On the order of the thermal transition in QCD as function of the number of quark flavours and their masses

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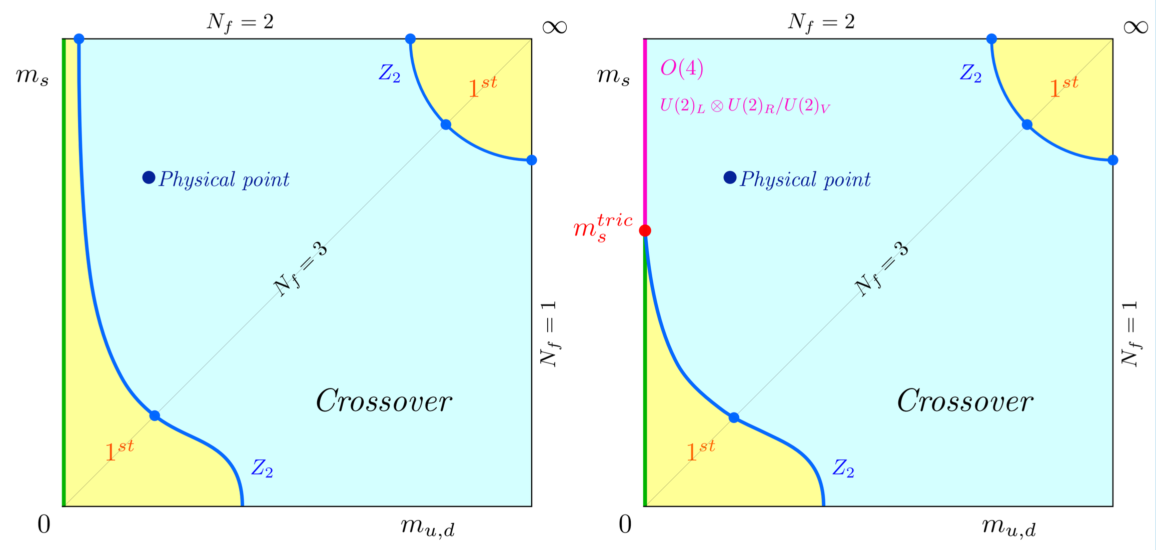
Introduction

Current knowledge of the lattice Quantum Chromodynamics (QCD) community on the order of the thermal phase transition in QCD as function of the two light (assumed degenerate) quark masses $m_{u,d}$ and the strange quark mass m_s is wrapped up in the *Columbia plot*. However, due to high simulation costs and large discretisation effects, we are not yet able to clarify which scenario for the QCD Columbia plot is realized in the continuum limit and there are at least two possibilities.



- The order of the transition at $\mu = 0$ and in the chiral limit for $N_f = 2$ quarks of degenerate mass $m_{u,d}$ is still under debate
- Direct investigations are hindered by the Dirac operator becoming more and more ill-conditioned for decreasing quark masses.

