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The Nature of the QCD Thermal Transition as a Function of Quark Flavours and Masses

Francesca Cuteri[1], **Owe Philipsen**[1,2], **and Alessandro Sciarra**[1]

[1] Institut für Theoretische Physik, Goethe Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany
E-mail: {cuteri, philipsen, sciarra}@th.physik.uni-frankfurt.de

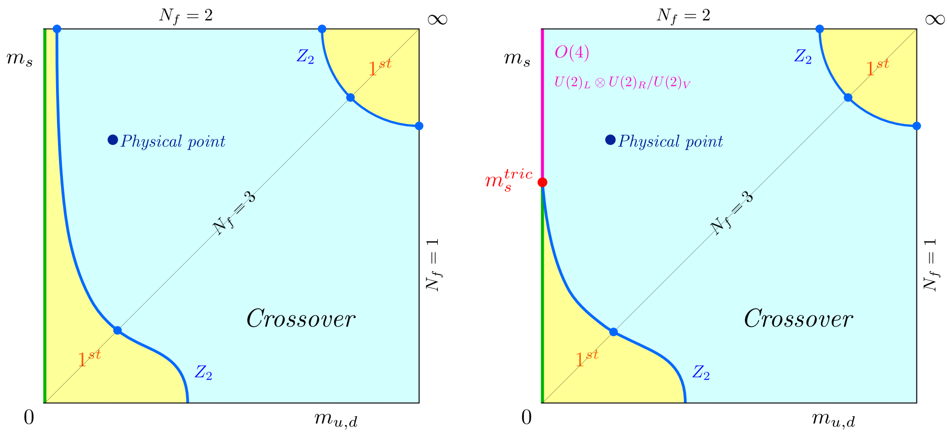
[2] John von Neumann Institute for Computing (NIC), GSI, Planckstr. 1, 64291 Darmstadt, Germany

Quantum Chromodynamics (QCD) is the fundamental theory of strongly interacting matter composed of quarks and gluons. The QCD phase diagram states in which form strongly interacting matter exists as a function of temperature and density. Because of a severe sign problem, finite densities are not amenable to standard Monte Carlo simulations and knowledge of the phase diagram remains scarce. Even the nature of the chiral phase transition at zero density and finite temperature is not yet known in the continuum limit, due to high simulation costs and large discretisation effects. We report from a long term project to determine the nature of the thermal QCD transition as a function of the quark masses, the number of flavours and the lattice spacing.

1 Introduction

Quantum Chromodynamics is the fundamental theory of the strong interactions governing the forces between nuclear and subnuclear particles. Its fundamental degrees of freedom are light u- and d-quarks, a heavier s-quark and gluons, which are the force carriers in this quantum field theory. The coupling strength of the interactions depends on the energy scale of a scattering process. For energies below a few GeV, the coupling is large and quarks and gluons combine into numerous tightly bound states, the hadrons, among them the familiar proton and neutron. On the other hand, at large temperatures or densities, the average energy per particle is higher and the theory enters a weak coupling regime, where the constituents form a so-called quark gluon plasma. The QCD phase diagram determines the form of matter under different conditions as a function of temperature, T, and matter density. Whether and where the hadronic phase and the quark gluon plasma are separated by true phase transitions has to be determined by first principle calculations and experiments. Since QCD is strongly coupled on scales of hadronic matter, a non-perturbative treatment is necessary. The most reliable approach is by Monte Carlo simulation of a reformulation of the theory on a space-time grid, lattice QCD.

Unfortunately, the so-called sign problem prohibits straightforward simulations at finite baryon density. For this reason, knowledge of the thermal phase transition at zero density as a function of the theory's parameters, also for unphysical values, is of great importance to constrain and anchor research in the finite density direction. It is well-known that the physical point of QCD (with quark mass values realised in nature) displays only an analytic, smooth crossover between the hadronic and the plasma regions, without a non-analytic phase transition[1]. However, the order of the finite temperature phase transition at zero density depends on the quark masses as is schematically shown in Fig. 1(a), where



(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 a function of the quarks masses.

