THREE-FLAVOR CHIRAL PHASE TRANSITION AND AXIAL SYMMETRY BREAKING WITH THE FUNCTIONAL RENORMALIZATION GROUP*

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The interplay of mesonic fluctuations with an axial $U(1)_A$-symmetry breaking and resulting effects on the location of a possibly existing critical endpoint in the QCD phase diagram are investigated in a framework of the functional renormalization group within a $N_f = 2 + 1$ flavor quark–meson model truncation. The axial $U(1)_A$-symmetry breaking is imposed by a mesonic Kobayashi–Maskawa–'t Hooft determinant. The quark mass sensitivity of the chiral phase transition with and without the $U(1)_A$-symmetry breaking is studied.

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1. Motivation

It is well-established knowledge that Quantum Chromodynamics (QCD) experiences a rapid crossover from a hadronic phase with broken chiral symmetry to a deconfined and chirally-symmetric quark–gluon plasma at high temperature and moderate baryon densities. In the chiral limit, *i.e.*, for

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N_f massless quark flavors the QCD Lagrangian is invariant under $\mathrm{U}(1)_\mathrm{V} \otimes \mathrm{U}(1)_\mathrm{A} \otimes \mathrm{SU}(N_\mathrm{f})_\mathrm{L} \otimes \mathrm{SU}(N_\mathrm{f})_\mathrm{R}$ transformations where for our discussion unimportant discrete subgroups have been ignored. The vector subgroup $\mathrm{U}(1)_\mathrm{V}$ corresponds to quark-number conservation and seems to be less important at the chiral transition. However, it is uncertain what happens to the anomalously broken $\mathrm{U}(1)_\mathrm{A}$-symmetry at the transition. If the $\mathrm{U}(1)_\mathrm{A}$-symmetry is broken, the relevant symmetry is reduced to the chiral $\mathrm{SU}(N_\mathrm{f})_\mathrm{L} \otimes \mathrm{SU}(N_\mathrm{f})_\mathrm{R}$ which is for two massless flavors isomorphic to the O(4) symmetry. For a continuous phase transition, this would lead to a three-dimensional O(4) universality class. However, the symmetry-breaking pattern changes significantly with a restored $\mathrm{U}(1)_\mathrm{A}$-symmetry leading to an essential impact on the nature of the chiral phase transition.

Recent experimental observations found a drop of at least 200 MeV in the anomalously large mass of the η'-meson close to the chiral crossover which might signal an effective restoration of the $\mathrm{U}(1)_\mathrm{A}$-symmetry [1, 2]. On the theoretical side, the situation is more controversial: A number of recent QCD lattice simulations found a substantial suppression of $\mathrm{U}(1)_\mathrm{A}$-anomaly related effects around the crossover [3–5] but there are also very recent results indicating a $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking in terms of chiral susceptibilities above the crossover [6]. Furthermore, some analytical studies show an effective $\mathrm{U}(1)_\mathrm{A}$-symmetry restoration at the transition in the chiral limit for three quark flavors but not for two flavors [7–10], see also [11]. Finally, the order and universality class of the chiral transition in the chiral limit for two quark flavors are not fully settled and depend on the behavior of $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking operators at the transition [12–14].

In the following, the role of the $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking at non-vanishing temperatures and quark chemical potentials is addressed. Fluctuations are taken into account by solving functional renormalization group (FRG) equations in a three flavor quark–meson model truncation. The $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking is implemented effectively by a mesonic Kobayashi–Maskawa–'t Hooft determinant in the truncation [15, 16]. Particular focus will be put on the interplay of mesonic fluctuations and $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking. Consequences for the location of a possibly existing critical endpoint in the QCD phase diagram are discussed and the quark mass sensitivity of the three flavor chiral transition with and without $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking is explored.

