Correlations among discontinuities in the QCD phase diagram

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Abstract

We show, in general, that when a discontinuity of either zeroth order or first order takes place in an order parameter such as the chiral condensate, discontinuities of the same order emerge in other order parameters such as the Polyakov loop. A condition for the coexistence theorem to be valid is clarified. Consequently, only when the condition breaks down, zeroth-order and first-order discontinuities can coexist on a phase boundary. We show with the Polyakov-loop extended Nambu–Jona–Lasinio model that such a type of coexistence is realized in the imaginary chemical potential region of the QCD phase diagram. We also present examples of coexistence of the same-order discontinuities in the real chemical potential region.

Exploring the phase diagram of quantum chromodynamics (QCD) is one of the most important subjects in hadron physics. Actually, many works have been done so far on this subject, and it is expected that there appears several interesting phases in hot and/or dense quark matter, for example, chiral symmetry broken and restored phases, confinement and deconfinement phases, two-flavor color superconducting and color-flavor locked phases, and so on; for example, see [1] and references therein. These phases are characterized in terms of some exact or approximate order parameters such as the chiral condensate, the diquark condensate, the Polyakov loop and so on. Therefore, correlations among these order parameters are to be investigated. In particular, the relation between orders of their discontinuities is essential. It was proven by Barducci, Casalbuoni, Pettini and Gatto (BCPG) [2] that different first-order phase transitions take place simultaneously. The theorem corresponds to a generalization of the Clausius–Clapeyron relation.

Studying these correlations directly in QCD is desired; however, in the finite chemical potential region, lattice QCD is still far from perfection because of the sign problem, for
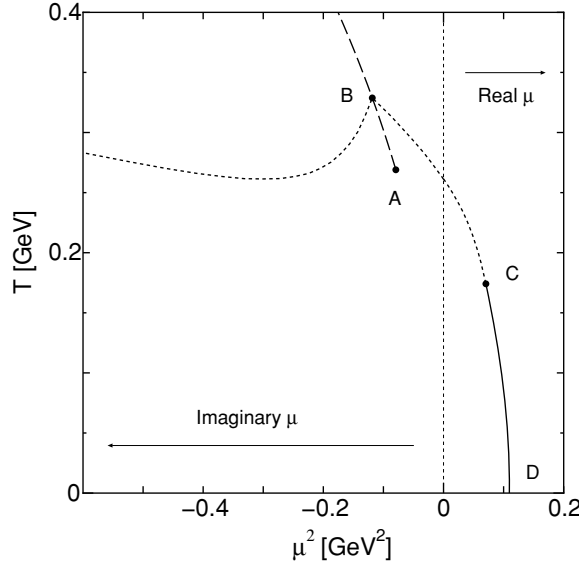
Figure 1. Phase diagram in the μ^2–T plane predicted by the PNJL model in the chiral limit.

example, see [3] and references therein. So the phase diagram was investigated with effective models. Recently, important progress has been made by the Polyakov-loop extended Nambu–Jona–Lasinio (PNJL) model [4–23]. This model can describe the chiral, the color superconducting and the confinement/deconfinement phase transitions.

Figure 1 shows the phase diagram in the chiral limit predicted by the two-flavor PNJL model without diquark condensate; the details of the calculation will be shown later. The diagram is drawn in the μ^2–T plane, where T stands for temperature and μ stands for quark chemical potential. The solid and dotted curves represent first- and second-order chiral phase transitions, respectively. In this paper, when an order parameter has a discontinuity in its value (zeroth order), we call it the first-order phase transition. Meanwhile, when an order parameter has a discontinuity in its derivative (first order) and its susceptibility is divergent, we refer to it as the second-order phase transition. However, our discussion is mainly concentrated on the relationship between zeroth- and first-order discontinuities.

On the solid curve between points C and D, two zeroth-order discontinuities emerge simultaneously in the Polyakov loop and the chiral condensate. This is a typical example of the BCPG theorem. As an interesting fact, on the dotted curves, two first-order discontinuities take place simultaneously in the chiral condensate and the Polyakov loop. This implies that the BCPG theorem on the zeroth-order discontinuity of order parameter can be extended to the case of the first-order one. As another interesting point, on the dashed curve between points A and B, a first-order discontinuity of the chiral condensate coexists with zeroth-order discontinuities of quark number density and other θ-odd quantities, where $\theta = -\mathrm{i}\mu/T$. On the dashed curve moving up from point B, furthermore, the quark number density still has a zeroth-order discontinuity, although the chiral condensate is always zero. Thus, the relation between orders of discontinuities of various quantities is much richer than that the BCPG theorem predicts.

In the left half plane of figure 1, μ is imaginary. However, the phase diagram in the region is also important, since in the region lattice QCD has no sign problem and then its results are

available. Hence, the validity of the PNJL model can be tested there by comparing the model results with the lattice ones. Actually, it has been shown for the case of finite quark mass that the results of the PNJL model are consistent with those of the lattice simulations [22]. Furthermore, the real μ system can be regarded as an image of the imaginary μ one, since the canonical partition function of real μ is the Fourier transform of the grand canonical partition function of imaginary μ [26].

The aim of this paper is to extend the BCPG theorem on the zeroth-order discontinuity of order parameter to the case of the first-order discontinuity, that is, we show that once a discontinuity of either zeroth order or first order takes place in an order parameter such as the chiral condensate, discontinuities of the same order appear in other order parameters such as the Polyakov loop. The original coexistence theorem of BCPG on the zeroth-order discontinuity and the present coexistence theorem on the first-order discontinuity are preserved, when the phase boundary is shifted in both the T- and μ-directions by varying values of external parameters such as the current quark mass; the condition will be shown later in (15) and (16). In other words, discontinuities in mutually different orders can coexist only when the condition breaks. Such a situation is not just a trivial exception but a physical relevance. Actually, we will show that the situation is realized in the Roberge and Weiss (RW) phase transition [26] appearing in the imaginary chemical potential region of the QCD phase diagram, and prove from the viewpoint of the coexistence theorem that the RW phase transition is a family of zeroth- and first-order discontinuities. This resolution of the RW phase transition is a principal subject of this paper. We present some examples of the coexistence by using the PNJL model for both real and imaginary chemical potential regions in the phase diagram.

