizations (cf. staggered Bonati et al. (2014), 10.1103/PhysRevD.90.074030)
- Expected shift of $\mu_i^{Z_2}(m_{u,d})$ to smaller $m_{u,d}$ as $a \to 0$

Outline

N_f continuous parameter in the path integral

- Partition function describing N_f flavours of degenerate mass m

$$Z_{N_f}(m, \mu, N_f) = \int \mathcal{D}A \, [\det M(A, m, \mu)]^{N_f} \, e^{-S_G}$$

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- Investigation of the phase diagram in the N_f *vs* m plane

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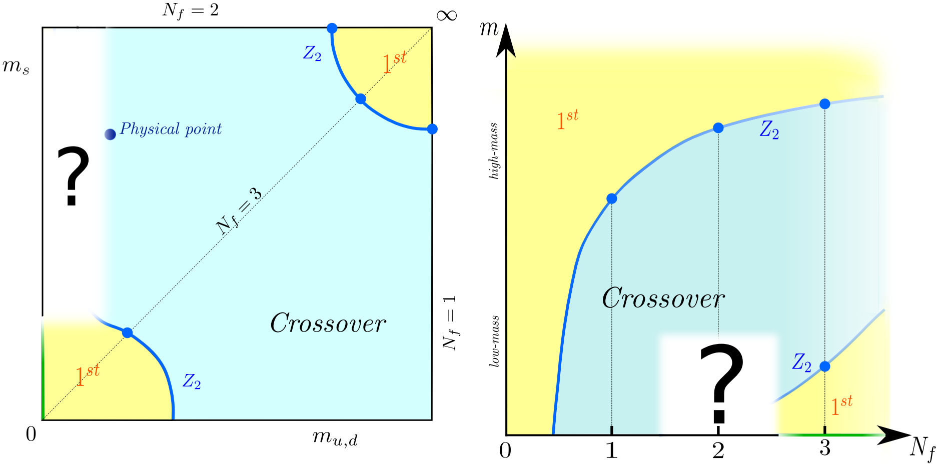
- Investigation of the phase diagram in the N_f *vs* m plane
  - mapping out the $m_{Z_2}(N_f)$ line
- Chiral limit extrapolation constrained by universality
  - tricritical scaling
  - Non-unique interpolation between $N_f = 2$ and $N_f = 3$;

$$\begin{aligned} Z_{N_f=2.\#} &= \int \mathcal{D}U \left[\det M(U, m, \mu)\right]^{2.\#} e^{-S_G} \\ Z_{N_f=2+1} &= \int \mathcal{D}U \left[\det M(U, m_1, \mu)\right]^{2} \left[\det M(U, m_2, \mu)\right] e^{-S_G} \end{aligned}$$

Further insights into the phase diagram

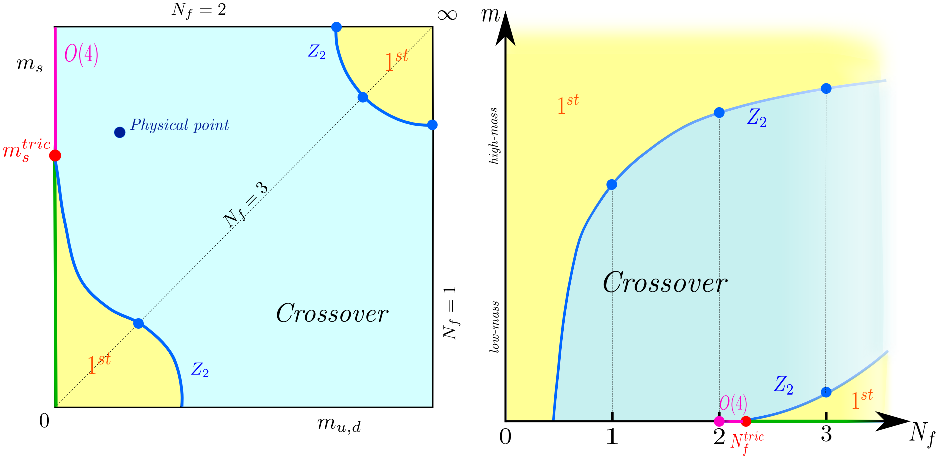
We still do not know the order of chiral transition for $N_f = 2$



Only two possible scenarios out of more are discussed (Vicari (2007), arXiv:0709.1014,...)