2. Flow equations for the three-flavor quark–meson model

Low-energy QCD with $N_\mathrm{f} = 3$ quark flavors can be described with an effective chiral quark–meson model which captures the degrees of freedom of strongly-interacting matter relevant for the chiral phase transition. The Euclidean Lagrangian [17]

$$\mathcal{L} = \bar{q}\left[\not{\partial} + \mu\gamma_4 + h\left(\sigma_b + i\gamma_5\pi_b\right)T^b\right]q + \mathrm{Tr}\left[\partial_\mu\Sigma^\dagger\partial_\mu\Sigma\right] + \tilde{U}(\rho_1,\tilde{\rho}_2)\,, \quad (1)$$

includes two degenerate light and one strange quarks q which are coupled through a flavor-independent Yukawa coupling h to scalar, σ_b, and pseudoscalar mesons π_b. Additionally, we have introduced a flavor symmetric quark chemical potential μ. The purely mesonic theory is parameterized with fields in matrix form $\Sigma = (\sigma_b + i\pi_b)T^b$, where T^b are the generators of the flavor U(3) group. The potential $\tilde{U}(\rho_1,\tilde{\rho}_2)$ parameterizes the interactions of all eighteen mesons in terms of the chiral invariants

$$\rho_1 = \mathrm{Tr}\left[\Sigma^\dagger\Sigma\right]\,, \qquad \tilde{\rho}_2 = \mathrm{Tr}\left[\left(\Sigma^\dagger\Sigma\right)^2\right] - \frac{\rho_1^2}{3}\,. \quad (2)$$

Non-vanishing quark masses can be implemented in the quark–meson model with explicit symmetry breaking terms that are linear in the uncharged scalar mesons σ_0, σ_3 and σ_8. Since the σ_3 term breaks the SU(2)-isospin symmetry explicitly, the $(2+1)$-flavor version of the quark–meson model is obtained by ignoring the σ_3 and consider only the σ_0 and σ_8 breaking. For explicit calculations, it is convenient to change the singlet-octet basis and perform a unitary rotation to the non-strange, σ_x, and strange, σ_y, scalar fields.

The Lagrangian defined in Eq. (1) respects the full chiral symmetry $\mathrm{U(1)_V}\times\mathrm{SU(3)_L}\times\mathrm{SU(3)_L}\times\mathrm{U(1)_A}$. The anomalous breaking of the $\mathrm{U(1)_A}$-symmetry can be taken into account by adding a Kobayashi–Maskawa–'t Hooft determinant [15, 16]

$$\xi = \det\Sigma + \det\Sigma^\dagger\,, \quad (3)$$

which is cubic in the (pseudo)scalar meson fields, to the Lagrangian Eq. (1). This interaction is invariant under $\mathrm{U(1)_V}\otimes\mathrm{SU(3)_L}\otimes\mathrm{SU(3)_L}$ and breaks the $\mathrm{U(1)_A}$-symmetry in Eq. (1). With this term, the proper mass splitting between η- and η'-meson as well as the pion mass can be reproduced but other implementations of the $\mathrm{U(1)_A}$-symmetry breaking are, in general, possible. The breaking term in Eq. (3) scales with the meson fields to the power N_f which leads to important N_f-dependent effects for the chiral phase transition. For three flavors, the mass splitting effects, caused by the cubic determinant, disappear in a symmetric phase of vanishing expectation values for all mesonic fields.

In total, the chirally invariant meson potential of the (2+1)-flavor quark–meson model $\tilde{U}$ in Eq. (1) is replaced by

$$\tilde{U}(\rho_1,\tilde{\rho}_2) \to \tilde{U}(\rho_1,\tilde{\rho}_2) - c\,\xi - c_x\sigma_x - c_y\sigma_y\,, \quad (4)$$

where two explicit chiral and one $\mathrm{U(1)_A}$-symmetry breaking terms have been added.

