PROCEEDINGS OF SCIENCE

Progress on the nature of the QCD thermal transition as a function of quark flavors and masses

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We investigate to which extent we can exploit the dependence of the order of the chiral transition on the number of light degenerate flavors N_f, re-interpreted as continuous parameter in the path integral formulation, as a means to perform a controlled chiral extrapolation and deduce the order of the transition for the case $N_\mathrm{f} = 2$, which is still under debate.

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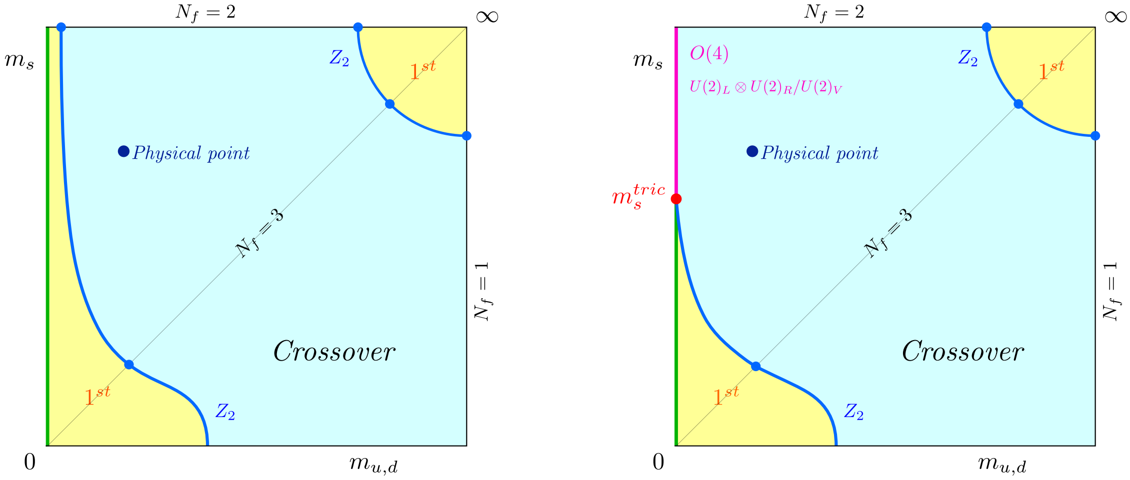


(a) First order scenario in the $m_s - m_{u,d}$ plane

(b) Second order scenario in the $m_s - m_{u,d}$ plane.

Figure 1: Two possible scenarios for the order of the QCD thermal phase transition as function of the masses of quarks. Indicated in Fig. 1(b) are also plausible universality classes for the second order line at $m_{u,d} = 0$.