Further insights into the phase diagram

$m_{Z_2}(N_f)$ according to the second order scenario



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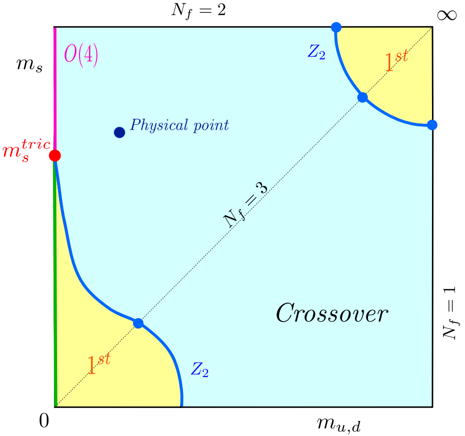

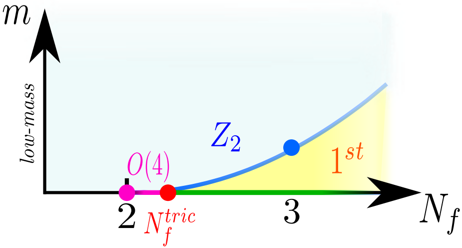

$N_f^{tric} > 2$

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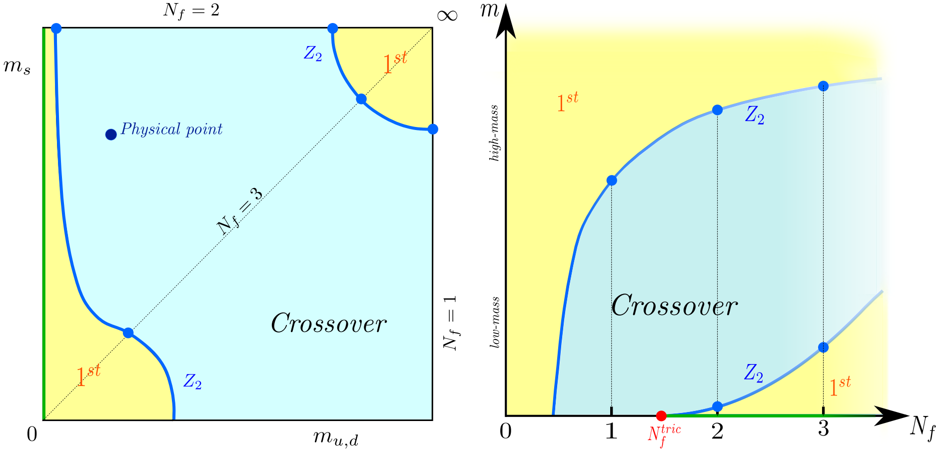

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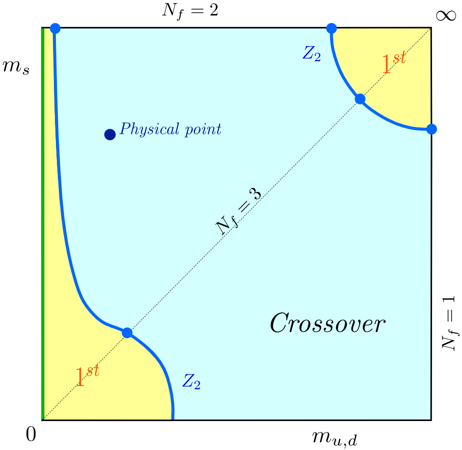