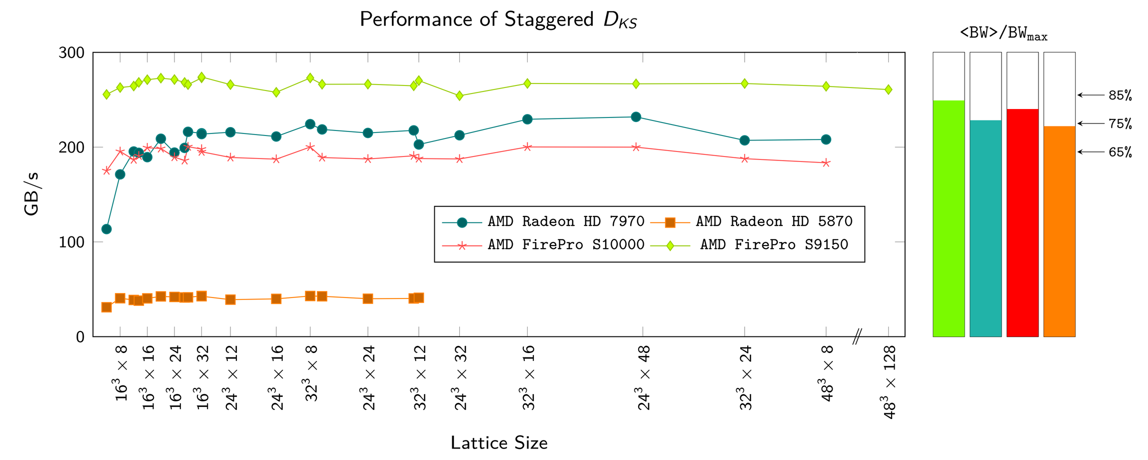
Motivation & general strategy

- Settling the order of the transition at $\mu = 0$ and in the $N_f = 2$ chiral limit is relevant for the pseudo-critical crossover region in the phase diagram of QCD, at physical values of the quark mass and low baryon-number density.
  - Physical transition might be affected by remnants of the chiral universality class due to the smallness of $m_{u,d}$
- The idea is to better constrain the first-order region by studying its extension in additional parameter directions, which allow for controlled extrapolations to the chiral limit.
  - A first-order transition in the chiral limit on a finite system represents a three-state coexistence.
  - If a continuous parameter X is varied to weaken the transition, the three-state coexistence may terminate in a tricritical point.
  - The functional behavior of the second-order boundary lines emanating from the tricritical point is governed by known critical exponents.
- Practical strategy consists in
  - Mapping out m_{Z_2} on a conveniently chosen $X - m_{u,d}$ plane
  - Safely extrapolating to the chiral limit as soon as the tricritical scaling region is entered, while varying X (e.g. $X = \mu_i$ [Bonati et al. (2014), Philipsen, Pinke (2016)]).

Simulation algorithm

- Standard Wilson action for $S_g[U]$ and standard staggered discretisation for the Dirac operator D_{KS}.
- Fermionic determinant to the power of $\frac{N_f}{4}$ in the Boltzmann weight.
- Appropriate algorithm, Rational Hybrid Monte-Carlo (RHMC).
  - Effective action embedded in a fictitious classical system evolved over a time τ according to the Hamiltonian equations of motion.
  - Rational approximation for the needed root of the determinant.

Benchmark for D_{KS} on LOEWE-CSC and L-CSC GPUs.



- D_{KS} high-dimensional and sparse matrix. Its inversion, via Iterative Krylov space methods, is the most cost-intensive operation. A well tuned D_{KS} implementation is crucial for performance.
- Numerical costs for the RHMC scale with some positive (negative) power of the volume V (pion mass m_π), which makes LQCD studies towards the chiral limit very cost-intensive.
- The employed simulation program is our publicly available[a] OpenCL-based code CL²QCD.

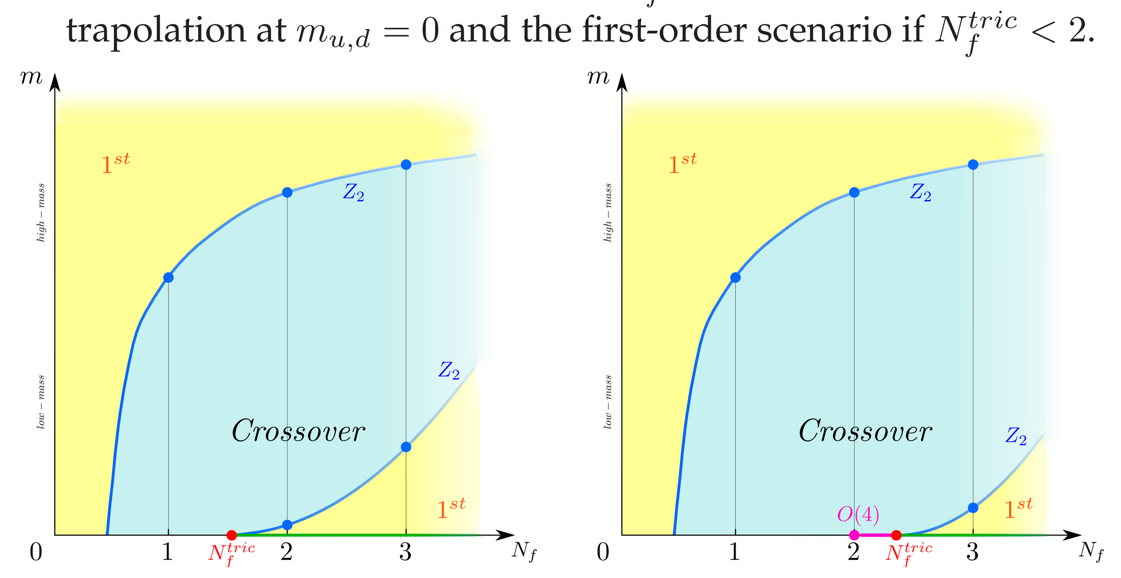
[a] See https://github.com/AG-Philipsen/cl2qcd/ .

