RHIC-BES seminar 07 November 2023

Lattice constraints on the QCD phase diagram

Owe Philipsen

- Chiral phase transition in massless limit constrains the QCD phase diagram
- 30+ years of common wisdom and inconclusive lattice results
- Resolution by a new lattice approach + data [Cuteri, O.P., Sciarra JHEP 21]
- Bounds on the phase diagram at finite density

CRC-TR 211 Strong-interaction matter under extreme conditions

ELEMENTS

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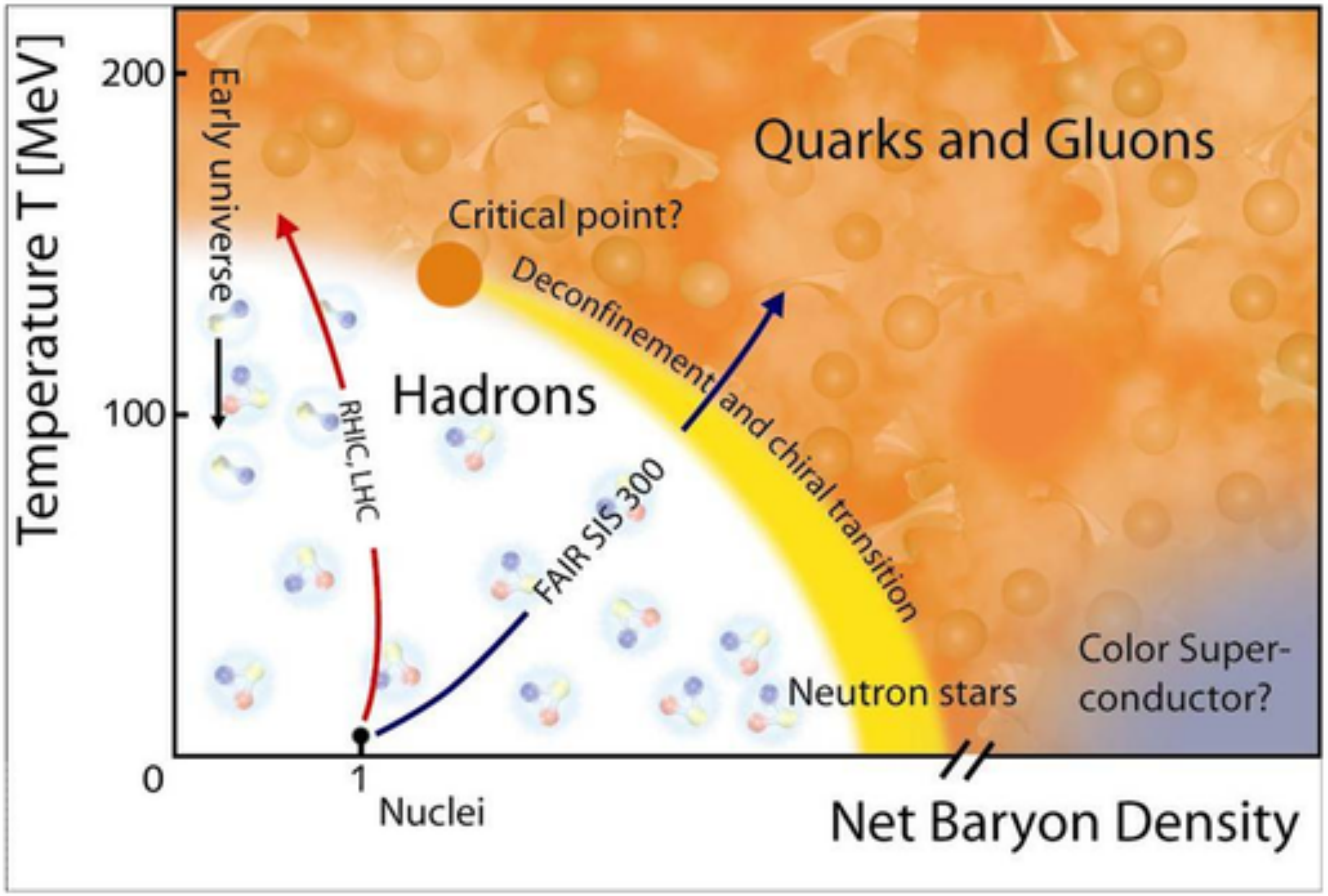
The expected QCD phase diagram



from GSI

- Fundamental for particle-, nuclear-, astro- physics, future textbook knowledge!
- Non-perturbative nature/confinement prevents perturbative solution
- “Sign problem” prevents Monte Carlo simulation (NP-hard problem?)

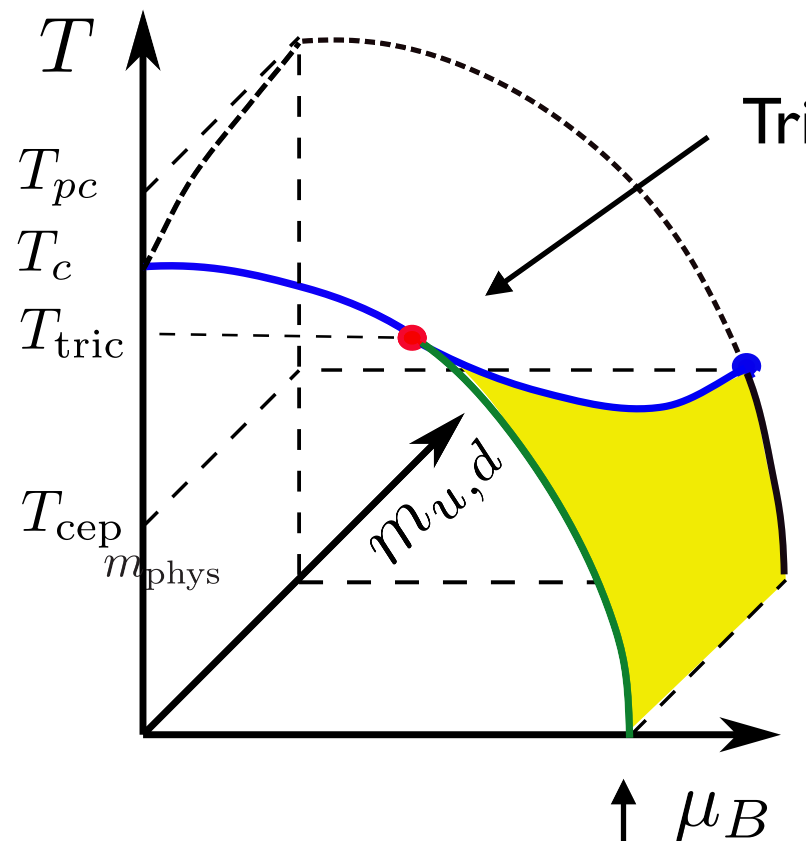
History: motivation for the critical endpoint

[Rajagopal 95, Halasz et al., PRD 98, Stephanov, Rajagopal, Shuryak PRL 98, Rajagopal, Wilczek 00, Hatta, Ikeda, PRD 03,…]

Breaking/restoration of exact chiral symmetry requires a (non-analytic) phase transition

$N_f = 2:$

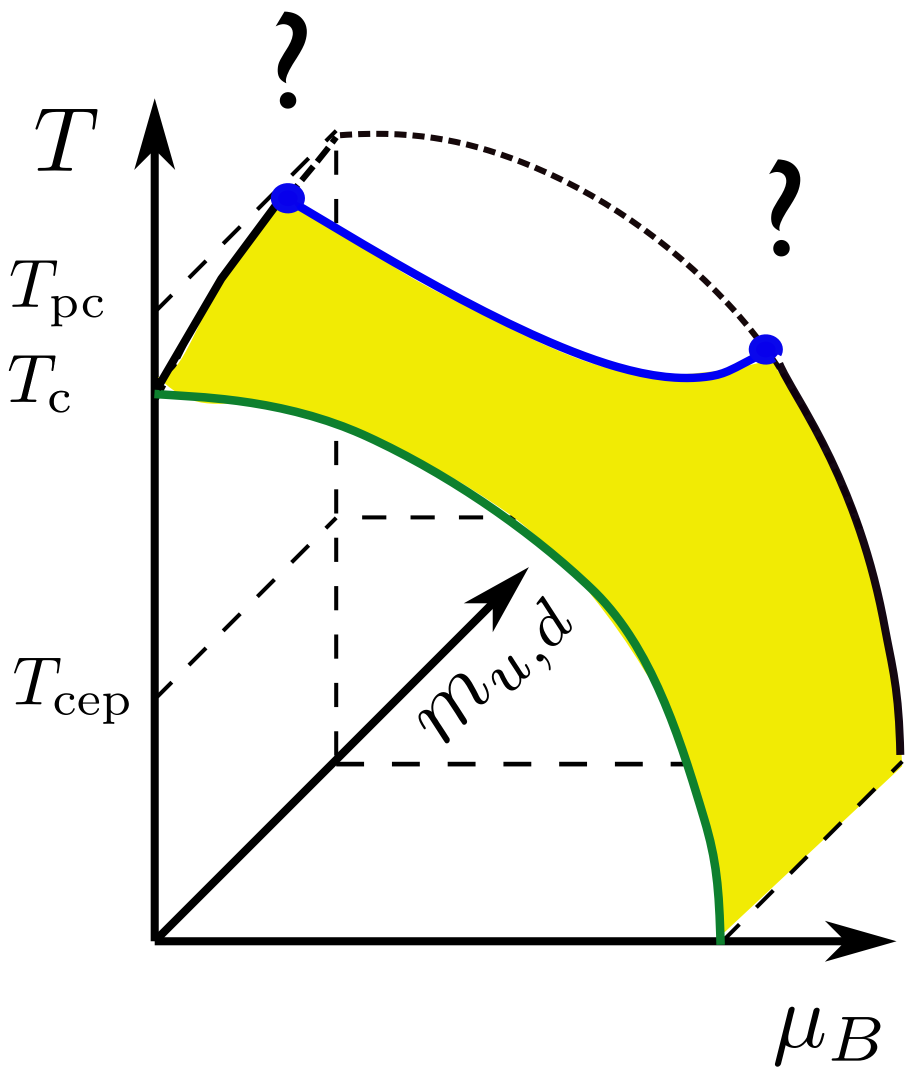
Model predictions, early lattice results →

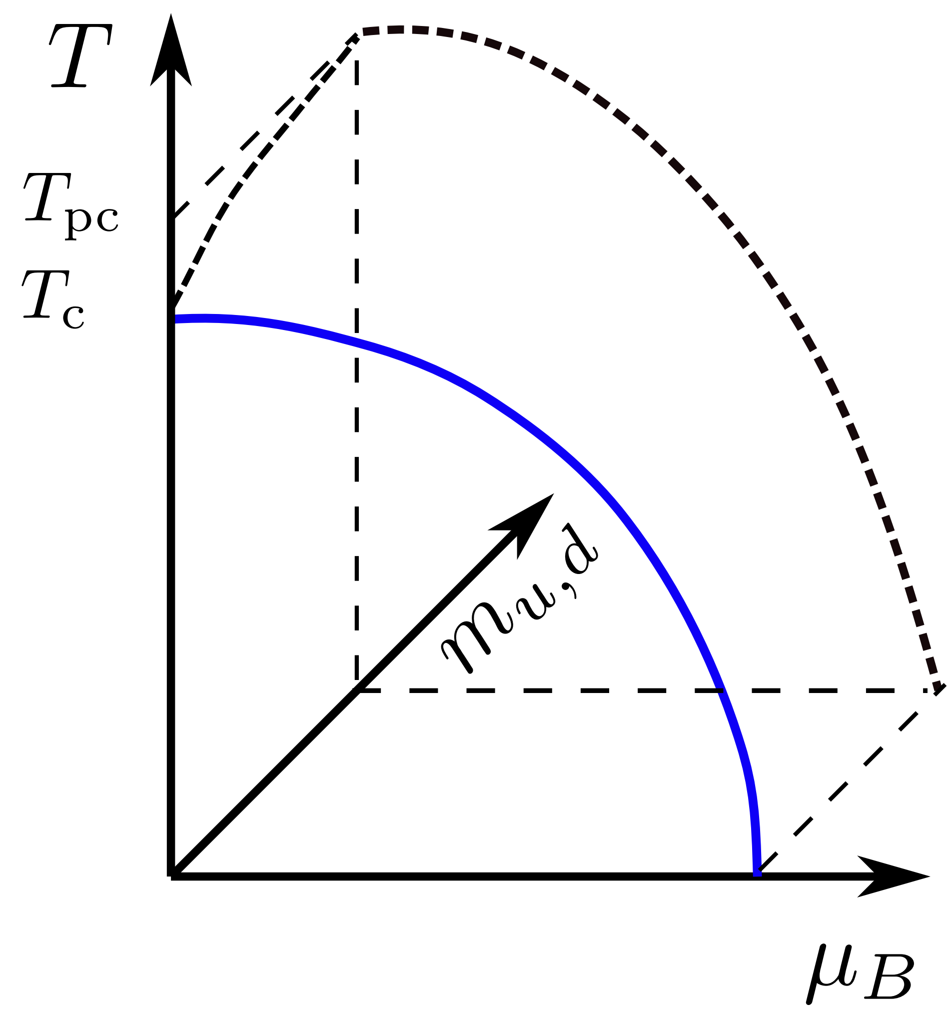


Tricritical point + wing line

Model predictions, no QCD information

Other (mostly ignored) possibilities



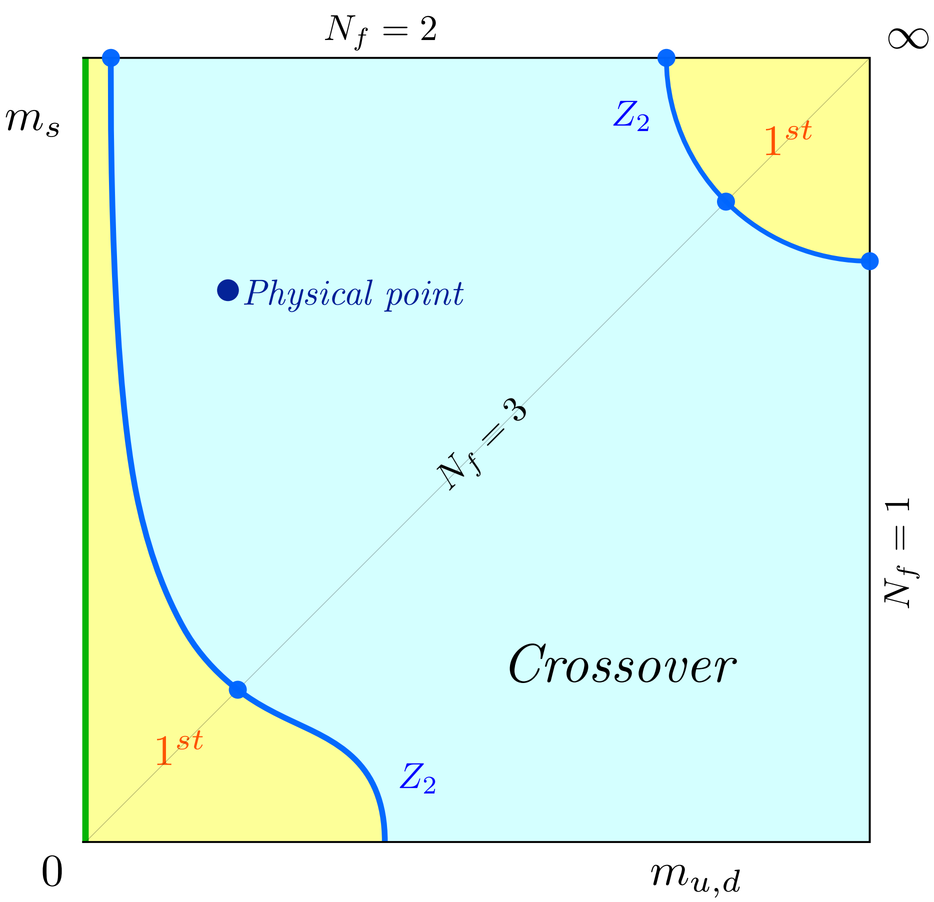


The order of the chiral phase transition at $\mu_B = 0$ narrows down possibilities

Nature of the QCD thermal transition at zero density

$N_f = 2+1$

deconfinement p.t.:
breaking of global $Z(3)$ symmetry

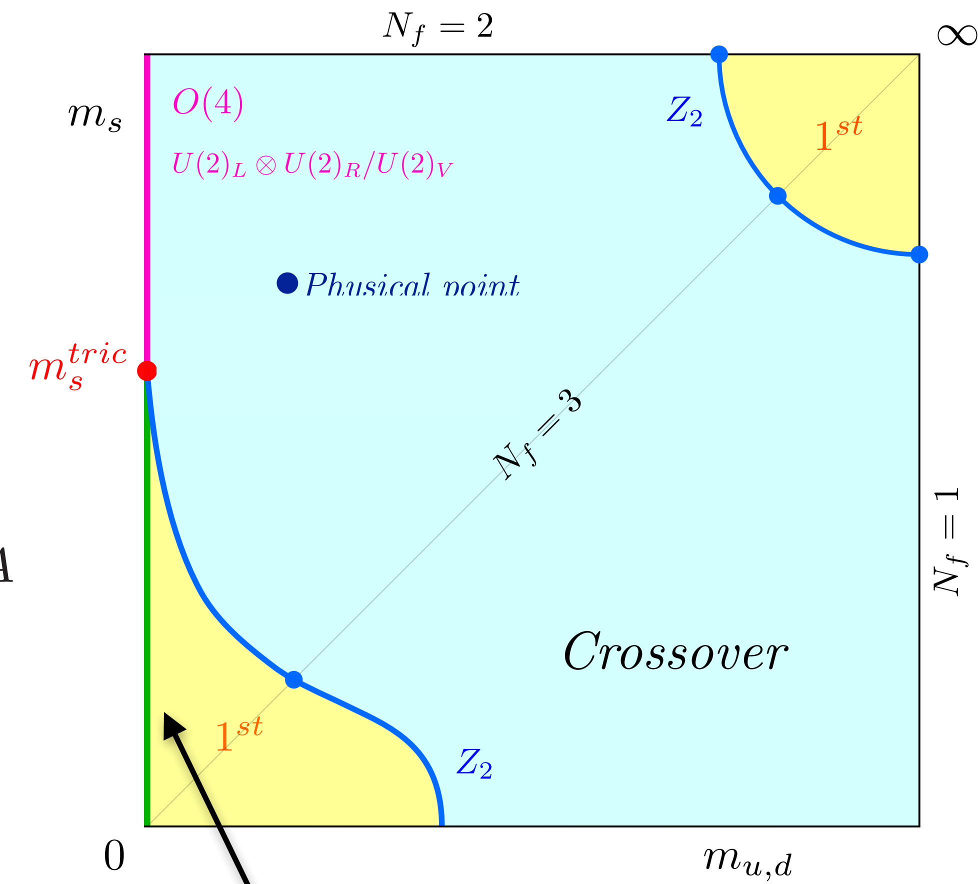


[Pisarski, Wilczek, PRD 84]:
(Linear sigma model in 3d)

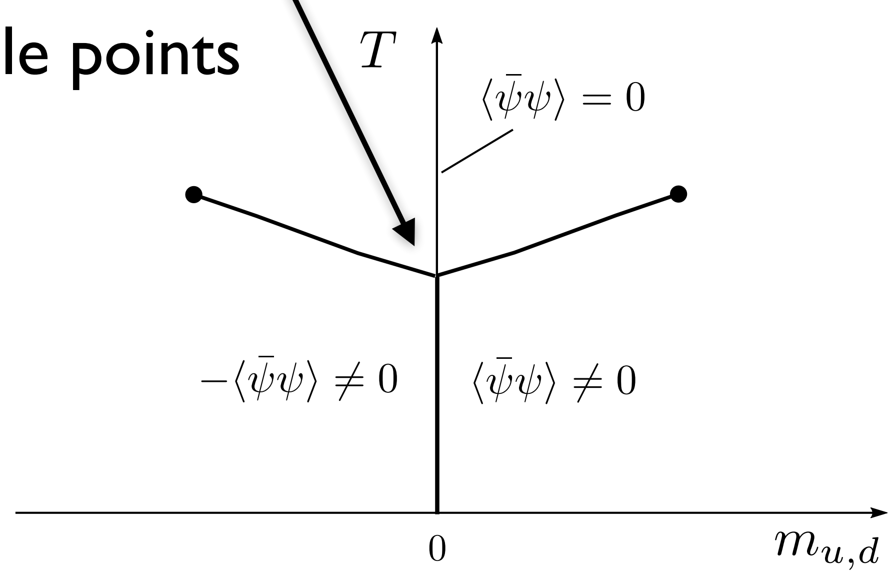
$N_f = 2$ depends on $U(1)_A$

restored broken

$N_f \geq 3$ 1st order



triple points



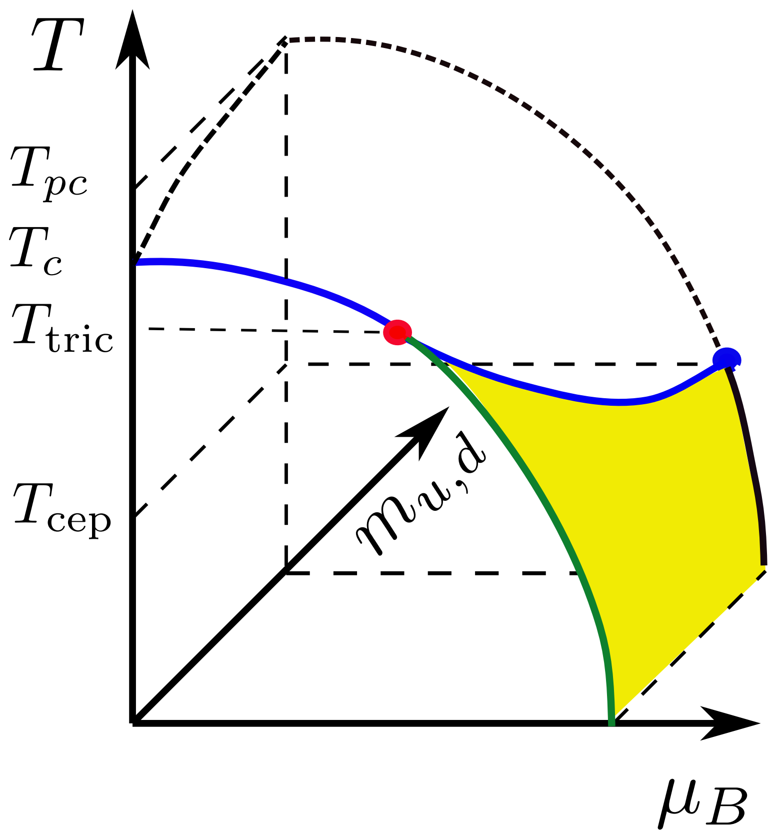
chiral p.t.
restoration of global symmetry in flavour space