We begin with the grand canonical partition function

$$Z(T, \mu) = \text{Tr} \exp[-\beta(\hat{H} - \mu\hat{N})] \tag{1}$$

with a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \sum_\alpha \lambda_\alpha \hat{\mathcal{O}}_\alpha, \tag{2}$$

where $\hat{H}_0$ determines the intrinsic system, λ_α are external parameters conjugate to the Hermitian operators $\hat{\mathcal{O}}_\alpha$ and $\beta = 1/T$, μ is the chemical potential and $\hat{N}$ is the particle number. The thermodynamical potential $\Omega(T, \mu)$ is given by

$$\Omega(T, \mu) = -\frac{T}{V} \ln Z(T, \mu) \tag{3}$$

with V being the three-dimensional volume, and the entropy density s and the particle number density n are also given by

$$s = -\left(\frac{\partial\Omega}{\partial T}\right)_{\mu,\lambda}, \qquad n = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,\lambda}, \tag{4}$$

where the subscripts mean that they are fixed in the partial differentiation as usual. The expectation value of the operator $\hat{\mathcal{O}}_\alpha$ per volume

$$o_\alpha = \frac{\langle\hat{\mathcal{O}}_\alpha\rangle}{V} = \frac{1}{VZ}\text{Tr}\{\hat{\mathcal{O}}_\alpha \exp[-\beta(\hat{H} - \mu\hat{N})]\} \tag{5}$$

is given by

$$o_\alpha = \left(\frac{\partial\Omega}{\partial\lambda_\alpha}\right)_{T,\mu,\lambda'}, \tag{6}$$

where the subscript λ' shows that all λ except λ_α are fixed in the partial differentiation. The subscripts of the partial differentiation will be suppressed for simplicity, unless any confusion arises.
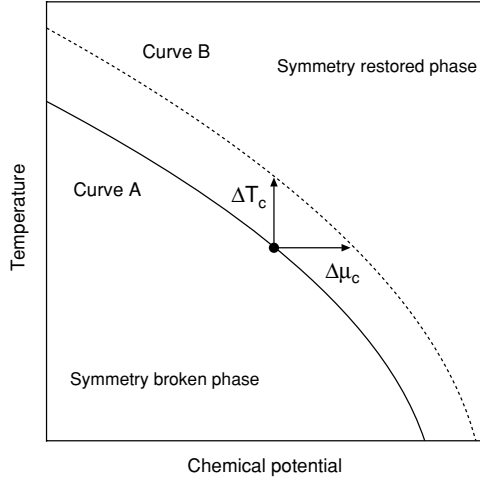
Figure 2. External parameter dependence of the phase boundary. Phase boundaries are projected on the μ–T plane from the λ_α–μ–T space.

First, we recapitulate the original BCPG theorem [2] on the zeroth-order discontinuity (the first-order phase transition) in order to know what is assumed in the proof. The proof is made as follows. We start with the assumption that there appears a discontinuity in o_γ, and show that the discontinuity propagates to other order parameters $o_{\alpha' \neq \gamma}$. Hereafter, α' stands for α except γ. Thus, no assumption is made beforehand on the property of discontinuities appearing in $o_{\alpha'}$. The first-order phase transition appearing in o_γ is drawn by the solid curve (μ_c, T_c) schematically in figure 2; its typical example is the chiral transition at low temperature shown in figure 1. The phase boundary (curve A) is shifted to curve B by taking different sets of external parameters, $\{\lambda_\alpha\}_B$. The thermodynamical potentials Ω_i of phases $i = 1$ and 2 on curve A satisfy the Gibbs condition

$$\Omega_1(T_c(\{\lambda_\alpha\}), \mu_c(\{\lambda_\alpha\}), \{\lambda_\alpha\}) = \Omega_2(T_c(\{\lambda_\alpha\}), \mu_c(\{\lambda_\alpha\}), \{\lambda_\alpha\}). \tag{7}$$

Differentiating the thermodynamical potentials with respect to λ_γ on the curve leads to

$$\left.\frac{\partial \Omega_1}{\partial \lambda_\gamma}\right|_c + \left.\frac{\partial \Omega_1}{\partial T}\right|_c \frac{\partial T_c}{\partial \lambda_\gamma} + \left.\frac{\partial \Omega_1}{\partial \mu}\right|_c \frac{\partial \mu_c}{\partial \lambda_\gamma} = \left.\frac{\partial \Omega_2}{\partial \lambda_\gamma}\right|_c + \left.\frac{\partial \Omega_2}{\partial T}\right|_c \frac{\partial T_c}{\partial \lambda_\gamma} + \left.\frac{\partial \Omega_2}{\partial \mu}\right|_c \frac{\partial \mu_c}{\partial \lambda_\gamma}, \tag{8}$$

where the subscript $|_c$ denotes that the quantities are evaluated at (μ_c, T_c). Hence we obtain

$$\delta o_\gamma = \frac{\partial T_c}{\partial \lambda_\gamma} \delta s + \frac{\partial \mu_c}{\partial \lambda_\gamma} \delta n, \tag{9}$$

where $\delta x = x_1 - x_2$ ($x = o_\gamma, s, n$) is evaluated on the phase boundary. In figure 2, the correspondence between each individual point on curve A and that on curve B is not unique. This means that one can define an infinitesimal variation of T_c in the T-direction with fixed μ_c,

$$T_c(\lambda_\gamma + \Delta\lambda_\gamma) - T_c(\lambda_\gamma) = \left.\frac{\partial T_c}{\partial \lambda_\gamma}\right|_{\mu_c} \Delta\lambda_\gamma, \tag{10}$$

and an infinitesimal variation of μ_c in the μ-direction with fixed T_c,

$$\mu_c(\lambda_\gamma + \Delta\lambda_\gamma) - \mu_c(\lambda_\gamma) = \left.\frac{\partial \mu_c}{\partial \lambda_\gamma}\right|_{T_c} \Delta\lambda_\gamma, \tag{11}$$

where the subscript $|_x$ denotes that x is fixed; these variations are illustrated by the arrows in figure 2. Using these variations, one can see from (9) that

$$\delta o_\gamma = \left.\frac{\partial T_c}{\partial \lambda_\gamma}\right|_{\mu_c} \delta s = \left.\frac{\partial \mu_c}{\partial \lambda_\gamma}\right|_{T_c} \delta n. \tag{12}$$