QCD with non-integer N_F

Path integral as a function of continuous N_f studied in the $N_f - m_{u,d}$ plane in the interesting range $N_f \in [2.0, 3.0]$

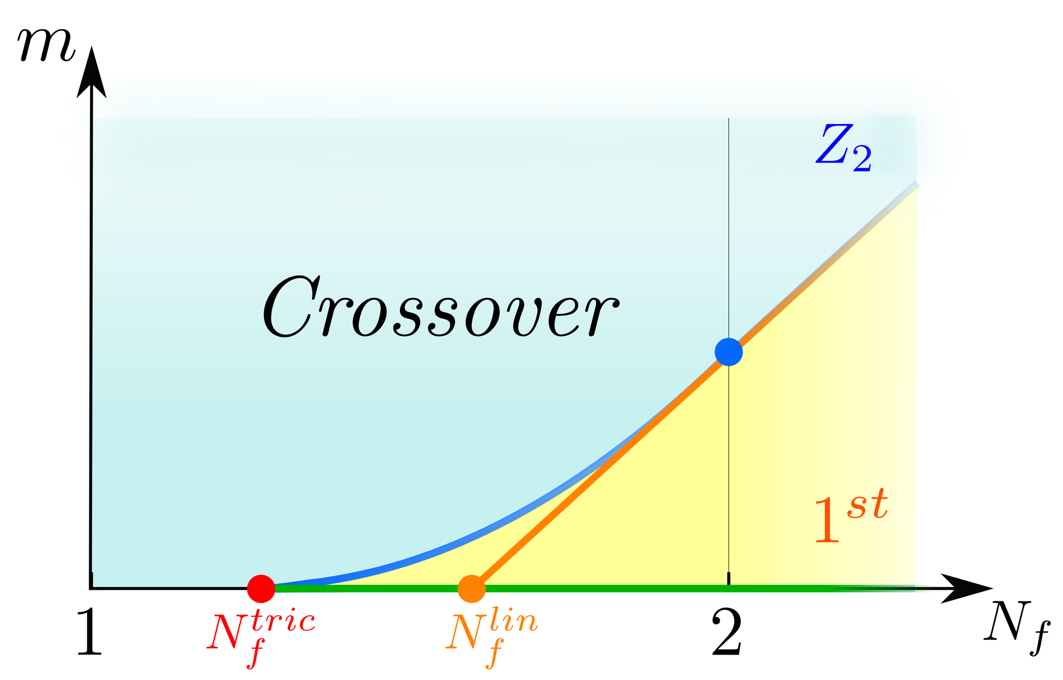
$$Z_{N_f}(m) = \int \mathcal{D}U\, [\det M(U,m)]^{N_f}\, e^{-\mathcal{S}_G}\,.$$