For a non-perturbative renormalization group analysis of the chiral phase transition, we employ the effective average action approach by Wetterich [18]. We truncate the effective action in form of a quark–meson model in a leading order derivative expansion. Recently, the relation of these truncations to full QCD has been affirmed by using dynamical hadronization. This approach introduces RG scale-dependent mesonic degrees of freedom that eliminate four-fermion interactions generated by gluon exchanges [19–22], see also [23]. Extending the formalism to finite temperature T, the flow equation for the RG-scale k-dependent and symmetrical potential $\tilde{U}_k$ with an optimized three-dimensional regulator [24] reads

$$k\frac{\partial \tilde{U}_k}{\partial_k} = \frac{k^5}{12\pi^2}\left[\sum_{b=1}^{2N_\mathrm{f}^2}\frac{1}{E_\mathrm{b}}\coth\left(\frac{E_\mathrm{b}}{2T}\right) -6\sum_{f=1}^{N_\mathrm{f}}\frac{1}{E_\mathrm{f}}\left\{\tanh\left(\frac{E_\mathrm{f}+\mu}{2T}\right)+\tanh\left(\frac{E_\mathrm{f}-\mu}{2T}\right)\right\}\right]. \quad (5)$$

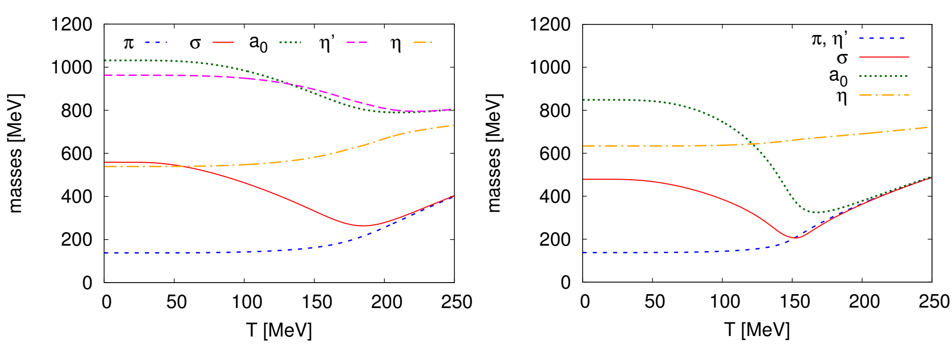
The fermionic (f) and bosonic (b) quasi-particle energies have the typical form $E_i = \sqrt{k^2+m_i^2}$. Explicit expressions for the corresponding meson masses m_b^2, calculated with the potential Eq. (4), can be found in [25]. In the non-strange–strange (x–y) basis the quark masses simplify to $m_x = h\sigma_x/2$ and $m_y = h\sigma_y/\sqrt{2}$.

The solution of this flow equation describes the scale evolution of the effective potential starting from an initial potential at some high ultraviolet scale Λ towards the full quantum effective potential in the infrared $k \to 0$ [26]. Evaluating the evolved potential at the minimum yields the grand potential as a function of temperature T and quark chemical potential μ which includes all quantum and thermal fluctuations. We adjust the initial potential $\tilde{U}_{k=\Lambda}$ at the UV scale Λ to reproduce known experimental observables in the infrared such as the pion mass or decay constants in the vacuum [25]. Concerning our implementation of $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking, we consider two different scenarios: one with a constant, *i.e.* temperature- and RG-scale-independent coupling for the Kobayashi–Maskawa–'t Hooft determinant and another without the determinant. In a future work, we will improve this truncation by considering a running version of this coupling [27] and in [28] the scale-dependency of the $\mathrm{U}(1)_\mathrm{A}$-anomaly induced determinant has already been analyzed in an RG context with QCD degrees of freedom in the vacuum.

For comparison, we also present results obtained with a standard mean-field approximation (MFA) where the mesonic fluctuations are completely neglected and a divergent vacuum contribution from the quark loop to the grand potential has been dropped. On the other hand, this divergent vacuum contribution is included in the flow equation (5). Hence, its influence on the phase transition can be investigated by solving the flow equation without mesonic fluctuations which is also called extended mean-field approximation.