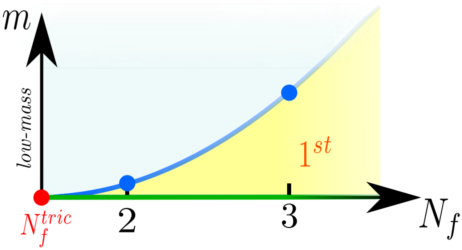

$N_f^{tric} < 2$

Code & investigated parameter space

- All simulations employ the OpenCL-based CL^{2}QCD code

  Philipsen et al. (2014) arXiv:1411.5219 https://github.com/CL2QCD/cl2qcd

  - Unimproved rooted staggered fermion discretization (RHMC algorithm)

- No. of flavours $\longrightarrow$ $N_f = 2.8, 2.6, 2.4, 2.2, 2.1, 2.0$
- Coarse lattices $\longrightarrow$ $N_\tau = 4$
- Chemical potential $\longrightarrow$ $\mu = 0$
- Scan in mass $\longrightarrow$ $m \in [0.0250, 0.0007]$
- Finite size scaling $\longrightarrow$ $N_\sigma = 8, 12, 16, 20$
- Scan in temperature $\longrightarrow$ $(3 - 5)$ β values
- Statistics $\longrightarrow$ $\sim (200k - 400k)$ per β

Checking the order of the transition...

- Chiral condensate $\langle\bar{\psi}\psi\rangle$ and moments of its distribution

$$B_n(\langle\bar{\psi}\psi\rangle, \beta, m, V) \equiv B_n(\beta, m, N_\sigma) = \frac{\left\langle \left(\bar{\psi}\psi - \langle\bar{\psi}\psi\rangle\right)^n \right\rangle}{\left\langle \left(\bar{\psi}\psi - \langle\bar{\psi}\psi\rangle\right)^2 \right\rangle^{n/2}}$$

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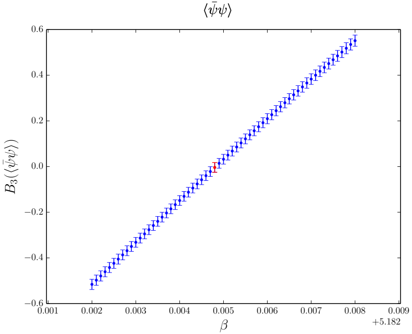

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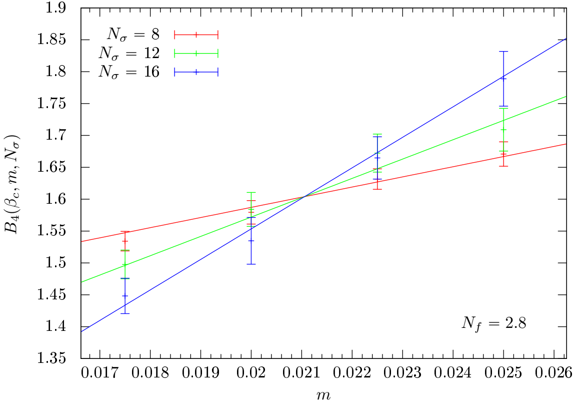
- $\forall m, N_\sigma$ identify β_c by the condition $B_3(\beta,m,N_\sigma)=0$
- $B_4(\beta_c,m,N_\sigma)$ to extract the order of the transition as function of m

$$B_4(\beta_c,m,N_\sigma) = \left.\frac{\left\langle \left(\bar{\psi}\psi - \langle\bar{\psi}\psi\rangle\right)^4 \right\rangle}{\left\langle \left(\bar{\psi}\psi - \langle\bar{\psi}\psi\rangle\right)^2 \right\rangle^{2}}\right|_{\beta_c} \underset{V\to\infty}{\sim} \begin{cases} 1, & 1^{st}\text{order;} \\ 1.604, & 2^{nd}\text{order}\, Z_2; \\ 3, & \text{crossover.} \end{cases}$$

...AND LOCATING $m_{Z_2}(N_f)$

Fitting $B_4(\beta_c, m, N_\sigma)$ at fixed N_f and various N_σ, as function of m

$$B_4(\beta_c, m, N_\sigma) = B_4(\beta_c, m_{Z_2}, \infty) + a(m - m_{Z_2})N_\sigma^{1/\nu} + \dots$$