N_f denotes the number of mass degenerate quark flavours. In the limits of zero and infinite quark masses (lower left and upper right corners), order parameters corresponding to the breaking of some global symmetry can be defined, and for three degenerate quarks one numerically finds, on rather coarse lattices, first order phase transitions at small and large quark masses at some finite temperatures $T_c(m)$. On the other hand, one observes an analytic crossover at intermediate quark masses, with second order boundary lines separating these regions. Both lines have been shown to belong to the $Z(2)$ universality class of the 3d Ising model[2–4]. The critical lines bound the quark mass regions featuring a chiral or deconfinement phase transition, and are called chiral and deconfinement critical lines, respectively. The former has been mapped out on $N_\tau = 4$ lattices[5] and puts the physical quark mass configuration in the crossover region. The chiral critical line recedes with decreasing lattice spacing[6,7], which is parametrised by increasing temporal lattice extent N_τ (see below): for $N_f = 3$, on the critical point, the quark masses correspond to pion mass values $m_\pi(N_\tau = 4)/m_\pi(N_\tau = 6) \sim 1.8$. Thus, in the continuum the physical point is deeper in the crossover region than on coarse lattices. An open question to this day remains the order of the transition in the limit of zero light quark masses, called the chiral limit. As explained below, this limit cannot be directly simulated. Consequently, it is still not known whether the chiral phase transition for two quark flavours is of first or second order. Hence an alternative scenario is Fig. 1(b). Clarifying this question is important because of the proximity of the critical line to the physical point.

2 Simulating Thermodynamical Lattice QCD

The central object in statistical physics is the partition function $\mathcal{Z}$ of a system. For lattice QCD it is expressed as a path integral over the gluon fields U, including a determinant of the Dirac operator for the quarks. An expectation value of some observable $\mathcal{O}$ then reads

$$\langle \mathcal{O} \rangle = \mathcal{Z}^{-1} \int \mathcal{D}U O \det D[U] \exp\left\{-S_g[U]\right\} \ , \tag{1}$$

where $S_g[U]$ is the discretised gauge action and $D[U]$ the discretised fermion Dirac operator (for detailed expressions see Ref. 8).

The bare parameters are the lattice gauge coupling $\beta = 6/g^2$, and the bare quark mass $m_{u,d} \equiv m$. A finite temperature T is specified by the inverse temporal lattice extent

$$T = (a(\beta)N_\tau)^{-1} \ . \tag{2}$$

On a lattice with given N_τ, temperature is tuned by changing the lattice spacing a indirectly via the running coupling $\beta(a)$. On the other hand, a continuum limit at fixed temperature implies $a \to 0, N_\tau \to \infty$, and larger values of N_τ imply smaller lattice spacings.

Expressing the determinant of the fermion matrix D in terms of pseudo fermions ϕ,

$$\det D[U] \sim \int \mathcal{D}\phi^\dagger \, \mathcal{D}\phi \exp\left\{-\phi^\dagger D^{-1}[U]\phi\right\} \ , \tag{3}$$

yields the effective action $S_{\text{eff}}[U,\phi] = S_{\text{gauge}}[U] + \phi^\dagger D^{-1}[U]\phi$. Importance sampling methods can, then, be used to evaluate this high-dimensional integral. Using the Boltzmann-weight $p[U,\phi] = \exp\left\{-S_{\text{eff}}[U,\phi]\right\}$ as probability measure, an ensemble of N gauge configurations $\{U_m\}$ is generated. Then, $\langle A \rangle$ may be approximated by

$$\langle A \rangle \approx \frac{1}{N}\sum_m A[U_m] \ . \tag{4}$$

The choice of the simulation algorithm to generate QCD gauge configurations depends on the employed discretisation for the QCD action. For our study we used, beside the standard Wilson action for $S_g[U]$, the standard staggered discretisation for the Dirac operator D_{KS}. A consequence of this choice is that the fermionic determinant appears raised to the power of $\frac{N_f}{4}$ in the analog of Eq. 1. So the appropriate algorithm, since we are simulating $N_f < 4$, is the Rational Hybrid Monte-Carlo (RHMC), where the effective action is embedded in a fictitious classical system evolved over a time τ according to the Hamiltonian equations of motion and a rational approximation is used to evaluate the fourth root of the determinant.

Since the fermion matrix D_{KS} is high-dimensional and sparse, iterative Krylov space methods are used for its inversion. This inversion is the most cost-intensive part of a simulation. Thus, for performance it is crucial to have a well tuned implementation, in particular of D_{KS}. The numerical costs for the RHMC scales with some positive power of the volume V and some negative power of m_π. This illustrates that LQCD studies are very cost-intensive, especially when going towards the chiral limit, and efficient simulation programs are needed. For the very largest lattices we thermalised configurations on JUQUEEN at NIC Jülich. For all others and production we employed our publicly available[a] OpenCL[b]-based code[9] CL^{2}QCD, which is optimised to run efficiently on the GPUs

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

[b]See `https://www.khronos.org/opencl/`.