We find from $\delta o_\gamma \neq 0$ that $\partial T_c/\partial \lambda_\gamma|_{\mu_c}$ and $\partial \mu_c/\partial \lambda_\gamma|_{T_c}$ are nonzero, since δs and δn never diverge.

When all λ_α's are fixed to zero, μ_c can be regarded as a function of T_c: $\mu_c = \mu_c(T_c)$. Differentiating (7) with respect to T_c, one can get

$$\frac{\mathrm{d}T_c}{\mathrm{d}\mu_c} = -\frac{\delta n}{\delta s}. \tag{13}$$

Equation (13) is the Clausius–Clapeyron relation between δs and δn [27], and equation (12) is a generalization of the relation to the case of nonzero λ_α.

A relation similar to (12) is obtainable for α':

$$\delta o_{\alpha'} = \left.\frac{\partial T_c}{\partial \lambda_{\alpha'}}\right|_{\mu_c} \delta s = \left.\frac{\partial \mu_c}{\partial \lambda_{\alpha'}}\right|_{T_c} \delta n. \tag{14}$$

Here, it should be noted that the curve (μ_c, T_c) is defined by a discontinuity appearing in o_γ. The discontinuity $\delta o_\gamma \neq 0$ induces a new discontinuity $\delta o_{\alpha'} \neq 0$ through $\delta s \neq 0$, when

$$\left.\frac{\partial T_c}{\partial \lambda_{\alpha'}}\right|_{\mu_c} \neq 0. \tag{15}$$

Similarly, the discontinuity $\delta o_\gamma \neq 0$ induces $\delta o_{\alpha'} \neq 0$ through $\delta n \neq 0$, when

$$\left.\frac{\partial \mu_c}{\partial \lambda_{\alpha'}}\right|_{T_c} \neq 0. \tag{16}$$

Thus, when the conditions (15) and (16) are satisfied, two first-order phase transitions take place simultaneously. In other words, the discontinuity of o_γ propagates to other physical quantity $o_{\alpha'}$ through those of s and n. The conditions mean that the phase boundary is shifted in both the T- and μ-directions in the μ–T plane by varying $\lambda_{\alpha'}$.

An early application of the BCPG theorem was to the case of a 2+1 flavor model in which two chiral condensations exist [28]. A similar situation is expected when an isospin chemical potential is introduced in two flavor models if a flavor mixing interaction is included [29].

Here, we show an example of the simultaneous occurrence of zeroth-order discontinuities of order parameters by using the PNJL model in the chiral limit. The formulation and the parameter set of the PNJL model are given in [18, 30], where the pure gauge part is obtained by reproducing lattice QCD data in the pure gauge theory [31, 32] as shown in [10]. In this paper, we put $m_0 = 0$ with keeping other parameters unchanged.

In the chiral limit, the chiral condensate $\sigma = \langle \bar{q}q \rangle$ is an exact order parameter of the spontaneous chiral symmetry breaking, namely, $o_\gamma = \sigma$ and $\lambda_\gamma = m_0$ for the quark field q and the current quark mass m_0. The Polyakov loop Φ is an exact order parameter of the spontaneous $\mathbb{Z}_3$ symmetry breaking in the pure gauge theory, but the symmetry is not exact anymore in the system with dynamical quarks. However, Φ still seems to be a good indicator of the deconfinement phase transition. We then regard Φ as an approximate order parameter of the deconfinement phase transition.

Figure 3(a) represents T dependence of σ, Φ and the charge-conjugated Polyakov loop $\bar{\Phi}$ at $\mu = 280$ MeV. These are discontinuous at the same temperature $T = 154$ MeV. This behavior is consistent with the BCPG theorem that guarantees the simultaneous occurrence of
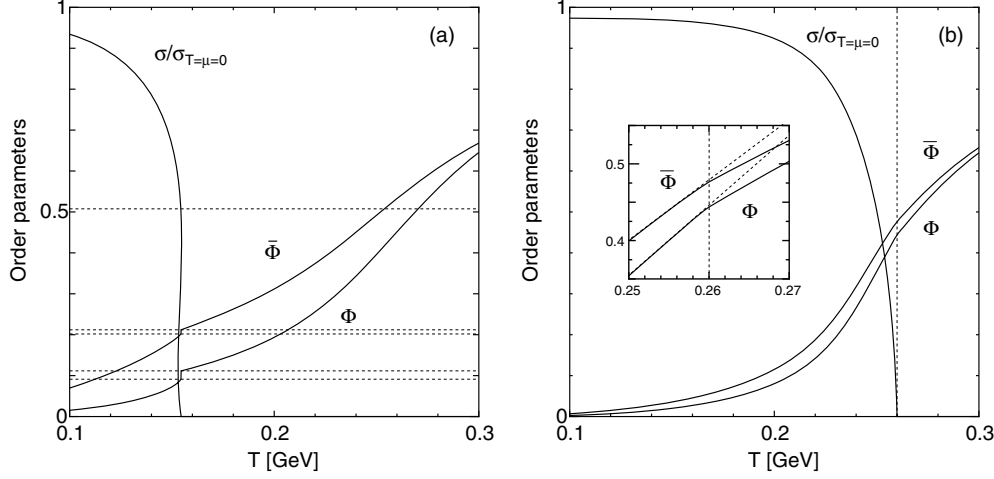
Figure 3. The temperature dependence of the chiral condensate σ, the Polyakov loop Φ and its conjugate $\bar{\Phi}$ at (a) $\mu = 280$ MeV and (b) $\mu = 50$ MeV in the chiral limit. The chiral condensate is normalized by the value at $T = \mu = 0$. The inset in (b) represents Φ and $\bar{\Phi}$ near $T = 260$ MeV that is the critical temperature.

zeroth-order discontinuities of order parameters. Here, one can also find that the μ dependence of Φ is similar to that of $\bar{\Phi}$. This is true for other real μ.

