

Fluctuations in QCD phase diagram
in the strong coupling limit of lattice QCD

for the degree of
Doctor of Science

Terukazu Ichihara
Department of Physics & Yukawa Institute for Theoretical Physics,
Kyoto University

February 12, 2016

Abstract

Phase diagram of Quantum Chromodynamics (QCD) at finite temperature and finite density would be related to heavy-ion collision experiments at zero or low density and neutron stars at sufficiently high density. Then the QCD phase diagram has attracted much attention from theoretical and experimental points of view. QCD exhibits two non-perturbative phase transitions: the chiral phase transition and the confinement-deconfinement phase transition. A first-principles method, lattice QCD, is an important tool to investigate the non-perturbative dynamics and it achieves great successes at zero density. However, it is not easy to apply lattice QCD to the finite density region due to the sign problem.

In this thesis, we investigate the QCD phase diagram and properties of QCD matter at finite temperature and finite density by using the strong coupling approach of lattice QCD. First, we show the QCD phase diagram with field fluctuation effects in the strong coupling and chiral limits. We utilize an effective action in the strong coupling limit derived from the lattice QCD action with one species of unrooted staggered fermion. In order to obtain the effective action, we take account of the leading order of the large dimensional expansion and apply the extended Hubbard-Stratonovich transformation to four Fermi interaction terms. We use the auxiliary field Monte Carlo (AFMC) method based on the obtained effective action beyond the mean field approximation. In fact, we include the field fluctuation effects numerically in AFMC. When we evaluate observables, we introduce a new method named as the chiral angle fixing (CAF) to obtain an appropriate order parameter, the chiral condensate, on a fixed size lattice in the symmetry breaking phase. After applying CAF, the order parameters show the phase transition behavior and we find that the obtained QCD phase diagram is almost consistent with that in the monomer-dimer-polymer simulation. We also study an origin of the sign problem in AFMC. We find that the high-momentum auxiliary fields give rise to the sign problem.

Next, we investigate net-baryon number cumulants in the strong coupling and chiral limits. Higher-order cumulants of the net-baryon number are con-

sidered to be good observables to detect the QCD critical phenomena at finite density. We find that the third and fourth-order cumulants show oscillatory behaviors as functions of temperature in the chiral limit due to the finite size effect. By comparison, the fourth-order cumulant positively diverges in the thermodynamic limit according to the scaling function analysis at finite density. We finally show the negative region of the fourth-order cumulant in the chiral limit, which would provide clear signals of criticality for theoretical or experimental studies. Our studies may be of help for constructing a finite size scaling function in the chiral limit. Once we can investigate the finite-size scaling function in the chiral limit, we obtain further insights into the scaling function with regard to both the finite size and the mass effects.

Contents

1	Introduction	5
1.1	Quantum Chromodynamics	5
1.1.1	Asymptotic freedom	6
1.1.2	Vacuum structure	7
1.2	QCD phase diagram	9
1.2.1	Overview of QCD phase diagram	9
1.2.2	Phase transition along the temperature axis	10
1.2.3	Phase transition at finite density	13
1.2.4	Theoretical studies of observables	17
1.3	Organization of this thesis	22
2	Lattice QCD approaches for QCD phase diagram	24
2.1	Lattice QCD	24
2.1.1	Lattice QCD action	25
2.1.2	Monte Carlo simulation	27
2.1.3	Sign problem in QCD	29
2.2	Strong coupling lattice QCD	31
2.2.1	Quark confinement at strong coupling	32
2.2.2	Chiral phase transition at strong coupling	33
2.2.3	QCD phase diagram at strong coupling	34
3	QCD phase diagram in the strong coupling limit with fluctuations	37
3.1	Strong coupling lattice QCD action	38
3.2	Effective action with auxiliary field fluctuations for mesonic fields	40
3.3	Order parameters and susceptibilities	42
3.3.1	Chiral angle fixing method	42
3.3.2	Observables in AFMC in the strong and chiral limits	45
3.4	QCD phase diagram in the strong coupling limit with mesonic fluctuations	48

3.4.1	Chiral susceptibility and effective potential analysis . .	48
3.4.2	QCD phase diagram in the strong coupling and chiral limits with fluctuations	49
3.5	Sign problem in AFMC	51
3.6	Short summary	53
4	Cumulant ratios in the strong coupling limit at finite density with/without mesonic field fluctuations	55
4.1	Net-baryon number cumulants in the mean field approximation	57
4.2	Net-baryon number cumulants with mesonic field fluctuations	59
4.2.1	Simulation details	59
4.2.2	(T, μ) dependence of $R_{3,2}^B$ and $R_{4,2}^B$	60
4.2.3	Lattice size dependence of $R_{3,2}^B$ and $R_{4,2}^B$	61
4.2.4	Discussion of cumulants in AMFC	63
4.2.5	$R_{4,2}^B$ in the QCD phase diagram in the strong coupling limit	65
4.3	Short summary	67
5	Summary and outlook	68
A	Mean field formulae at strong coupling	73
A.1	Effective action in the mean field analysis	73
A.2	Matsubara frequency	75
A.3	Some formulae for cumulants in MF analysis	77
B	Formulae with fluctuation effects	86
B.1	Fermion determinant with fluctuations	86
B.1.1	Fermion determinant and recursion formulae	86
B.1.2	Order parameters and Susceptibilities	87
B.2	Higher order derivatives of the baryon chemical potential in the auxiliary field Monte Carlo method	89
B.3	Cumulants in AMFC	91
C	Review of $O(N)$ ($N=2,4$) scaling function	93

Chapter 1

Introduction

In this chapter, we review the basic properties of QCD based on Refs. [1, 2, 3] and prepare for discussions in the following chapters. In Sect. 1.1, we review natures of QCD: the asymptotic freedom, chiral symmetry breaking, and quark confinement. Current understanding of the QCD phase diagram is reviewed in Sect. 1.2.

1.1 Quantum Chromodynamics

Quantum chromodynamics (QCD) describes the strong interaction of quarks and gluons. Nowadays, six flavors ($N_f = 6$) of quarks are found: up (u), down (d), strangeness (s), charm (c), bottom (b), and top (t). Quarks and gluons have color degrees of freedom [4] ($N_c = 3$) and are confined in hadrons at low energy. The hadron is observed as a color singlet state: a baryon (e.g. nucleon) is made of three quarks and a meson (e.g. pion) is made of a quark and an antiquark in a simple quark-model picture [5, 6].

