Charge Fluctuations along the QCD phase boundary

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Abstract. We discuss the properties of the net–quark and isovector fluctuations along the chiral phase transition line in the plane spanned by temperature and baryon chemical potential. Our results are obtained in terms of the Nambu–Jona-Lasinio (NJL) model within the mean-field approximation. The model is formulated at the finite temperature and for non-vanishing net–quark and the isospin chemical potentials. The fermion interactions are controlled by the strength of the scalar and vector couplings in the iso-scalar and iso-vector channels of constituent quarks. We explore properties and differences in the behavior of the net–quark number and isovector susceptibilities for different values of thermal parameters near the phase transition. We argue that any non-monotonic behavior of the net–quark number susceptibility along the phase transition boundary is an excellent probe of the existence and the position of the second order endpoint in the QCD phase diagram.

One of the essential predictions of QCD is the existence of the boundary line in the temperature and net–quark chemical potential, \((T,\mu_q)\)–plane that separates the confined, chirally broken hadronic phase from the deconfined quark–gluon plasma phase. The existence of such a boundary line for \(\mu_q/T \leq 1\) has been recently established by the first principle calculations in the Lattice Gauge Theory (LGT) formulated at finite baryon density \([1, 2, 3, 4]\).

Arguments based on effective models \([5, 6, 7, 8, 9, 10, 11, 12, 13]\) indicate that at large \(\mu_q\) the transition along the boundary line is the first order. For small \(\mu_q\) and for two massless flavor QCD the chiral transition was argued \([14]\) to be second order with the critical exponents of the O(4) spin model. For the finite quark mass, due to the explicit chiral symmetry breaking, this transition is likely to be replaced by the rapid crossover. Such a different nature of the phase transition at low and high \(\mu_q\) suggests that the QCD phase diagram should exhibit a critical endpoint at which the line of the first order phase transition matches that of the second order or analytical crossover \([15]\). The critical properties of this second order chiral endpoint are expected to be determined by the three-dimensional Ising model universality class \([10, 16]\).

The existence of a critical endpoint in QCD has been recently studied in the lattice calculations at the non-vanishing chemical potential by either considering the location of Lee–Yang zeros in \((2+1)\)–flavor QCD \([4, 17]\) or by analyzing the convergence radius of the Taylor series in \(\mu_q/T\) expansion of the free energy \([2, 18, 19]\). Recent results \([18]\) based on the first approach suggest that a critical endpoint indeed exists in QCD phase diagram and might occur at \(T \simeq 164\) and \(\mu_q \simeq 120\) MeV. In the 2–flavor QCD and with a relatively large quark mass used in the actual lattice calculations \([18]\) no direct evidence for the existence of the critical endpoint has been found for \(\mu_q < T\) where the Taylor expansion method is applicable.

The critical behavior and the position of the chiral endpoint can be possibly identified by observables that are sensitive to singular part of the free energy \([20]\). One such observable is the quark susceptibility \(\chi_{ij}\) defined as the second order derivative of the thermodynamical-potential \(\Omega(T,\vec{\mu},V)\) with respect to quark–flavor chemical potentials, \(\chi_{ff'} = -\partial^2\Omega/\partial\mu_f\partial\mu_{f'}\), where for two light \((u,d)\)–quarks, \(\vec{\mu} = (\mu_u,\mu_d)\). To identify the chiral critical endpoint in the QCD phase diagram, the properties of the net–quark number susceptibility \(\chi_q\) are of particular interest \([21, 22, 23]\). In two–flavor QCD, \(\chi_q\) is expressed as the sum of \(u\) and \(d\) quarks susceptibilities: \(\chi_q = 2(\chi_{uu} + \chi_{ud})\). The universality argument predicts that independent of the values of the quark masses the \(\chi_q\) should diverge at the chiral endpoint.