The BCPG theorem does not necessarily mean that there cannot exist a quarkyonic phase [33] defined in the limit of large number of colors as a phase that has a finite value of the baryon number density n but is confined. This is understandable as follows. The quarkyonic phase has recently been investigated with the PNJL model [7, 21, 34] and the strong coupling QCD [35]. The PNJL analysis of [21] shows the simultaneous occurrence of zeroth-order discontinuities of σ, Φ and n. However, the discontinuity in Φ is only a jump from a small value to another small one, while that in n is a jump from almost 0 to a value larger than the nuclear saturation density. As mentioned above, Φ is only an approximate order parameter of the deconfinement phase transition, and then such a small jump is possible. Such a small jump could be just a propagation of the discontinuity in σ. Thus, we cannot say necessarily from the small jump of Φ that a first-order deconfinement phase takes place together with the chiral phase transition and the phase transition of n. A plausible definition of a critical temperature of the deconfinement phase transition is a temperature that gives $\Phi = 0.5$. In this definition, the deconfinement transition is a crossover, and then the BCPG theorem is no longer applicable.

Next, we proceed to the case that an order parameter has a first-order discontinuity. In this case, since a first-order discontinuity becomes continuous by a change of external parameters, the boundary must be defined in terms of a susceptibility as follows. Here, we take the chiral transition in two flavor systems at high temperature, shown by the dotted curve in figure 1, as a typical example: namely, $\lambda_\gamma = m_0$ and $o_\gamma = \sigma = \langle \bar{q}q \rangle$. The second-order chiral phase transition at $m_0 = 0$ becomes a crossover whenever m_0 is finite [22]. It is possible to define the phase boundary of such a crossover with the chiral susceptibility $\chi_\sigma = -\partial\sigma/\partial m_0$ so that the T dependence of χ becomes maximum on the boundary. This definition works also in the chiral limit, although the maximum is infinity. In this case, curves A and B in figure 2 are reinterpreted as phase boundaries so defined and correspond to the chiral limit ($m_0 = 0$) and

to the case of small m_0, respectively. Curve A can move continuously and reach curve B by varying m_0 from 0 to a finite value. The chiral susceptibility χ_σ is divergent on boundary A, since the chiral phase transition is of second order there.

Now, we consider curve A defined above and its vicinity. The system concerned has no zeroth-order discontinuity, $\delta s = \delta n = 0$. Differentiating $\delta s = 0$ with respect to λ_γ on the boundary (μ_c, T_c) leads to

$$\delta\left(\frac{\partial s}{\partial \lambda_\gamma}\right) + \frac{\partial T_c}{\partial \lambda_\gamma}\delta\left(\frac{\partial s}{\partial T}\right) + \frac{\partial \mu_c}{\partial \lambda_\gamma}\delta\left(\frac{\partial s}{\partial \mu}\right) = 0. \tag{17}$$

Using the relation $\partial s/\partial \lambda_\gamma = -\partial o_\alpha/\partial T$ and the variations in the T- and μ-directions mentioned above, one can get

$$\delta\left(\frac{\partial o_\gamma}{\partial T}\right) = \frac{\partial T_c}{\partial \lambda_\gamma}\bigg|_{\mu_c}\delta\left(\frac{\partial s}{\partial T}\right) = \frac{\partial \mu_c}{\partial \lambda_\gamma}\bigg|_{T_c}\delta\left(\frac{\partial s}{\partial \mu}\right). \tag{18}$$

Taking the same procedure for $\delta n = 0$, one also obtains

$$\delta\left(\frac{\partial o_\gamma}{\partial \mu}\right) = \frac{\partial T_c}{\partial \lambda_\gamma}\bigg|_{\mu_c}\delta\left(\frac{\partial n}{\partial T}\right) = \frac{\partial \mu_c}{\partial \lambda_\gamma}\bigg|_{T_c}\delta\left(\frac{\partial n}{\partial \mu}\right). \tag{19}$$

Other order parameters $o_{\alpha'}$ satisfy the same equations as (18) and (19). Note that all the equations are evaluated in the chiral limit $\lambda_\gamma = m_0 = 0$. It is found from (18) and (19) for o_γ and the corresponding equations for $o_{\alpha'}$ that discontinuities $\delta(\partial o_\gamma/\partial T) \neq 0$ and $\delta(\partial o_\gamma/\partial \mu) \neq 0$ induce new ones $\delta(\partial o_{\alpha'}/\partial T) \neq 0$ and $\delta(\partial o_{\alpha'}/\partial \mu) \neq 0$, when the conditions (15) and (16) are satisfied. Thus, two first-order discontinuities of order parameters can coexist under the conditions (15) and (16). Furthermore, it is found from (18) and (19) that $\delta(\partial o_\gamma/\partial \mu)$ is not zero whenever $\delta(\partial o_\gamma/\partial T)$ is not zero, because of $\partial n/\partial T = \partial s/\partial \mu$. Accordingly, the first-order discontinuity of o_γ emerges in both $\partial o_\gamma/\partial T$ and $\partial o_\gamma/\partial \mu$.