QCD is a non-Abelian gauge theory based on the Yang-Mills theory [7] with color $N_c = 3$. The QCD lagrangian is given as

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\mathcal{D} - m_0)\psi - \frac{1}{2} \text{Tr} F_{\mu\nu} F^{\mu\nu} , \quad (1.1)$$

with the covariant derivative $D_\mu = \partial_\mu + igA_\mu$ and the field strength $F_{\mu\nu} = [D_\mu, D_\nu]/(ig) = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu]$. Here we define $\mathcal{D} = \gamma^\mu D_\mu$, ($\mu, \nu = 0, 1, 2, 3$). The quark field ψ belongs to the fundamental representation of $\text{SU}(N_c)$ and the gluon (gauge) field $A_\mu = A_\mu^a T_a$ ($a = 1, \dots, N_c^2 - 1$) belongs to the adjoint representation of $\text{SU}(N_c)$. The coupling constant in QCD and the quark mass matrix are given as g and m_0 , respectively. The gamma matrix γ^μ satisfies anti-commutation relation $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\mathbf{1}$. The traceless

hermitian matrix T^a is the generator of the Lie group, which satisfies the relations,

$$[T^a, T^b] = if_{abc}T^c, \quad \text{Tr}(T^a T^b) = \frac{1}{2}\delta^{ab}. \quad (1.2)$$

Here, f_{abc} is the structure constant of the Lie group. The QCD lagrangian is invariant under the gauge transformation:

$$\psi(x) \rightarrow g(x)\psi(x), \quad \bar{\psi}(x) \rightarrow \bar{\psi}(x)g^\dagger(x), \quad (1.3)$$

$$A_\mu(x) \rightarrow g(x)A_\mu(x)g^\dagger(x) + \frac{1}{ig}g(x)\partial_\mu g^\dagger(x), \quad (1.4)$$

where $g(x) = \exp(-i\theta^a(x)T^a)$ with $\theta^a(x) \in \mathbb{R}$.

The QCD lagrangian has the chiral symmetry in the case of massless quarks. In order to find the chiral symmetry, we can define left- and right-handed quarks,

$$\psi_{L,R} = \frac{1 \mp \gamma_5}{2}\psi, \quad \gamma_5\psi_{L,R} = \mp\psi_{L,R}. \quad (1.5)$$

By using the right- and left-handed quarks, the QCD lagrangian is rewritten as

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}_L i \not{D} \psi_L + \bar{\psi}_R i \not{D} \psi_R - (\bar{\psi}_L m \psi_R + \bar{\psi}_R m \psi_L) - \frac{1}{2} \text{Tr} F_{\mu\nu} F^{\mu\nu}. \quad (1.6)$$

When we consider the chiral transformation,

$$\psi_L \rightarrow g_L \psi_L, \quad \psi_R \rightarrow g_R \psi_R, \quad (1.7)$$

where $g_L = \exp(i\theta_L^a T_a) \in \text{SU}(N_f)_L$ and $g_R = \exp(i\theta_R^a T_a) \in \text{SU}(N_f)_R$. The QCD lagrangian in Eq. (1.6) is invariant in the chiral limit (massless case), which is referred to as the chiral symmetry.

The above QCD lagrangian has $\text{U}(1)_B \times \text{U}(1)_A \times \text{SU}(N_f)_L \times \text{SU}(N_f)_R \times \text{SU}(N_c)$ symmetry for massless N_f flavors. $\text{U}(1)_B$ is related to the baryon number conservation. Due to the axial anomaly (See [8, 9] for example), $\text{U}(1)_A$ is explicitly broken to $\text{Z}(2N_f)$ [10, 11, 12]. We assume $\text{U}(1)_B \times \text{SU}(N_c)$ is not broken throughout this thesis while it can be broken in the color superconducting phase at sufficiently high density [2, 13, 14].

1.1.1 Asymptotic freedom

One of the characteristic features of QCD is the asymptotic freedom [15, 16, 17]. The interaction becomes weak in the high energy region and then we

can apply the perturbative calculation at high energy. In the high temperature region, the hard thermal loop perturbation theory (See Ref. [18] for example) is a useful tool. The color superconductivity can be realized at low temperature and sufficiently high density (See Refs. [13, 14] for example).

In order to see the asymptotic freedom explicitly, we consider the beta function obtained by the 1-loop diagrams as

$$\beta(g) = \mu_R \frac{dg(\mu_R)}{d\mu_R} = -b_0 g^3 - \dots, \quad (1.8)$$

where $b_0 = (11N_c/3 - 2N_f/3)/(4\pi)^2$ [15, 16] and μ_R denotes the renormalization scale. The coupling constant reads $g^2(\mu_R) = 1/\{b_0 \ln(\mu_R^2/\Lambda_{\text{QCD}}^2)\}$, where $\Lambda_{\text{QCD}} \simeq 200$ MeV is the scale parameter in QCD. This relation between the coupling constant and the renormalization scale tells us the asymptotic freedom, $g \rightarrow 0$ at $\mu_R \rightarrow \infty$.

At low energy, the interaction becomes strong and non-perturbative features appear: the spontaneous breaking of the chiral symmetry and the quark confinement. In order to describe these features, non-perturbative frameworks are required such as lattice QCD as reviewed in Sect. 2.1.

1.1.2 Vacuum structure

As introduced in Sect. 1.1.1, non-perturbative features appear at low temperature and characterize the vacuum structure. In the following, we review two non-perturbative aspects, the spontaneous chiral symmetry breaking and the quark confinement based on Refs. [1, 2, 3].

Spontaneous breaking of chiral symmetry

In this subsection, we discuss the spontaneous chiral symmetry breaking [19, 20, 21]. In the vacuum, the chiral symmetry is spontaneously broken as $\text{SU}(N_f)_R \times \text{SU}(N_f)_L \rightarrow \text{SU}(N_f)_V$, where $\psi \rightarrow \exp(i\theta_V^a T^a)\psi$, ($\theta_V^a = \theta_L^a = \theta_R^a$). One of the order parameters of this chiral symmetry breaking is the chiral condensate $\langle \bar{\psi}\psi \rangle = \langle \bar{\psi}_L\psi_R + \bar{\psi}_R\psi_L \rangle$ which mixes the left- and right-handed quarks. Quarks obtain the effective mass with the finite chiral condensate and form hadrons as constituent quarks. It should be noted that when the symmetry is broken spontaneously, the massless particles appear as the Nambu-Goldstone (NG) modes [20, 21, 22, 23].