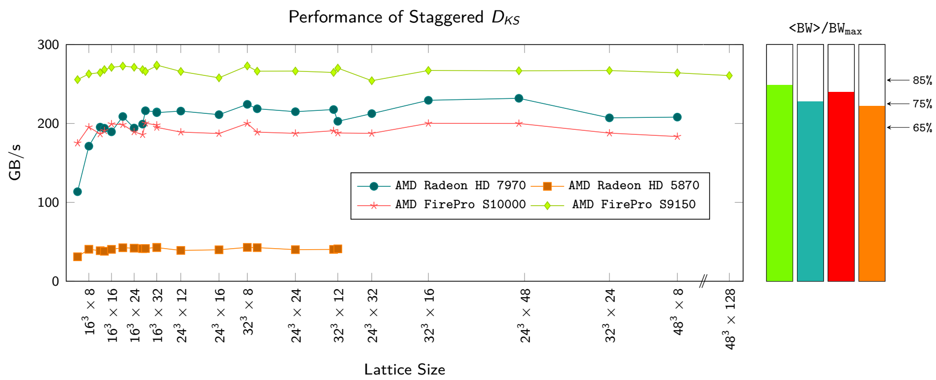


Figure 2. Benchmark for D_{KS} on LOEWE-CSC and L-CSC GPUs (see also `https://github.com/AxelKrypton/PhD_Thesis`).

of the LOEWE-CSC[10] at Goethe-University Frankfurt and the L-CSC[11] at GSI in Darmstadt. The latter was ranked as the most energy efficient computing cluster in the world[c]. Fig. 2 shows the performance of the D_{KS} and underlines the efficient implementation.

3 QCD with Non-Integer N_f

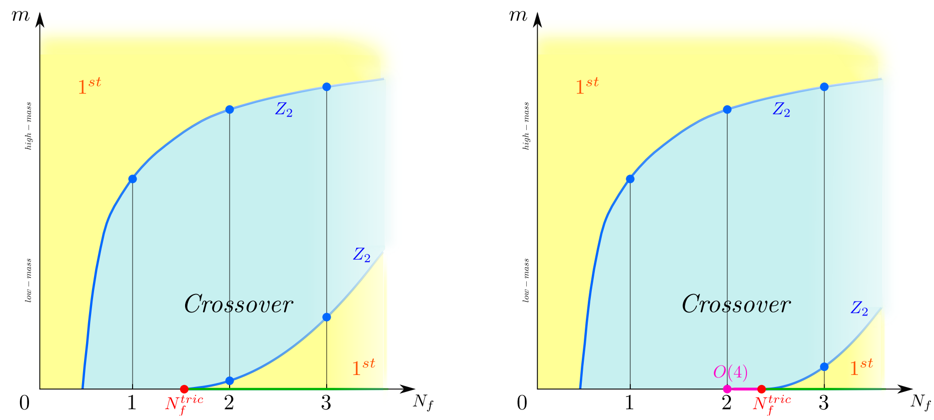
The impossibility to simulate the chiral or continuum limits directly motivates attempts to better constrain the first-order region by studying its extension in additional parameter directions, which might allow for controlled extrapolations. The idea is based on the fact that a first-order transition in the chiral limit on a finite system represents a three-state coexistence (with chiral condensate being positive, negative or zero). If a continuous parameter is varied such as to weaken the transition, like increasing the strange quark mass m_s in Fig. 1(b), the three-state coexistence terminates in a tricritical point, which governs the functional behaviour of the second-order boundary lines emanating from it by known critical exponents. Thus, if such a boundary line can be followed into the tricritical scaling regime, an extrapolation becomes possible. This kind of approach has been successfully tested adding a imaginary chemical potential, where there is no sign problem[12].

Here, we consider QCD with N_f mass-degenerate quarks of mass m at zero density and the partition function reads

$$Z_{N_f}(m) = \int \mathcal{D}U \, [\det D_{KS}(U,m)]^{N_f/4} \, e^{-S_G} \; . \tag{5}$$

Ignoring, for the moment, that it originates from QCD, we can formally view this as a partition function of some statistical system characterised by a continuous parameter N_f. Our question then is for which (tricritical) value of N_f the phase transition displayed by this system changes from first-order to second-order. Of course, the extension of $Z_{N_f}(m)$ to non-integer values of N_f is not unique, with infinitely many possibilities to "fill in"

[c] See `https://www.top500.org/green500/list/2014/11/`.