Here, we show an example of the simultaneous occurrence of two discontinuities by the PNJL model in the chiral limit. Figure 3(b) represents T dependence of σ, Φ and $\bar{\Phi}$ at $\mu = 50$ MeV. Obviously, Φ and $\bar{\Phi}$ are not smooth at $T_c = 260$ MeV. In the inset of figure 3(b), the solid curves show Φ and $\bar{\Phi}$ near $T_c = 260$ MeV, and two dotted lines do tangential lines of the solid curves at $T = T_c - 0$. The deviations between the solid curves and the corresponding dotted lines indicate that Φ and $\bar{\Phi}$ are not smooth at $T_c = 260$ MeV. Thus, $\partial\sigma/\partial T$, $\partial\Phi/\partial T$ and $\partial\bar{\Phi}/\partial T$ are discontinuous at the same temperature, as expected from the coexistence theorem on the first-order discontinuity of order parameter.

As shown in figure 3(b), $\delta(\partial\sigma/\partial T)$ diverges at $T = T_c$, because $\partial\sigma/\partial T|_{T=T_c-0} = \infty$ and $\partial\sigma/\partial T|_{T=T_c+0} = 0$; note that $\sigma \leqslant 0$. A similar divergence is also seen on the second-order chiral phase transition line (dotted curves) in figure 1. This divergence indicates from (18) that $\partial T_c/\partial m_0|_{\mu_c}$ and/or $\delta(\partial s/\partial T)$ diverge on the second-order chiral phase transition curve. If $\delta(\partial s/\partial T)$ is infinite there, the divergence will propagate to other quantities $\delta(\partial o_{\alpha'}/\partial T)$ when the condition (15) is satisfied. As shown below, this is not the case of the second-order chiral phase transition. Figure 4 presents the T dependence of $\partial s/\partial T$, the chiral susceptibility χ_σ and the Polyakov-loop susceptibility $\chi_{\Phi\bar{\Phi}}$ at $\mu = m_0 = 0$ in panel (a) and the m_0 dependence of T_c at $\mu = 0$ in panel (b); definition of $\chi_{\Phi\bar{\Phi}}$ is shown below. As shown in panel (a), χ_σ (the dotted curve) diverges at $T = 261.4$ MeV, but $\partial s/\partial T$ (the solid curve) has a finite gap there. Meanwhile, panel (b) shows that the gradient $\partial T_c/\partial m_0$ is divergent at $m_0 = 0$. In the present case, thus, the divergence in $\delta(\partial\sigma/\partial T)$ does not propagate to other quantities $\delta(\partial o_{\alpha'}/\partial T)$. Accordingly, the coexistence of first-order discontinuities of order parameters takes place, but the coexistence of second-order phase transitions does not occur necessarily, because there is a possibility that $\partial T_c/\partial \lambda_\gamma|_{\mu_c}$ and $\partial \mu_c/\partial \lambda_\gamma|_{T_c}$ diverge. In other words, when $\partial T_c/\partial \lambda_\gamma|_{\mu_c}$
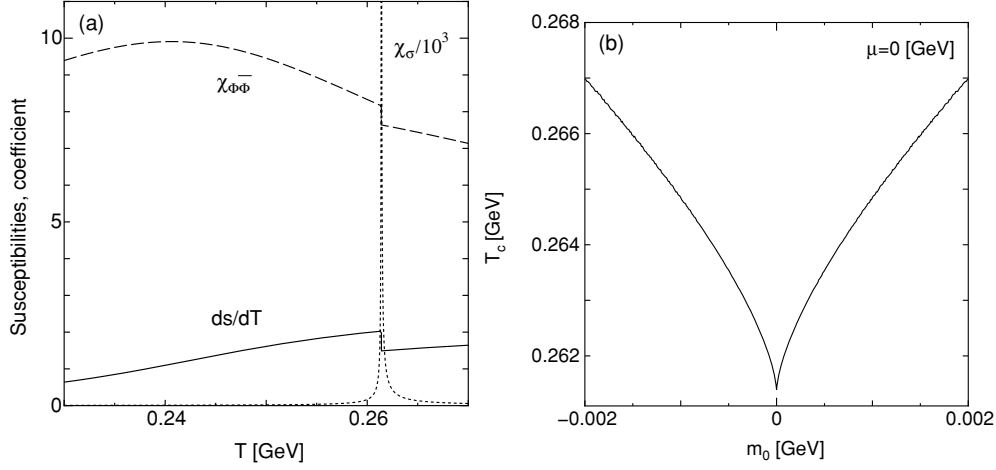
Figure 4. Properties of thermal quantities at $\mu = 0$: (a) T dependence of chiral and Polyakov-loop susceptibilities and $\partial s/\partial T$ at $m_0 = 0$, and (b) quark-mass dependence of the critical temperature. In panel (a), the solid, dashed and dotted curves represent $\partial s/\partial T$, $\chi_{\Phi\bar{\Phi}}$ and χ_σ, respectively. The chiral susceptibility χ_σ has a divergent peak at $T = T_c = 261.4$ MeV.

and $\partial T_c/\partial\lambda_{\alpha'}|_{\mu_c}$ are nonzero and finite, or when $\partial\mu_c/\partial\lambda_\gamma|_{T_c}$ and $\partial\mu_c/\partial\lambda_{\alpha'}|_{T_c}$ are nonzero and finite, the coexistence of second-order phase transitions takes place.