In the realistic cases, the chiral symmetry is approximately realized since the current quark masses of u and d ($m_u \sim 3$ MeV, $m_d \sim 5$ MeV [24]) are small enough compared with the typical scale $\Lambda_{\text{QCD}} \simeq 200$ MeV; the symmetry is governed by $\text{SU}(2)_L \times \text{SU}(2)_R$. In addition to the u and d

quarks, we often consider the strange quark contribution ($m_s \sim 100$ MeV [24]) and the symmetry becomes $SU(3)_L \times SU(3)_R$ in this case. Because of the spontaneous chiral symmetry breaking, the chiral condensate is realized as $\langle \bar{\psi}\psi \rangle \sim -(250\text{MeV})^3$ and the constituent quark masses are found to be $M_{u,d} \sim 350$ MeV and $M_s \sim 550$ MeV for u , d and s quarks, respectively [1]. One can identify approximate NG particles as pions, kaons, and eta in the 3 flavor case.

Quark confinement

We here review properties of the quark confinement based on Refs. [1, 2, 3]. In the low energy region, the typical degrees of freedom are hadrons and we cannot directly observe quarks. This phenomenon is called the quark confinement [25, 26, 27].

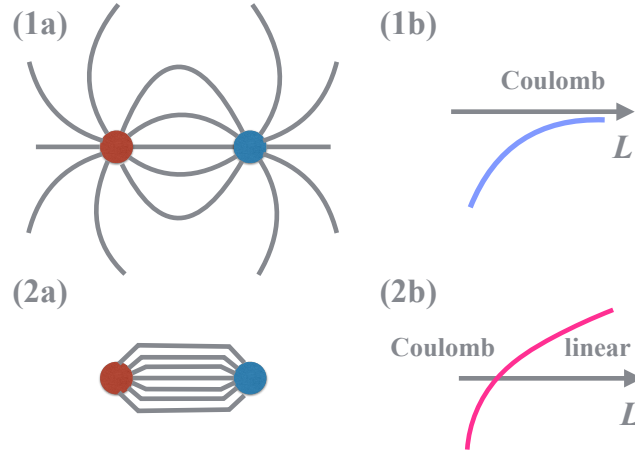


Figure 1.1: Schematic pictures of electric or color field lines of force in QED and QCD. The top panels show the QED case and the bottom panels show the QCD case. The electric line of force between e^+ and e^- is shown in Fig. (1a) and the color line of force between a quark and an antiquark is given in Fig. (2a). The right panels are the potential in QED in Fig. (1b) and that in QCD in Fig. (2b).

In the quantum electrodynamics (QED), electric field lines start from a positive electric charge radially and the potential between two charges is given by the Coulomb potential as in Figs. 1.1 (1a) and (1b). The color field lines in QCD are squeezed along the line between a quark and an antiquark in Fig. 1.1

(2a). The static-quark potential between heavy quarks is well described by $V(L) = -C/L + \sigma_{\text{string}}L + \text{const.}$, with the distance between two quarks L , the string tension σ_{string} , and a constant value C , respectively [25, 26, 27]. The first term and the second term correspond to a Coulomb potential and a linear potential, respectively, as shown in Fig. 1.1 (2b). The linear potential at long distance tells us that one needs an infinite energy in order to put a quark far from the other quark, and then quarks are confined in mesons. Similarly, three quarks are confined in baryons [28, 29]. In the realistic case, the quark masses are finite and the quark-antiquark pair creation occurs at sufficiently large distance; and then quarks are confined in hadrons again.

1.2 QCD phase diagram

In this section, we review the conjectured QCD phase diagram at finite temperature and density based on Refs. [1, 2, 3, 30, 31, 32, 33, 34].

1.2.1 Overview of QCD phase diagram

We show a schematic picture of the QCD phase diagram in Fig. 1.2. In the low temperature and low chemical potential region, quarks and gluons are confined in hadrons, and the chiral symmetry is spontaneously broken (*Nambu-Goldstone (NG) phase*). At high temperature, the Quark-Gluon-Plasma (QGP) is realized, and the chiral symmetry is restored (*Wigner phase*) via crossover [39, 40]; the relevant degrees of freedom (DOF) become quarks and gluons. At finite chemical potential, the crossover is expected to turn to the first-order phase transition at a critical point (CP) [35]. In the low temperature and large chemical potential region, the color superconducting phase or other phases are expected (See [2, 3] for example).

In order to investigate the non-perturbative phenomena, the lattice QCD approach is applied as a first-principles method at zero chemical potential as reviewed in Sect. 2.1. Quantitative understanding such as the critical temperature [41, 42, 43] and the order of the phase transition [39] is well established at vanishing chemical potential by using lattice QCD. At finite density, it is not easy to investigate the QCD phase diagram due to the sign problem in lattice QCD especially for $\mu/T > 1$ (See [37] for example) and then effective models are applied (See [30] for example). In order to find the CP location experimentally, the Beam Energy Scan (BES) program has been recently performed at Relativistic Heavy Ion Collider (RHIC) and higher-order cumulants¹ of conserved charges and a proxy for the net-baryon

¹We can find fluctuation properties through higher-order cumulants as reviewed in