The quark susceptibilities have been recently obtained \([3, 18, 19, 24]\) within the lattice QCD for two light quark flavors using p4–improved staggered fermion action with the quark mass \(m_q/T = 0.4\) \([24, 18]\). The
Monte Carlo simulations have been done at the finite quark chemical potential via Taylor series expansion. The susceptibilities were calculated up to the $O(\mu_q^4)$ order in the quark chemical potential \cite{18, 25, 20}. The lattice results \cite{18, 25} for the net–quark number susceptibility $\chi_q$ and isovector susceptibility $\chi_I$ as a function of the temperature for different values of $\mu_q$ are shown in Fig. 1. There is a strong suppression of the $\chi_q$ fluctuations in confined phase and the cusp-like structure in the near vicinity of the transition temperature $T_0$. A rather strong increase of $\chi_q$ at the transition temperature $T_0$ with increasing quark chemical potential is also observed on the lattice. The lattice results confirmed that the quark fluctuation in the isovector channel $\chi_I$ contrary to $\chi_q$ does not exhibit a peak structure at $T_0$ and shows a rather weak dependence on $\mu_q$ as seen in Fig. 1–right. Such a properties of $\chi_q$ and $\chi_I$ can be also quantified by the regular part of the free energy due to the enhanced contribution of resonances in the near vicinity of the transition temperature \cite{18, 20, 25, 26}. The above became clear in Fig. 1 where the LGT results on $T$ and $\mu_q$ dependence of different quark susceptibilities in confined phase are seen to be quite successfully described by the resonance gas partition function \cite{25}. The apparent agreement of the LGT results with the hadron resonance gas on the level of the equation of state and the susceptibilities in the temperature range $T < T_0$ indicate that increase of the $\chi_q$ fluctuations observed in Fig. 1 with increasing $\mu_q$ at $T_0$ is a necessary but not sufficient condition to verify the existence of the chiral endpoint. In the following we will argue in model calculations that to verify the appearance of the TCP in the QCD phase diagram would require a non-monotonic behavior of the $\chi_q$ when going along the phase boundary.

Having in mind the importance of the quark number fluctuations as a probe of phase structure of QCD as well as the above lattice results the main scope of this article is to consider the properties of different quark susceptibilities in terms of an effective chiral model. Of particular interest is the behavior of the quark number correlations in different channels along the boundary line and in the near vicinity of the chiral endpoint. The calculations will be done in terms of two-flavor Nambu–Jona-Lasinio (NJL) model \cite{27} formulated at the finite temperature and chemical potentials related with baryon number and isospin conservation.
**Figure 2.** The NJL model phase diagram in the chiral limit for $G_V^{(S)} = 0, 0.3$ and $0.6 G_S$. The dashed (solid) line denotes the second-order (first-order) transition line. The tricritical point indicated by a dot ($\bullet$) is located at $(T, \mu_q) = (65, 275)$ MeV for $G_V^{(S)} = 0$ and $(T, \mu_q) = (42, 305)$ MeV for $G_V^{(S)} = 0.3 G_S$. The results are shown for vanishing isovector chemical potential.

1. The net–quark and isovector fluctuations in the NJL model

The thermodynamics of the NJL model at the finite temperature and non vanishing net–quark and isospin chemical potentials is obtained from the partition function $Z(T, \mu_q, \mu_I, V)$ formulated as a generating functional in the Euclidean space. In the mean field approximation the partition function is obtained from the effective Lagrangian

$$L = \bar{\psi} (i \partial - M + \bar{\mu} \gamma_0) \psi - \frac{1}{4G_S} (M - m)^2 + \frac{1}{4G_V^{(S)}} (\bar{\mu}_q - \mu_q)^2 + \frac{1}{4G_V^{(V)}} (\bar{\mu}_I - \mu_I)^2, \quad (1)$$

in which the thermal averages $\langle \bar{\psi} \gamma^\tau \gamma_0 \psi \rangle$ have been neglected. The strength of the constituent quarks interactions in scalar and vector channels are parameterized by the effective coupling $G_S$ and $G_V$ respectively which have dimensions of length square. To distinguish quark-antiquark interactions in the iso-scalar and iso-vector channels we have defined two independent couplings $G_V^{(S)}$ and $G_V^{(V)}$ respectively. In Eq. (1) we have also introduced a dynamical mass $M$ and shifted chemical potential $\bar{\mu}$ which are obtained from

$$M = m - 2G_S \langle \bar{\psi} \psi \rangle, \quad \bar{\mu} = \bar{\mu}_q + \bar{\mu}_I \tau^3, \quad (2)$$

with

$$\bar{\mu}_q = \mu_q - 2G_V^{(S)} \langle \bar{\psi} \gamma_0 \psi \rangle, \quad \bar{\mu}_I = \mu_I - 2G_V^{(V)} \langle \bar{\psi} \tau^3 \gamma_0 \psi \rangle. \quad (3)$$