Susceptibilities χ_{ij} of σ, Φ and $\bar{\Phi}$ can be written as [6, 15, 18]

$$\chi_{ij} = (K^{-1})_{ij} \qquad (i, j = \sigma, \Phi, \bar{\Phi}), \tag{20}$$

where

$$K = \begin{pmatrix} \dfrac{\beta}{4G_s^2\Lambda}\dfrac{\partial^2\Omega}{\partial\sigma^2} & -\dfrac{\beta}{2G_s\Lambda^2}\dfrac{\partial^2\Omega}{\partial\sigma\partial\Phi} & -\dfrac{\beta}{2G_s\Lambda^2}\dfrac{\partial^2\Omega}{\partial\sigma\partial\bar{\Phi}} \\[3mm] -\dfrac{\beta}{2G_s\Lambda^2}\dfrac{\partial^2\Omega}{\partial\Phi\partial\sigma} & \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\Phi^2} & \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\Phi\partial\bar{\Phi}} \\[3mm] -\dfrac{\beta}{2G_s\Lambda^2}\dfrac{\partial^2\Omega}{\partial\bar{\Phi}\partial\sigma} & \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\bar{\Phi}\partial\Phi} & \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\bar{\Phi}^2} \end{pmatrix} \tag{21}$$

is a symmetric matrix of curvatures of Ω and $(K^{-1})_{ij}$ is an (i, j) element of the inverse matrix K^{-1}. In the chiral limit, Ω is invariant under the transformation $\sigma \rightarrow -\sigma$ [18] and hence σ-even. In the case that the chiral phase transition is the second order, as shown in figure 3, Ω becomes minimum at $\sigma = 0$ when $T \geqslant T_c$. Therefore, $K_{\sigma\Phi}$ and $K_{\sigma\bar{\Phi}}$ are zero at $T \geqslant T_c$, because they are σ-odd. In this situation, χ_{ij} at $T \geqslant T_c$ are reduced to

$$\chi_\sigma \equiv \chi_{\sigma\sigma} = \frac{1}{K_{\sigma\sigma}}, \qquad \chi_{ij} = \left(K_2^{-1}\right)_{ij} \qquad (i, j = \Phi, \bar{\Phi}), \tag{22}$$

where

$$K_2 = \begin{pmatrix} \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\Phi^2} & \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\Phi\partial\bar{\Phi}} \\[3mm] \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\bar{\Phi}\partial\Phi} & \dfrac{\beta}{\Lambda^3}\dfrac{\partial^2\Omega}{\partial\bar{\Phi}^2} \end{pmatrix}. \tag{23}$$

Thus, the susceptibilities of Φ and $\bar{\Phi}$ are decoupled from that of σ. In particular at $T = T_c$, the curvature $K_{\sigma\sigma}$ is zero and then χ_σ is divergent, while at $T > T_c$ the curvature $K_{\sigma\sigma}$

is positive and then χ_σ is a positive finite value. This divergence makes no influence on other susceptibilities $\chi_{ij}(i, j = \Phi, \bar{\Phi})$, since $K_{\sigma\Phi}$ and $K_{\sigma\bar{\Phi}}$ are zero; see [24, 25] for details. Figure 4(a) is a typical example of this situation; χ_σ has a divergent peak, while $\chi_{\Phi\bar{\Phi}}$ does not.

　　In the imaginary chemical potential region ($\mu^2 < 0$), as shown by the dashed curve between points A and B of figure 1, there coexists a zeroth-order discontinuity of quark number density n and a first-order discontinuity of chiral condensate σ. The coexistence is consistent with the proofs mentioned above, as shown below. This is the principal subject of this paper.

　　It is convenient to introduce a new variable $\theta = -\mathrm{i}\mu/T$ instead of μ. The conditions (15) and (16) are then changed into

$$\left.\frac{\partial T_{\mathrm{c}}}{\partial \lambda_{\alpha'}}\right|_{\theta_{\mathrm{c}}} \neq 0, \tag{24}$$

$$\left.\frac{\partial \theta_{\mathrm{c}}}{\partial \lambda_{\alpha'}}\right|_{T_{\mathrm{c}}} \neq 0. \tag{25}$$

As shown later in figure 7, the coexistence of $\delta n \neq 0, \delta\sigma = 0$ and $\delta(\partial\sigma/\partial\theta) \neq 0$ always appears on vertical lines $\theta = (2k+1)\pi/3$ in the θ–T plane, where k is an integer. This indicates that $\partial\theta_{\mathrm{c}}/\partial m_0 = 0$ and then the condition (25) breaks down. Taking the new variable θ also changes (9) into

$$\delta\tilde{\sigma} = \frac{\partial T_{\mathrm{c}}}{\partial m_0}\delta\tilde{s} + \frac{\partial \theta_{\mathrm{c}}}{\partial m_0}\delta\tilde{n} = \frac{\partial T_{\mathrm{c}}}{\partial m_0}\delta\tilde{s} \tag{26}$$

with

$$\tilde{s} = -\left(\frac{\partial\Omega}{\partial T}\right)_{\theta,\lambda}, \qquad \tilde{n} = -\left(\frac{\partial\Omega}{\partial\theta}\right)_{T,\lambda} = \mathrm{i}nT, \tag{27}$$

$$\tilde{\sigma} = \left(\frac{\partial\Omega}{\partial m_0}\right)_{\theta,T,\lambda'} = \sigma, \tag{28}$$

where use has been made of $\partial\theta_{\mathrm{c}}/\partial m_0 = 0$ in the second equality of (26). Thus, even if $\delta\tilde{n}$ is not zero, one can keep $\delta\sigma = 0$ in (26) when $\delta\tilde{s}$ is zero.

　　The discontinuity $\delta\tilde{n} \neq 0$ was first pointed out by Roberge and Weiss (RW) [26], and is often called the RW transition. Here, we consider how the discontinuity $\delta\tilde{n} \neq 0$ influences other order parameters o_α. In this case, curve A in figure 2 is defined by the discontinuity $\delta\tilde{n} \neq 0$. The quantity $\delta\tilde{n}$ is a function of $T_{\mathrm{c}}, \theta_{\mathrm{c}}$ and λ_α, but θ_{c} does not depend on λ_α, namely, $\delta\tilde{n} = -f(T_{\mathrm{c}}(\{\lambda_\alpha\}), \theta_{\mathrm{c}}, \{\lambda_\alpha\})$. Differentiating $\delta\tilde{n} + f = 0$ with respect to λ_α leads to

$$\delta\left(\frac{\partial\tilde{n}}{\partial\lambda_\alpha}\right) + \frac{\partial T_{\mathrm{c}}}{\partial\lambda_\alpha}\delta\left(\frac{\partial\tilde{n}}{\partial T}\right) + \left.\frac{\partial f}{\partial\lambda_\alpha}\right|_{\tilde{c}} + \left.\frac{\partial f}{\partial T}\right|_{\tilde{c}}\frac{\partial T_{\mathrm{c}}}{\partial\lambda_\alpha} = 0 \tag{29}$$

because of $\partial\theta_{\mathrm{c}}/\partial\lambda_\alpha = 0$, where the subscript $|_{\tilde{c}}$ denotes that the quantities are evaluated at $(\theta_{\mathrm{c}}, T_{\mathrm{c}})$. Using $\partial\tilde{n}/\partial\lambda_\alpha = -\partial o_\alpha/\partial\theta$ and taking the variation in the θ-direction with fixed T_{c}, one can obtain

$$\delta\left(\frac{\partial o_\alpha}{\partial\theta}\right) = \left.\frac{\partial f}{\partial\lambda_\alpha}\right|_{\tilde{c}}. \tag{30}$$