$B_4(\beta_c, m_{Z_2}, \infty) = 1.604$

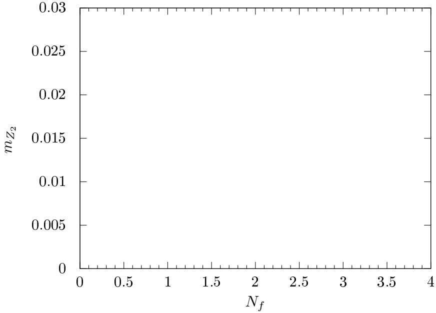
$a = 0.59(5)$

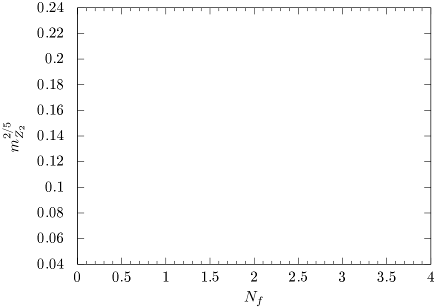
$\nu = 0.6301$

$m_{Z_2} = 0.0211(3)$

$\chi^2_{ndf=10} = 0.27$

How (~~wide~~) small is the tricritical scaling region in $m_{Z_2}(N_f)$?





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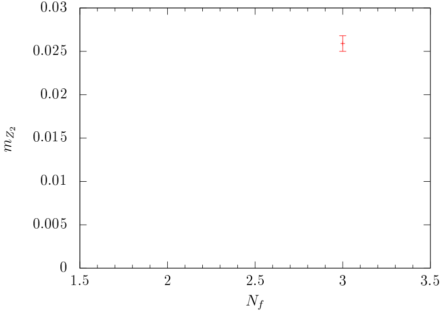

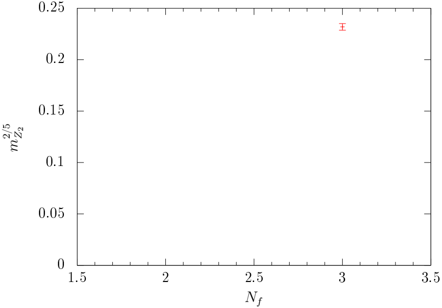

de Forcrand and Philipsen (2003), 10.1016/j.nuclphysb.2003.09.005

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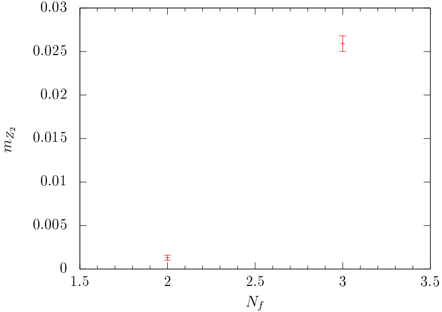

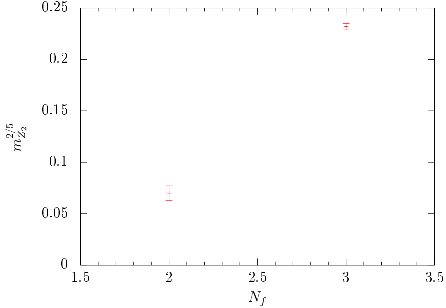

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Bonati et al. (2014), 10.1103/PhysRevD.90.074030