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

Figure 3. The two considered possible scenarios for the order of the QCD thermal phase transition as a function of the light-quarks mass and the number of fermion flavours.

values such that in the limits $N_f \to 2, 3$ the respective QCD partition functions are recovered. In general such interpolations using non-integer powers of the determinant will not correspond to local quantum field theories. However, for our study this is not of too much interest. Rather, for any given lattice spacing, we are just considering a statistical system that represents one particular interpolation between two quantum field theories with integer N_f. Accordingly, the precise value of N_f^{tric}, which we seek to determine, has no meaning in itself other than being located between two particular integer N_f's. Whichever prescription one considers for the interpolation, this relative position of N_f^{tric} with respect to the integer N_f remains the same. In particular, for each lattice spacing the nature of the chiral phase transition for $N_f = 2$ can be decided by whether the extrapolated N_f^{tric} is between $N_f = 1, 2$ or between $N_f = 2, 3$, as in Fig. 3.

4 Determining the Order of the Chiral Phase Transition

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

$$B_n(\beta, m, N_\sigma) = \frac{\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^n \rangle}{\left\langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \right\rangle^{n/2}}. \tag{6}$$

Being interested in the thermal phase transition in the chiral limit, we measured the chiral condensate $\langle \overline{\psi}\psi \rangle$ as approximate order parameter. In order to extract the order of the transition as a function of the quark mass and number of flavours, we considered the kurtosis $B_4(\beta, m)$[13] of the sampled $\langle \overline{\psi}\psi \rangle$ distribution, evaluated at the coupling β_c for which we have vanishing skewness $B_3(\beta = \beta_c, m, N_\sigma) = 0$, i.e. on the phase boundary. In the thermodynamic limit $N_\sigma \to \infty$, the kurtosis $B_4(\beta_c, m, N_\sigma)$ 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, where, if the transition is in the $3D$ Ising universality class, it takes the value[14] 1.604.

The discontinuous step function is smeared out to a smooth function as soon as a finite volume is considered. However, in the vicinity of a critical point, the kurtosis can be expanded in powers of the scaling variable $(m - m_{Z_2})N_\sigma^{1/\nu}$, and, for large enough volumes, the expansion can be truncated after the linear term,

$$B_4(\beta_c, m, N_\sigma) \simeq B_4(\beta_c, m_{Z_2}, \infty) + c(m - m_{Z_2})N_\sigma^{1/\nu}. \tag{7}$$

In our case, the critical value for the mass m_{Z_2} corresponds to a second order phase transition in the 3D Ising universality class, so that one can fix $B_4 \approx 1.604$ and $\nu \approx 0.6301$. Our simulated values for $B_4(\beta_c, m, N_\sigma)$ are then fitted to Eq. 7 and the fit parameters c and m_{Z_2} are extracted. We are particularly interested in m_{Z_2} indicating the position in mass of the Z_2 critical boundary in the $m_{Z_2} - N_f$ plane. We varied the spatial extent of the lattice N_σ such that the aspect ratios, governing the size of the box in physical units at finite temperature, were in the range $L/T = N_\sigma/N_\tau \in [2-5]$. The whole study has been repeated for 5 different N_f values, $N_f = 2.8, 2.6, 2.4, 2.2, 2.1$. For each parameter set

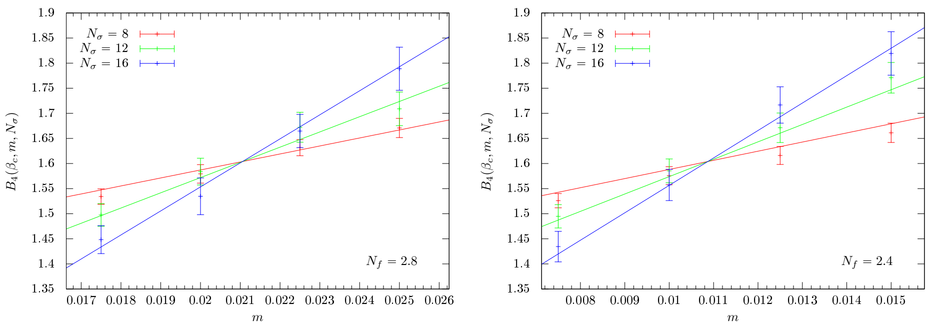


Figure 4. Finite size scaling of B_4 and fit.