$SU(2)_L \times SU(2)_R \times U(1)_A$

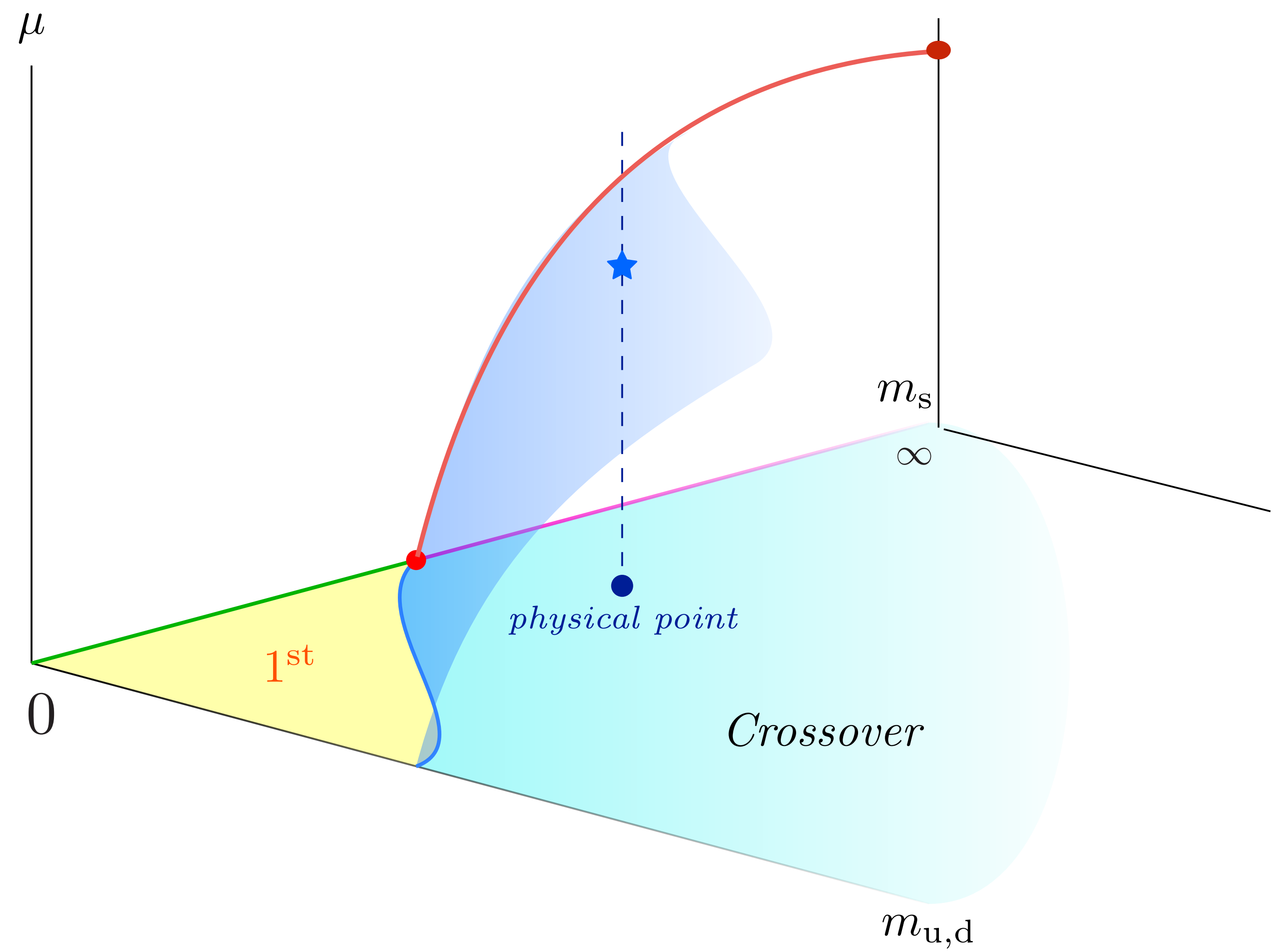
anomalous

The Columbia plot with chemical potential

$N_f = 2$



$N_f = 2+1$

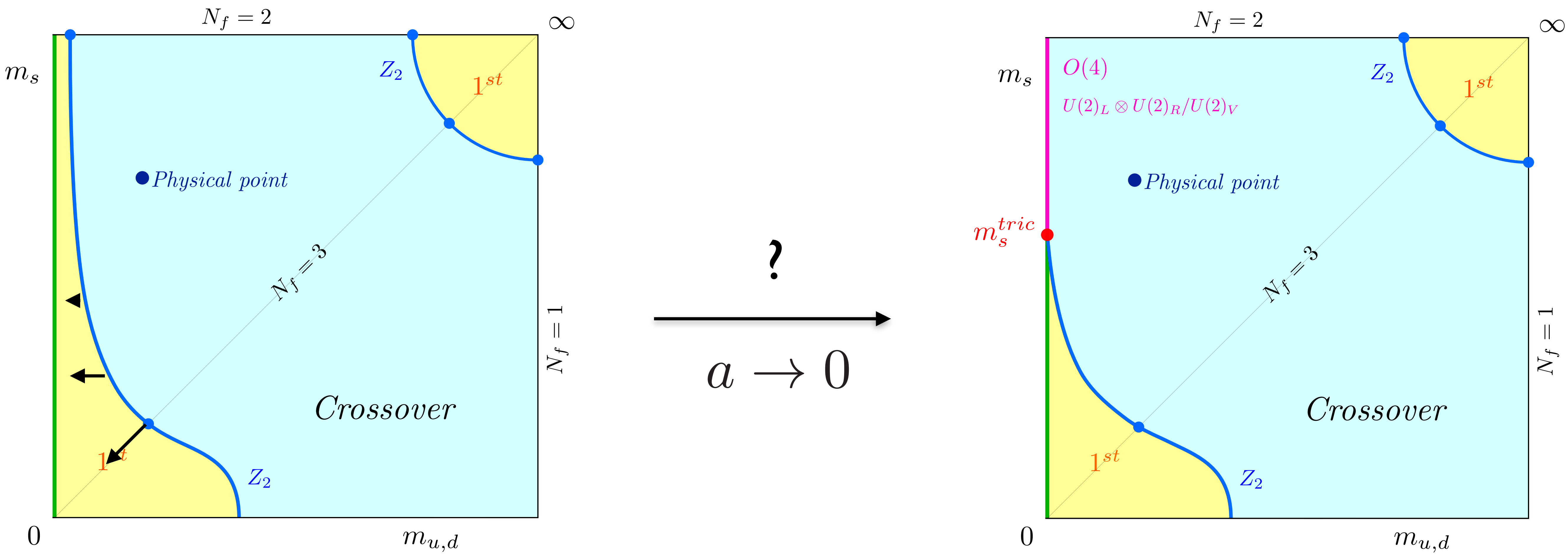


[Stephanov, Rajagopal, Shuryak PRL 98]: (based on models, early lattice)

"As m_s is reduced from infinity, the tricritical point … moves to lower μ until it reaches the T-axis and can be identified with the tricritical point in the (T, m_s)-plane"

The nature of the QCD chiral transition at zero density

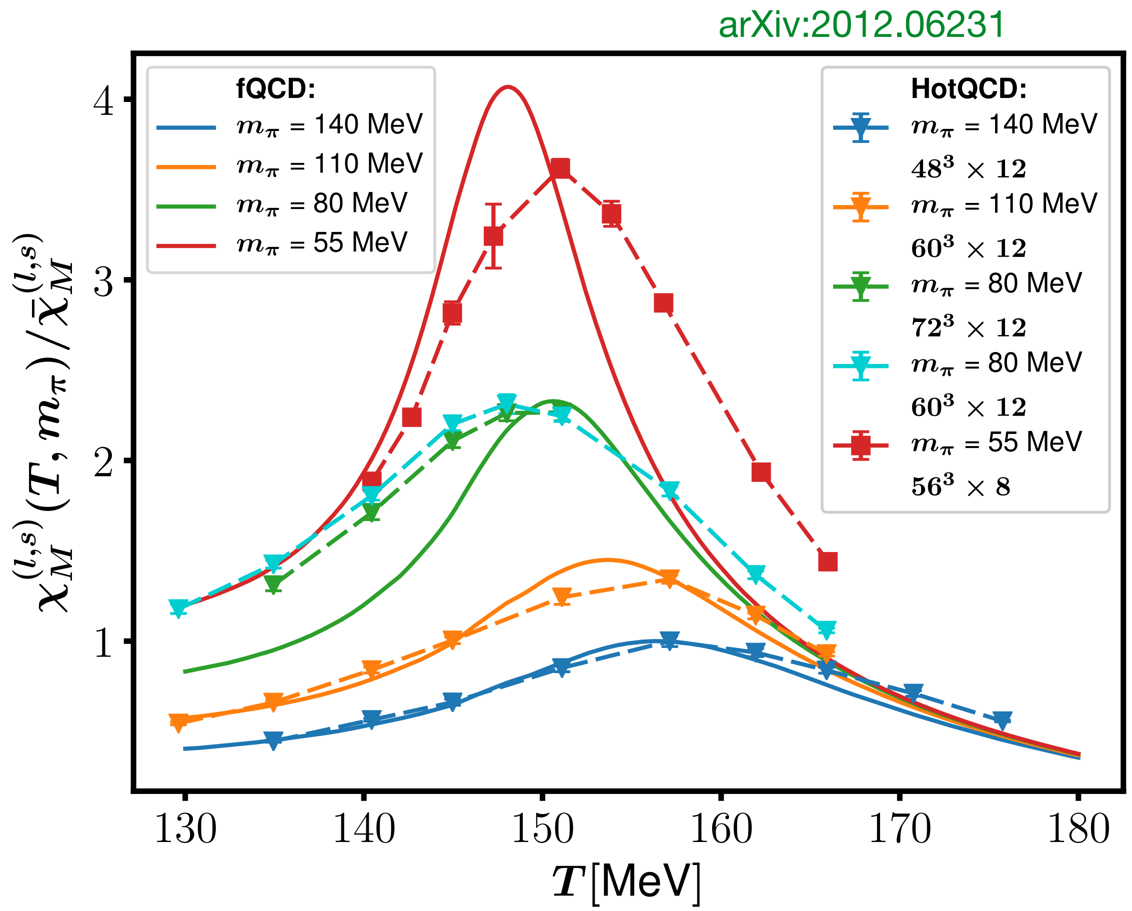
…is elusive, massless limit not simulable!

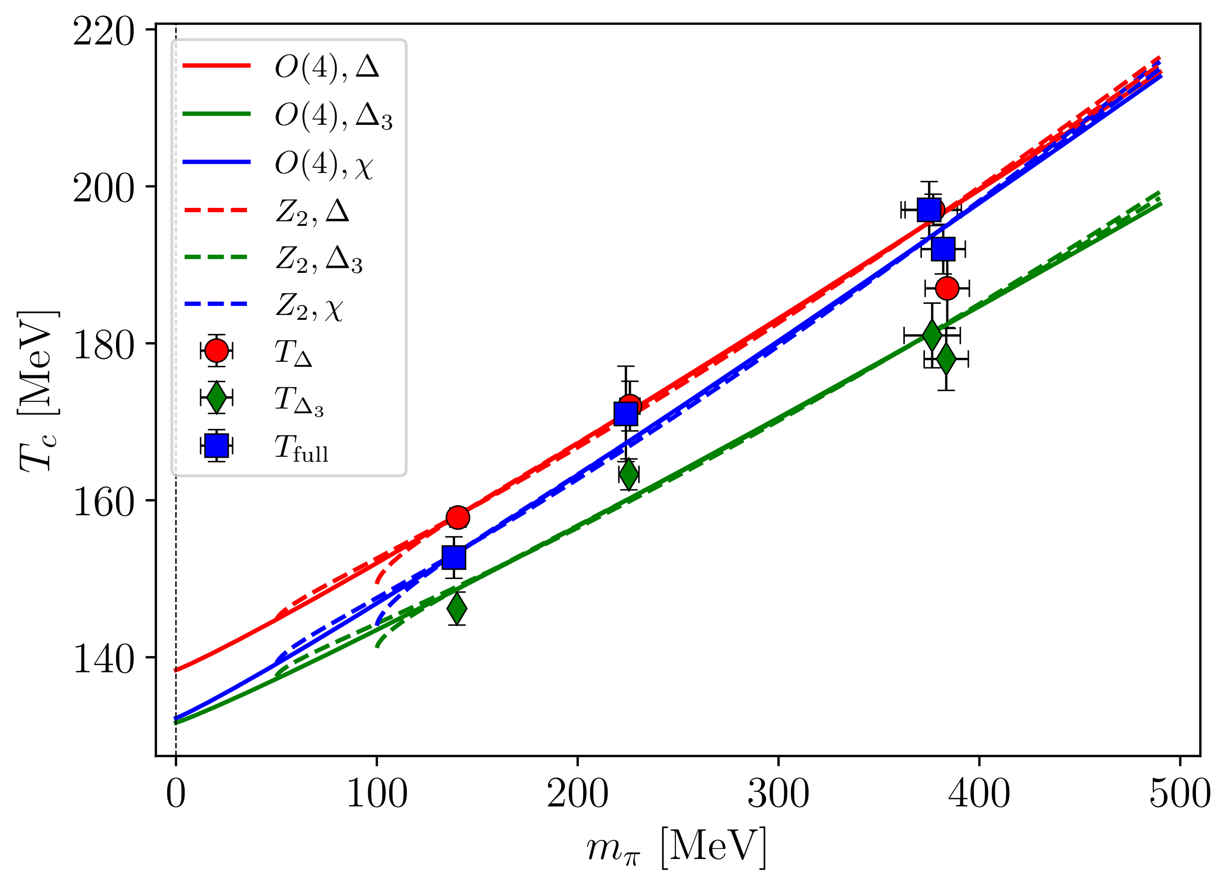


- Coarse lattices or unimproved actions: 1st order for $N_f = 2, 3$
- 1st order region shrinks rapidly as $a \to 0$
- For fixed lattice spacing: apparent contradictions between different lattice actions

Details and references: [O.P., Symmetry 13, 2021]

From the physical point to the chiral limit





[HotQCD, PRL 19] HISQ (staggered)

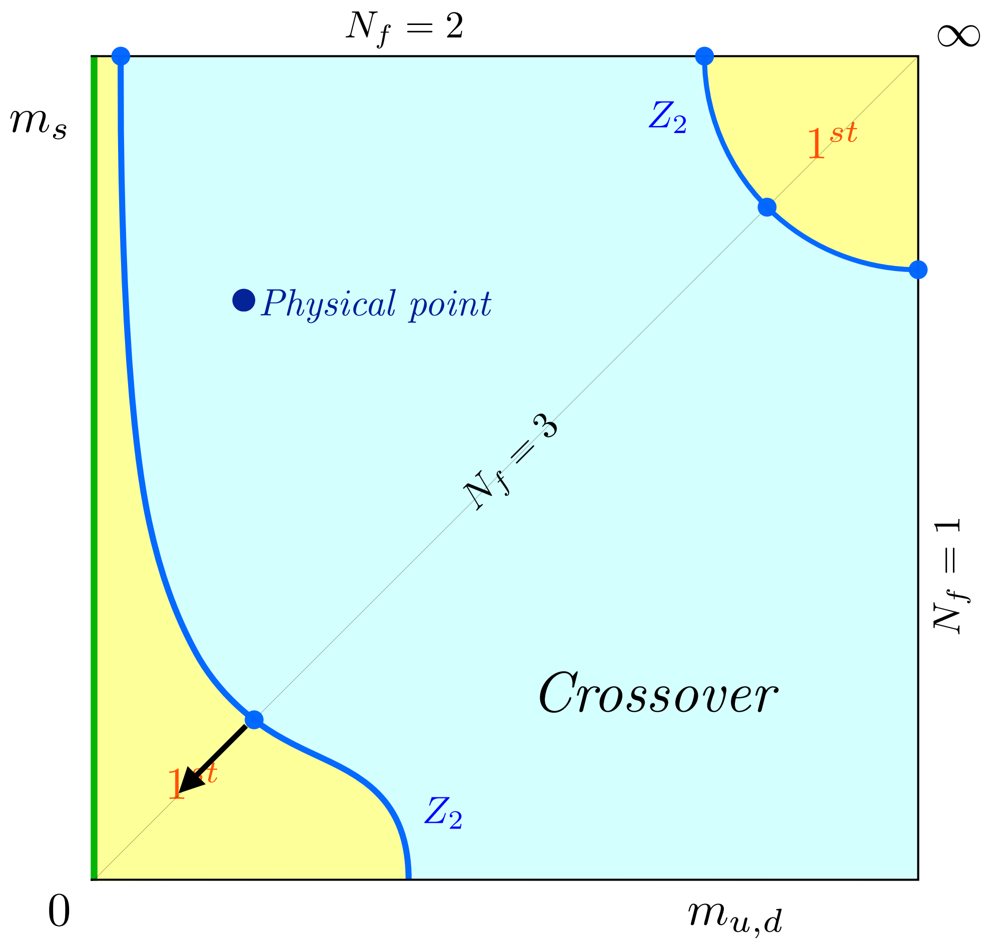
[Kotov, Lombardo, Trunin, PLB 21] Wilson twisted mass

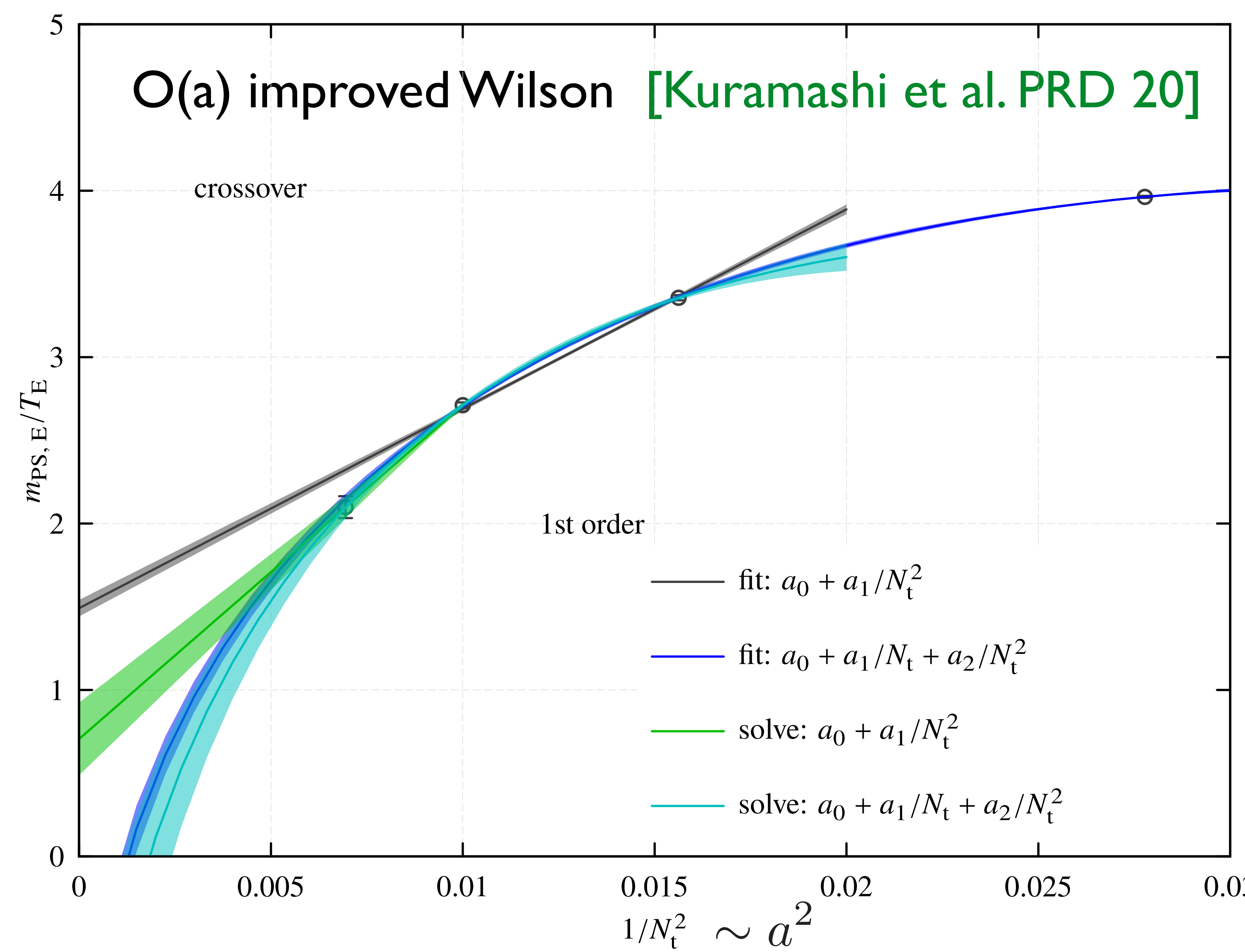
$$T_c^0 = 132^{+3}_{-6} \text{ MeV} \qquad T_{pc}(m_l) = T_c^0 + K\, m_l^{1/\beta\delta} \qquad T_c^0 = 134^{+6}_{-4} \text{ MeV}$$

- Strange quark mass fixed, crossover sharpens as chiral limit approached, no 1st o. seen
- Cannot distinguish between Z(2) vs. O(4) exponents, need exponential accuracy!
- Comparison with fRG: $T_c^0 \approx 142\text{MeV}$ [Braun et al., PRD 21] Scaling window tiny $m_\pi \leq 5\text{MeV}$ (!!) [Braun et al., arXiv:2310.19853]

The nature of the QCD chiral transition, Nf=3

…has enormously large cut-off effects!