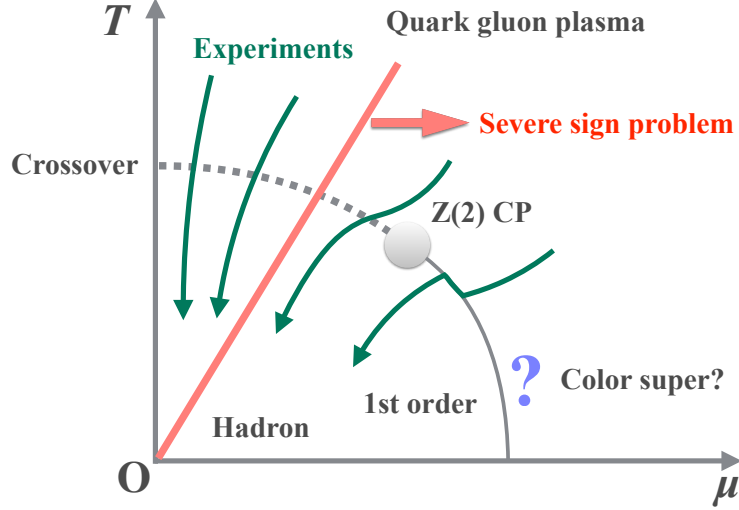


Figure 1.2: A schematic QCD phase diagram with the temperature T and the quark chemical potential μ axes. In the hadron phase, typical degrees of freedom (DOF) are hadrons. The important DOF become quarks and gluons in the quark-gluon plasma (QGP) phase. The crossover and first-order phase transition are expected at low and high densities, respectively. A critical point (CP) is located at the end point of the first-order phase transition line [35, 36]. A first-principles method, lattice QCD, is not reliable for $\mu/T > 1$ due to the sign problem [37]. The heavy-ion collision experiments are carried out and higher-order cumulants of conserved charges are measured in order to determine the CP location [38].

number are investigated [38, 44, 45].

We review the phase transition along the temperature axis in Sect. 1.2.2 and the phase transition at finite density in Sect. 1.2.3.

1.2.2 Phase transition along the temperature axis

In the early time of the QCD phase transition study, Hagedorn argued about what is going on at high temperature. He implied that there should be a transition at high temperature from the usual hadron phase [46]. Current understanding of the phase transition may be summarized as follows [1, 2, 3, 30, 42]. At low temperature, the chiral symmetry is spontaneously broken,

Sect. 1.2.4.

and quarks and gluons are confined in hadrons. They are released from hadrons at high temperature via crossover [39] and the relevant DOF are quarks and gluons. The chiral symmetry is restored in this QGP phase. Above the phase transition temperature, the energy and pressure increase rapidly since the number of DOF in QGP is larger than that in the hadron phase [32, 42, 47].

At sufficiently high temperature, the dynamics of quarks and gluons can be described approximately by free particles according to the asymptotic freedom. We can expand pressure by g^2 . The leading order of the expansion corresponds to the Stefan-Boltzmann (SB) limit, and one can obtain the higher-order corrections as discussed in Refs. [1, 48, 49, 50, 51, 52, 53].

Confinement-deconfinement phase transition

We here review some natures of the confinement-deconfinement phase transition based on Refs.[1, 2, 3]. At finite temperature, one of the order parameters of the confinement-deconfinement phase transition with infinite quark masses is the Polyakov loop which is related to the $Z(N_c)$ symmetry [54, 55, 56];

$$P(\mathbf{x}) = \frac{1}{N_c} \text{Tr} \mathcal{P} \exp \left[-ig \int_0^\beta dx_4 A_4(\mathbf{x}, x_4) \right] , \quad (1.9)$$

where $\mathcal{P}$ denotes the time ordered product, T is the temperature with $\beta = 1/T$, and the spacetime is defined in the Euclidean coordinate. The periodic boundary condition is imposed on the gauge fields. The expectation value of the Polyakov loop is related to the free energy F_q of a static quark [57, 58, 59] as $\langle P(\mathbf{x}) \rangle \sim \exp(-F_q/T)$. In the confined phase, the free energy is infinite and the expectation value of the Polyakov loop vanishes, then the $Z(N_c)$ symmetry is realized. By comparison, the free energy is finite in the deconfined phase and the expectation value of $P(\mathbf{x})$ is finite, then the $Z(N_c)$ symmetry is spontaneously broken. The order of the phase transition is the first for $N_c = 3$ [55, 60, 61, 62] and is the second for $N_c = 2$ [63, 64, 65]. When we consider the finite mass effect, the Polyakov loop is an approximate order parameter due to the explicit breaking of the center symmetry [55, 56].

In order to include the confinement-deconfinement dynamics, we consider the Polyakov loop effect in the effective models [66].

Chiral phase transition

Pisarski and Wilczek studied the order of the chiral phase transition by using the Ginzburg-Landau theory with the renormalization group flow [11]. In the massless case without axial anomaly, the phase transition is of

- the second order for $N_f = 1$ due to $O(2)$ symmetry ,
- the first order for $N_f \geq 2$,

In the massless case with axial anomaly, the phase transition is

- crossover for $N_f = 1$,
- of the second order for $N_f = 2$ due to $O(4)$ symmetry ,
- of the first order for $N_f \geq 3$,

In the presence of an isospin symmetry for u and d quarks, $m_{ud} \equiv m_u = m_d$, we can obtain insights into the order of the phase transition from the famous Columbia plot [67, 68, 69]. A schematic picture of the Columbia plot is given in Fig. 1.3. The right-top corner in the Columbia plot corresponds to

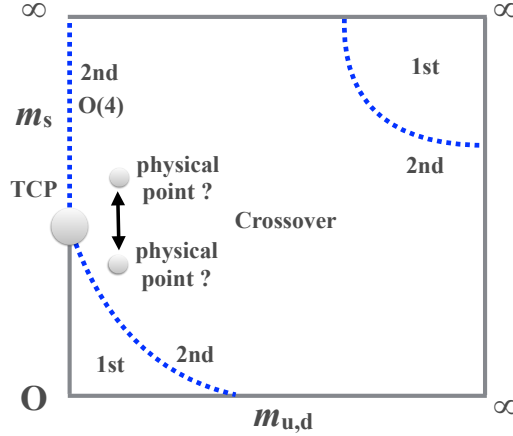


Figure 1.3: Phase transition order at finite temperature in the (m_{ud}, m_s) plane (Columbia plot) [67, 68, 69]. TCP denotes tricritical point. Actual location of the physical point is under debate [70, 71].

no-dynamical quark case (static quark limit) $(m_{ud}, m_s) = (\infty, \infty)$, and the phase transition is of the first order for $N_c = 3$ [55, 60, 61, 62]; the theory becomes the pure Yang-Mills theory and the Polyakov loop is the exact order parameter of the $Z(3)$ symmetry. In the lower mass region, there are a first order region and a crossover region, separated by the second order boundary. On the left-top corner, the dynamics is characterized by massless 2 flavors, $(m_{ud}, m_s) = (0, \infty)$, and the symmetry is $SU(2)_L \times SU(2)_R \simeq O(4)$, so the phase transition is of the second order [11]. Along the m_s axis, there is a

tricritical point and the first-order phase-transition region is realized at lower masses, including massless 3 flavor case on the left-bottom corner [11] in the Columbia plot.