Taking the same procedure for $\delta\tilde{s} = 0$ leads to

$$\delta\left(\frac{\partial o_\alpha}{\partial T}\right) = \left.\frac{\partial\theta_{\mathrm{c}}}{\partial\lambda_\alpha}\right|_{T_{\mathrm{c}}}\left.\delta\left(\frac{\partial\tilde{s}}{\partial\theta}\right)\right|_{\tilde{c}} = 0 \tag{31}$$
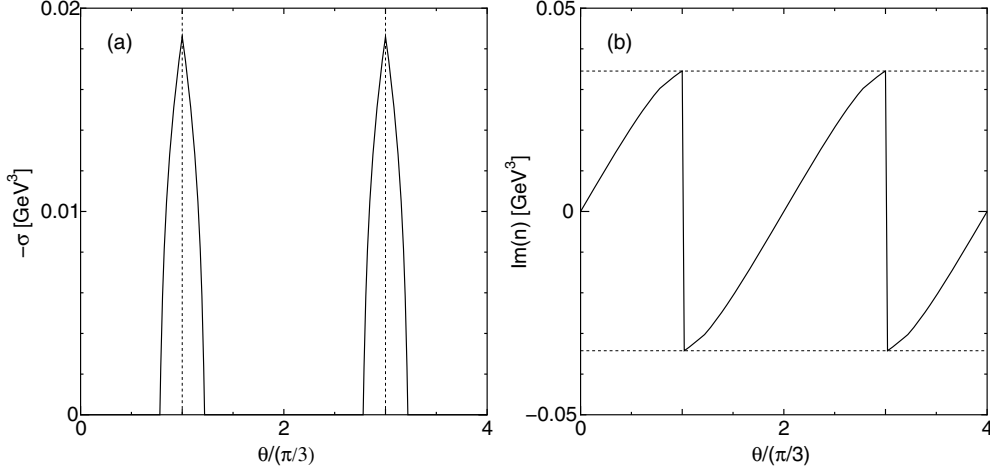
Figure 5. The θ dependence of the chiral condensate and the imaginary part of the quark number density at $T = 300$ MeV in the chiral limit.

because of $\partial\theta_c/\partial\lambda_\alpha|_{T_c} = 0$. Equations (30) and (31) indicate that order parameters are discontinuous in $\partial o_\alpha/\partial\theta$ but not in $\partial o_\alpha/\partial T$. This property is different from that of the ordinary second-order chiral phase transition, shown by the dotted curve of figure 1, that is discontinuous in both $\partial o_\alpha/\partial\theta$ and $\partial o_\alpha/\partial T$. The coexistence of the zeroth-order discontinuity of n and the first-order one of σ is originated from the fact that the RW transition line is vertical in the θ–T plane and does not move in the θ-direction by changing the external parameter $\lambda_\alpha = m_0$. The influence of the RW discontinuity of n on the Polyakov loop is discussed in the following.

In the imaginary μ region, physical quantities have a periodicity of $2\pi/3$ in θ, when these are invariant under the extended $\mathbb{Z}_3$ transformation [22],

$$e^{\pm i\theta} \to e^{\pm i\theta}\, e^{\pm i\frac{2\pi k}{3}}, \qquad \Phi(\theta) \to \Phi(\theta)\, e^{-i\frac{2\pi k}{3}}, \qquad \bar{\Phi}(\theta) \to \bar{\Phi}(\theta)\, e^{i\frac{2\pi k}{3}}. \qquad (32)$$

This is called the RW periodicity [26]. The thermodynamical potential Ω_{PNJL} and σ, s and n are invariant under the extended $\mathbb{Z}_3$ symmetry, but Φ and $\bar{\Phi}$ are not [22]. However, this can be cured by introducing the modified Polyakov loop $\Psi = \Phi \exp(i\theta)$ invariant under the extended $\mathbb{Z}_3$ transformation. We then consider a period $0 \leqslant \theta \leqslant 2\pi/3$ without loss of generality.

Figure 5 shows the θ dependence of the chiral condensate σ and the imaginary part of n, Im[n], at $T = 300$ MeV; note that n is pure imaginary for imaginary μ by definition. The chiral condensate has a cusp at $\theta = \pi/3$, while n is discontinuous there. Thus, the first-order discontinuity of σ and the zeroth-order discontinuity of n coexist, as predicted above.

Next, we consider the relation between the discontinuity of n and the Polyakov loop transition by using Re[Ψ] = $(\Psi(\theta) + \bar{\Psi}(\theta))/2$. In the PNJL model, $\Psi(\theta)$ and $\bar{\Psi}(\theta)$ are treated as classical variables, and it is found from the expression for Ω_{PNJL} in (13) of [18] that $\bar{\Psi}(\theta)$ is the complex conjugate of $\Psi(\theta)$ for the case of imaginary μ. Figure 6(a) shows the θ dependence of the real part Re[Ψ] at $T = 300$ MeV. There appears a first-order discontinuity also in Re[Ψ] on the line $\theta = \pi/3$, as expected from (30).