1. Introduction

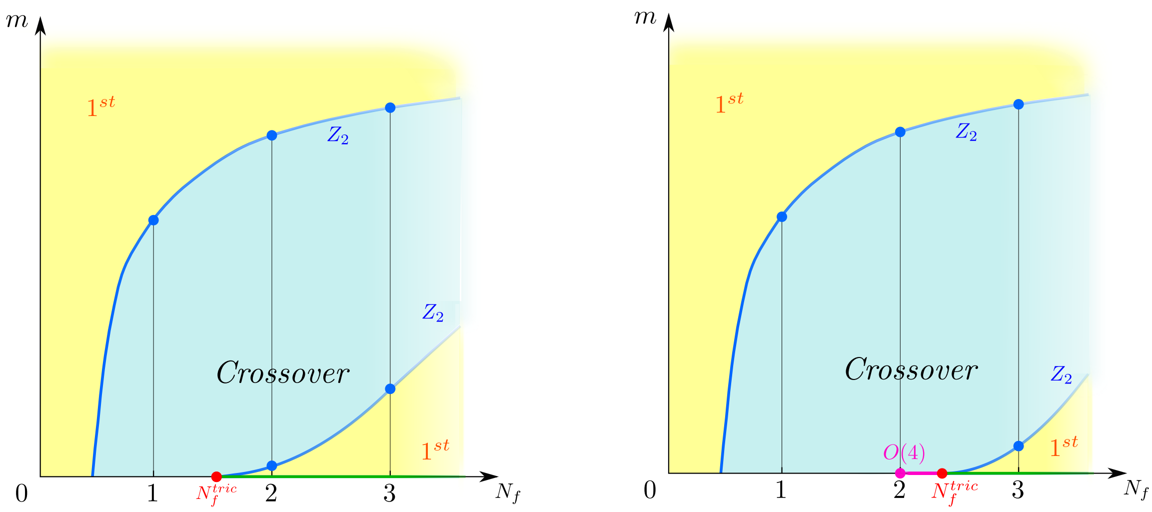
The *Columbia plot*, of which we show in Figure 1 two possible versions based on current findings, encapsulates our still very limited knowledge about the order of the thermal phase transition in QCD as function of the two light (assumed degenerate) quark masses $m_{u,d}$ and the strange quark mass m_s. Continuum extrapolated results are so far only available at the physical point. Elsewhere, using different unimproved [1–6] and improved [7–10] fermion discretizations, seemingly contradicting results have been obtained, in particular in what concerns the case of $N_\mathrm{f} = 2, 3$ degenerate light flavors in the limit of small masses corresponding to the top and bottom left corners in the Columbia plot, respectively.

This motivated us to push forward with studies aiming at elucidating, in particular, the picture for $N_\mathrm{f} = 2$ degenerate light flavors, by exploiting the dependence of the chiral transition on the number of light degenerate flavors N_f as a means to perform controlled chiral extrapolations. To this end, we treated N_f as a continuous real parameter, of some statistical system behaving, at any integer N_f value, as QCD at zero density, with N_f mass-degenerate fermion species [11]

$$Z_{N_\mathrm{f}}(m) = \int \mathscr{D}U \, [\det M(U,m)]^{N_\mathrm{f}} \, e^{-\mathscr{S}_\mathrm{G}} \,. \tag{1.1}$$

Within this framework, the two considered scenarios for the Columbia plot can be put in one-to-one correspondence with the two sketches for the order of the thermal phase transition in the (m, N_f)-plane displayed in Figure 2.

Our original strategy was to find out for which (tricritical) value $N_\mathrm{f}^\mathrm{tric}$ the phase transition displayed by this system changes from first-order to second-order, by mapping out the Z_2 phase boundary. The extrapolation to the chiral limit with known tricritical exponents can then decide between the two scenarios, depending on whether $N_\mathrm{f}^\mathrm{tric}$ is larger or smaller than 2.



(a) First order scenario in the $m - N_\mathrm{f}$ plane (b) Second order scenario in the $m - N_\mathrm{f}$ plane

Figure 2: The two considered possible scenarios for the order of the QCD thermal phase transition as function of the mass of the quarks and the number of degenerate fermion flavors.

While the tricritical scaling region was found to be very narrow already on coarse lattices, results at larger m and N_f were found to feature, over a much wider region, a remarkable linear behavior, which was not expected on universality grounds.

What our findings suggest is that, if it is reasonable to expect both linearity within some range in N_f and tricritical scaling more in the chiral limit, then one would be able to make use of a linear extrapolation to $m = 0$, to at least get $N_\mathrm{f}^\mathrm{lin}$ as an upper bound for $N_\mathrm{f}^\mathrm{tric}$, out of much more affordable simulations and possibly without even simulating at noninteger numbers of flavors.

For as long as the upper bound from the linear extrapolation keeps lying at $N_\mathrm{f} < 2$, while one simulates at larger and larger N_τ values towards the continuum limit, one can infer that the transition in the $N_\mathrm{f} = 2$ chiral limit is of first order. However, should our linear extrapolation give $N_\mathrm{f}^\mathrm{lin} \gtrsim 2$, then knowledge of the size of the scaling region is necessary to draw conclusions.