At the physical point, there is no sharp phase transition i.e. crossover, which is confirmed by the lattice QCD simulation [39]. The phase transition temperature is found to be about 172 MeV for $N_f = 2$ [41, 42, 43] and about 154 MeV for $N_f = 3$ [41, 42] from the lattice QCD calculations. The physical point in the Columbia plot is not determined yet [70, 71].

Regarding the massless 2 flavor case without anomaly, numerical and theoretical studies beyond the Pisarski and Wilczek's argument have been carried out motivated by the effective restoration of $U(1)_A$ symmetry (See, for example Ref. [72] and references there in) and further studies are required to determine the phase transition order.

1.2.3 Phase transition at finite density

We review the QCD phase diagram at finite density based on Refs. [1, 2, 3, 30, 38, 73], where we face the sign problem in lattice QCD.

Phase transition at zero temperature along the chemical potential axis

We here discuss the phase structure at zero temperature $T = 0$ and finite chemical potential $\mu > 0$ based on Ref. [73]. The vacuum state is realized at vanishing chemical potential in which the baryon density is zero. The first order phase transition occurs when the value of the chemical potential takes the critical value of the chemical potential $\mu_0 \sim 924$ MeV: $m_N \sim 939$ MeV (the nucleon mass) $- 16$ MeV (the binding energy in the isospin-symmetric nuclear matter) [73]. In QCD, the baryon density jumps to the saturation density of nuclear matter, $\rho_0 \simeq 0.17 \text{ fm}^{-3}$ at $\mu = \mu_0$. Thus, the baryon density is the order parameter and this phase transition is the liquid-gas type phase transition [2]². One expects that the chiral phase transition can be realized at higher μ than μ_0 and the order is expected to be the first according to effective model calculations [30, 35]. It should be noted that the crossover phase transition can be realized due to the strong vector interactions [75] and another mechanism [76, 77].

²This liquid-gas type phase transition ends at a second-order phase transition point at finite T [74].

Chiral phase transition in QCD phase diagram

We briefly introduce the current understanding of the QCD phase diagram with regard to the chiral phase transition based on Refs. [1, 2, 3, 30, 37]. The QCD phase diagram has been investigated by using effective models, lattice QCD with methods evading the sign problem, and so forth [30, 37]. A schematic QCD phase diagram is shown in Fig. 1.4.

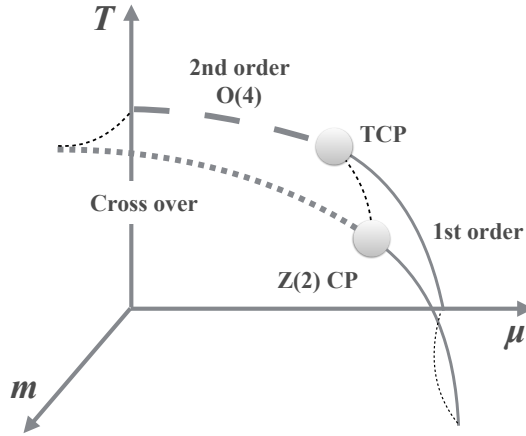


Figure 1.4: Schematic picture of QCD phase diagram with the quark mass axis regarding the chiral phase transition [78]. A tricritical (critical point) is expected to exist between the second-order (crossover) and the first-order phase transition in the chiral limit (at finite mass). This figure is basically taken from Ref. [78]

First, we introduce the conjectured QCD phase diagram in the chiral limit ($m_0 \rightarrow 0$). As mentioned in previous subsections, the second-order phase transition occurs at low chemical potential for $N_f = 2$, which belongs to the $O(4)$ universality class [11]. The second-order phase transition line turns into the first-order phase transition line at the tricritical point (TCP) in the finite chemical potential region [35]. Around TCP, the behavior of the chiral phase transition is well described by the mean field theory [79].

At finite mass, the phase transition is crossover at zero and small chemical potentials as confirmed by lattice QCD simulations [39, 40]. Since there is no sharp phase transition for crossover, we call the boundary the pseudo-critical line³. From the lattice QCD calculations, the curvature of the pseudo-critical

³One often defines the phase boundary as a peak position of the chiral susceptibility, which is the second-order derivative of $\log Z_{\text{QCD}}$ with respect to m_0 .

line is obtained as $T_c(\mu)/T_c(0) = 1 - \kappa(N_c\mu/T)^2 + \mathcal{O}((N_c\mu/T)^4)$ with small curvature κ [40, 80, 81, 82, 83]. TCP becomes the critical point (CP) at finite density [35], where the transition is characterized by Z(2) universality. In the large chemical potential region, the first-order phase transition starts at Z(2) CP from effective model calculations [35, 79, 84, 85] (See, for example [30] as a review).

At finite chemical potential, the effect of the baryon (quark) number density is important [79, 86, 87, 88, 89]; the chiral condensate (an order parameter of the chiral phase transition) can be mixed with the baryon (quark) number density [86, 87, 88]. The soft mode is the number density $\langle\psi^\dagger\psi\rangle$ rather than the chiral condensate at finite mass around the critical point (CP) [86, 87, 88]. In Sect. 1.2.4, we will review the fluctuation properties of the baryon (quark) number density.

The location of CP [35, 36] provides a key information to deduce the phase boundary. Then the CP location has been suggested in/beyond the mean field approximation by using the effective models (See, for example [35, 66, 79, 84, 85, 90, 91, 92]). Because of the model dependence (See, for example [30] as a review), we cannot determine the CP location in model calculations, so the first-principles method, the lattice QCD, is demanded while we face the sign problem at finite chemical potential. In lattice QCD calculations, there are some attempts to investigate the location of CP. By using the reweighting method in lattice QCD, the CP location is suggested [93, 94, 95], but it is pointed out that the signal can be accidentally observed because of the sign problem [96]. Most of methods based on MC simulations are currently not reliable for $\mu_q/T > 1$ due to the sign problem (See, for example [37] as a review); then we need further developments from theoretical and experimental points of view.