- **Disclaimer:**
  - Infinitely many $\mathcal{Z}$ such that for $N_f \to 2, 3$ the partition function for N_f degenerate flavours of mass m is recovered (e.g. $N_f = 2+1$).
  - Manifest locality lost due to non-integer power of $\det M(U,m)$.
- **However:**
  - Z_{N_f} at non-integer N_f: statistical system that represents one of the infinitely many interpolations between $N_f = 2$ and $N_f = 3$;
  - Physics at $N_f = 2, 3$ is fixed: relative position of N_f^{tric} with respect to $N_f = 2$ has to be fixed.
  - Effective locality, i.e. the exponential decay of all n-point functions is sufficient for universal scaling to be observed.
- **Yet at least two possible scenarios:**
  - Second-order scenario realized if $N_f^{tric} > 2$ is found from the extrapolation at $m_{u,d} = 0$ and the first-order scenario if $N_f^{tric} < 2$.



Scaling towards the chiral limit

- Both tricritical scaling in the range $N_f \in [2.0, 2.2]$ and linearity in the range $N_f \in [2.4, 3.0]$ observed in our study on coarse $N_\tau = 4$ lattices [Cuteri, Philipsen, Sciarra (2018)]
- If it is reasonable to expect both linearity within some range in N_f and tricritical scaling closer to the chiral limit
  - make use of a linear extrapolation to $m = 0$ to get an upper bound for N_f^{tric}, without the need to enter the tricritical scaling region
    - ∗ Lower cost.
    - ∗ Possibly no need for simulations at non-integer N_f values.



- If $N_f^{lin} < 2$, while one simulates at larger and larger N_τ towards the continuum limit
  - Transition in the $N_f = 2$ chiral limit keeps being a first order one.
- As soon as $N_f^{lin} \gtrsim 2$
  - No conclusion can be drawn.

Location of the chiral phase transition

Finite size scaling analysis of the third and fourth standardized moments of the distribution of the (approximate) order parameter to locate m_{Z_2}. The n[th] standardized moment for a generic observable $\mathcal{O}$ is

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

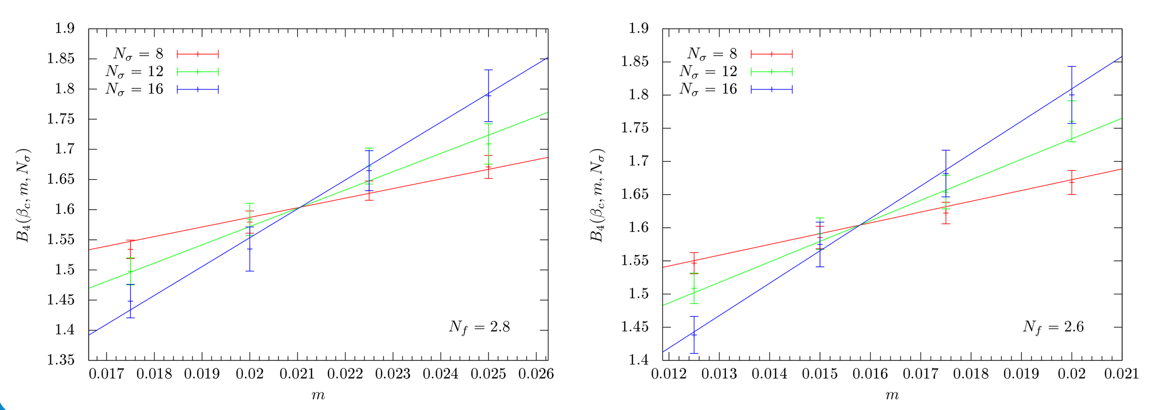
- We study the kurtosis $B_4(\beta, m)$ of the sampled $\langle \bar\psi\psi \rangle$ distribution, evaluated at the coupling β_c for which $B_3(\beta = \beta_c, m, N_\sigma) = 0$ knowing that

$$\lim_{N_\sigma \to \infty} B_4(\beta_c, m, N_\sigma) = \begin{cases} 1, & 1^{st} \text{ order} \\ 1.604, & 2^{nd} \text{ order } Z_2 \\ 3, & \text{crossover} \end{cases}.$$