3. Chiral transition and axial anomaly

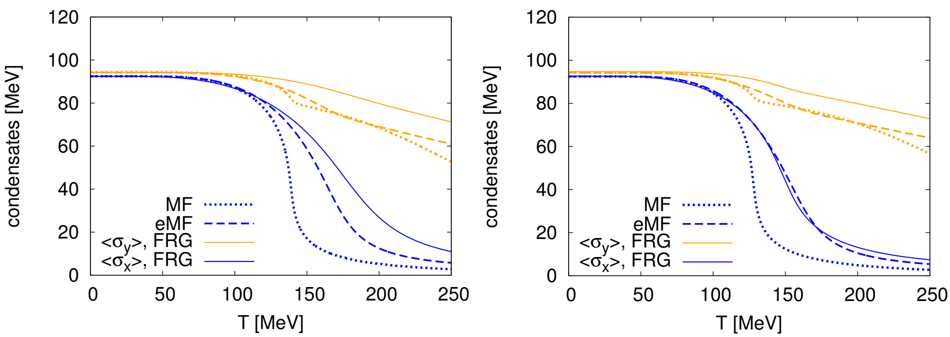
We start with a discussion of the three-flavor chiral phase transition at finite temperature and flavor symmetric chemical potential μ and investigate the interplay of fluctuations with the anomalous $\mathrm{U}(1)_{\mathrm{A}}$-symmetry breaking. The finite-temperature behavior of the (pseudo)scalar non-strange and η-, η'-meson screening masses obtained with the FRG are shown in Fig. 1 for $\mu = 0$ with (left panel) and without (right panel) $\mathrm{U}(1)_{\mathrm{A}}$-symmetry breaking. Without breaking, the η'-meson degenerates with the pion mass and the two sets of light chiral partners $(\sigma, \vec{\pi})$ and $(\vec{a}_0, \eta')$ merge in the chirally symmetric high-temperature phase. On the other hand, for a constant temperature- and scale-independent $\mathrm{U}(1)_{\mathrm{A}}$-symmetry breaking, a mass gap between the two sets of the chiral partners is obtained and the η'-meson mass drops about 200 MeV near the chiral crossover in agreement with experimental observations [1, 2]. Since the anomalous contribution to the η'- and η-meson masses is proportional to the condensates, this behavior is a consequence of the melting of the light condensate $\langle \sigma_x \rangle$ at the chiral crossover. Furthermore, the melting of the light condensate entails that the η-meson is dominantly strange and the η'-meson dominantly non-strange above the crossover temperature [17]. The remaining difference between η'-meson and pions is then directly proportional to the strange condensate $\langle \sigma_y \rangle$ which decreases much slower.



(a) with $\mathrm{U}(1)_{\mathrm{A}}$-symmetry breaking (b) without $\mathrm{U}(1)_{\mathrm{A}}$-symmetry breaking

Fig. 1. Scalar and pseudoscalar meson masses for $\mu = 0$.

The melting of both condensates as a function of temperature is demonstrated for $\mu = 0$ in Fig. 2, again, with (left panel) and without $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking (right panel). In addition to the FRG results (solid lines), we also show results obtained with a standard MFA (dotted lines) and extended MFA (dashed lines). In analogy to similar two flavor investigations [29], we find generally that fluctuations wash out the transition and the condensates decrease faster in the standard MFA. However, this behavior cannot be solely attributed to mesonic fluctuations. Comparing the FRG non-strange condensate $\langle\sigma_x\rangle$ with the one obtained in the renormalized model (eMFA), the influence of the $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking term becomes visible. Without the breaking term both non-strange condensates agree well, whereas with a $\mathrm{U}(1)_\mathrm{A}$-breaking term the melting of $\langle\sigma_x\rangle$ is further softened if mesonic fluctuations are added. In other words, the chiral transition is considerably affected by the Kobayashi–Maskawa–'t Hooft term only if mesonic fluctuations are taken into account, whereas the mean-field investigations show only a weak dependence on the $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking.



(a) with $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking (b) without $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking

Fig. 2. Non-strange $\langle\sigma_x\rangle$ and strange $\langle\sigma_y\rangle$ chiral condensates for $\mu = 0$.