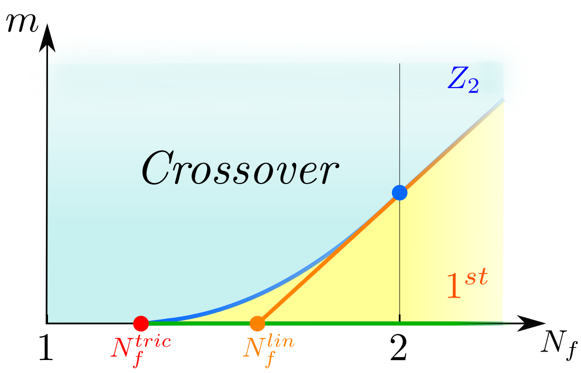


Figure 3: Sketch showing how, via a linear extrapolation to the chiral limit, $N_\mathrm{f}^\mathrm{lin}$ as an upper bound for $N_\mathrm{f}^\mathrm{tric}$ can be extracted, with the first order scenario being realized for as long as $N_\mathrm{f}^\mathrm{lin} < 2$.

2. Numerical strategy

We employ unimproved staggered fermions and use the RHMC algorithm [12] to simulate any number N_f of degenerate flavors, with $\frac{N_\mathrm{f}}{4}$ being the power to which the fermion determinant is

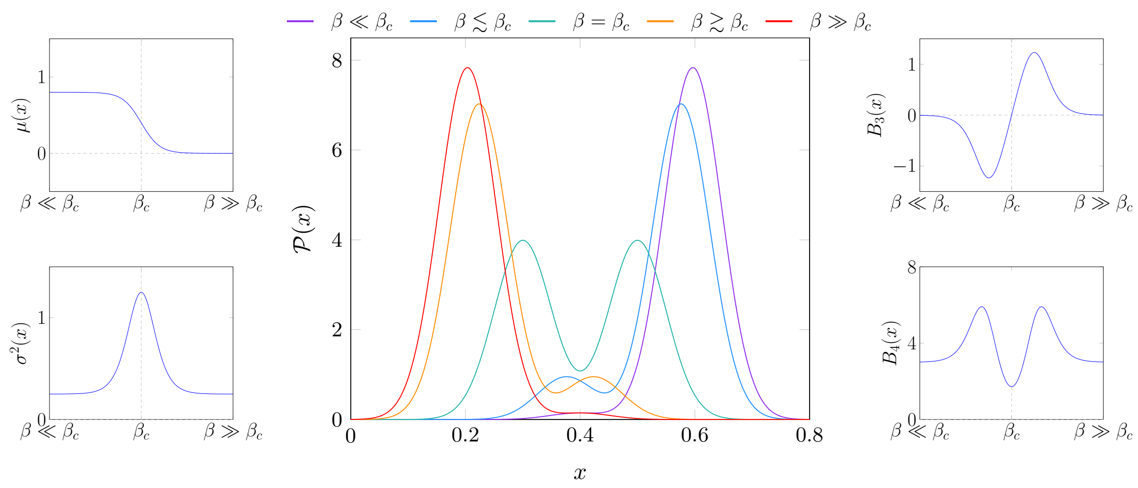


Figure 4: The chiral condensate distribution according to a model $\mathscr{P}(x)$ based on our numerical findings at various β values and the corresponding moments as function of β. Details on the model are discussed in [11].

raised in $Z_{N_f}(m)$. All numerical simulations are performed using the publicly available OpenCL-based code CL^{2}QCD [13] of which a version 1.0 has been recently released [14]. We consider temporal extents $N_\tau = 4,6$ to check for the cutoff dependence of N_f^{lin}. The ranges in mass m and gauge coupling constant β of the investigated parameter space are dictated by our purpose of locating the chiral phase transition for values of the mass m around the critical m_{Z_2} value, with the temperature related to the coupling according to $T = 1/(a(\beta)N_\tau)$.