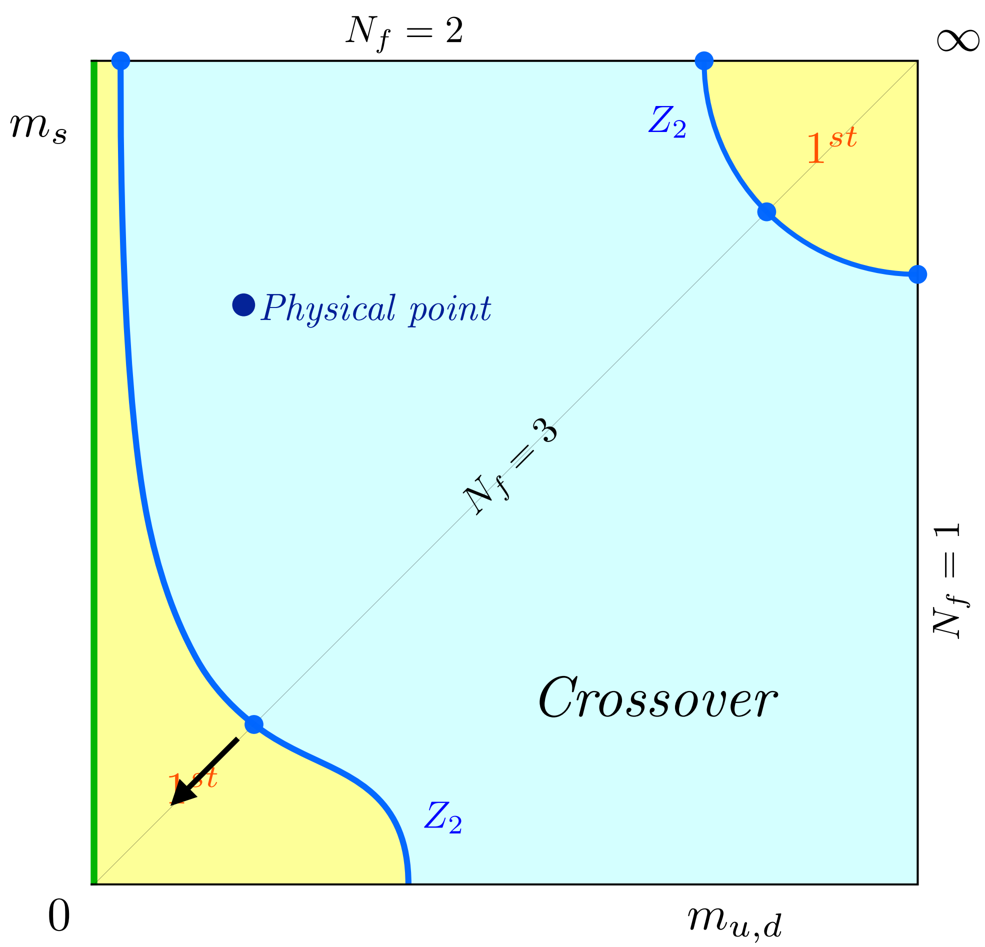


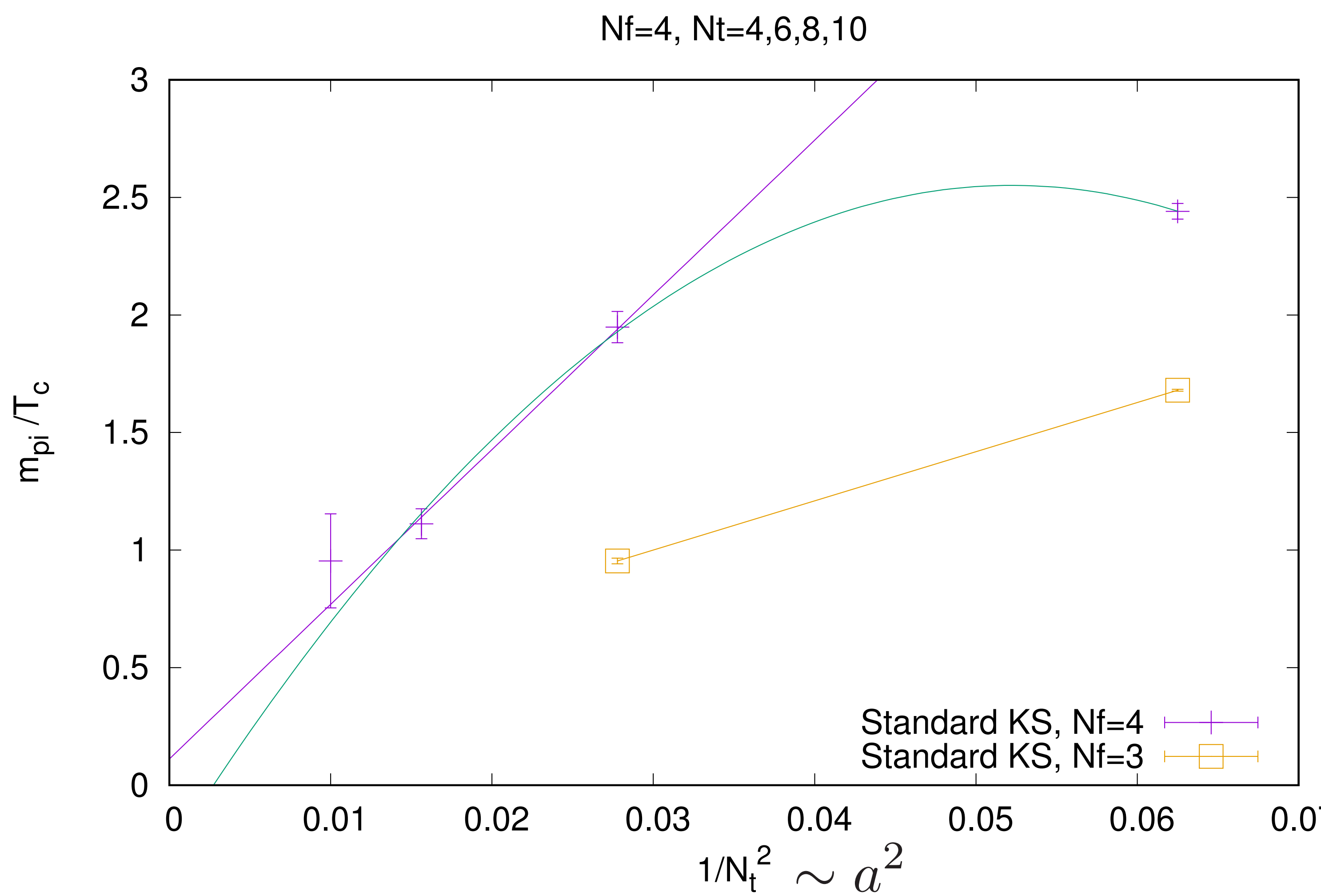
O(a)-improved Wilson:
1st order region shrinks for $a \to 0$

$m_\pi^c \leq 110$ MeV $\quad N_\tau = 4, 6, 8, 10, 12$

The nature of the QCD chiral transition, Nf=3,4

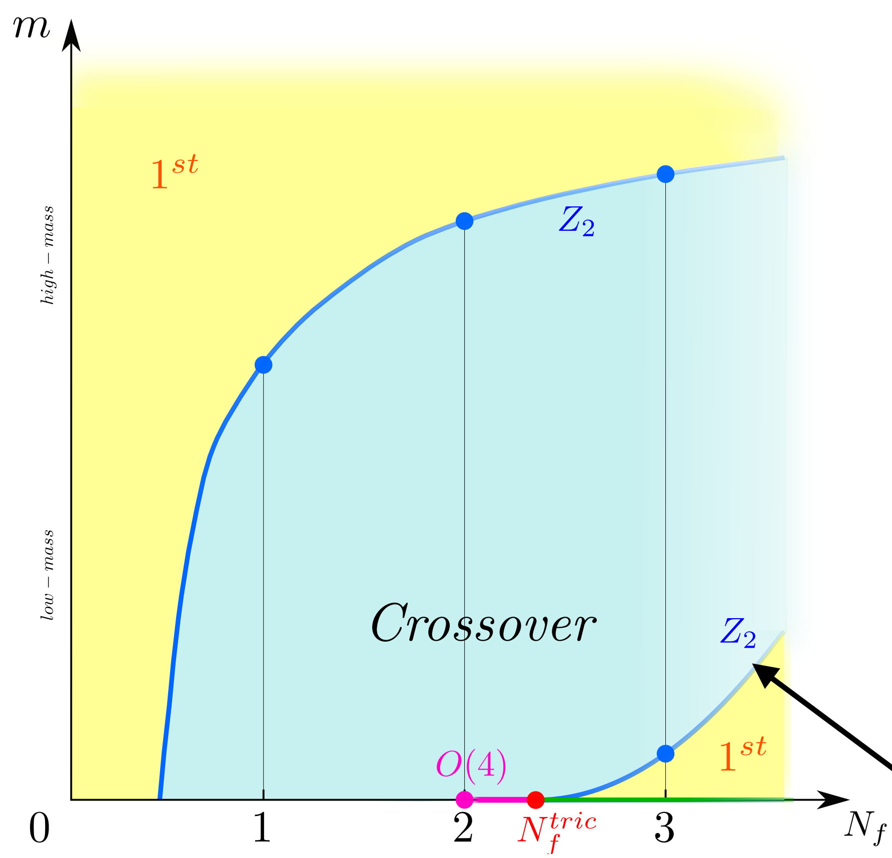
…has enormously large cut-off effects!

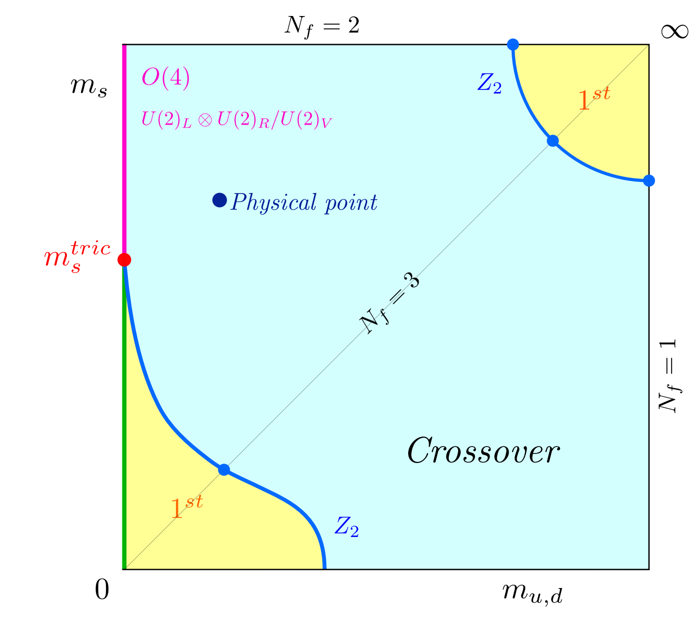




Unimproved staggered:
1st order region shrinks for $a \to 0$, both for $N_f = 3, 4$ [de Forcrand, D'Elia, PoS LAT 17]

Different view point: mass degenerate quarks





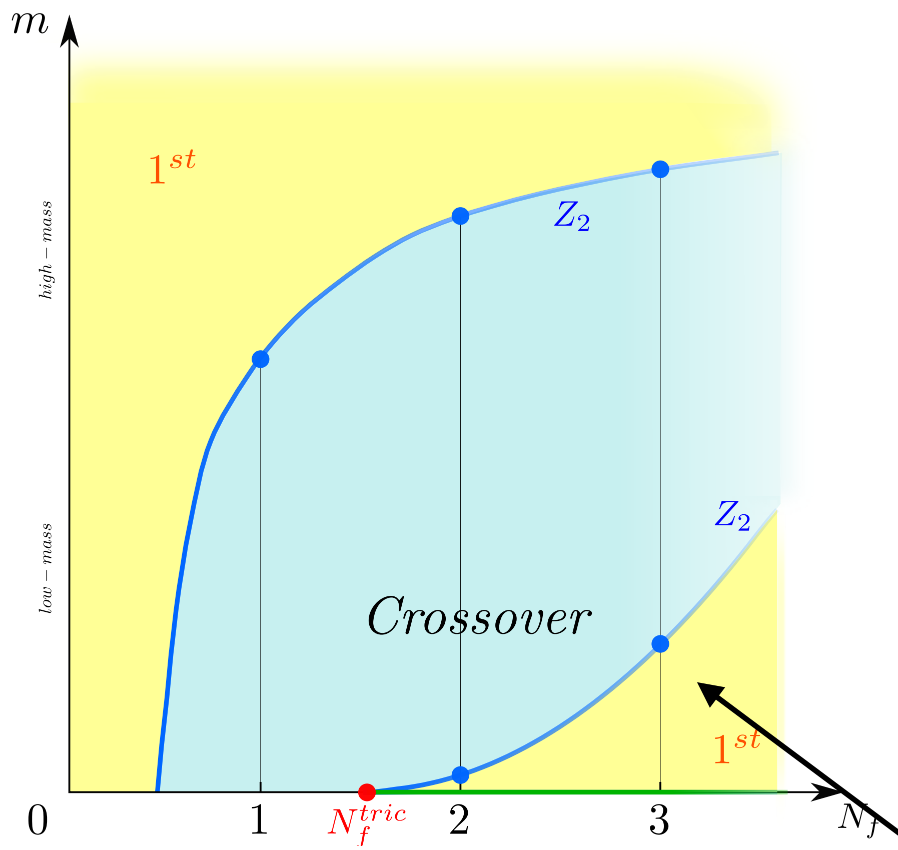
$$Z(N_\mathrm{f}, g, m) = \int \mathcal{D}A_\mu \, (\det M[A_\mu, m])^{N_\mathrm{f}} \, e^{-\mathcal{S}_\mathrm{YM}[A_\mu]}$$

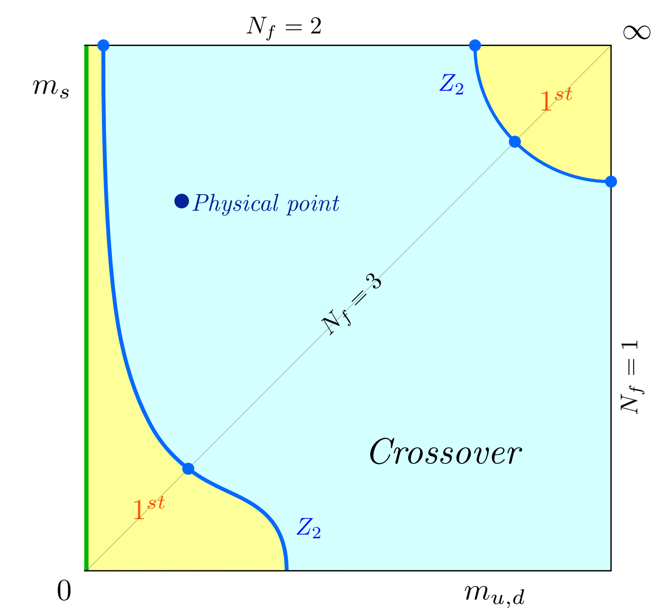
$$N_\mathrm{f}^c(am) = N_\mathrm{f}^\mathrm{tric} + \mathcal{B}_1 \cdot (am)^{2/5} + \mathcal{O}\left((am)^{4/5}\right)$$

- Consider analytic continuation to continuous N_f
- Tricritical point guaranteed to exist if there is 1st order at any N_f
- Known exponents for critical line entering tric. point!
- Continuation to $a \neq 0$: Z(2) surface ends in tricritical line

[Cuteri, O.P., Sciarra PRD 18]

Different view point: mass degenerate quarks





$$Z(N_{\rm f}, g, m) = \int \mathcal{D}A_\mu \, (\det M[A_\mu, m])^{N_{\rm f}} \, e^{-\mathcal{S}_{\rm YM}[A_\mu]}$$

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[Cuteri, O.P., Sciarra PRD 18]

Methodology to determine order of transition

Finite size scaling of generalised cumulants

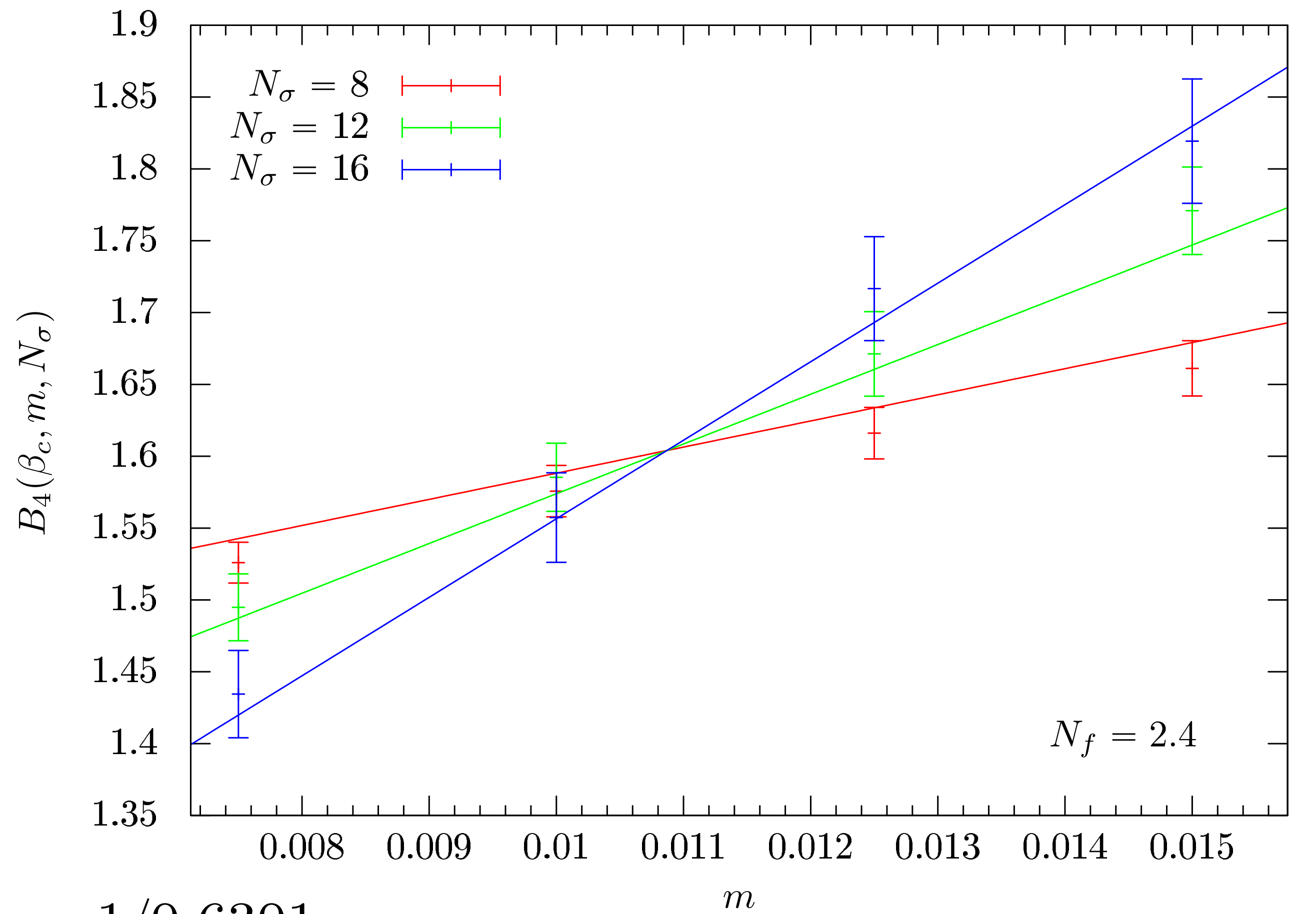
$$B_n = \frac{\langle (\bar\psi\psi - \langle\bar\psi\psi\rangle)^n\rangle}{\langle (\bar\psi\psi - \langle\bar\psi\psi\rangle)^2\rangle^{n/2}}$$

Standard staggered fermions, bare parameters: β, am, N_f, N_τ

(Pseudo-critical) phase boundary: $B_3 = 0$ 3d manifold

Second-order 3d Ising:

2d chiral critical surface separates 1st order from crossover



$$B_4(\beta_c, am, N_\sigma) \approx 1.604 + c\,(am - am_c)\,N_\sigma^{1/0.6301}$$

Machines and computing approach

Goethe-HLR (Goethe U.) and VIRGO cluster (GSI),   AMD-GPU cluster

Scans of parameter space parallel, one lattice per GPU, strictly zero communication overhead

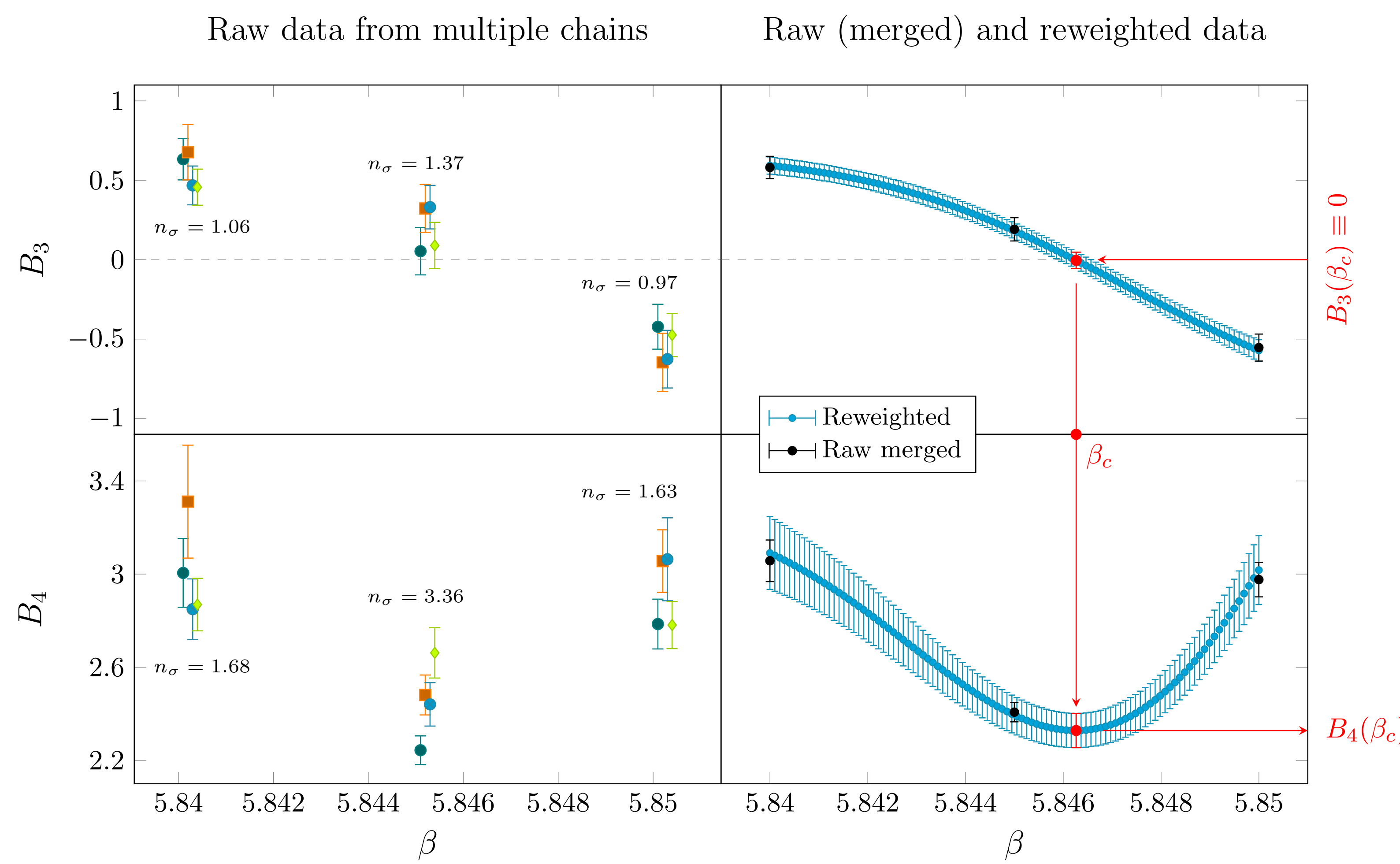
Search for phase boundary:

3-4 coupling values with multiple simulation chains

Good control over autocorrelation; merge independent chains

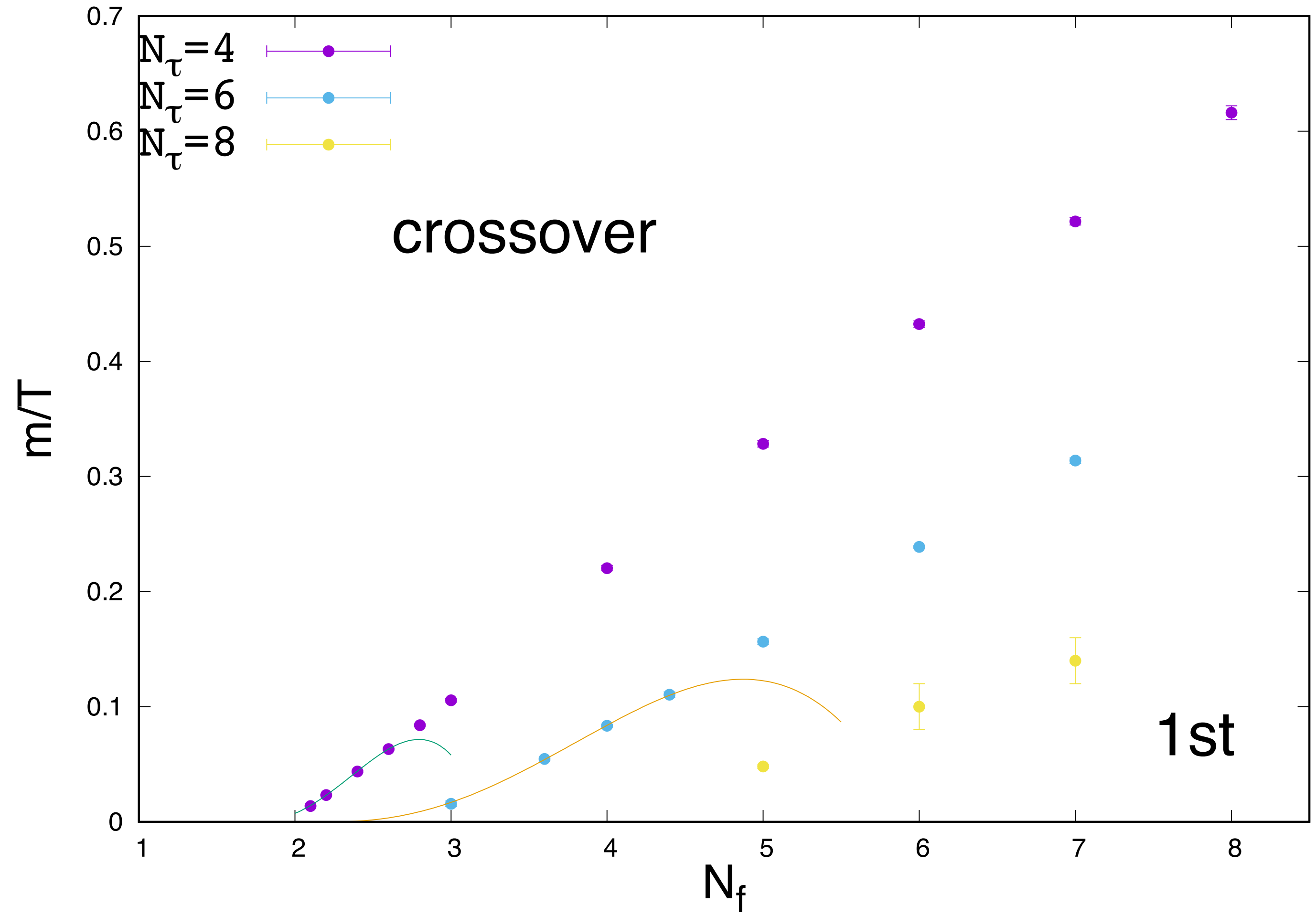
Repeat for different masses

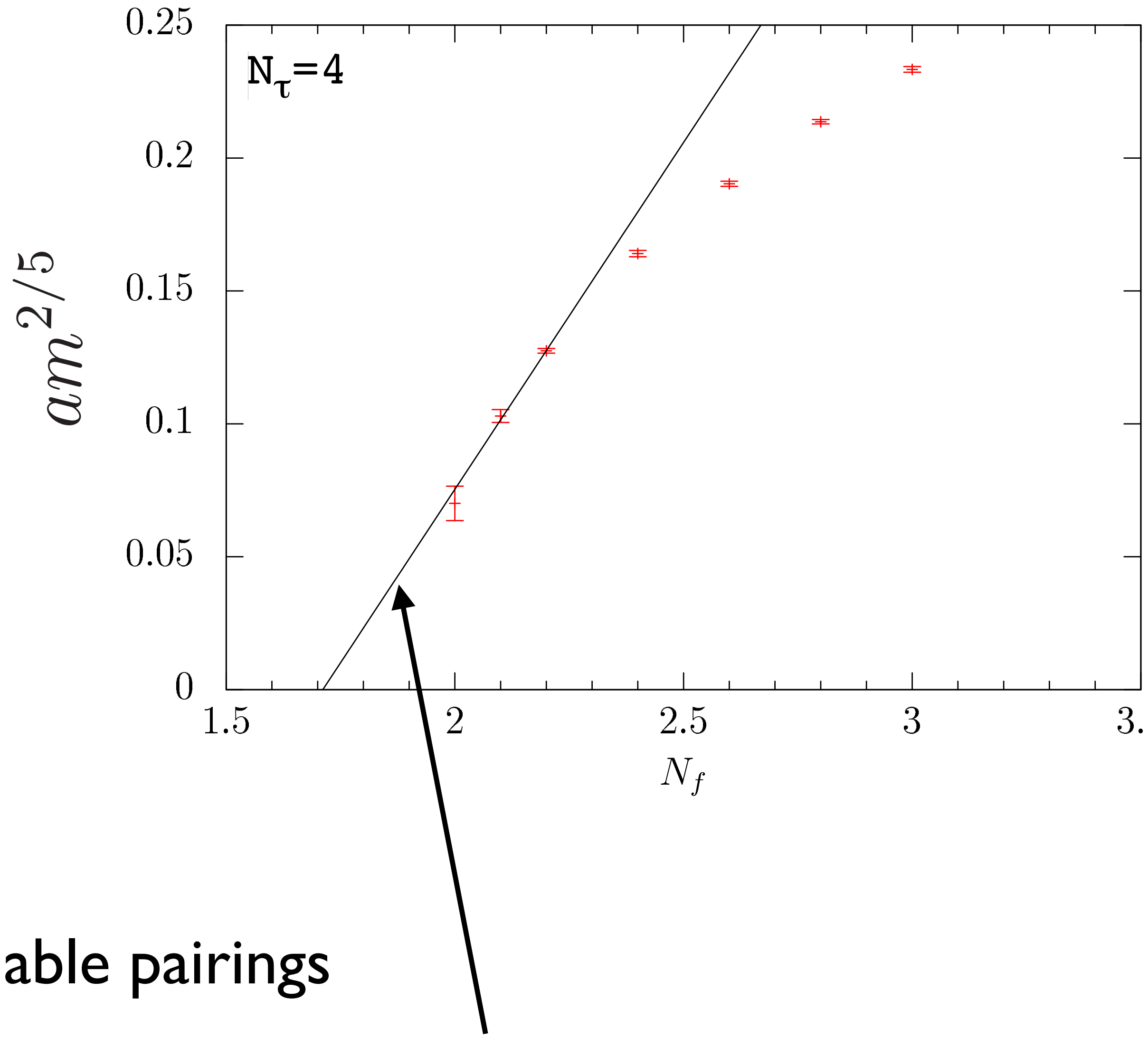
Repeat for different volumes



Bare parameter space of unimproved staggered LQCD

[Cuteri, O.P., Sciarra 21] ~120 M Monte Carlo trajectories with light fermions, aspect ratios 3,4,5

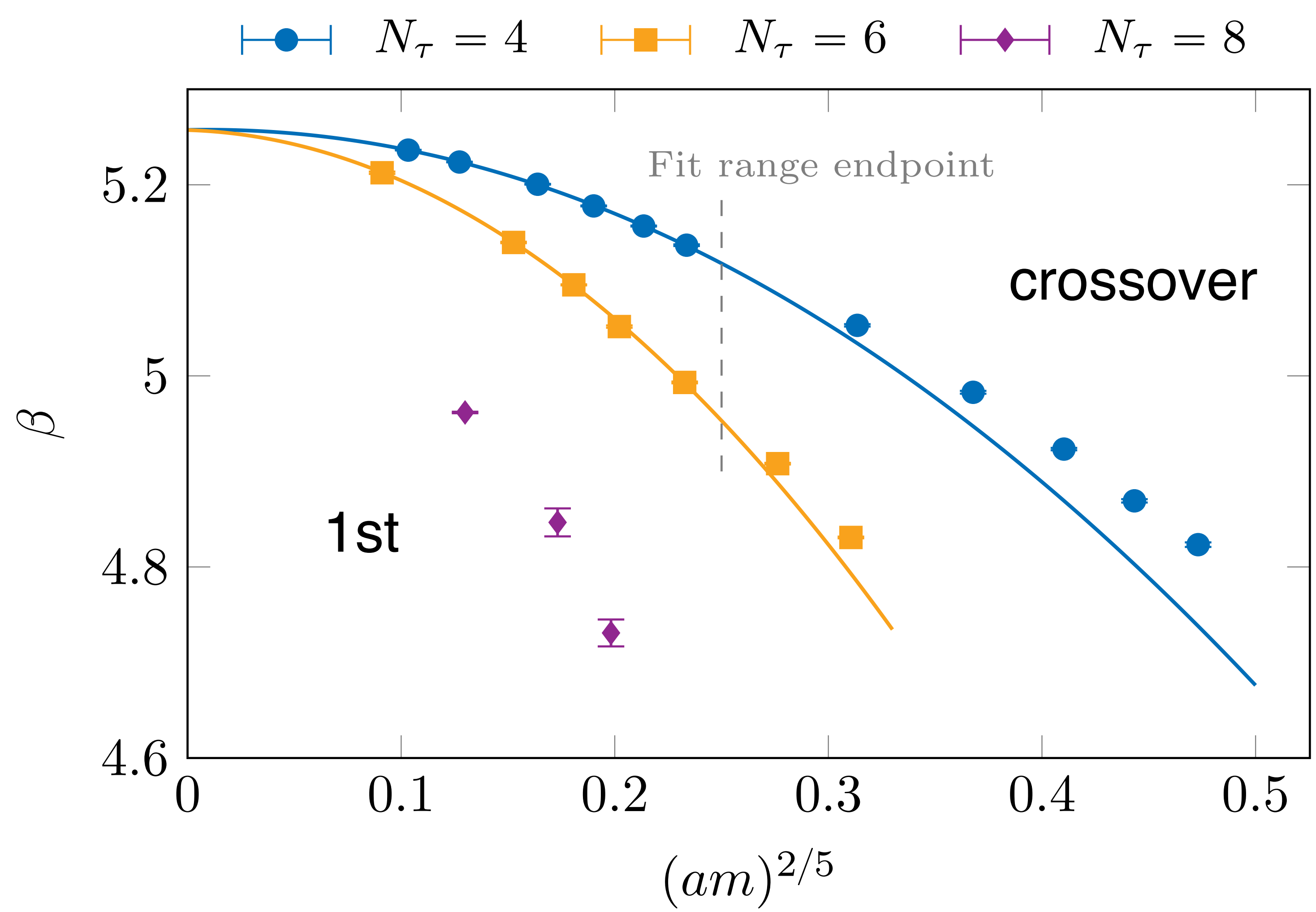




- Tricritical scaling observed in different variable pairings
- Consistent with tric. scaling from finite imaginary μ [Bonati et al. PRD 14]
- Old question: $m_c/T = 0$ or $\neq 0$? Answered for $N_f = 2$
- New question: will $N_f^{\rm tric}$ slide beyond $N_f = 3$?

Bare parameter space of unimproved staggered LQCD

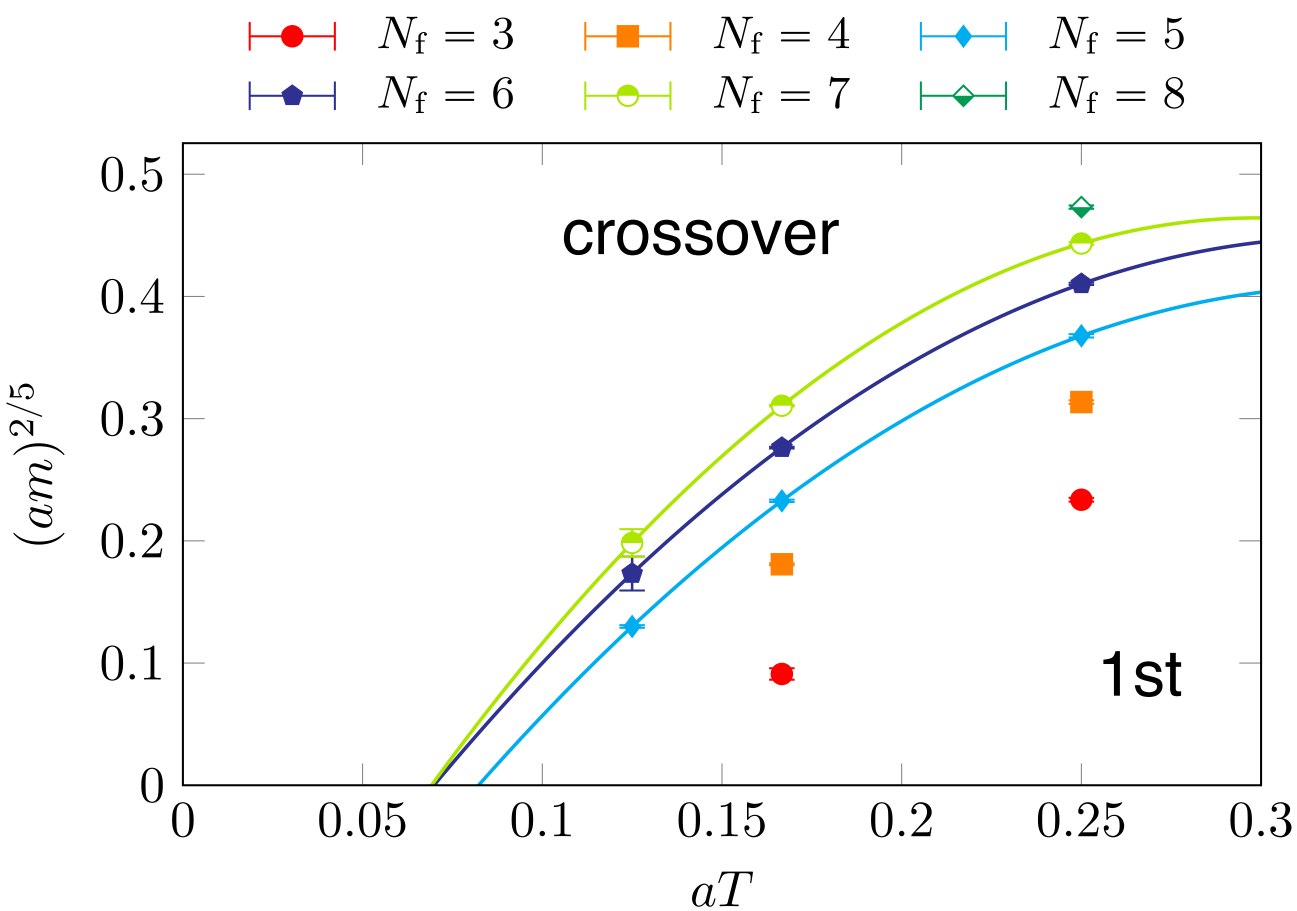
[Cuteri, O.P., Sciarra JHEP 21] ~120 M Monte Carlo trajectories with light fermions, aspect ratios 3,4,5



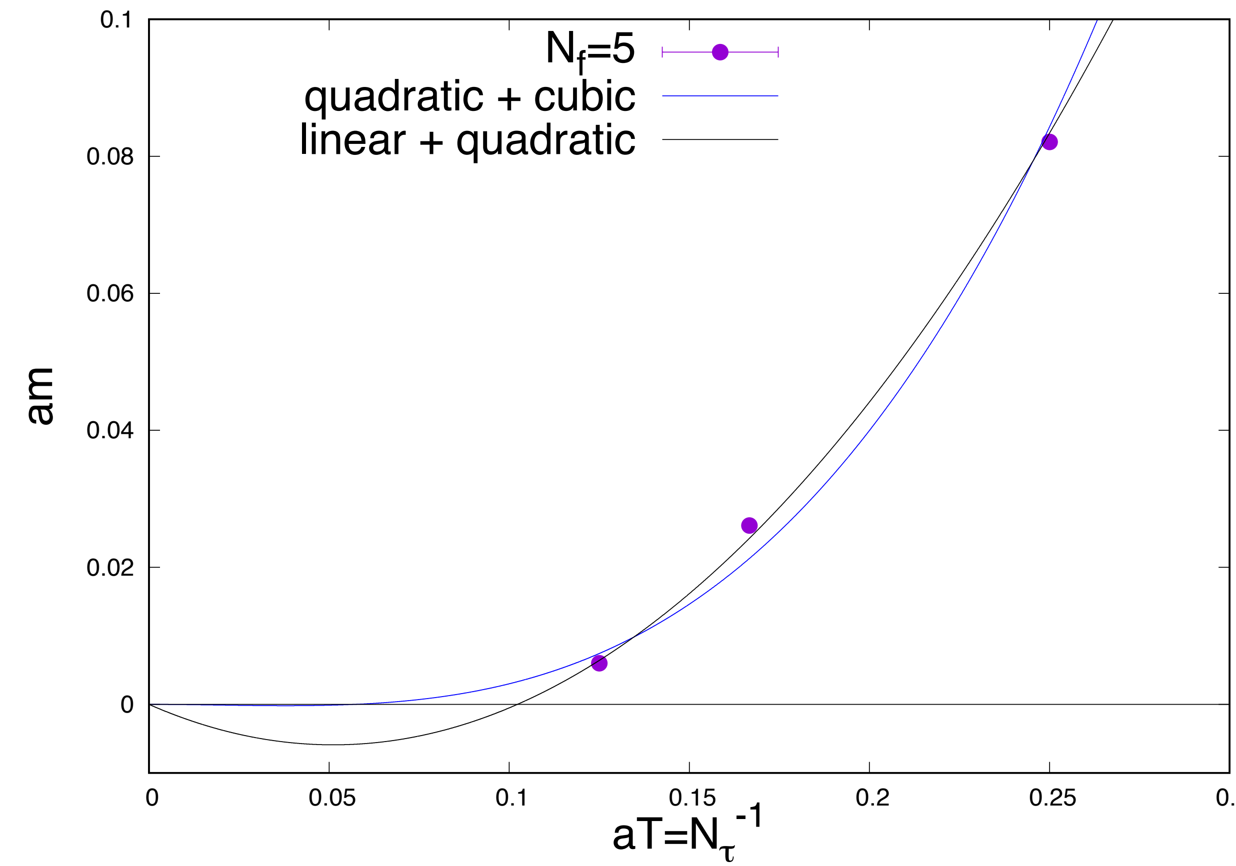
- Data points implicitly labeled by Nf
- Tricritical scaling observed in lattice bare parameter space
- Tricritical extrapolation always possible!

Bare parameter space of unimproved staggered LQCD

[Cuteri, O.P., Sciarra 21]



1st order scenario does not fit!