- For $N_\sigma^3 \times N_\tau$ large enough and $\beta \sim \beta_c$, the kurtosis can be expanded in powers of the scaling variable $x = (m - m_{Z_2}) N_\sigma^{1/\nu}$, and the expansion can be truncated after the linear term according to

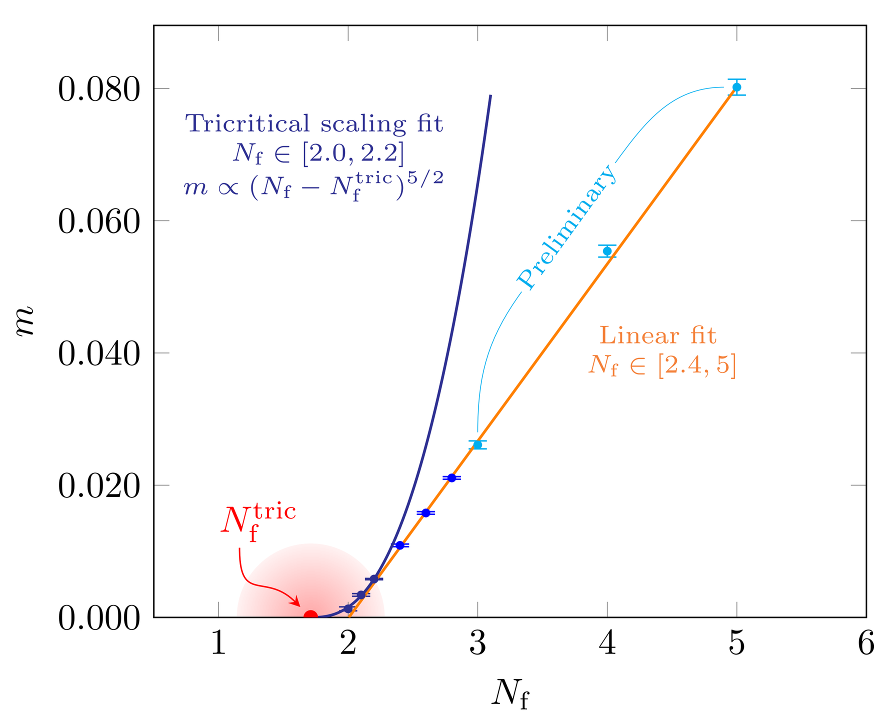
$$B_4(\beta_c, m, N_\sigma) = B_4(\beta_c, m_{Z_2}, \infty) + c(m - m_{Z_2}) N_\sigma^{1/\nu} + \ldots\,,$$
$$\text{with} \quad B_4(\beta_c, m_{Z_2}, \infty) = 1.604 \quad \text{and} \quad \nu = 0.63\,.$$

- Simulated values for $B_4(\beta_c, m, N_\sigma)$ are fitted and c and m_{Z_2} are extracted from the fit. m_{Z_2} being the position in mass of the Z_2 critical boundary.



Results

In the vicinity of a tricritical point, m_{Z_2} displays a power law dependence with known critical exponents $m_{Z_2}^{2/5}(N_f) = C\left(N_f - N_f^{tric}\right)$, while linear scaling is observed at larger N_f values further away from the chiral limit. Both N_f^{tric} and N_f^{lin} can be extracted from fits.