At non-vanishing chemical potential the impact of mesonic fluctuations including a $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking has similar consequences. For this purpose, we investigate the existence and location of the critical endpoint (CEP) in the (T, μ)-plane obtained with the FRG and mean-field approximations with and without the Kobayashi–Maskawa–'t Hooft determinant. The results are collected in the left panel of Fig. 3. An endpoint labeled with a star is the corresponding result including the determinant and a cross denotes the results without a $\mathrm{U}(1)_\mathrm{A}$-symmetry breaking term. Since the location of the endpoints also depends considerably on the chosen value of the σ-meson mass [17], we have fixed the value to $m_\sigma = 480$ MeV in all calculations. At the critical point, the quark-number susceptibiliy diverges because the chiral transition is of second order. This is shown in the right panel of Fig. 3.

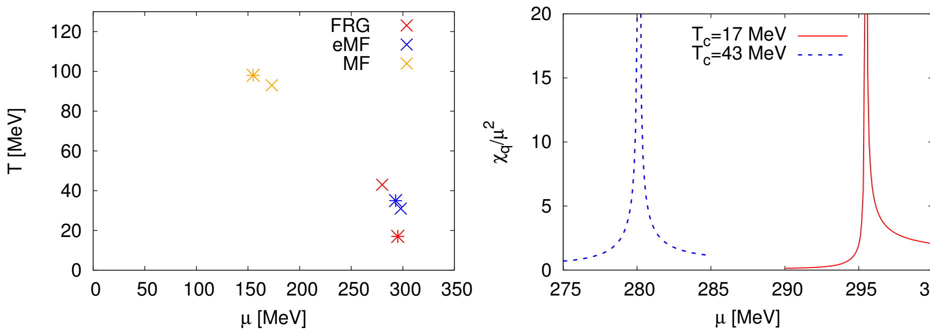
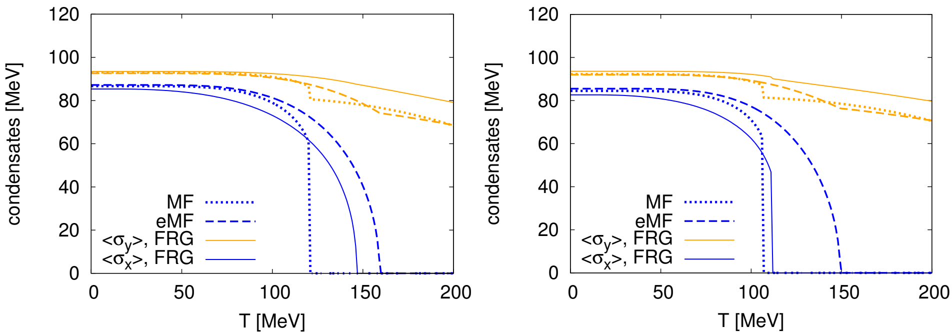


Fig. 3. Charts of critical endpoints. Left panel: stars $U(1)_A$-symmetry breaking included, crosses: no $U(1)_A$-symmetry breaking term. Right panel: FRG quark number susceptibilities, dashed lines without and solid lines with $U(1)_A$-symmetry breaking term.

Similar to the $\mu = 0$ results, we see that the inclusion of the fermionic vacuum term (eMF) makes the system less critical and, therefore, the location of the CEP is pushed towards larger chemical potentials and smaller temperatures as compared to the standard mean-field approximation. In both mean-field approximations, the influence of $U(1)_A$-symmetry breaking is rather weak and we find that the CEP without a breaking term is always at slightly smaller temperatures and larger chemical potentials. Adding mesonic fluctuations with the FRG leads to a qualitative change. With a $U(1)_A$-symmetry breaking, the mesonic fluctuations push the CEP to even larger chemical potentials and smaller temperatures in contrast to the mean-field approximations. This behavior is in agreement with observations in two-flavor O(4)-symmetric investigations [29], which implicitly assume a maximal $U(1)_A$-symmetry breaking if the remaining chiral (pseudo)scalar multiplets, the η and $\vec{a}$ fields, are neglected. Interestingly, without the determinant, the endpoint is moved in the opposite direction towards smaller chemical potentials and larger temperatures if additionally mesonic fluctuations are taken into account.