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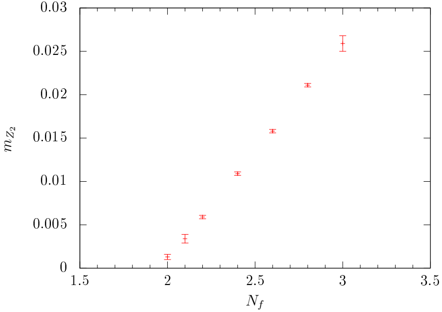
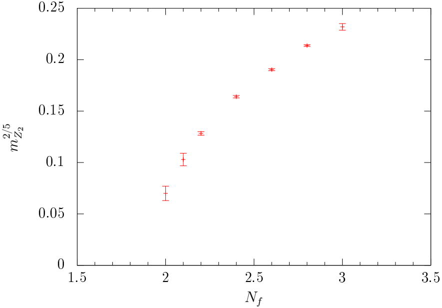
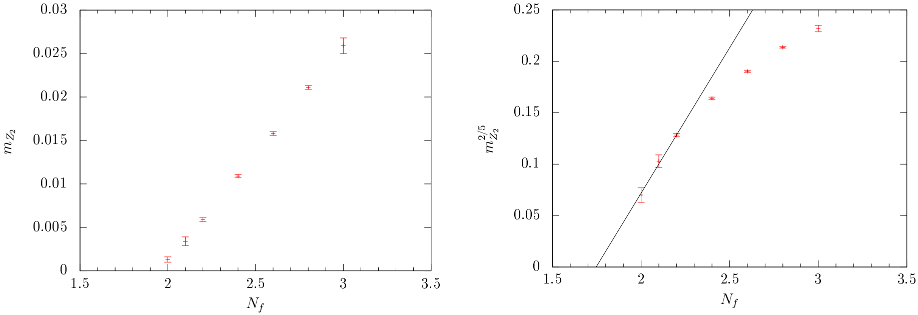




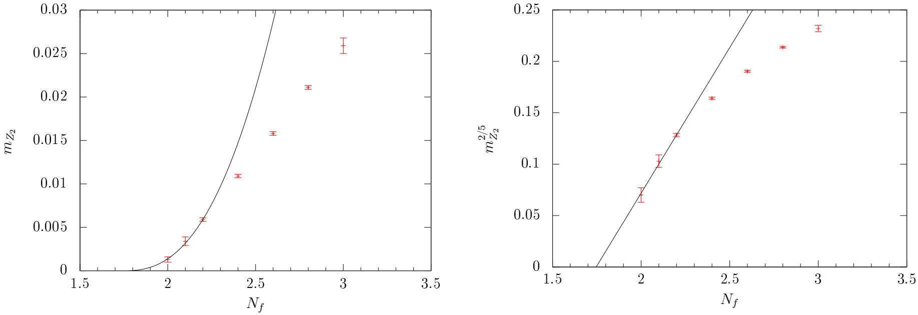
$$m_{Z_2}^{2/5}(N_f) = C\left(N_f - N_f^{tric}\right)$$

$N_f = 2.2 \in$ TRICRITICAL SCALING REGION?



$m_{Z_2}^{2/5}(N_f) = C\left(N_f - N_f^{tric}\right)$ $\chi^2_{ndf=1} = 0.28$

$N_f = 2.2 \in$ TRICRITICAL SCALING REGION?



- Assuming that the tricritical scaling sets in at $N_f = 2.2$
  - Same scaling window in m as found in the extrapolation from μ_i
  - $N_f^{tric} = 1.75(32)$
- Waiting for ongoing simulations at $N_f = 2.0$...

Outline

Outlook

- First investigation
  - Just entered the scaling region...
  - Coarse $N_\tau = 4$ lattices explored
  - Rooted staggered fermion discretization: cross check needed
- Theoretical caveat: at non-integer N_f our theory lacks locality and does NOT correspond to a well defined QFT in the CL
- Theoretical caveat: ∞ many interpolations between $N_f = 2$ and $N_f = 3$ $\lim_{N_f \to 2,3} \mathcal{Z}(N_f = 2.\#) = \mathcal{Z}(N_f = 2, 3)$
- However
  - the relative position of N_f^{tric} w.r.t. $N_f = 2$ has to be uniquely determined by every interpolation
  - possible matching among interpolations
- In view of a continuum limit: the width of scaling regions fixed in physical units will shrink in lattice units
  - Which extrapolation is more expensive?
    - ★ from imaginary chemical potential μ_i at $N_f = 2$
    - ★ from non-integer N_f at $\mu = 0$
    - ★ from $N_f = 2 + 1$ while increasing m_s at $\mu = 0$

THANK YOU!