Higher-order fluctuations (cumulants) of the conserved charges are expected to be a good signal to find the QCD critical phenomena and the CP location [97, 98, 99, 100]. Once the singular behavior is smeared by some effects (e.g. finite mass and volume effects), the divergent behavior of the second-order cumulant (or the susceptibility) is not very useful to identify the critical behavior especially in experiments [98, 99, 100, 101, 102]. Higher-order cumulants than the third-order one are proposed to be better observables to see the phase transition phenomena. Higher-order cumulants are considered to remain sensitive to the correlation length [98]. In addition, the sign changes of the third-order [97, 100] and the fourth-order cumulants [99, 100] would be useful tools since the sign changes of cumulants can be detected unambiguously. We will review aspects of the cumulants in Sect. 1.2.4.

Experiments at heavy-ion collider

The heavy-ion collision experiments have been performed to investigate properties of QCD at RHIC in Brookhaven National Laboratory and at Large Hadron collider (LHC) in CERN. Heavy-ions are accelerated and collided with each other. QGP, which is a deconfined system of quarks and gluons, may be created in the reaction region at RHIC and LHC.

One of the QGP evidences is the jet quenching [103, 104, 105]. This is the phenomenon of the energy loss of jets. Jets created in the primary hard scatterings would lose energy by the strong interaction with the medium. For example, a jet with the back-to-back correlation loses its energy significantly and thus disappears. Also, the nuclear modification factor provides a evidence of QGP [105, 106, 107, 108]. This factor is the ratio of hadron yields produced in QGP to those from superpositions of nucleon-nucleon collisions. The nuclear modification factor shows the suppression behavior at high transverse momentum, which is not observed in pA collisions. This phenomenon may be related to the energy loss in the medium. Another evidence is the quark number scaling [109, 110, 111, 112]. In order to see the scaling, we first introduce the elliptic flow (v_2). The elliptic flow is the second Fourier component of the azimuthal distribution of particles and reflects the geometric property of the medium. If particles in the medium are partons (quarks and gluons), quarks may coalesce to form hadrons. The elliptic flow is expected to scale with the number of constituent quarks as, $v_2^h(\mathbf{p}_T) = n_q v_2^q(\mathbf{p}_T/n_q)$ with the elliptic flow for hadrons (quarks) v_2^h (v_2^q), the transverse momentum $\mathbf{p}_T$, and the number of constituent quarks n_q . This phenomenon is called the quark number scaling and is observed in heavy-ion collision experiments [111, 112].

The creation of QGP has been confirmed at small chemical potential, where the transition is crossover [39, 40]. The next grand step is to find CP and the first-order phase transition, which are expected to exist at finite chemical potential [30, 35]. Once we can fix the CP location by experiments, we expect that one can deduce the phase boundary in the large chemical potential region; and then BES has been carried out to investigate the phase boundary and CP [38]. In BES, we explore the finite density region by varying the colliding energy [113]. One of the promising observables for the critical behavior at finite density are the event-by-event fluctuations such as the higher-order cumulants: *e.g.* the net-proton number (as a proxy for baryon number), charge, and strangeness cumulants (See, for example [38]).

In experiments, the whole system is finite and is characterized by the non-equilibrium dynamics. It is not easy to find the divergent behavior of the second-order cumulant or susceptibility due to the smeared singular behavior

[98, 99, 100, 101, 102]. Alternatively, the sign changes of the higher-order cumulants are considered to be more suitable to study critical phenomena [97, 99, 100]. Furthermore, the higher-order cumulants are more sensitive to the correlation length than the second-order cumulant [98]. Then, the higher-order cumulants and their ratios have been measured by using the multiplicity distribution [44, 45, 114, 115]. According to the arguments that the higher-order cumulants of the net-baryon number can be negative from theoretical view points [97, 99, 100], the net-proton number cumulants as a function of the colliding energy have been obtained as a proxy for the net-baryon number. Their ratios are found to behave non-monotonically, deviating from the expected behavior of non-interacting hadrons [44, 45, 114]. Origins of this deviation are under debate; one of the reasons might be a signal of the phase transition phenomena as reviewed in Sect. 1.2.4. We can expect that some features of the QCD phase diagram will be revealed by BES and its second stage of BES in the future.

The cumulant ratios of the net-baryon number can be different from the ratios obtained from the net-proton number. In Refs. [116, 117], the relations between the net-baryon and net-proton number are discussed based on simple models. More realistic cases are studied in Refs. [118, 119].

1.2.4 Theoretical studies of observables

From now on, we discuss the theoretical approaches to obtain observables: the order parameters, the susceptibilities, and the cumulants.

The behaviors of the chiral condensate and its susceptibility are standard observables to identify the chiral phase boundary in the static and infinite volume case. In addition, it is proposed that fluctuation observables are important to observe the signatures of the phase transition and of the existence of CP [31, 97, 98, 120, 121, 122, 123]. In this subsection, we review the phase transition phenomena appearing in the cumulants by focusing on the chiral phase transition based on Refs. [31, 33, 34, 124].

Order parameters and susceptibilities

We here consider a partition function as [31, 33, 124]

$$Z_{\text{QCD}} = \text{Tr} \left[\exp \left\{ - \left(\hat{H}_{\text{QCD}}(m_0) - \sum_i \mu_i N_i \right) / T \right\} \right], \quad (1.10)$$

where $\hat{H}_{\text{QCD}}$, μ_i , and Q_i are the QCD hamiltonian, the chemical potential, and the conserved charge, respectively. i denotes the corresponding conserved

quantity: for example, $i = q, B, Q$, and s are for the quark number, baryon number, electric charge, and strangeness in QCD.

As mentioned in Sect. 1.2.3, an order parameter of the chiral phase transition is the chiral condensate σ ,

$$\sigma = -\langle \bar{\psi}\psi \rangle = \frac{T}{V} \frac{\partial \log Z_{\text{QCD}}}{\partial m_0} . \quad (1.11)$$

Around CP, the baryon (quark) number density is the soft mode of the phase transition [86, 87, 88], which can be defined by

$$n_B = \frac{1}{V} \frac{\partial \log Z_{\text{QCD}}}{\partial (\mu_B/T)} \left(n_q = \frac{1}{V} \frac{\partial \log Z_{\text{QCD}}}{\partial (\mu_q/T)} \right) , \quad (1.12)$$

for $\mu_B = N_c \mu_q$. The susceptibilities of the chiral condensate and the baryon number density are the second-order derivative of the $\log Z_{\text{QCD}}$:

$$\chi_\sigma = \frac{T}{V} \frac{\partial^2 \log Z_{\text{QCD}}}{\partial m_0^2} , \quad (1.13)$$

and

$$\chi_B = \frac{T}{V} \frac{\partial^2 \log Z_{\text{QCD}}}{\partial \mu_B^2} , \quad (1.14)$$

respectively. These susceptibilities indicate the fluctuations of the corresponding observables. From the combination of the different type of the derivatives, one can obtain insights into the connection between order parameters. For example, the off diagonal part of the susceptibility of the chiral condensate and baryon number ($\chi_{\mu,m} \propto \partial^2 \log Z_{\text{QCD}} / (\partial m_0 \partial \mu_B)$) shows the correlation between the chiral condensate and baryon number [31].