It is enlightening to extend the analysis and study the quark mass sensitivity of the chiral transition with a focus on the role of fluctuations together with the axial $U(1)_A$-symmetry. In an RG context with an ϵ-expansion, it has been argued that in a purely bosonic theory for vanishing anomaly the chiral phase transition should be of fluctuation-induced first order for $N_f \geq 2$ in the SU(3)-symmetric chiral limit [12]. Including the anomaly term, the order does not change and the phase transition remains first order for $N_f \geq 3$. However, the case of $N_f = 2$ massless flavors is special. If the temperature-dependence of the coupling of the, in this case quadratic, Kobayashi–Maskawa–'t Hooft determinant is negligible the phase transition can be second order with O(4) criticality. In other words, a temperature-independent $U(1)_A$-symmetry breaking can smoothen the transition from first to second order in the two-flavor chiral limit, see also [13, 14] for recent investigations. The opposite happens for three flavors and the first-order transition can become even stronger in the three-flavor chiral limit.

In Fig. 4 we show the non-strange and strange condensates in the light chiral limit, $c_x \to 0$ and $c_y \neq 0$ for $\mu = 0$ similar to Fig. 2. In agreement with previous works [17], a first-order transition is found independent of the $U(1)_A$-symmetry breaking in the standard mean-field approximation. Going beyond mean-field by including the fermionic vacuum contribution (eMF), the transition changes to second order. With the FRG the $U(1)_A$ anomaly has a significant influence: with the determinant we find a second-order transition and without a first-order transition.



(a) with $U(1)_A$-symmetry breaking (b) without $U(1)_A$-symmetry breaking

Fig. 4. Condensates for $\mu = 0$ similar to Fig. 2 for the light chiral limit $c_x \to 0$.

The results on the quark mass sensitivity of the chiral transition with and without the $U(1)_A$-symmetry are consistent with the results of [12] under the assumption that the Kobayashi–Maskawa–'t Hooft determinant behaves qualitatively like a two-flavor determinant in the case of a physical strange quark mass. This is also indicated by the fact that the strange condensate is affected only mildly at the light chiral transition. As a consequence, the cubic determinant for $N_f = 3$ behaves like the quadratic two-flavor Kobayashi–Maskawa–'t Hooft term. Furthermore, these findings elucidate why the system is "more critical" in the absence of the determinant, *i.e.*, why, in this case, the critical endpoint is pushed towards larger temperature and smaller chemical potential if mesonic fluctuations are taken into account.

Finally, we want to point out that a first-order transition emerges in the chiral limit only if the chiral invariant $\tilde{\rho}_2$ is taken into account which is most important for similar two-flavor investigations.

4. Summary and conclusions

The influence of quantum and thermal fluctuations on the chiral three-flavor phase transition with and without an axial $U(1)_A$-symmetry breaking is investigated in the framework of the functional renormalization group with a quark–meson model truncation. Different mean-field approximations where certain fluctuations are neglected, are confronted to the full FRG analysis. The $U(1)_A$-symmetry breaking is effectively implemented by a Kobayashi–Maskawa–'t Hooft determinant with a constant coupling strength.

We find a strong dependence of the location of the critical endpoint on the $U(1)_A$-symmetry breaking if mesonic fluctuations are taken into account. With a broken $U(1)_A$-symmetry the endpoint is pushed towards smaller temperature and larger quark chemical potentials which is in contrast to corresponding investigations within mean-field approximations.

In the limit of vanishing light quark masses with a physical strange quark mass, the transition is first order for a $U(1)_A$-symmetric theory but second order with a constant $U(1)_A$-symmetry breaking Kobayashi–Maskawa–'t Hooft determinant. It will be fascinating to see the results for an improved truncation with a temperature- and scale-dependent $U(1)_A$-symmetry breaking implementation whose outcomes should lie in between our two findings.

Both findings, the influence of the determinant on the location of the critical endpoint as well as the order of the chiral transition, can be traced back to an effective mass term induced by the $U(1)_A$-symmetry breaking term in the light flavor sector of the theory.

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