Finally, we consider the imaginary part of Ψ, Im[Ψ] = $(\Psi(\theta) - \bar{\Psi}(\theta))/2i$. This is also real, but θ-odd (odd under the interchange of $\theta \leftrightarrow -\theta$), because $\Psi(\theta) = \bar{\Psi}(-\theta)$ [22]. One cannot use λ_αIm[Ψ] as a source term $\lambda_\alpha\mathcal{O}_\alpha$, since it breaks θ-evenness, $\Omega_{\text{PNJL}}(\theta) = \Omega_{\text{PNJL}}(-\theta)$, that is the charge-conjugation symmetry of Ω_{PNJL} [36]. To avoid this problem, we introduce a
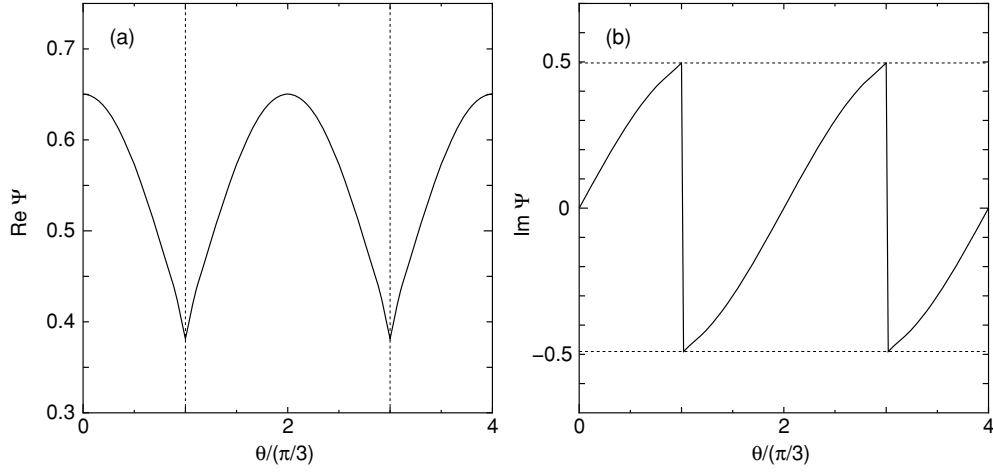
10

Figure 6. The θ dependence of Ψ at $T = 300$ MeV in the chiral limit: (a) the real part and (b) the imaginary part.
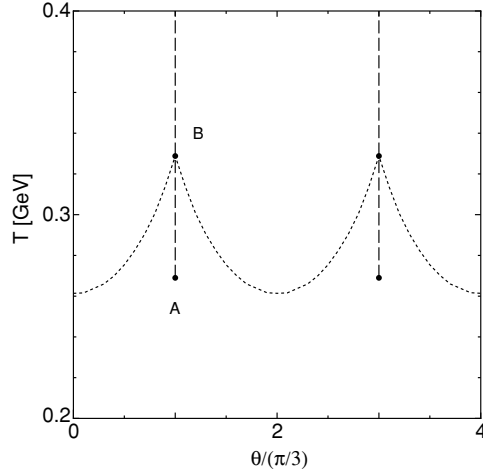

Figure 7. Phase diagram on the θ–T plane predicted by the PNJL model in the chiral limit.

source term, $\lambda_\alpha \sin(3\theta)\mathrm{Im}[\Psi]$, designed to keep θ-evenness and the RW periodicity. This is just an example of operators having the two properties. For this source term, (30) is reduced to

$$\delta(\mathrm{Im}[\Psi]) = -\frac{1}{3}\frac{\partial f}{\partial \lambda_\alpha}\bigg|_{\tilde{c}}. \tag{33}$$

Thus, $\delta(\mathrm{Im}[\Psi])$ is finite on the RW phase transition line $\theta = \pi/3$ because of $\partial f/\partial \lambda_\alpha|_{\tilde{c}} \neq 0$. This indicates that the zeroth-order discontinuity of n induces that of $\mathrm{Im}[\Psi]$, as shown in figure 6(b).

Throughout all the analyses, we can conclude that the zeroth-order discontinuity of a θ-odd quantity n induces zeroth-order ones in θ-odd quantities and simultaneously first-order ones in θ-even quantities; see [22] for the proof of the even/odd property of n, σ, $\mathrm{Re}[\Psi]$, $\mathrm{Im}[\Psi]$, $|\Psi|$

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and arg[Ψ]. As shown in figure 5, $\partial\sigma/\partial\theta$ is finite on both sides of the critical chemical potential θ_c. This means that the chiral susceptibility χ is finite. Hence, there is no second-order phase transition on the RW line. Therefore, the RW phase transition is a first-order phase transition and a family of zeroth- and first-order discontinuities.

Figure 7 shows the phase diagram on the θ–T plane that corresponds to the $\mu^2 < 0$ part of figure 1. On the dashed line between points A and B, the RW phase transition mentioned above emerges. The transition comes out also on the dashed line going up from point B, although σ is zero there and then no discontinuity takes place in σ. The dotted curves represent ordinary chiral phase transitions of second order.

To summarize, we showed that once a zeroth- or first-order discontinuity takes place in a quantity o_γ, discontinuities of the same order emerge in other quantities $o_{\alpha\neq\gamma}$, if the conditions (15) and (16) are satisfied, that is, if the phase boundary is shifted in both the directions of T and μ in the T–μ plane by varying values of external parameters λ_α conjugate to o_α. This coexistence theorem is an extension of the BCPG theorem on the zeroth-order discontinuity of order parameter (the first-order phase transition). When the conditions break, first- and second-order discontinuities can coexist on the same phase boundary. The RW phase transition in the θ–T plane, composed of zeroth-order discontinuities of θ-odd quantities and first-order discontinuities of θ-even ones, is a typical example of the coexistence of zeroth- and first-order discontinuities. The RW phase transition line is vertical and does not move in the θ-direction, even if any external parameter varies. Thus, the shape of the phase boundary and its variation with external parameters are essential in determining which type of coexistence is realized.

Acknowledgments

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