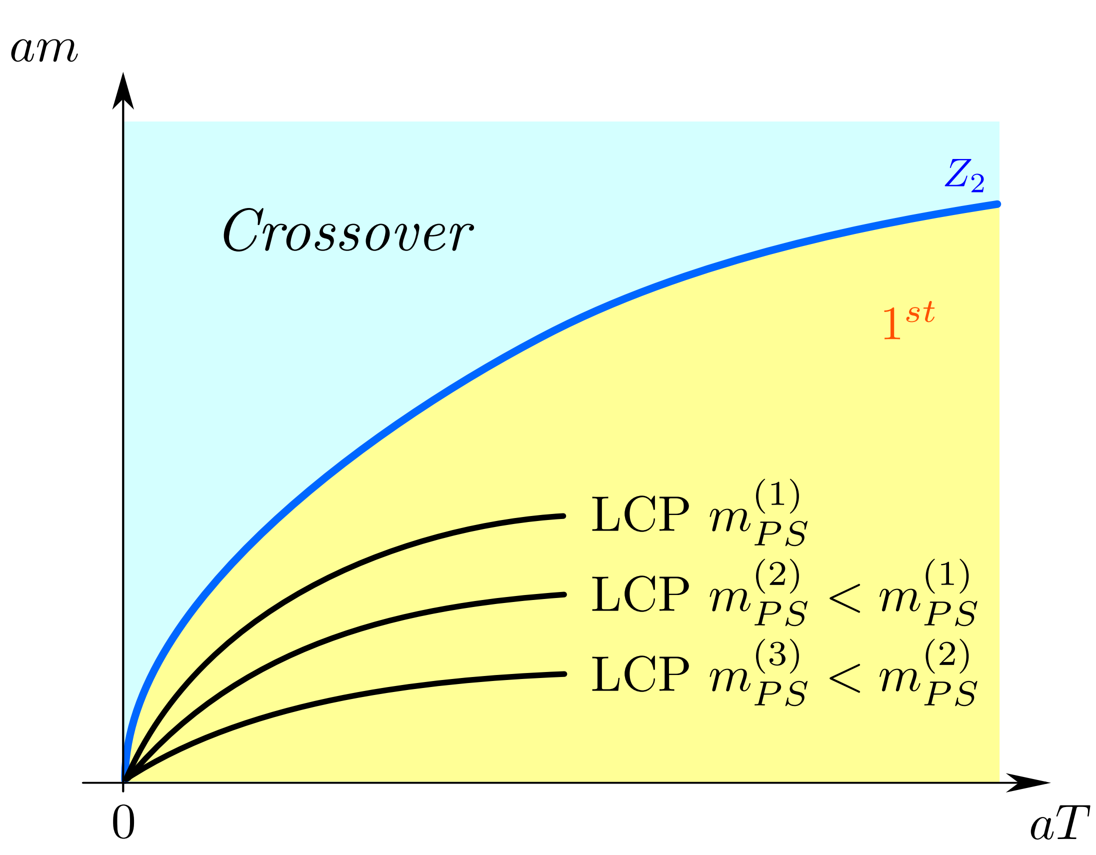


- Tricritical scaling observed also in plane of mass vs. lattice spacing
- Allows extrapolation to lattice chiral limit, tricritical points $N_\tau^{\mathrm{tric}}(N_f)$
- 1st order scenario: $m_c(a) = m_c(0) + c_1(aT) + c_2(aT)^2 + \ldots$

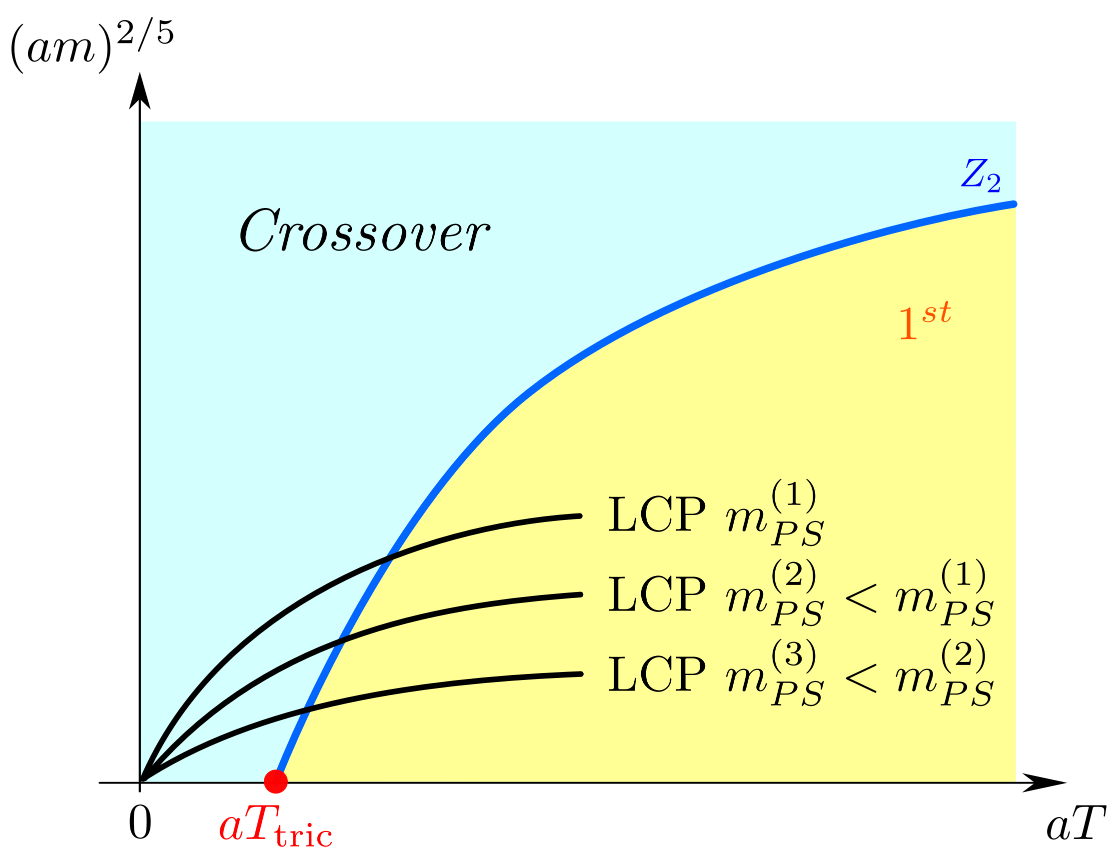
Incompatible with data! $\chi^2_{\mathrm{dof}} > 10$

Implications for the continuum

- Finite $N_\tau^{\text{tric}}(N_f)$ implies that 1st order transition is not connected to continuum
- Approaching continuum first, then chiral limit:
  Continuum chiral phase transition second-order!



1st order scenario

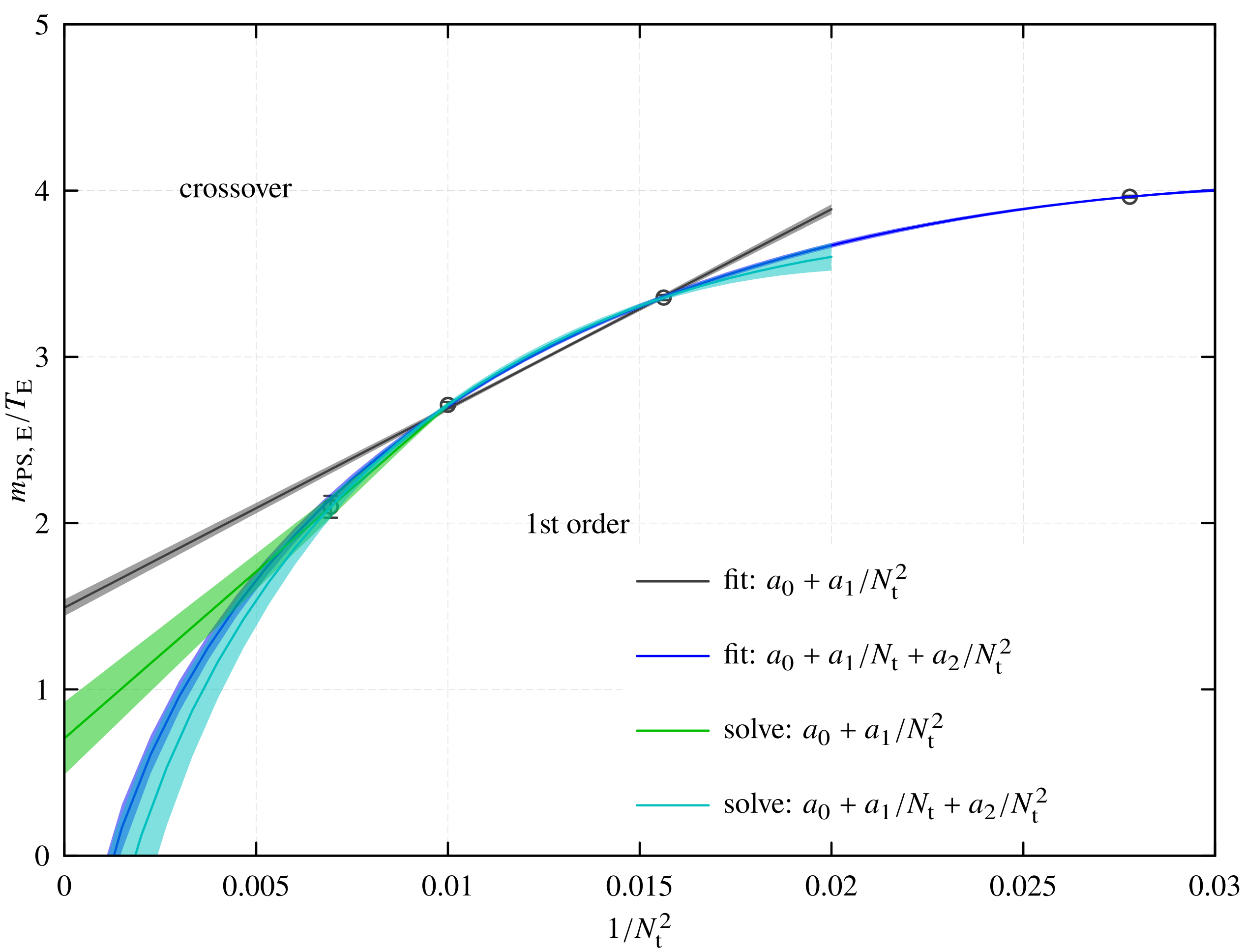


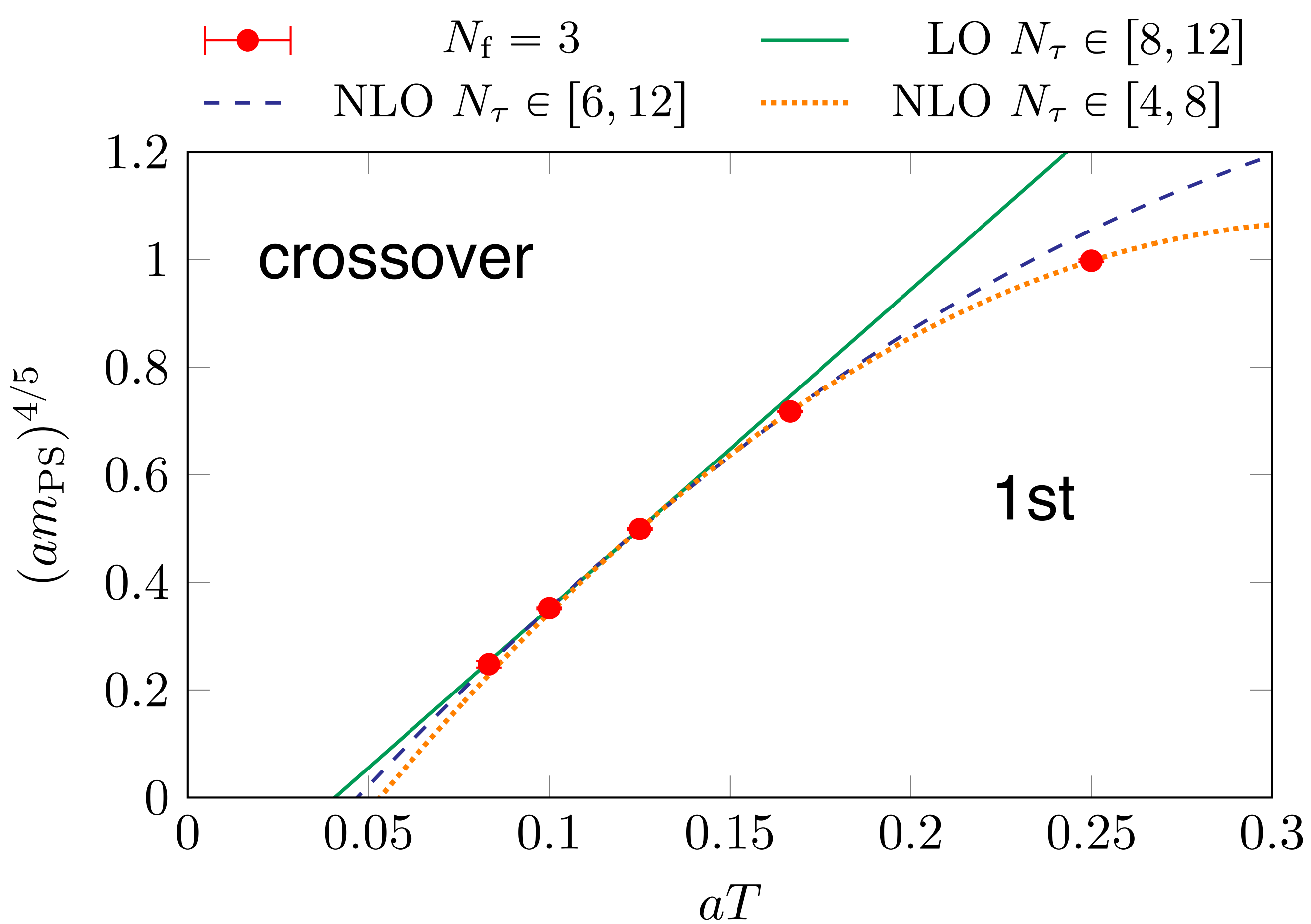
2nd order scenario

Nf=3 O(a)-improved Wilson fermions

[Kuramashi et al. PRD 20] $m_\pi^c \leq 110\ \mathrm{MeV} \quad N_\tau = 4, 6, 8, 10, 12$

Re-analysis using: $am_{PS}^2 \propto am_q$



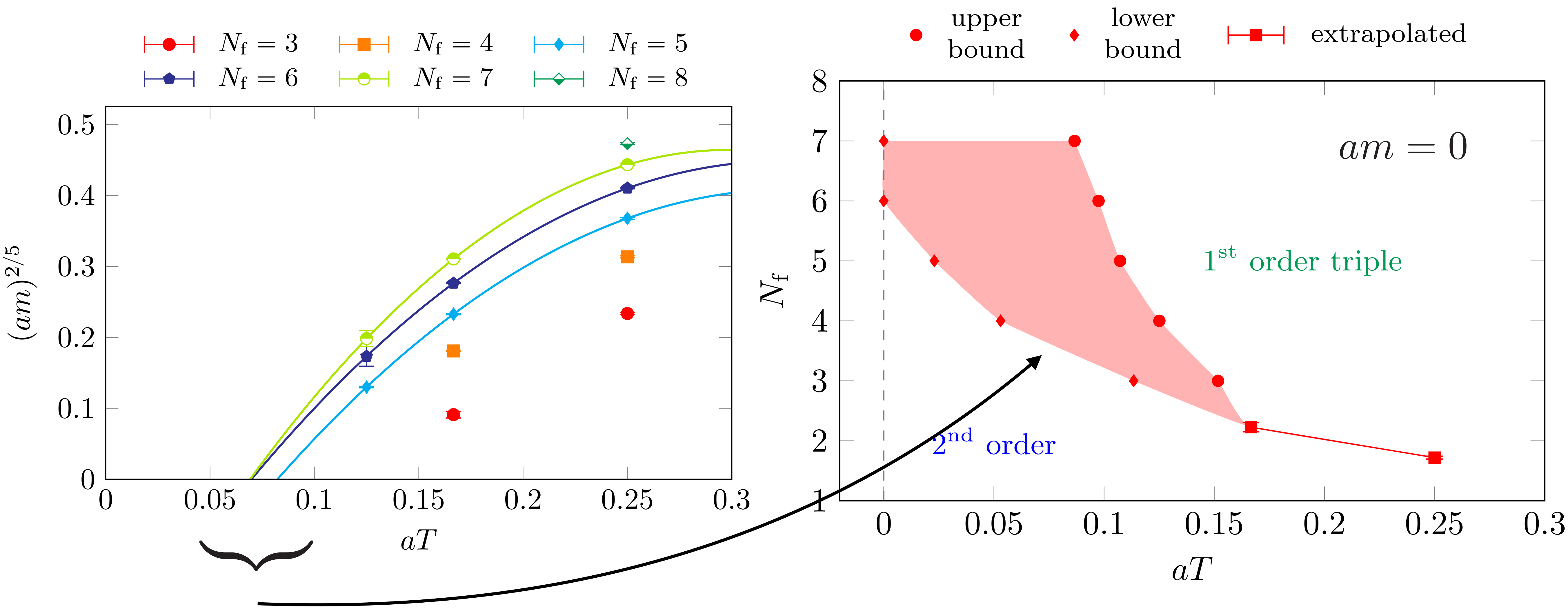


[Cuteri, O.P., Sciarra, JHEP 21]

Tricritical scaling!

Nf=3 consistent with staggered, 2nd order in chiral continuum limit!

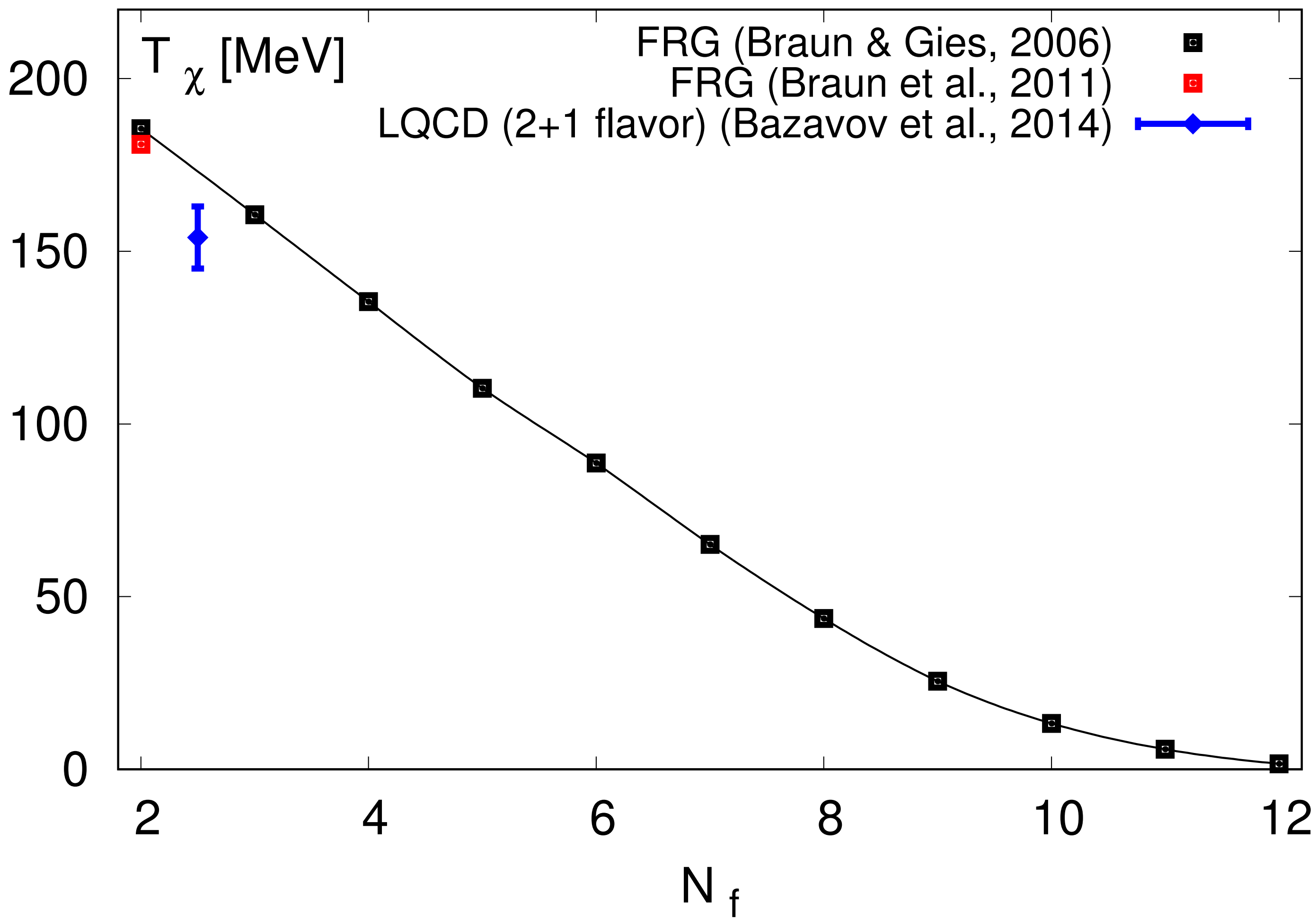
Digression: tricritical points as function of Nf



- $N_\tau^{\mathrm{tric}}(N_f)$ increasing function
- Tricritical line in the plane of the lattice chiral limit, separates 1st from 2nd
- Is there a tricritical point in the continuum?