In the mean field approximation the thermodynamic potential of the NJL model is obtained in the following form

$$\Omega(T, \mu; M, \bar{\mu}) = \sum_{f=u,d} \Omega_f(T, \mu; M_f, \bar{\mu}_f) +$$

$$\frac{1}{4G_S} (M - m)^2 - \frac{1}{4G_V^{(S)}} (\bar{\mu}_q - \mu_q)^2 - \frac{1}{4G_V^{(V)}} (\bar{\mu}_I - \mu_I)^2, \quad (4)$$
in the $(T, \mu_{T,\mu})$-plane and isovector chemical potentials. 

The location of the boundary line that separates chirally broken from the symmetric phase was found from the requirement of vanishing dynamical quark mass $M(T, \mu_{q}) = 0$ when approaching from the side of the broken phase. Along the boundary line the order of the chiral symmetry restoration transition is

\[
\Omega_f(T, \mu; M_f, \tilde{\mu}_f) = -2N_c \int \frac{d^3p}{(2\pi)^3} \left[ E_f - T \ln(1 - n_f^{(+)}(T, \tilde{\mu}_f)) - T \ln(1 - n_f^{(-)}(T, \tilde{\mu}_f)) \right],
\]

where $E_f = \sqrt{p^2 + M_f^2}$ is a quasiparticle energy and $n_f^{(\pm)}(T, \tilde{\mu}_f) = \left(1 + \exp\left[(E_f \mp \tilde{\mu}_f)/T\right]\right)^{-1}$ is the distribution function for the particle $(+)$ and anti-particle $(-)$.

The condensates appearing in Eqs. (2)-(4) are obtained from the conditions to minimize the thermodynamic potential with respect to the dynamical mass and the shifted chemical potentials, $\partial \Omega/\partial M_f = \partial \Omega/\partial \tilde{\mu}_f = 0$. From the above stationary conditions and from Eqs. (2)-(4) one calculates the quark condensates as the solution of the following gap equations:

\[
M_f = m_f + 4G_S N_c \sum_{f=u,d} \frac{d^3p}{(2\pi)^3} \frac{M_f}{E_f} \left[1 - n_f^{(+)}(T, \tilde{\mu}_f) - n_f^{(-)}(T, \tilde{\mu}_f)\right],
\]

\[
\mu_q = \tilde{\mu}_q + 4G_V^{(S)} N_c \sum_{f=u,d} \frac{d^3p}{(2\pi)^3} \left[n_f^{(+)}(T, \tilde{\mu}_f) - n_f^{(-)}(T, \tilde{\mu}_f)\right],
\]

\[
\mu_I = \tilde{\mu}_I + 4G_V^{(V)} N_c \int \frac{d^3p}{(2\pi)^3} \left[\left(n_u^{(+)}(T, \tilde{\mu}_u) - n_u^{(-)}(T, \tilde{\mu}_u)\right) - (u \rightarrow d)\right].
\]

The above gap equations together with the potential (4) are sufficient to describe within the NJL model the thermodynamics and the phase structure of an effective quark medium at the finite temperature and the net–quark and isovector chemical potentials.

Fig. 2 represents the phase diagram of the NJL model related with the chiral symmetry restoration in the $(T, \mu_q)$-plane obtained in the isospin symmetric system and in the limit of vanishing current quark masses. The location of the boundary line that separates chirally broken from the symmetric phase was found from the requirement of vanishing dynamical quark mass $M(T, \mu_q) = 0$ when approaching from the side of the broken phase. Along the boundary line the order of the chiral symmetry restoration transition is...
not unique. In the high quark density regime the phase transition is of the first order and terminates at the finite $T$ and $\mu_q$ as the second order transition corresponding to the position of the tricritical point (TCP). In the NJL model under the mean field approximation the location of the TCP is determined by the condition of vanishing of the second and the fourth order coefficients in the Taylor expansion of the thermodynamical potential: $\Omega(M, \mu_q, T) = a_0 + a_2 M^2 + a_4 M^4 + O(M^6)$ applicable in the limit of $M \to 0$. For temperatures above the TCP the transition stays of the second order as expected in the Ginzburg–Landau theory.