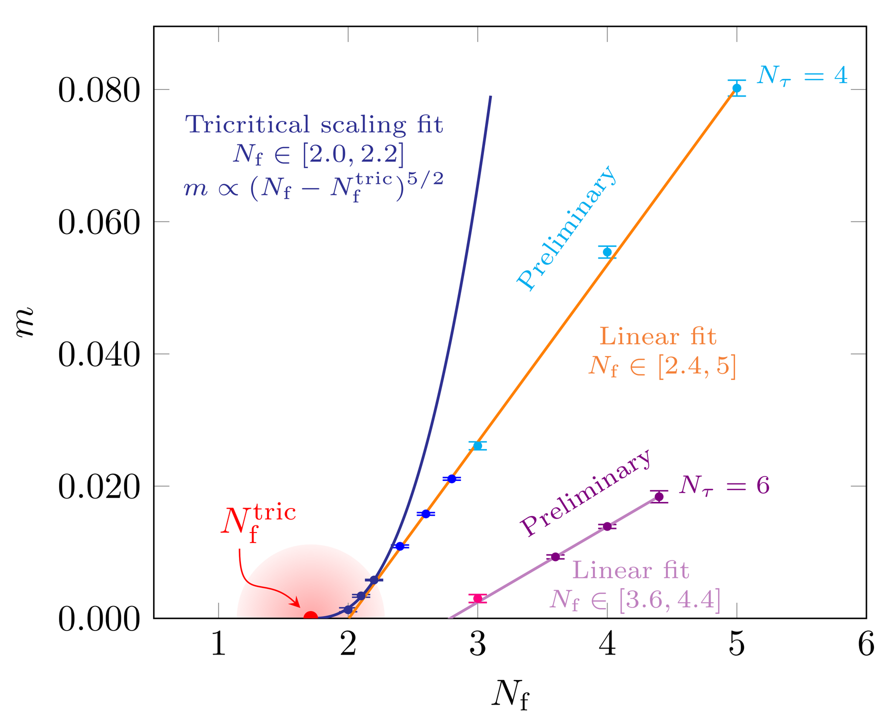


Tricritical extrapolation at $N_\tau = 4$

- Data, consistent with the tricritical scaling relation for $N_f \leq 2.2$, provide an extrapolation to the chiral limit resulting in $N_f^{tric} < 2$.
- Simulated results for $N_f = 2.2, 2.1$ fully aligned with the result for $N_f = 2.0$, based on the tricritical extrapolation from imaginary chemical potential, the width in mass of the tricritical scaling window being roughly the same in both extrapolations.

Linear extrapolation at $N_\tau = 4$

- Data exhibit linear scaling within the range $N_f \in [2.4, 5.0]$, provide an extraplation to the chiral limit resulting in $N_f^{lin} = 2$ within errors.



Tricritical extrapolation at $N_\tau = 6$

- Data produced within the range $N_f \in [3.6, 4.4]$ do not fall in the tricritical scaling region.

Linear extrapolation at $N_\tau = 6$

- Data exhibit linear scaling within the range $N_f \in [3.6, 4.4]$, provide an extraplation to the chiral limit resulting in $N_f^{lin} > 2$ within errors.
- Result for $N_f = 3$ from [de Forcrand, Kim, Philipsen (2007)] fully consistent with linear extrapolation.

Conclusions

Proposed and tested an alternative approach, w.r.t. the extrapolation from μ_i, to clarify the order of the thermal transition in the chiral limit of QCD at zero chemical potential with two dynamical flavours of quarks.

- Extrapolation in the $m - N_f$ plane with N_f promoted to a continuous parameter in the path integral formulation of the theory;
- If the transition for $m \to 0$ changes with N_f from 1^{st} order (triple) to 2^{nd} by reducing N_f, there exists a tricritical point at some N_f^{tric}.
- A linear extrapolation to $m = 0$ can also provide an upper bound N_f^{lin} for N_f^{tric}, without the need to enter the tricritical scaling region.
- On our coarse lattices the conclusion for $N_f = 2$ is that
  - the first order scenario seems to be realized on $N_\tau = 4$ lattices, in agreement with earlier results using imaginary chemical potential, instead of N_f, in the same strategy.
  - already on $N_\tau = 6$ lattices the first order scenario looks more improbable.
- Considered the size of the shift in the Z_2 critical boundary from $N_\tau = 4$ to $N_\tau = 6$, the first order scenario would look more and more contrived with larger and larger N_τ values.
- Approaches based on linear/tricritical extrapolations might provide useful tools on finer lattices, to help resolving the "$N_f = 2$ puzzle".