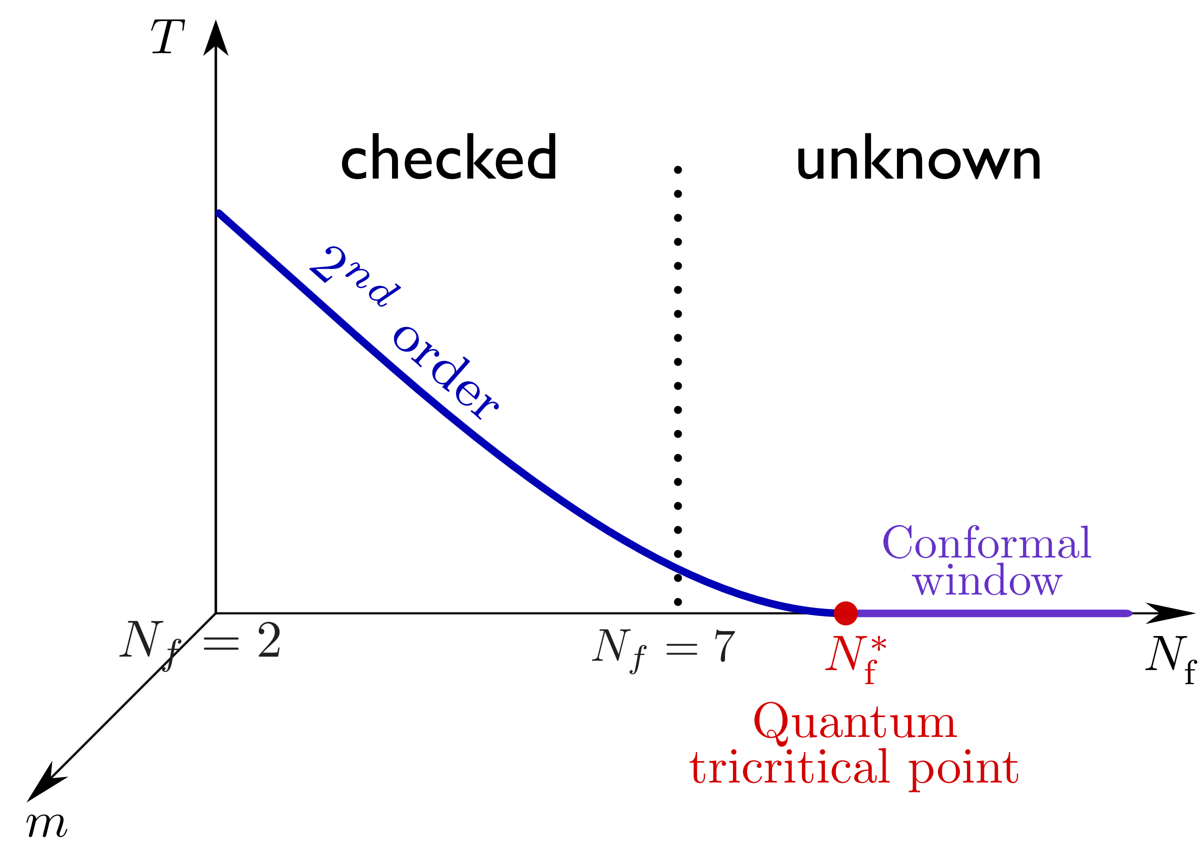
The chiral phase transition for different N_f

Temperature dependence:



For lattice, see [Miura, Lombardo, NPB 13]

Order of the transition:



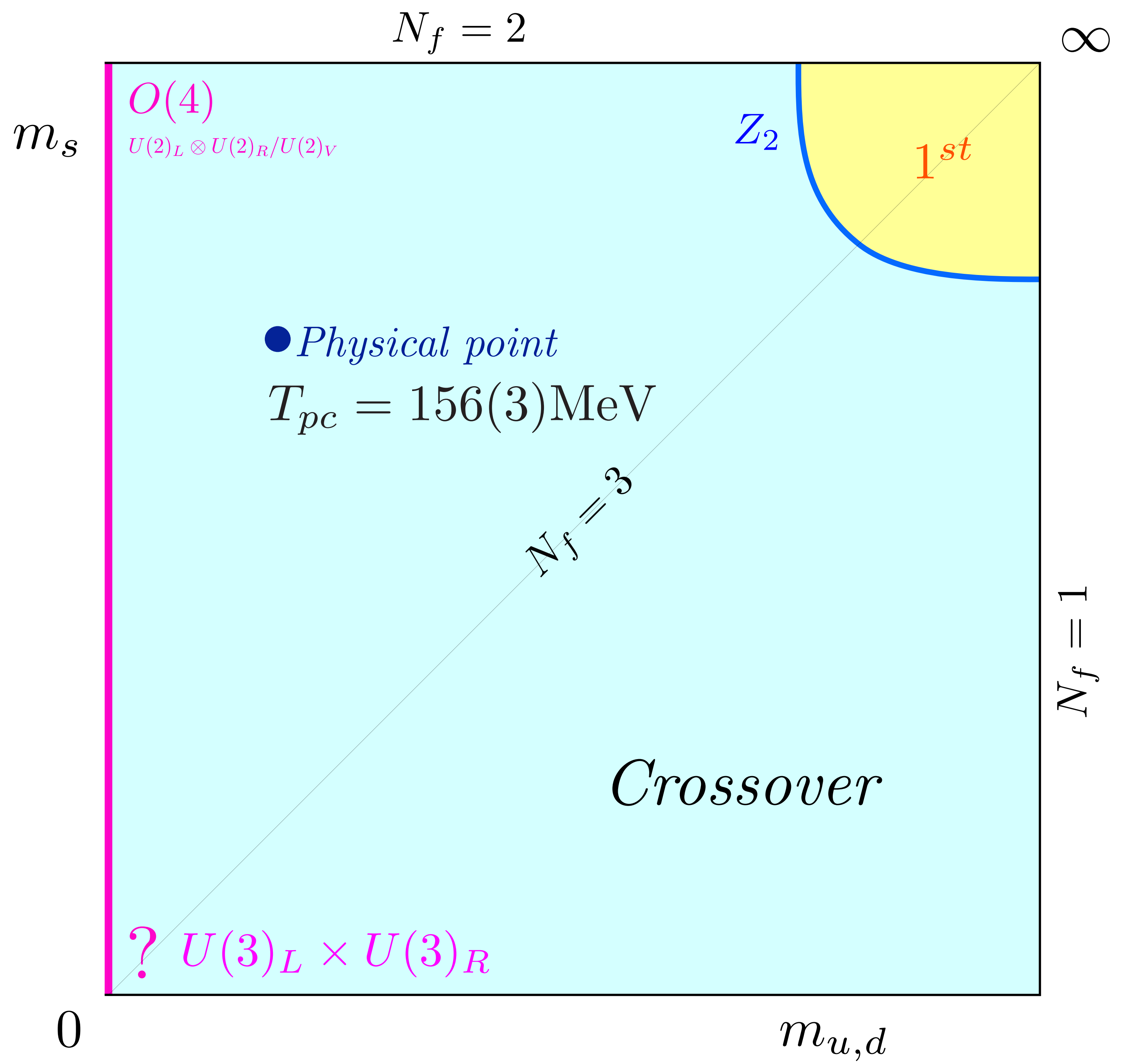
[Cuteri, O.P., Sciarra, JHEP 21]

The chiral phase transition in the massless limit is likely second-order for all N_f

The Columbia plot in the continuum

[Cuteri, O.P., Sciarra JHEP 21]

Universality class?



What about Pisarski, Wilczek 1984?

- 3d ϕ^4 - Ginzburg-Landau-Wilson theory for chiral condensate plus t'Hooft term
- Epsilon expansion about $\epsilon = 1$
- All conclusions confirmed by [Butti, Pelisetto, Vicari, JHEP 03]
  (High order perturbative expansion in fixed d)
- Support also from simulation of 3d sigma model [Gausterer, Sanielovici, PLB 88]

Suggested resolution: ϕ^6 term, in 3d renormalisable; even higher powers…..?

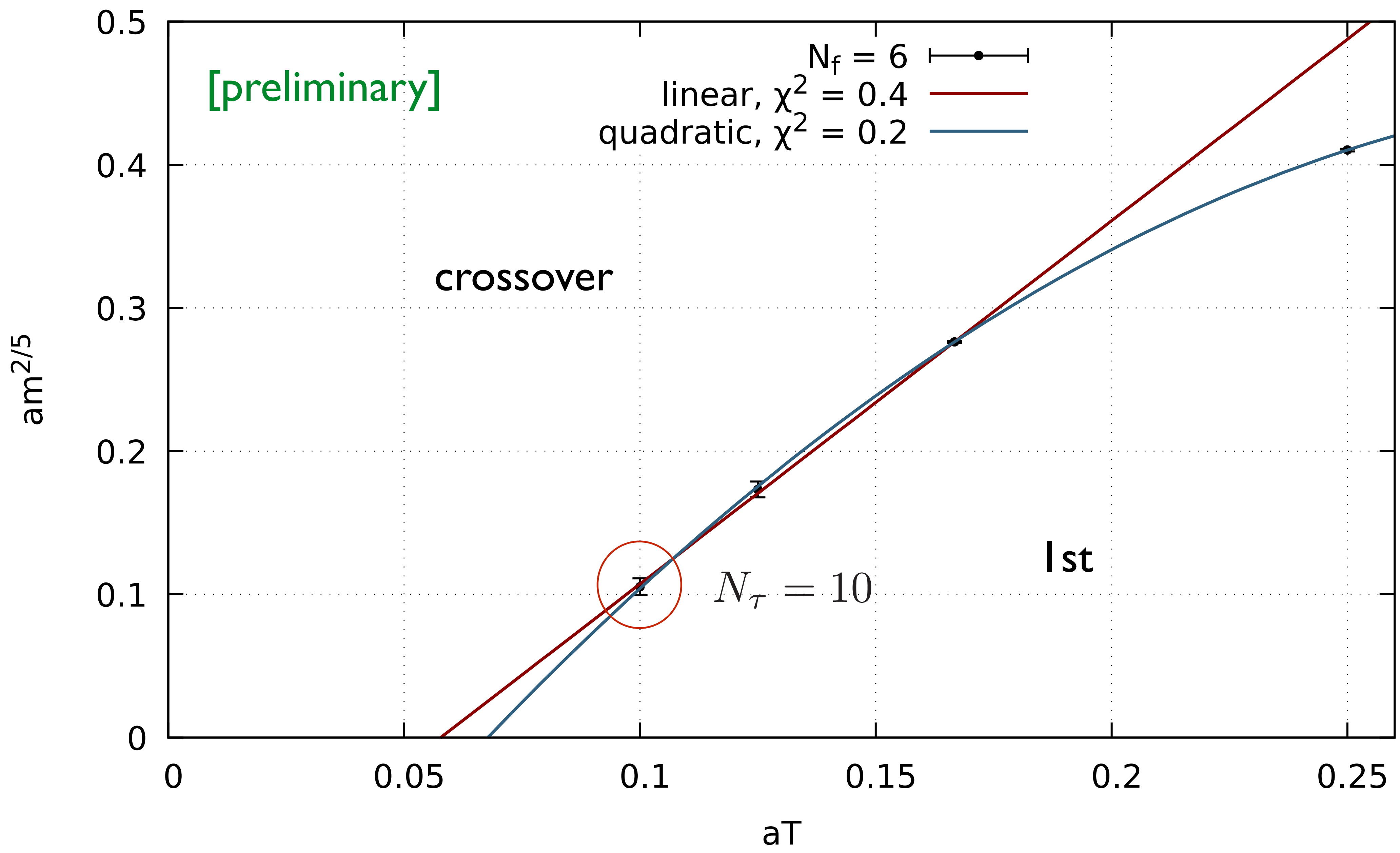
[Fejos, PRD 22] 3d ϕ^6 with t'Hooft term, functional RG study:
IR-stable fixed point, 2nd order transition for restored anomaly

[Kousvos, Stergiou, SciPost 23] Numerical conformal bootstrap:
U(3)xU(3) displays IR stable fixed point

No contradictions!

Meanwhile in Frankfurt...

progressing to finer lattices



New $N_\tau = 10$ result on predicted scaling curve!

The Columbia plot in the continuum

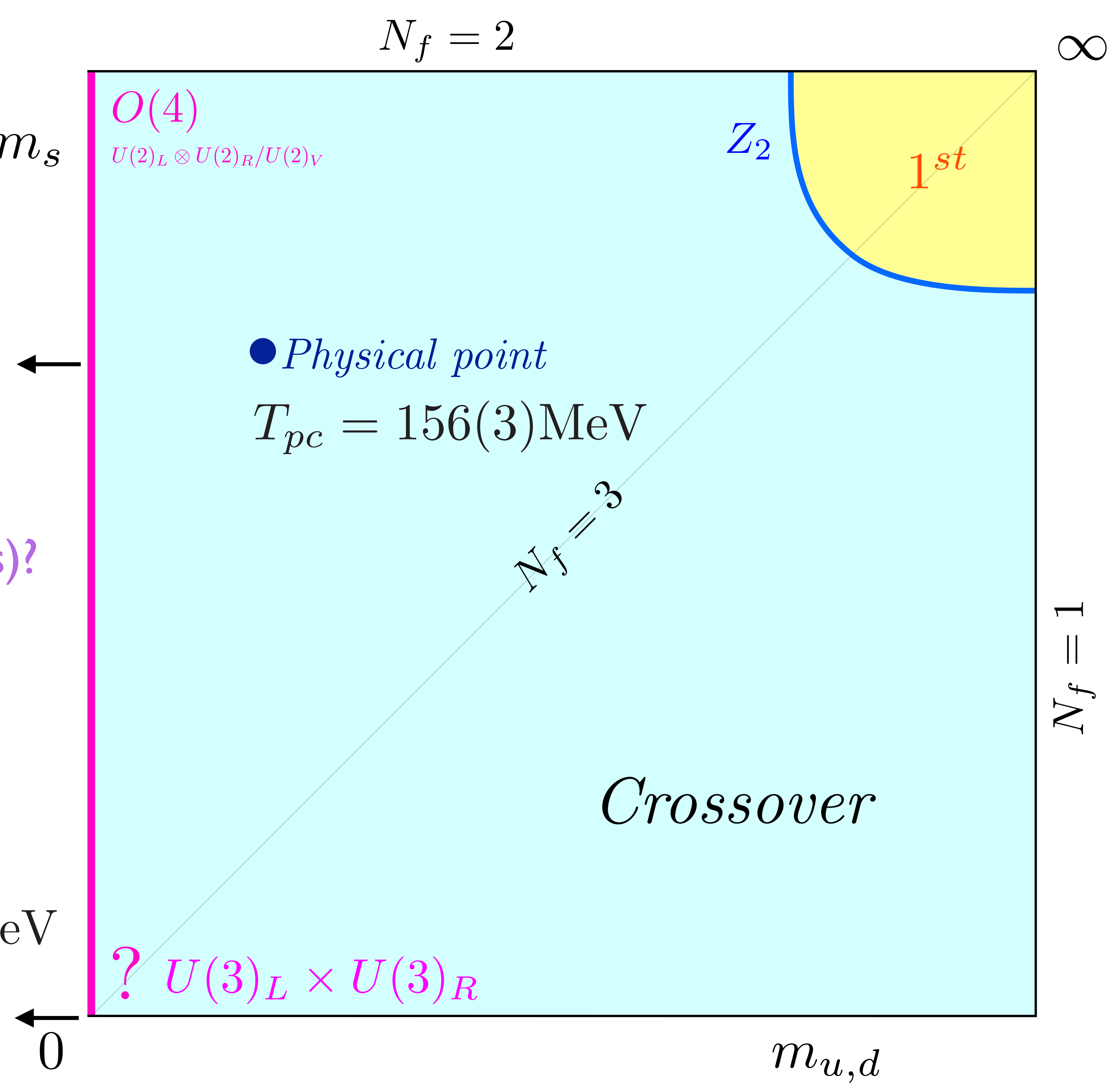
[Cuteri, O.P., Sciarra JHEP 21]

[HotQCD PRL 19]
$T_c^0 = 135(8)\text{MeV}$

Universality class(es)?

[HotQCD PRD 22]

HISQ, crossover
down to $m_\pi \approx 45\text{MeV}$
$T_c^0 = 98(6)\text{MeV}$



Crossover for DW fermions, Nf=3, $m_q \sim m_{phys}$ [Zhang et al., PoS LAT22]

QCD with imaginary chemical potential

Motivation: no sign problem!

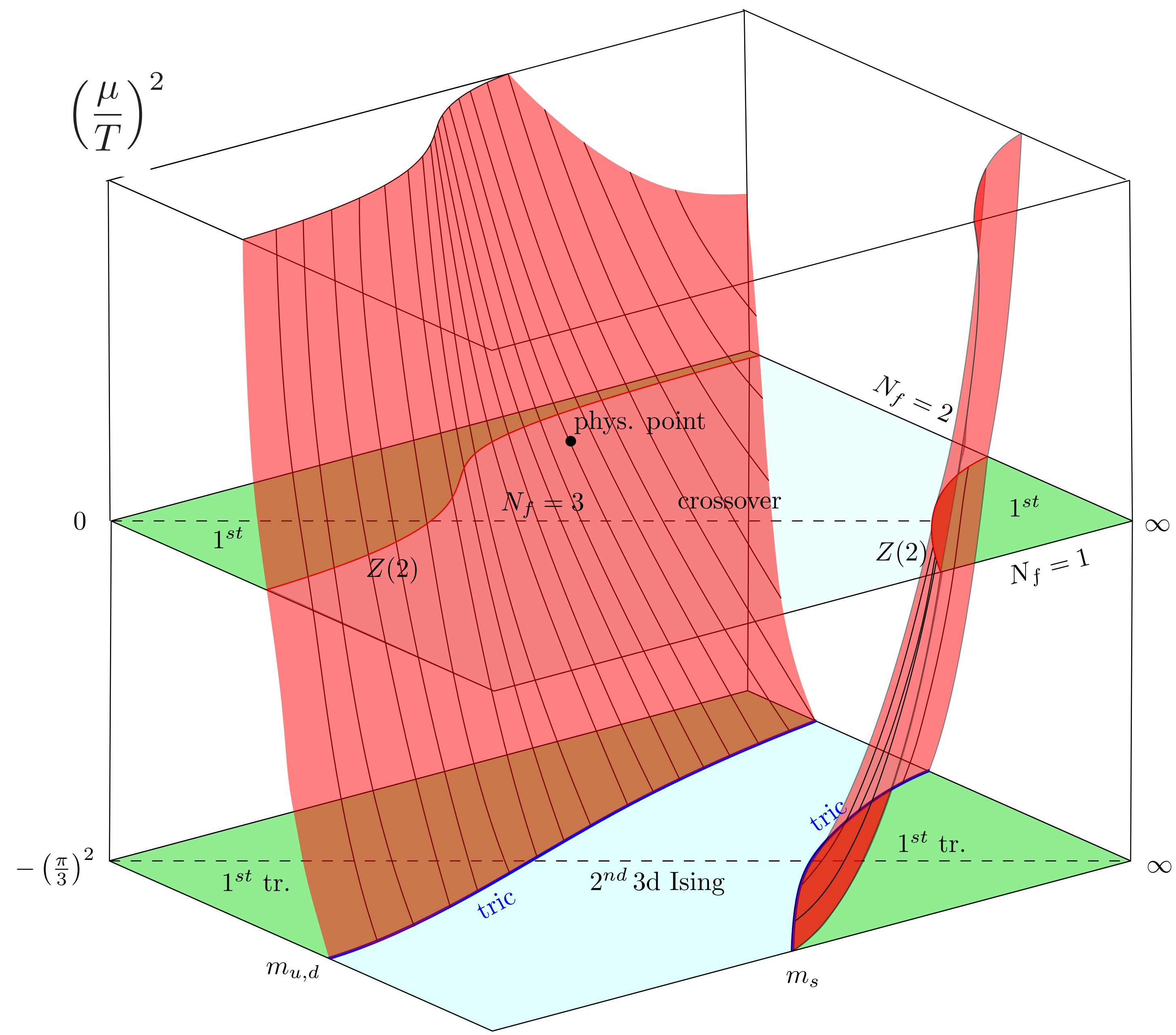
Roberge-Weiss (center) symmetry: $Z\left(T, i\frac{\mu_i}{T}\right) = Z\left(T, i\frac{\mu_i}{T} + i\frac{2n\pi}{N_c}\right)$

Results from coarse lattices: $N_\tau = 4$

Chiral critical surface analytic around $\mu_B = 0$, negative curvature

[de Forcrand, O.P. 07]

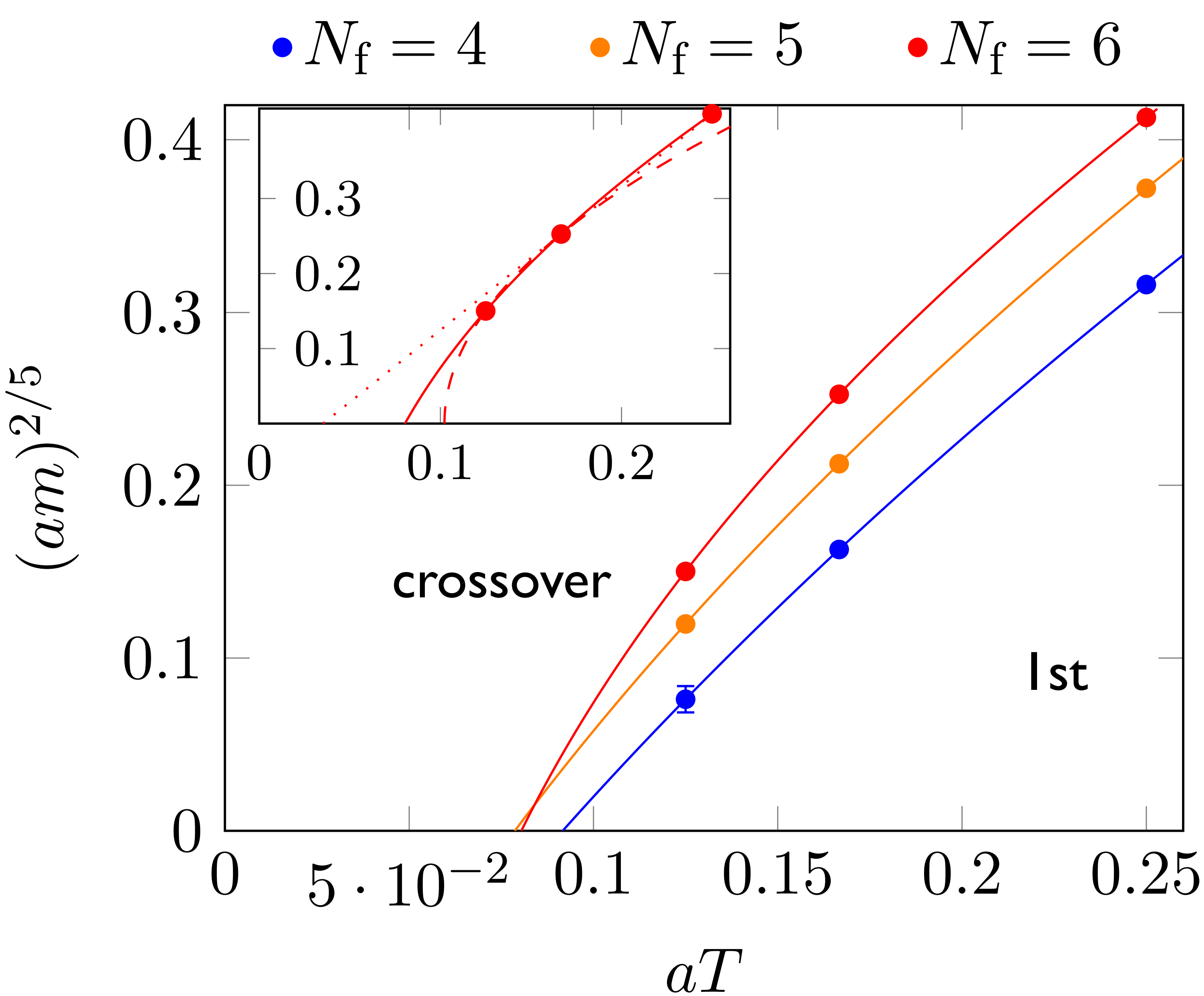
Details and reference list:
[O.P., Symmetry 13, 2021]



Imaginary chemical potential: cutoff effects

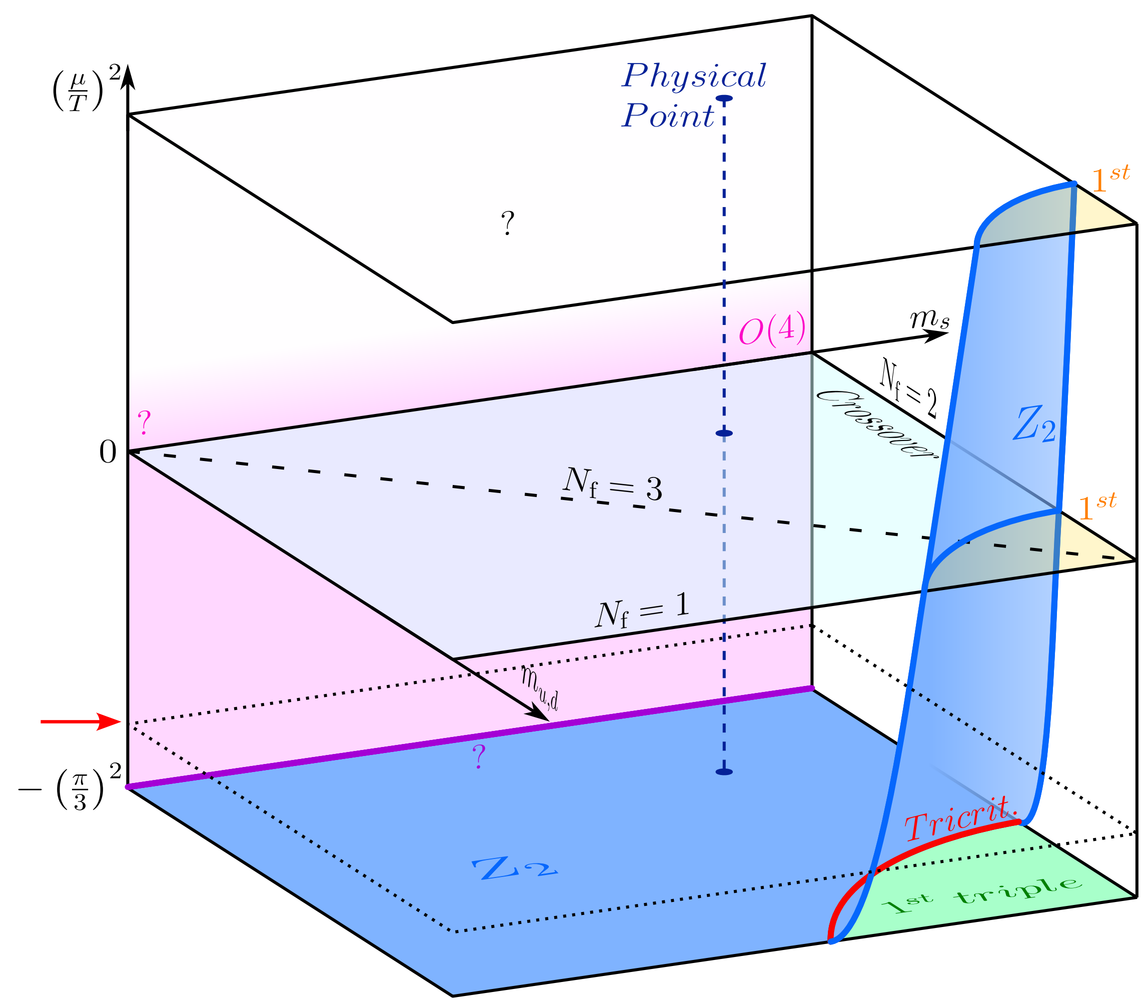
[D'Ambrosio, Fromm, Kaiser, O.P., in progress]

Repeat study of Columbia plot with $\mu = i\,0.81\pi T/3$



Same situation as $\mu = 0$

1st-order region not connected to continuum limit!