Higher-order cumulants of conserved charges

The n th-order cumulants with respect to a chemical potential can be defined as

$$c_i^{(n)} = \frac{1}{VT^3} \frac{\partial^n \log Z}{\partial \hat{\mu}_i^n} , \quad (1.15)$$

where $\hat{\mu}_i = \mu_i/T$ and $i = q, B, Q$, and s denote the net-quark number, net-baryon number, charge, and strangeness, respectively. The first-order cumulant reads

$$c_i^{(1)} = \frac{\langle N_i \rangle}{VT^3} = \frac{n_i}{T^3} , \quad (1.16)$$

where

$$\langle N_i \rangle = \frac{\partial \log Z}{\partial \hat{\mu}_i} , \quad (1.17)$$

and n_i denotes the corresponding number density. Higher-order cumulants are given as

$$\begin{aligned} c_i^{(2)} &= \frac{1}{VT^3} \langle (\delta N_i)^2 \rangle , \\ c_i^{(3)} &= \frac{1}{VT^3} \langle (\delta N_i)^3 \rangle , \\ c_i^{(4)} &= \frac{1}{VT^3} \left[\langle (\delta N_i)^4 \rangle - 3 \langle (\delta N_i)^2 \rangle^2 \right] , \end{aligned} \quad (1.18)$$

where $\delta N_i = N_i - \langle N_i \rangle$ [124]. These higher-order cumulants indicate the fluctuation properties of the corresponding order parameter.

In order to investigate critical phenomena around the phase transition, it is useful to introduce cumulant ratios as

$$R_{m,n}^i = \frac{c_i^{(m)}}{c_i^{(n)}} , \quad (1.19)$$

since we can omit the trivial volume and temperature dependence.

Higher-order cumulants of net-baryon number

At finite chemical potential, $c_B^{(1)} \propto n_B$ is finite and increases rapidly around the phase transition; the first-order cumulant of the net-baryon number plays important roles to investigate the phase transition [79, 86, 87, 88, 89, 97, 100] as shown in the left top panel of Fig. 1.5, and the second-order cumulant or susceptibility exhibits a peak structure at large chemical potential [36, 79, 90, 126, 127]. In addition, the sign flip of higher-order cumulants is a useful tool to detect the phase transition as well as the divergent or growing behavior of the second-order cumulant [97, 99, 100]. Then we review properties of the higher-order net-baryon number cumulants at finite density in this subsection.

The behavior of the cumulants at high and low temperature can be deduced as follows. At $T < T_c$, the hadron resonance gas (HRG) model well describes the pressure and energy density in lattice QCD [128, 129], and then cumulants are also expected to be well described by the HRG model at low temperature. In HRG [130, 131, 132], we include interaction effects by introducing all hadron and resonance contributions as non-interacting particles. It

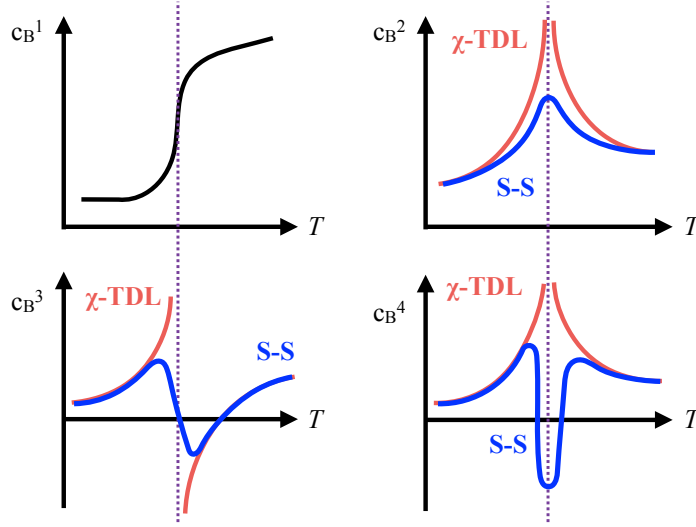


Figure 1.5: Expected behavior of cumulants for net-baryon number at finite density [79, 97, 100, 124, 125]. The first, second, third, and fourth order cumulants are shown in top left, top right, bottom left, and bottom right panels, respectively. The second and fourth-order cumulants positively diverge and third one exhibits a positive and a negative divergences in the chiral and thermodynamic limits (χ -TDL). At finite mass and/or in finite volume (smeared singularity, S-S), the singular behavior is masked and a downward convex region (or a negative valley) appears. The third-one changes its sign and it is useful to investigate critical phenomena [97].

is argued that HRG well describes the pressure given by interacting particles due to the cancellation between attractive and repulsive phase shifts of particles [132]. At $T \gg T_c$, we expect that the asymptotic value of observables becomes closer to the Stefan-Boltzmann (SB) value.

When the phase transition occurs, the higher-order cumulants show non-monotonic behavior around the phase transition temperature. In the chiral and thermodynamic limits, the second- and fourth-order cumulants are expected to positively diverge around TCP (and the phase transition for the fourth-order one) as shown in Fig. 1.5 labeled as χ -TDL [79, 100, 125]. The third-order one positively and negatively diverges below and above the phase transition in χ -TDL, respectively [100].

Once the singular behavior is smeared by some effects such as the finite mass effect and/or the finite volume effect, higher-order cumulants show

different behavior [100, 133]. The divergent behavior of $c_B^{(2)}$ is smeared and it has a positive peak as shown in Fig. 1.5 labeled by S - S [133]. In addition, the third- and fourth-order cumulants oscillate around the phase transition [133]. The third one has a positive peak below T_c and has a negative valley above T_c [97, 100, 133]. $c_B^{(3)}$ oscillates also as a function of $\hat{\mu}$. Then $c_B^{(4)} = \partial c_B^{(3)} / \partial \hat{\mu}$ should have a negative region around the phase transition. In fact, it would have a negative valley between two positive peaks at small mass [100, 133]. According to $Z(2)$ universality, the fourth-order cumulant may have the negative region around CP [99].