The position of the boundary line and the TCP clearly depends on the values of the model parameters. In Fig. 2 the critical line was calculated for different strength of the vector coupling $G_V$ at fixed values of $G_S$ and the momentum cut-off $\Lambda$. As can be seen in Fig. 2, an increase of $G_V$ results a decrease of $T_c$ and a shift of $\mu_q^c$ towards larger values. This is to be expected as the vector couplings $G_V^{(S)}$ and $G_V^{(V)}$ are related with repulsive interactions of constituent quarks. The position of the TCP is also shifted to the lower temperature and higher $\mu_q$, with increasing coupling in the vector channel. A similar modification of position of the phase diagram and the TCP is observed with change of the scalar coupling $G_S$ and the cut–off $\Lambda$. It is interesting to see that for a sufficiently large $G_V$ the TCP disappears from the phase diagram and in the whole parameter range the phase transition is of the second order.

1.0.1. Quark susceptibilities near the phase boundary With the thermodynamic potential and the self-consistent gap equations one can calculate the net–quark number and isovector susceptibilities and study their sensitivity and behavior near the phase transition.

To calculate $\chi_q$ and $\chi_I$ from Eq. 4 we have to take into account that the dynamical masses $M_I$ and the shifted chemical potentials $\tilde{\mu}_I$ are implicitly dependent on $\mu_q$, $\mu_I$ and $T$. Consequently the susceptibilities $\chi_q, I$ are controlled by derivatives of $M_I$ and $\tilde{\mu}_I$:

$$\chi_q = \frac{2N_c}{T} \sum_{f=u,d} \int \frac{d^3p}{(2\pi)^3} \left[ - \frac{M_f}{E_f} \frac{\partial M_f}{\partial \mu_q} \left( n_f^{(+)} (1 - n_f^{(+)} - n_f^{(-)} (1 - n_f^{(-)})) \right) + \frac{\partial \tilde{\mu}_f}{\partial \mu_q} \left( n_f^{(+)} (1 - n_f^{(+)} + n_f^{(-)} (1 - n_f^{(-)})) \right) \right],$$

$$\chi_I = \frac{2N_c}{T} \sum_{f=u,d} \int \frac{d^3p}{(2\pi)^3} \left[ - \frac{M_u}{E_u} \frac{\partial M_u}{\partial \mu_I} \left( n_u^{(+)} (1 - n_u^{(+)} - n_u^{(-)} (1 - n_u^{(-)})) \right) + \frac{\partial \tilde{\mu}_u}{\partial \mu_I} \left( n_u^{(+)} (1 - n_u^{(+)} + n_u^{(-)} (1 - n_u^{(-)})) \right) - (u \to d) \right],$$

where we have suppressed for simplicity the $T$ and $\mu_f$ dependence of $n_f^{(+)}$ distributions.

The NJL model does not exhibit confinement properties of QCD. Thus, there are no hadronic bound states and resonances in the chirally broken phase in the NJL medium. Instead, we are dealing with constituent quarks which can be viewed as quasi-particles with the temperature and density dependent composition of the medium in the NJL model is not changed. At the chiral transition the dynamical quark masses $M_I$ vanish and above $T_c$ the medium is populated by interacting massless quarks. In addition, due to the momentum cut-off there is a suppression of large momentum quark modes which is particularly efficient at high temperature. The differences in the mass spectrum of the NJL model and the QCD as well as suppression of the particle thermal phase-space will result in different quantitative properties of quark number fluctuations. However, this does not exclude some possible common features of susceptibilities in QCD and in the NJL model related with the restoration of the chiral symmetry.