Imaginary chemical potential, improved actions

$\mu = i\pi T/3$ Roberge-Weiss boundary

- [Bonati et al., PRD 19]
  stout-smeared staggered $N_\tau = 4$

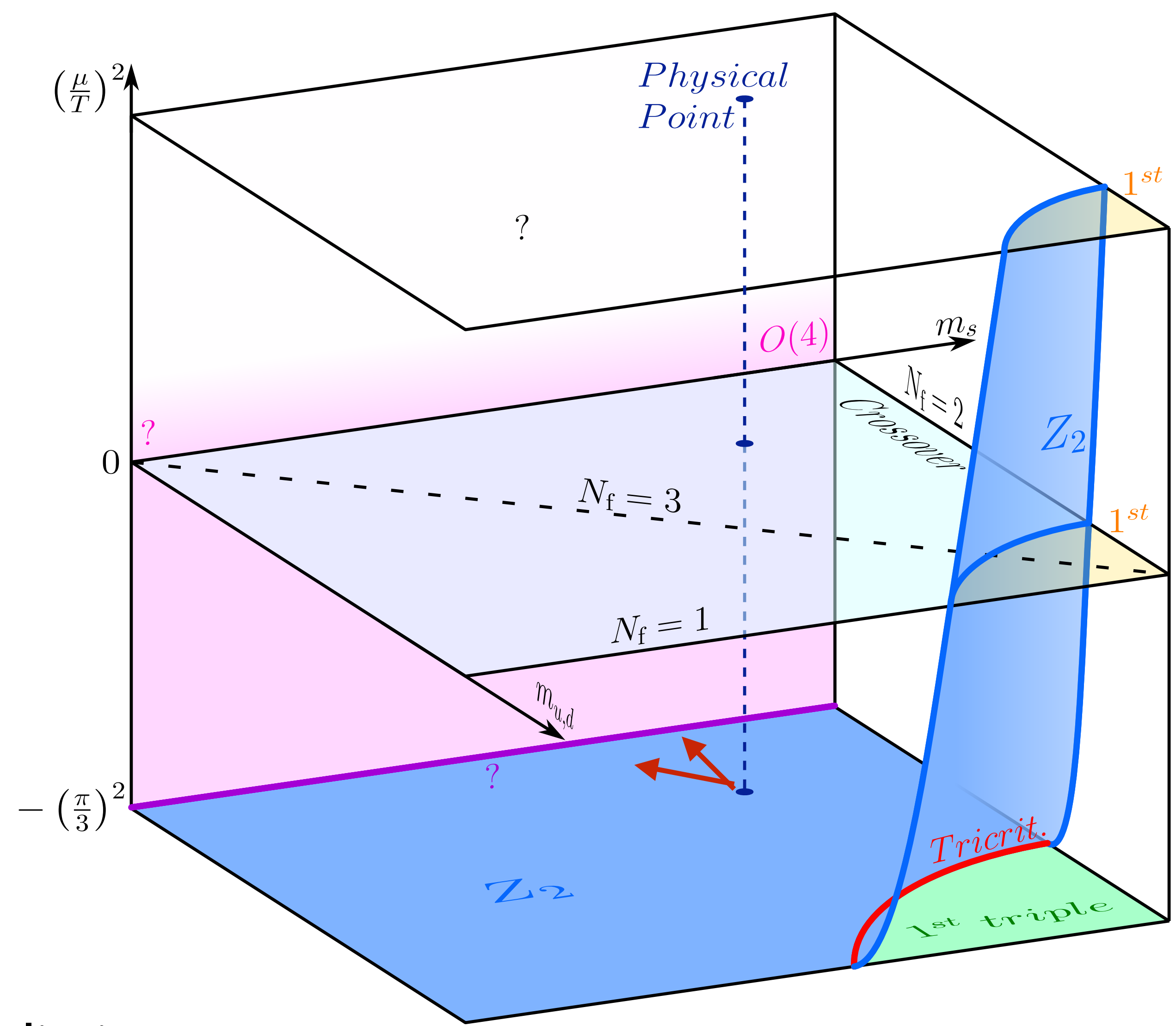
  quark mass scan down to $m_\pi \approx 50\ \mathrm{MeV}$
  fixed m_{ud}/m_s

- [Bielefeld+Frankfurt, PRD 22]
  HISQ $N_\tau = 4$

  quark mass scan down to $m_\pi \approx 55\ \mathrm{MeV}$
  fixed m_s

- No sign of 1st-order phase transition!

- Entire chiral critical surface moves to massless limit



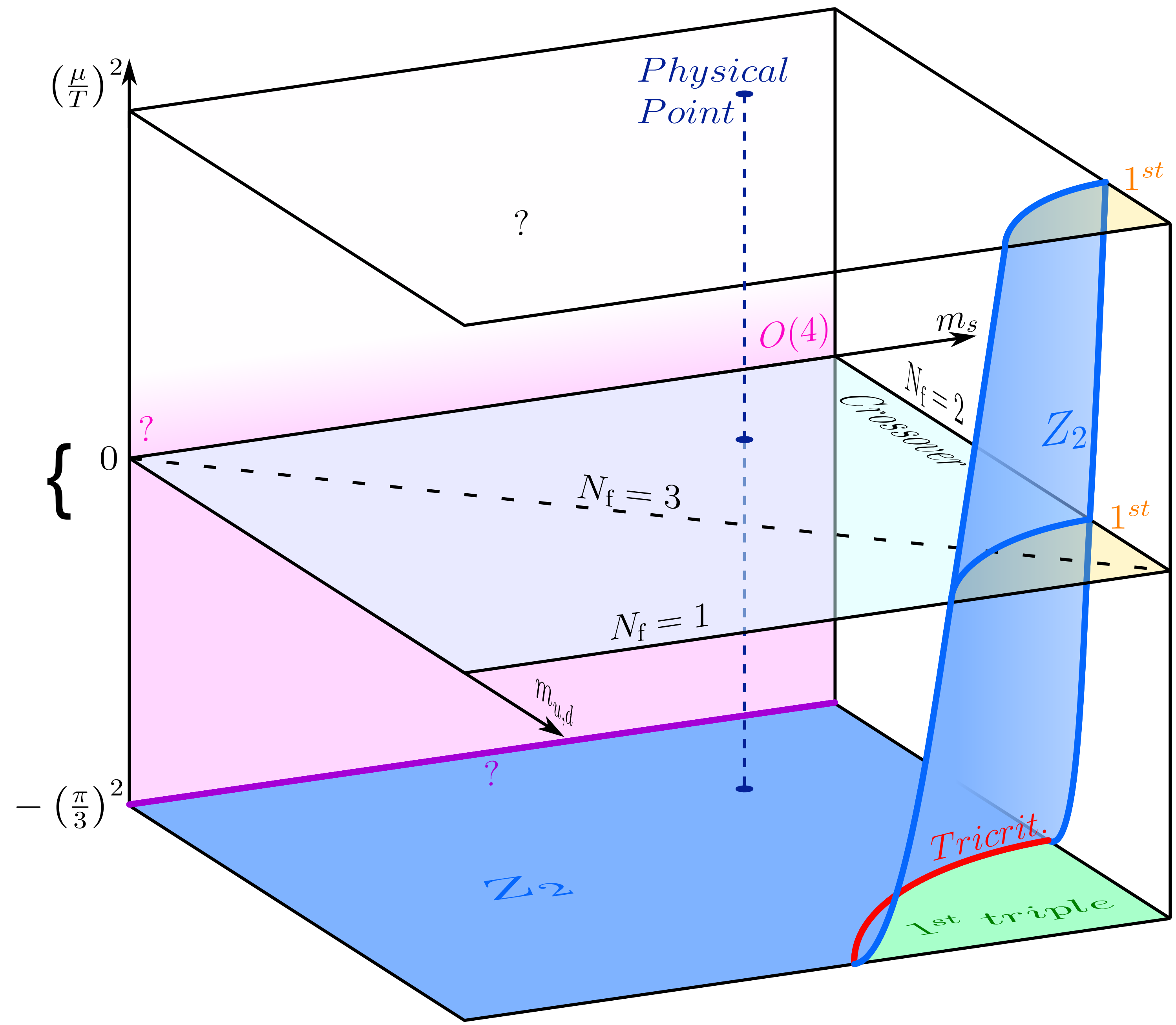
Columbia plot with chemical potential, continuum

[Bernhardt, Fischer, arXiv:2309.06737]

Dyson-Schwinger eqs. $|\mu| \leq 30\text{MeV}$

Same picture

Columbia plot analytic around $\mu = 0$

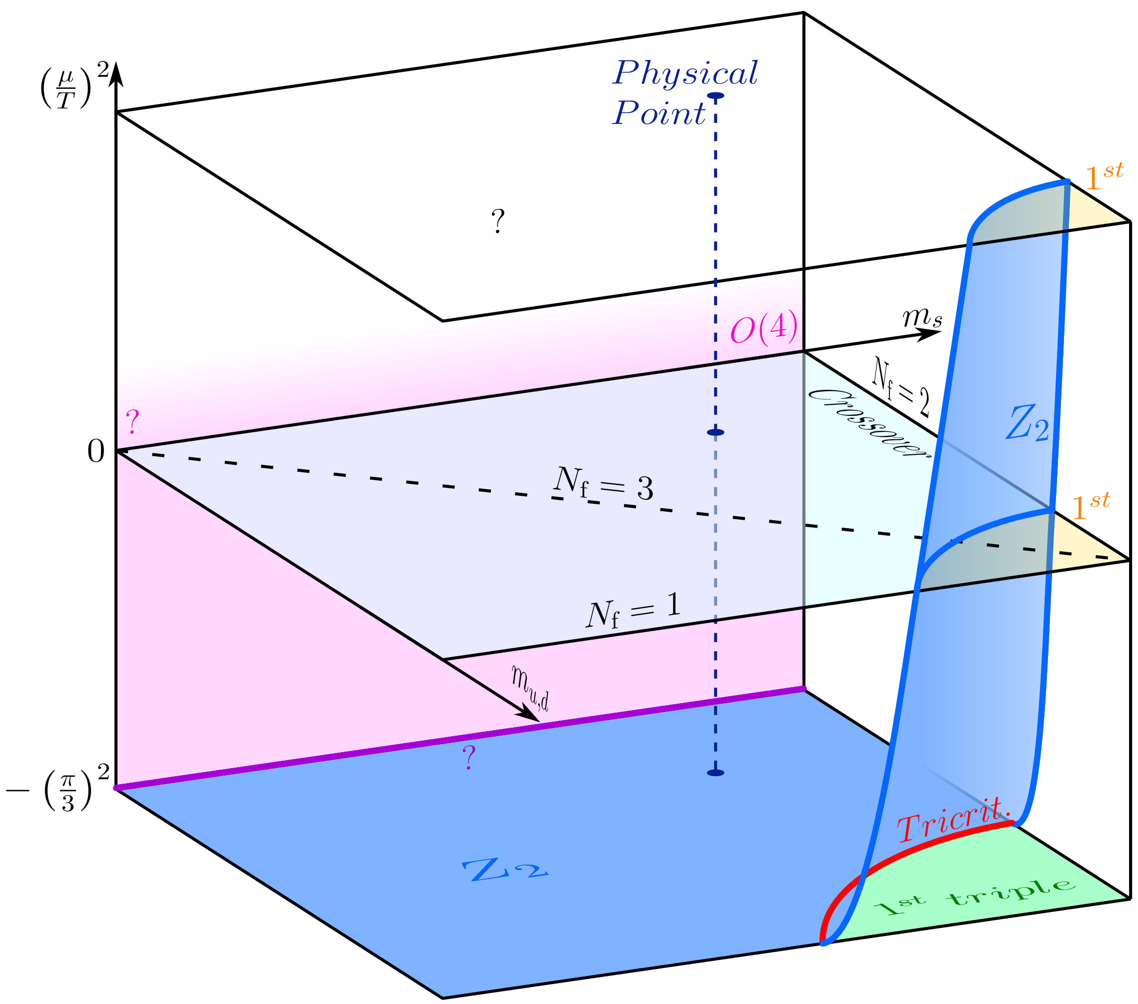


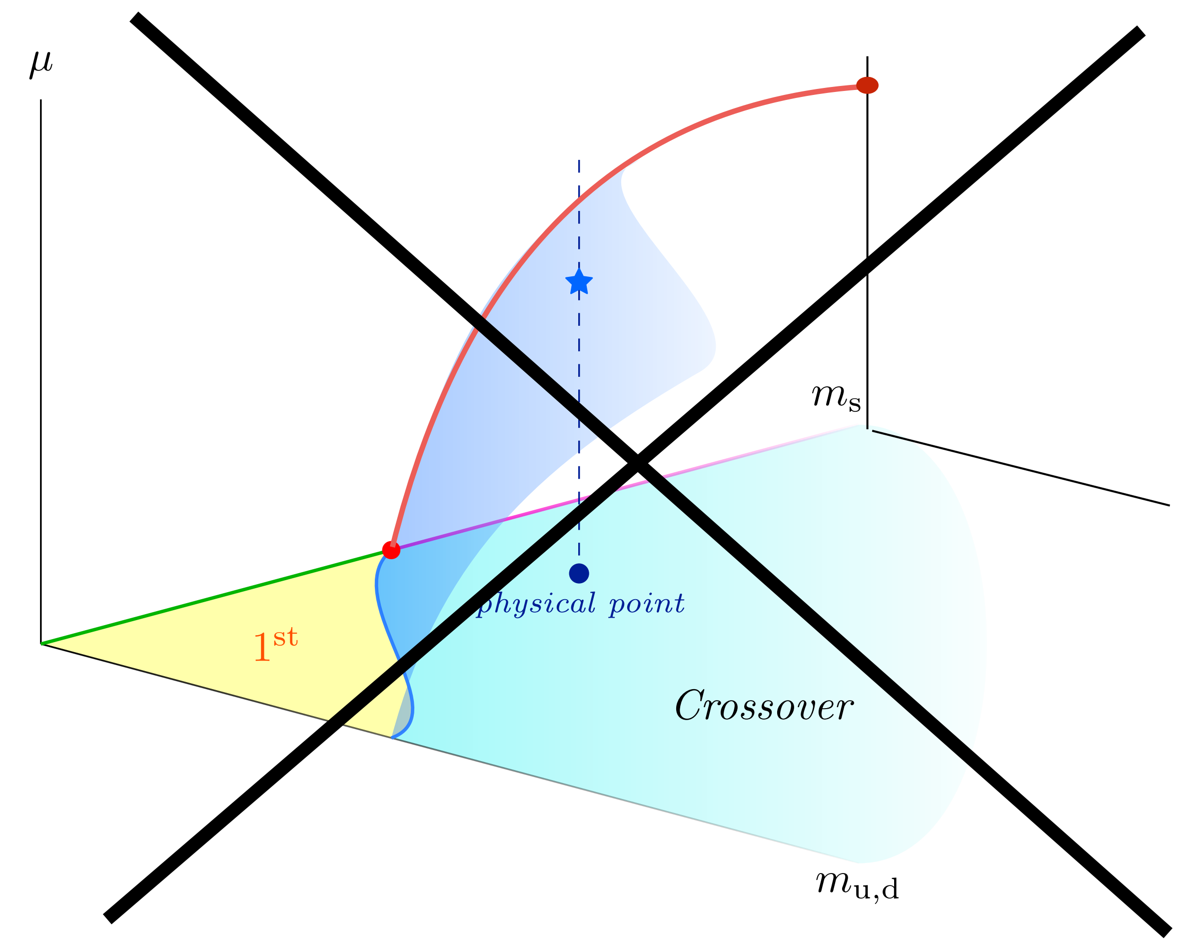
Columbia plot with chemical potential, continuum

Critical point not ruled out

But requires additional critical surface

Class of low energy models now ruled out

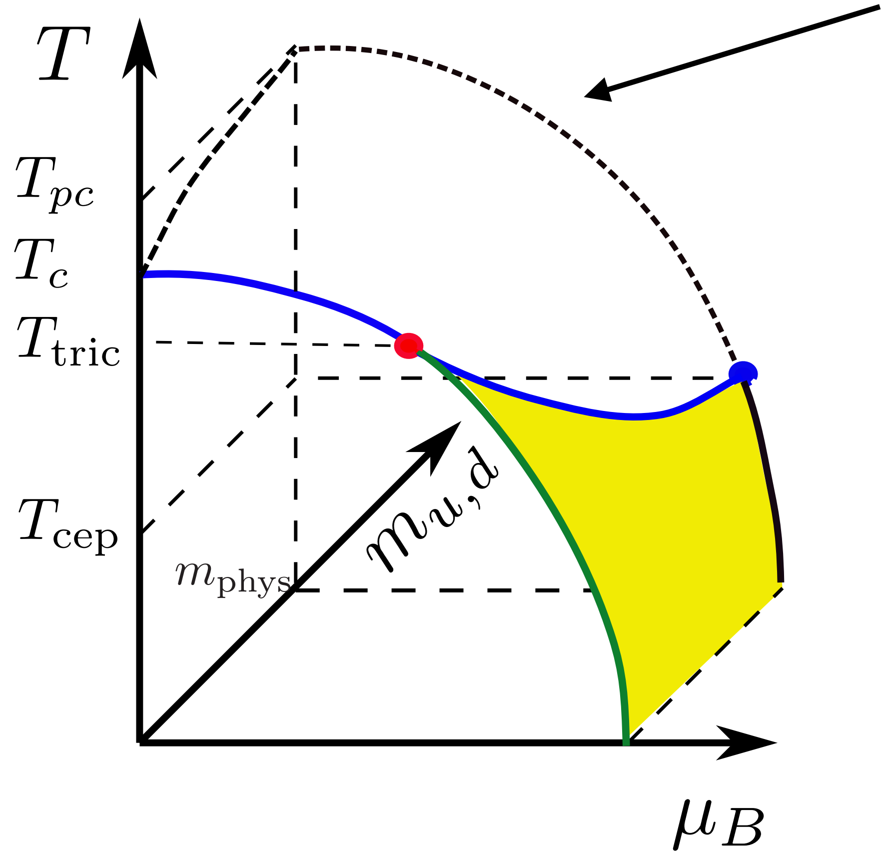




No tuning of parameters in $N_f = 2+1$ theory with critical point at $\mu = 0$

From the chiral limit back to the physical point

The "standard scenario":



$$\frac{T_{pc}(\mu_B)}{T_{pc}(0)} = 1 - \kappa_2 \left(\frac{\mu_B}{T_{pc}(0)} \right)^2 + \dots$$

κ_2	Action	
0.0158(13)	imag. μ, stout-smeared staggered	[Bellwied et al, PLB 15]
0.0135(20)	imag. μ, stout-smeared staggered	[Bonati et al, NPA 19]
0.0145(25)	Taylor, stout-smeared staggered	[Bonati et al, PRD 18]
0.016(5)	Taylor, HISQ	[HotQCD, PLB 19]

$T_{pc} > T_c > T_{\rm tric} > T_{\rm cep}$ → $\mu_B^{\rm cep} > 3.1\ T_{pc}(0) \approx 485$ MeV

Physical point: modelling lattice fluctuations

$$\frac{p(T,\mu_B)}{T^4} = \frac{p(T,0)}{T^4} + \sum_{n=1}^{\infty} \frac{1}{2n!} \chi_{2n}^B(T) \left(\frac{\mu_B}{T}\right)^{2n}$$

search for radius of convergence

Example: baryon number density at imag. μ_B

$$\left. \frac{\rho_B(T,\mu_B)}{T^3} \right|_{\mu_B = i\,\theta_B\,T} = i \sum_{k=0}^{\infty} b_k(T) \sin\left(\frac{k\mu_B}{T}\right)$$