To locate and identify the order of the chiral phase transition we rely on a finite size scaling analysis of the third and fourth standardized moments of the distribution of the (approximate) order parameter. The n$^{\text{th}}$ standardized moment for a generic observable $\mathscr{O}$ is expressed as

$$B_n(\beta,m,N_\sigma) = \frac{\langle(\mathscr{O}-\langle\mathscr{O}\rangle)^n\rangle}{\left\langle(\mathscr{O}-\langle\mathscr{O}\rangle)^2\right\rangle^{n/2}} \,. \tag{2.1}$$

Being interested in the order of the thermal phase transition in the chiral limit, we consider the kurtosis $B_4(\beta,m)$ [15] of the sampled $\langle\bar{\psi}\psi\rangle$ distribution, evaluated at the coupling β_c for which $B_3(\beta=\beta_c,m,N_\sigma)=0$, i.e. on the phase boundary.

In the thermodynamic limit $N_\sigma \to \infty$, the kurtosis $B_4(\beta_c,m)$ takes the values of 1 for a first order transition and 3 for an analytic crossover, respectively, with a discontinuity when passing from a first order region to a crossover region via a second order point. For the $3D$ Ising universality class, which is the relevant one for our case, the kurtosis takes the value 1.604 [16]. The discontinuous step function is smeared out to a smooth function as soon as a finite volume is considered. In the lattice box, the distribution of the approximate order parameter and its higher moments behave, depending on β, as illustrated in Figure 4. Moreover, in the vicinity of a critical point, the kurtosis $B_4(\beta_c,m,N_\sigma)$ can be expanded in powers of the scaling variable $x \equiv (m-m_{Z_2})N_\sigma^{1/\nu}$, and, for large enough volumes, the expansion can be truncated after the linear term,

$$B_4(\beta_c,m,N_\sigma) \simeq B_4(\beta_c,m_{Z_2},\infty) + c\,(m-m_{Z_2})N_\sigma^{1/\nu} \,. \tag{2.2}$$