Fig. 3 shows the quark number susceptibility $\chi_q$ as a function of $T$ for different values of $\mu_q$. The calculations correspond to the chiral limit and were done for the fixed value of the vector coupling constant $G_V^{(S)} = 0.3G_S$. The net–quark fluctuations are normalized to that one for an ideal quark gas $\chi_q^{(\text{free})} = N_c N_f (T^2/3 + \mu_q^2/\pi^2)$. 

\[\text{Charge Fluctuations along the QCD phase boundary}\]
There are generic features in the temperature dependence of $\chi_q$ for different values of $\mu_q$. From Fig. 4 it is clear that the model exhibits a phase transition for all values of $\mu_q$. The transition temperature is strongly $\mu_q$-dependent and decreases with increasing $\mu_q$. However, there is an essential difference between the critical behavior of $\chi_q$ at vanishing and at the finite $\mu_q$. For $\mu_q \neq 0$ the susceptibility exhibits discontinuity at $T_c$ which increases with increasing $\mu_q$. For $\mu_q = 0$ such a discontinuous structure disappears and instead at $T_c$ the susceptibilities shows a non-analytic structure which results as discontinuity in higher moments of net–quark number fluctuations. Such a properties of $\chi_q$ are consistent with that expected if the phase transition is of second order and belongs to universality class of three-dimensional $O(4)$ symmetric spin models [21, 25]. To see it, let us construct an effective thermodynamic potential in the near vicinity to the chiral transition. The relevant field is here a constituent quark that carries the dynamical mass $M$. Performing the Taylor expansion of $\Omega(M, T, \mu_q)$ as power series around $M \approx 0$ one gets:

$$\Omega(M, T, \mu_q) = \Omega_0(T, \mu_q) + \frac{1}{2}a(T, \mu_q)M^2 + \frac{1}{4}b(T, \mu_q)M^4.$$ (11)

Thus, $\Omega$ has a structure of the Ginzburg–Landau (GL) potential where the effective quark mass acts as the sigma field. Following the GL theory and applying the mean field approximation the effective potential (11) is rewritten as

$$\Omega(T, \mu_q; M_0) = \Omega_0(T, \mu_q) - \frac{a^2(T, \mu_q)}{4b(T, \mu_q)}.$$ (12)

where we have used the stationary condition $\partial\Omega/\partial M |_{M_0} = 0$ and introduced the stationary point $M_0 = \sqrt{-a/b}$. Approaching the critical line from the symmetric phase with $M = 0$, the quark number susceptibility $\chi_q$ is obtained from Eq. (11) as

$$\chi_q^{(\text{sym})} = \frac{\partial^2\Omega_0}{\partial \mu_q^2}.$$ (13)

In the GL theory the second-order phase transition line (the $O(4)$ critical line) is determined by the requirement that the coefficient $a = 0$ and $b \neq 0$ in Eq. (11). In the near vicinity to the critical point $(T_c, \mu_q^c)$...
the coefficient $a(T, \mu_q)$ can be parameterized in the MF approximation as
\[ a(T, \mu_q) \approx C(T - T_c) + D(\mu_q - \mu_q^c), \tag{14} \]
where $C$ and $D$ are independent of $T$ and $\mu_q$. Approaching the $O(4)$ critical line from the broken phase, the quark susceptibility is calculated from Eqs. (12) and (14) as:
\[ \chi_q^{\text{(broken)}} = \frac{\partial^2 \Omega_0}{\partial \mu_q^2} - \frac{D^2}{2b(T, \mu_q)}. \tag{15} \]
Comparing Eqs. (12) and (15) it is clear that the second term in (15) gives just a discontinuity of $\chi_q$ across the $O(4)$ critical line at the finite $\mu_q$. While at $\mu_q = 0$ the coefficient $D = 0$ and $\chi_{q}^{\text{(sym)}} = \chi_{q}^{\text{(broken)}}$ at $T = T_c$.