Coefficients computable on the lattice
[Wuppertal-Budapest, Vovchenko et al., PLB 2017]

$$b_k(T) = \frac{2}{\pi} \int_0^{\pi} \mathrm{Im}\left[\frac{\rho_B(T, i\theta_B T)}{T^3}\right] \sin(k\,\theta_B)\, d\theta_B$$

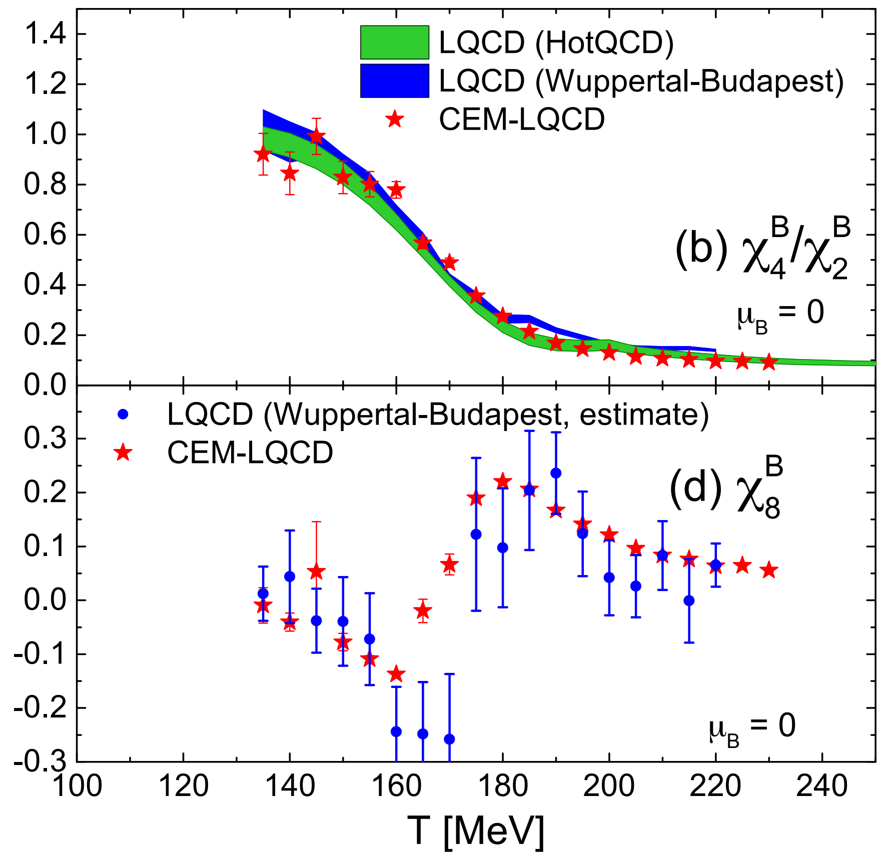
Cluster expansion model (CEM) [Vovchenko et al., PRD 2018]:

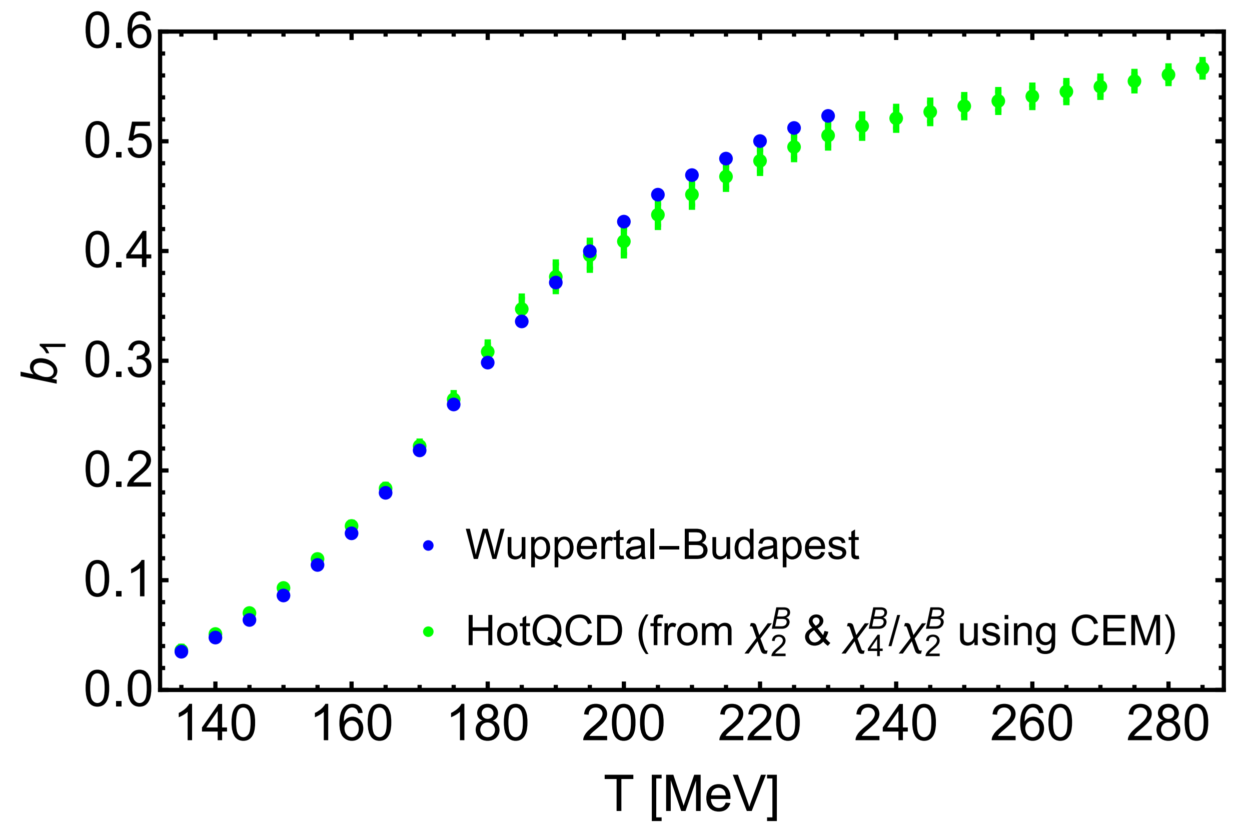
$$b_k(T) = \alpha_k^{\mathrm{SB}} \frac{[b_2(T)]^{k-1}}{[b_1(T)]^{k-2}}, \qquad k = 3, 4, \ldots$$

b_1, b_2 input from the WB-lattice data, α_k^{SB} fixed to Stefan-Boltzmann,
all higher coefficients are model predictions

Physical point: modelling fluctuations

[Vovchenko et al., PoS Corfu 2018; NPA 2018]

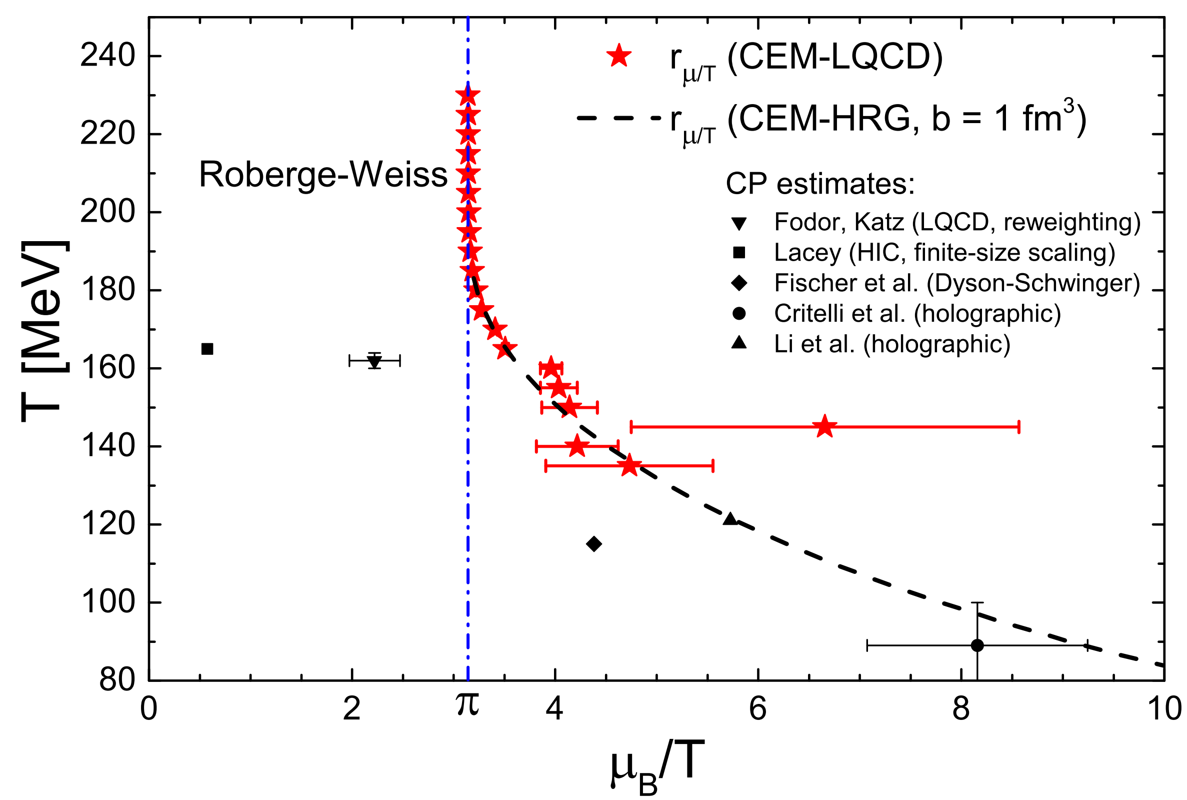




CEM prediction: [Vovchenko et al. PRD 18]

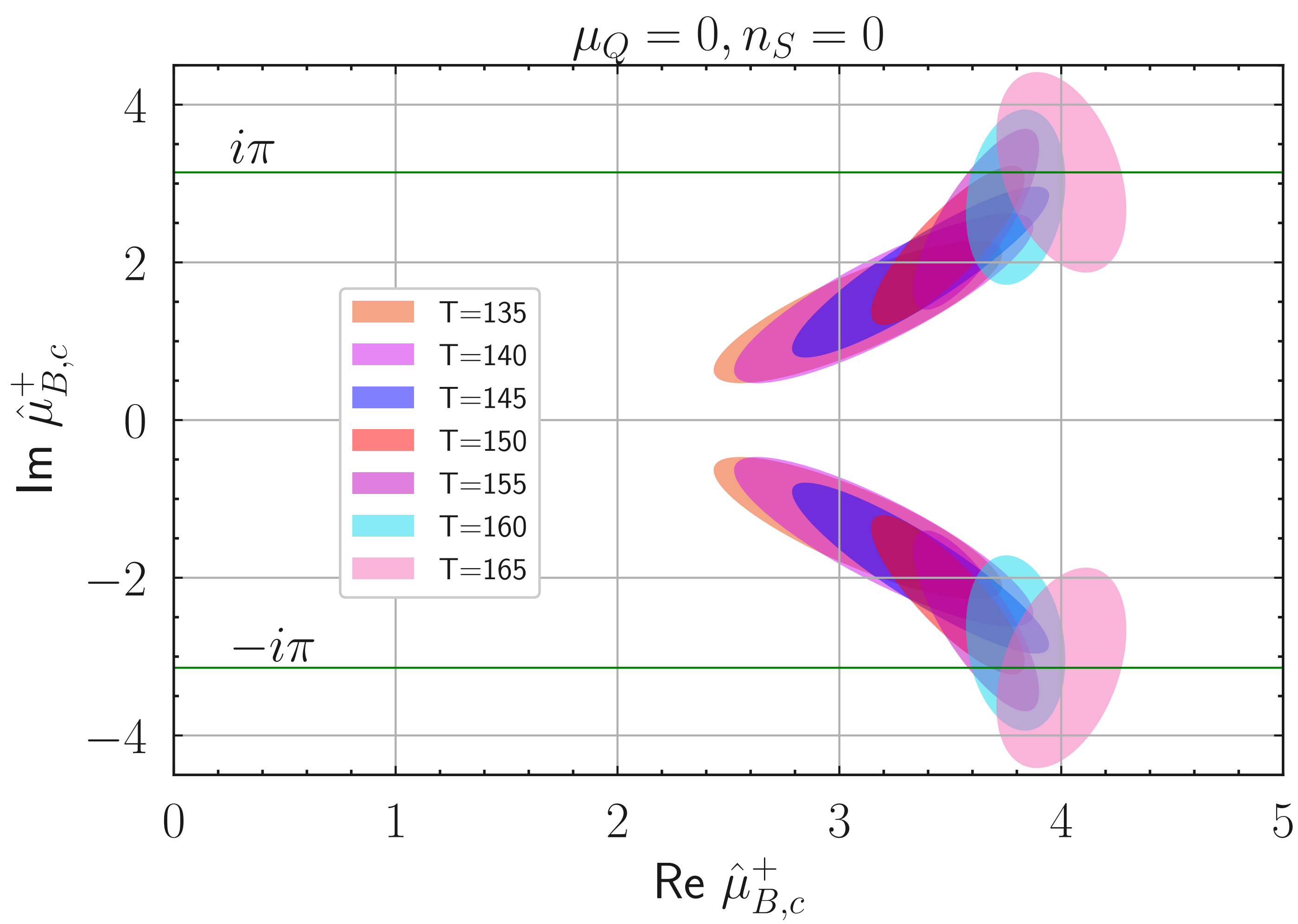
Closest singularity in complex plane is Roberge-Weiss transition

$$\mu_B^{\rm cep} > \pi T$$



Search for Lee-Yang zeroes

LY zeros (in infinite volume) at real parameter values signal non-analytic phase transition

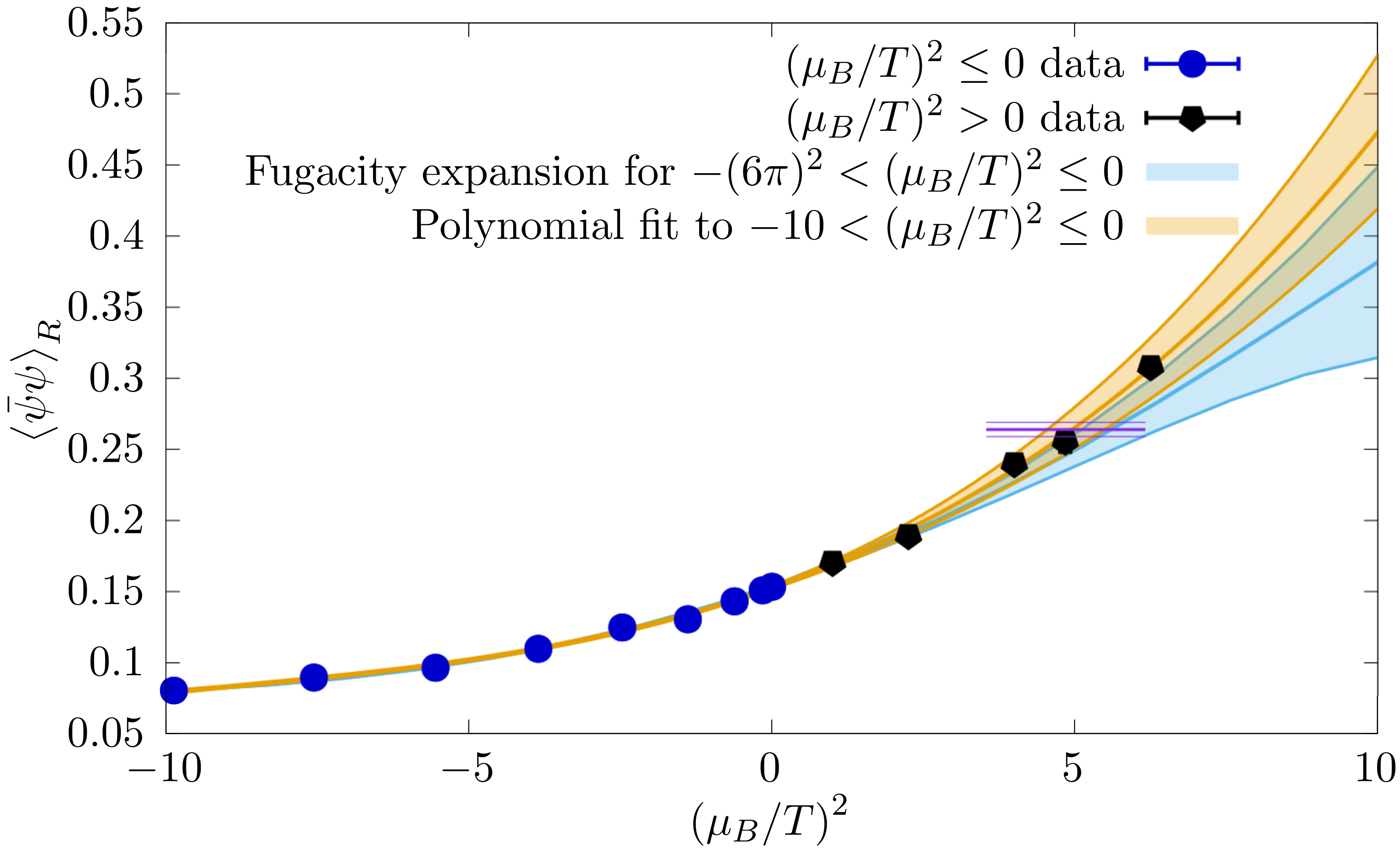


From lattice coeffs up to μ_B^8 , Pade resummation

$$\mu_B^{\rm cep} > 2.5T, T < 125 \text{ MeV}$$

[HotQCD PRD 22]

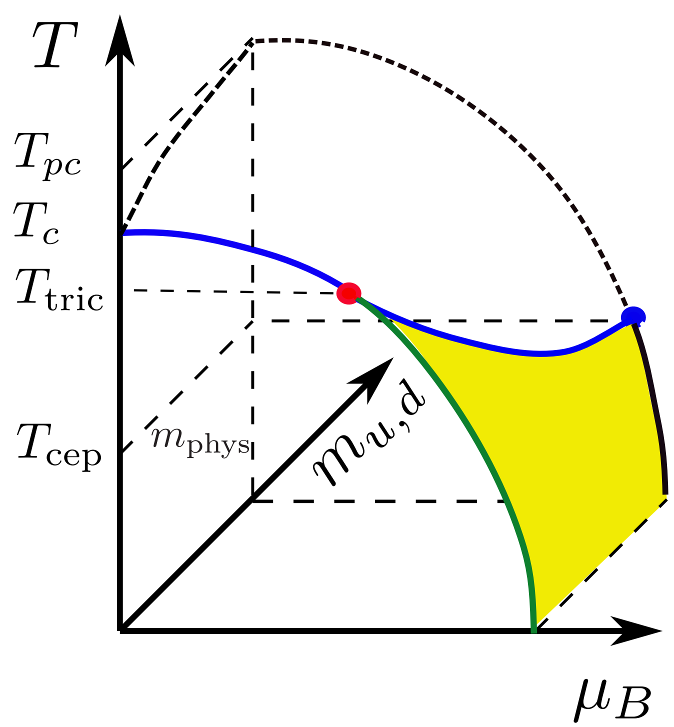
Physical point: reweighting LQCD revisited



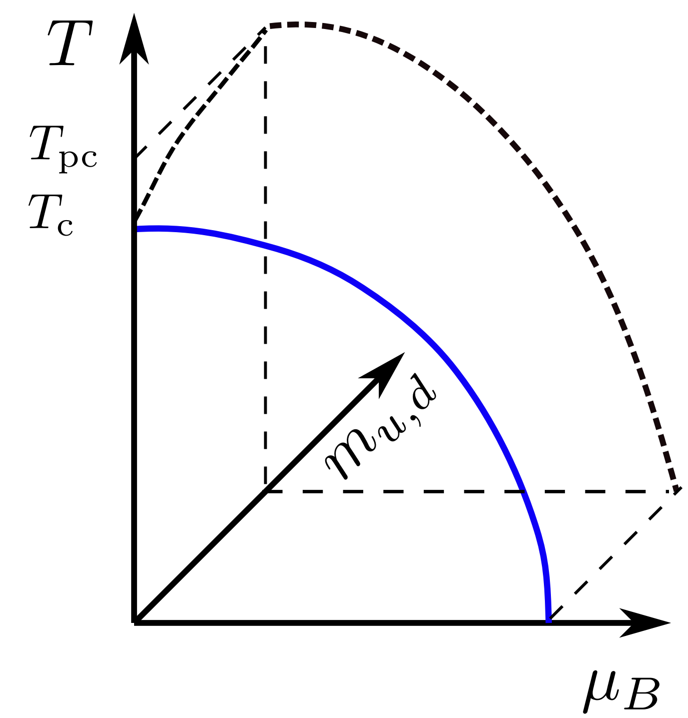
[Borsanyi et al., PRD 22]

- New treatment: rooted determinant + reweighting in sign only [Giordano et al. JHEP 20]
- Simulation with stout-sm. staggered action, $N_\tau = 6$: no sign of criticality for $\mu_B < 2.5T$

Summary: constraints on the critical point



?



- Ordering of critical temperatures $\mu_B^{\rm cep} > 3.1\ T_{pc}(0) \approx 485\ \text{MeV}$ [O.P. Symmetry 21]
- Cluster expansion model of lattice fluctuations $\mu_B^{\rm cep} > \pi T$ [Vovchenko et al. PRD 18]
- Singularities, Pade-approx. fluctuations $\mu_B^{\rm cep} > 2.5T, T < 125\ \text{MeV}$ [Bollweg et al. PRD 21]
- Direct simulations with refined reweighting $\mu_B^{\rm cep} > 2.5T$ [Wuppertal-Budpest collaboration, PRD 21]

- Consistent with DSE, fRG [Fischer PPNP 19; Fu, Pawlowski, Rennecke PRD 20; Gao, Pawlowski PRD 21]

CEP seen at larger density, but "not yet controlled" $(T_{\rm CEP}, \mu_{B_{\rm CEP}}) = (98, 643)\,\text{MeV}$

Conclusions

- Chiral transition at zero density is second order
  for Nf=2,3 massless quark flavours

- So far consistent between all lattice discretisations + DSE

- Imaginary chemical potential has no effect on the order
  of the chiral transition

- Lesson from cutoff effects:

  Correct UV sector of a theory is crucial for its phase diagram!

  “Low energy effective models” can be deceiving