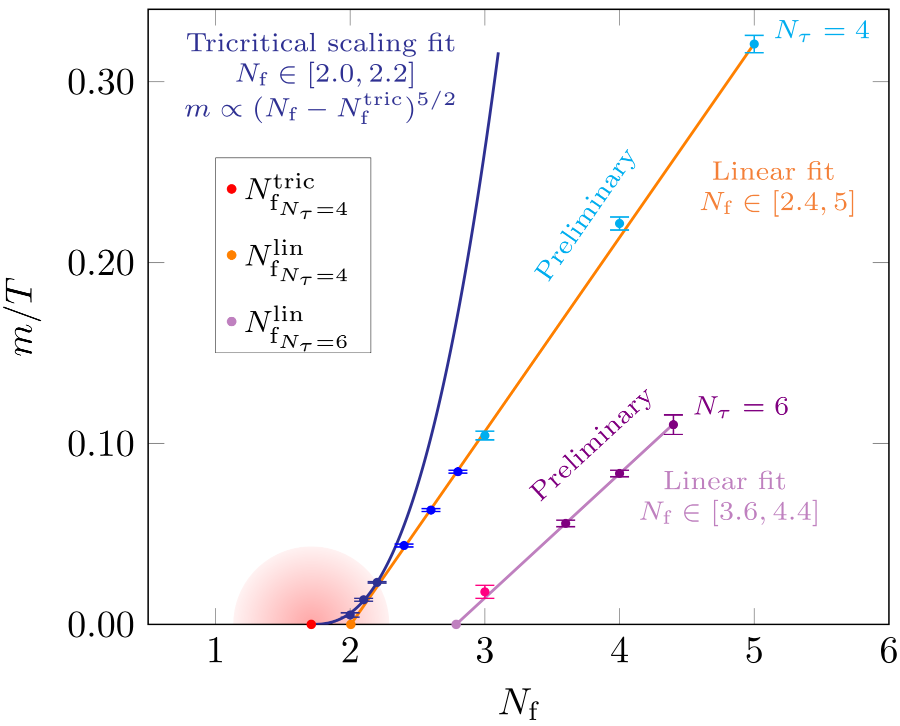


Figure 5: The Z_2 boundary in the $m/T - N_f$ plane for $N_\tau = 4, 6$. The dark blue line represents the tricritical extrapolation to the chiral limit as in [11]. The orange line represents a linear extrapolation based on m_{Z_2} in the N_f range 2.4-5 using also newly simulated points. The violet line represents a linear extrapolation on the basis of m_{Z_2} in the N_f range 3.6-4.4. The magenta point at $N_\tau = 6$ and $N_f = 3$ is borrowed from [3].

As already mentioned, in our case, the critical value for the mass m_{Z_2} is known to correspond to a second order phase transition in the 3D Ising universality class, so we fix $B_4(\beta_c, m_{Z_2}, \infty) = 1.604$ and $\nu = 0.6301$ to better constrain the fit.

Our simulated values for $B_4(\beta_c, m, N_\sigma)$ are then fitted to Eq. (2.2) and the fit parameters c and m_{Z_2} are extracted. The whole study has been repeated for $N_f \in \{3, 4, 5\}$ at $N_\tau = 4$ and $N_f \in \{3.6, 4.0, 4.4\}$ at $N_\tau = 6$.

3. Results and conclusions

Our results are reported in Figure 5. The first important thing to observe is that, while tricritical extrapolation for $N_\tau = 4$ resulted in $N_f^{tric} < 2$, providing a confirmation for the first order scenario being realized on coarse lattices, a linear extrapolation to the chiral limit using those data which exhibit linear scaling within the range $N_f \in [2.4, 5.0]$, results in $N_f^{lin} = 2$ within errors. Strictly speaking, by just considering $N_\tau = 4$ results, one would conclude that the linear extrapolation alone cannot give conclusive answers on the order of the $N_f = 2$ transition in the chiral limit. However, results on finer lattices were produced as well. On $N_\tau = 6$, what we observe is that data within the range $N_\mathrm{f} \in [3.6, 4.4]$ certainly do not fall in the tricritical scaling region, but they do exhibit linear scaling. Moreover, if we consider the result for $N_\mathrm{f} = 3$ for the same discretization from the literature [3], we can see it is fully consistent with our linear extrapolation. Finally, the most important aspect of this result is that, linearly extrapolating at $N_\tau = 6$, we get $N_\mathrm{f}^\mathrm{lin} \lesssim 3$, namely quite far to the right of $N_\mathrm{f} = 2$.

To conclude, we have proposed and tested an approach, to clarify the order of the thermal transition in the chiral limit of QCD at zero chemical potential with two dynamical flavors of quarks. Specifically, a controlled chiral extrapolation in the $m - N_f$ plane with N_f promoted to a continuous parameter in the path integral formulation of the theory is possible, given that if the transition for $m \to 0$ changes with N_f from 1^{st} order (triple) to 2^{nd} by reducing N_f, there has to exist a tricritical point at some $N_\mathrm{f}^\mathrm{tric}$. Moreover, the linearity featured by the Z_2 boundary over a wide N_f region suggests that a linear extrapolation to $m = 0$ can also provide an upper bound $N_\mathrm{f}^\mathrm{lin}$ for $N_\mathrm{f}^\mathrm{tric}$, which may become useful to discriminate between first and second order scenario and help resolving the "$N_\mathrm{f} = 2$ puzzle".

Based on our numerical findings, the shift in the Z_2 critical boundary from $N_\tau = 4$ to $N_\tau = 6$ points towards a behavior consistent with that from improved actions on sufficiently fine lattices.

4. Acknowledgements

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