Considering the phase diagram in Fig. 2 we have already indicated that for large $\mu_q$ the NJL model experiences the TCP. The right panel of Fig. 2 shows the properties of the quark number susceptibility in the near vicinity and at TCP. In the GL theory the position of the TCP is characterized by the condition of vanishing $a(T, \mu_q)$ and $b(T, \mu_q)$ coefficients in the effective potential (11). Consequently, from Eq. (15) it is clear that the quark fluctuations $\chi_q$ should diverge at TCP. These expected properties of $\chi_q$ are clearly seen in Fig. 3. With the present choice of parameters the TCP is located at $(T_c, \mu_q^c) = (42, 305)$ MeV where $\chi_q \to \infty$. Crossing TCP towards larger $\mu_q$ the second order $O(4)$ chiral phase transition is converted to the first order where $\chi_q$ is finite and has a gap at the critical temperature.

From the perspective of heavy ion experiments the properties of different susceptibilities are of particular interest. This is because, fluctuations related with the conserved charges are experimentally directly accessible. Since these are also observables that are sensitive to the critical behavior, knowledge of the properties of susceptibilities along the phase boundary line could give insights how to verify the QCD phase transition experimentally. Clearly, the quantitative structure of the phase diagram and the position of the chiral endpoint is model dependent. Thus, also the position of the QCD boundary line could be very different than that found in the NJL model. However, the model study could still answer a phenomenologically relevant question how to observe and how large is the critical region along the phase transition where the fluctuations are sensitive to the singular structure at the tricritical or chiral endpoint.

Fig. 3 shows the net–quark susceptibility $\chi_q$ along the phase boundary line from Fig. 2. The $\chi_q$ is quantified as a function of the chiral phase transition temperature $T_c$. The appearance of the TCP in the phase diagram results in a non-monotonic behavior of $\chi_q$ along the transition line. There is a window of $\Delta T_c \simeq 30$ MeV above and $\Delta \mu_q^c \simeq 10$ MeV around TCP where the fluctuations are sensitive to the appearance of the tricritical point. If the TCP was absent in the phase diagram then the $\chi_q$ would be a monotonic function of $T_c$ along the phase boundary as shown by a dashed–dotted line in Fig. 2. Such a behavior is seen in Fig. 4–right in the isovector susceptibility which is not sensitive to the appearance of the TCP in the phase diagram 33. The non-monotonic behavior of $\chi_q$ is only seen from the side of the chirally broken phase. Approaching $T_c$ from the chirally symmetric phase results in continuous behavior of $\chi_q$ along the boundary line. This is because the $\chi_q^{\text{(sym)}}$ is finite at the chiral transition in the whole parameter range as seen in Fig. 3. A difference between $\chi_q^{\text{(sym)}}$ and $\chi_q^{\text{(broken)}}$ calculated along the phase transition line measures the magnitude of discontinuity at the phase transition. Fig. 3 shows that at $\mu_q^c = 0$ this discontinuity vanishes and at $T_c = 0$ would be the largest if the phase diagram did not experience the TCP.

In nucleus–nucleus collisions any change of the temperature and chemical potential is correlated with the corresponding change of the c.m.s collision energy $\sqrt{s}$ 34. An increase of $\sqrt{s}$ results in increasing the temperature $T$ and decreasing the quark chemical potential $\mu_q$. Thus, the critical region around tricritical or chiral endpoint ($\Delta \mu_q^c, \Delta T_c$) can be converted to that in the c.m.s. $\sqrt{s}$–energy in A–A collisions. Admitting that the relation of $\mu_q^c$ and $T_c$ with $\sqrt{s}$ are the same as for chemical freezeout parameters extracted from experimental data 34 the $\Delta T_c \simeq 30$ MeV window around the TCP would correspond to $\Delta s \sim 1$ A-GeV. Thus, within our crude estimates, we can expect that to observe any remnant of critical fluctuations in A–A collisions one would need the $\sqrt{s}$ energy step to be within a range of 1 AGeV.
We have discussed the properties of quark fluctuations in terms of Nambu–Jona-Lasinio (NJL) model. The model was formulated at finite temperature and chemical potentials related with the conservation of baryon number and isospin. Applying the mean field approach, we have shown how the fluctuations of different quark flavors are changing across the phase boundary. Such a study is interesting from the perspective of heavy ion phenomenology and the lattice gauge theory. In the first case we have indicated and quantified the non-monotonic structure of the net-quark number susceptibility along the phase boundary as the method to identify the position of the chiral endpoint. We have also discussed the critical region around this point in the context of heavy ion phenomenology.

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