N_f	am - range	m_{Z_2}	c	χ^2
3.0	[0.0250:0.0450]	0.0259(9)	0.51(6)	0.19
2.8	[0.0175:0.0250]	0.0211(3)	0.59(5)	0.27
2.6	[0.0125:0.0200]	0.0158(2)	0.60(5)	0.18
2.4	[0.0075:0.0150]	0.0109(2)	0.67(5)	0.55
2.2	[0.0025:0.0100]	0.0059(2)	0.74(6)	0.28
2.1	[0.0015:0.0045]	0.0034(5)	0.84(26)	0.22

Table 1. Results for fits to Eq. 7 for $N_f = 3.0, 2.8, 2.6, 2.4, 2.2, 2.1$. The $N_f = 3.0$ result is taken from Ref. 16. $B_4(m_{Z_2}, \infty)$ and ν have been set to 1.604 and 0.6301, respectively.

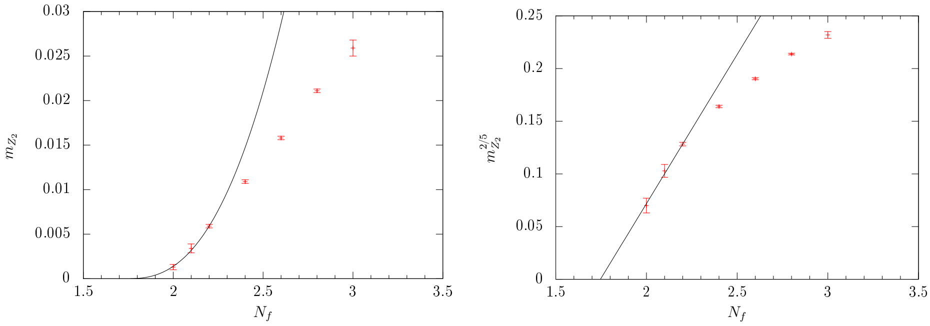


Figure 5. A linear fit in the range $[2.0, 2.2]$ is displayed in the rescaled plot (right) and the corresponding curve is also drawn in the unscaled plot (left). For $N_f = 2.0$ we use the result from the extrapolation from imaginary chemical potential[12].

$\{N_f, m, N_\sigma, \beta\}$, statistics of about $(200k - 400k)$ trajectories has been accumulated over 4 Markov chains, subject to the requirement that the skewness of the chiral condensate distribution is compatible within 2 to 3 standard deviations between the different chains. Examples of our procedure, for the cases $N_f = 2.8, 2.4$, are plotted in Fig. 4. From the Figure we observe how the ordering of kurtosis values for a fixed mass m as function of the volume depends on whether m lies in the crossover region (B_4 increases with N_σ) or in the first order region (B_4 decreases with N_σ), m_{Z_2} being the mass at which sets of B_4 values for different volumes cross in one point (provided we are effectively in the thermodynamic limit).

From Tab. 1 we observe how, as N_f is lowered, m_{Z_2} decreases towards zero and now we use that the critical line, in the vicinity of a tricritical point, is known to display a power law dependence with known critical exponents[15]. The scaling law in our case is

$$m_{Z_2}^{2/5}(N_f) = C\left(N_f - N_f^{tric}\right). \tag{8}$$

The plots of m_{Z_2} as a function of N_f and of the rescaled mass $m_{Z_2}^{2/5}$ as a function of N_f are displayed in Fig. 5. The solid line in the mass-rescaled plot shows that the simulated results for $N_f = 2.2, 2.1$ are aligned with the result for $N_f = 2.0$ taken from literature[12]. Our results indicate agreement with the expected scaling relation for $N_f \leq 2.2$.

5 Conclusion and Discussion

Our study indicates that the first order chiral phase transition of QCD, when it is considered as a function of non-integer number of quark flavours, ends in a tricritical point N_f^{tric}, which because of its known scaling behaviour allows for a controlled extrapolation. This confirms an earlier analogous observation when imaginary chemical potential is introduced and varied[12]. Mapping out the second-order boundary line for a number of lattice spacings thus offers, at least in principle, a path to a controlled chiral and continuum limit. Unfortunately, even on the coarse lattices used for this work, the computing cost is extremely high, while the lattice spacing needs to be reduced by at least a factor of three before a continuum extrapolation becomes possible. This observation underlines the crucial importance of high performance computing at its highest capacity for the progress of nuclear and particle physics.

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