There are attempts to see the explicit critical behavior of the higher-order cumulants at finite density by using models [90, 97, 100, 125, 134, 135, 136, 137, 138]. We find oscillatory behavior of higher-order cumulants and their ratios around the phase transition as functions of μ and T . At sufficiently large μ , the fourth-order cumulant can be negative. The sign changes of cumulants might be good signals to investigate the QCD phase transition, and need to be confirmed theoretically beyond the model calculations.

Higher-order cumulants have been investigated also in lattice QCD at finite density [139, 140, 141, 142, 143, 144, 145, 146], but it is not easy to find the negative $c_B^{(4)}$ region in lattice QCD. In the Taylor expansion method, for example, we expand dimensionless free energy as $f/T^4 = c_B^{(0)}|_{\hat{\mu}=0} + c_B^{(2)}|_{\hat{\mu}=0}\hat{\mu}^2/2! + c_B^{(4)}|_{\hat{\mu}=0}\hat{\mu}^4/4! + c_B^{(6)}|_{\hat{\mu}=0}\hat{\mu}^6/6! + \dots$ and the fourth-order cumulant reads $c_B^{(4)}(\hat{\mu}) = c_B^{(4)}|_{\hat{\mu}=0} + c_B^{(6)}|_{\hat{\mu}=0}\hat{\mu}^2/2! + \dots$ at finite density. $c_B^{(4)}|_{\hat{\mu}=0}$ should be positive [100], then we need $c_B^{(6)}|_{\hat{\mu}=0}$ and higher-order cumulants than sixth order, $c_B^{(6)}|_{\hat{\mu}=0}$, which can take negative values, to describe negative $c_B^{(4)}$ at finite μ . These higher-order cumulant contributions need statistics and $c_B^{(6)}|_{\hat{\mu}=0}$ has been obtained recently [140, 141, 146]. There is a possibility that we observe the negative region in lattice QCD, but we have not yet concluded the existence of the region because of large error bars, a small number of data points, heavier masses than the physical one, and so on [139, 142, 143, 144, 145].

In this thesis, we investigate the higher-order cumulants on various size lattices systematically. Due to the sign problem, it is difficult to see the oscillatory behavior of cumulants quantitatively in standard lattice QCD simulations [139, 142, 143, 144, 145]. In addition, we need calculations at sufficiently small quark mass to find the critical behavior from $O(N)$ universality [100, 133]. Then we need another way of observing them systematically at finite density near the chiral limit on a lattice in order to investigate whether the negative cumulant region exists or not based on the lattice QCD formalism. We here apply the strong coupling approach to study the finite

density region. We find the oscillatory behavior and negative region of cumulants around the phase transition due to the finite size effect, which would be consistent with $O(N)$ spin-model analyses in a finite system [133].

Remarks on the relation to experimental data

In experiments, the QGP medium created by a heavy-ion collision is finite volume. As mentioned in previous section, finite volume can affect the singular behavior of cumulants [133]. According to Ref. [147], the size of QGP created in experiments may be evaluated by a dimensionless quantity $LT \simeq 2.4 - 3.6$ ($1/(LT) \simeq 0.28 - 0.42$), where L is a box length. By comparison, the finite mass effect may be characterized by a dimensionless quantity $m_0/T \simeq 0.03$, provided that $m_0 \simeq 5$ MeV and $T \simeq 160$ MeV at a freeze-out temperature [147]⁴. Then, the finite size effect plays important role to cumulants and their ratios with regard to the chiral phase transition (See, for example [133, 148, 149, 150, 151, 152, 153, 154, 155, 156]). It should be noted that the finite size effect in lattice QCD and that in experiments may be different from each other: e.g. boundary conditions, but we can expect that the finite size effect is basically the same between each other.

In previous subsections, we focus on the fluctuations in terms of the grand canonical ensembles while fluctuation effects in experiments are different. There are arguments that fluctuations of conserved charges in the experimental system are somewhat similar to the grand canonical ensembles in the thermal system [31]. Supposing that we focus on the fluctuations of the conserved charges, the conserved charges do not fluctuate when we consider the whole phase space. The conserved charges will fluctuate if a subsystem is measured since particles can move to other subsystems, which is the similar to the grand canonical ensemble case [119]. The above interpretation may be supported by the success of the statistical thermal model [157], but we need careful treatments to compare experimental results with theoretical results.

1.3 Organization of this thesis

Critical behavior has key information on the QCD phase diagram. One of the powerful first-principles methods, lattice QCD, gives insights into the critical phenomena in QCD. However, it has a notorious sign problem in the finite chemical potential region [37]. Thus, we need other approaches to investigate the phase diagram. One of the ways to attack such a region is the

⁴According to the scaling function analysis [100], the mass term appears as m_0/T , which should be small enough to investigate QCD phase transition phenomena.

strong coupling lattice QCD (SC-LQCD), where we assume that the coupling constant is sufficiently large [158, 159, 160, 161]. There are several works for the QCD phase diagram using SC-LQCD in the mean-field approximation [162, 163, 164, 165, 166, 167, 168]. Nowadays, it becomes possible to evaluate observables beyond the mean field approximation and to include field fluctuation effects in SC-LQCD [78, 169, 170, 171, 172]. This theoretical development is a vital step since it is important to evaluate observables exactly and critical phenomena are governed by critical exponents, which generally requires studies beyond the mean-field approximation. We here perform the Monte Carlo simulation and then we evaluate the field fluctuation effects in the QCD phase diagram [172].

We can further consider the fluctuation observables: higher-order cumulants of the net-baryon number [78]. These observables give significant insights into the critical phenomena around the phase transition [31, 33, 34, 124]. Particularly, we can confirm the finite size effect on cumulants at finite density, which may be useful to interpret heavy-ion collision data in view of finite size effect [133, 147]. By investigating cumulants in the chiral limit on a finite size lattice, we can omit the finite mass effect and investigate the finite size effect on higher-order cumulants [133]. For example, the fourth-order cumulant positively diverges around the phase transition in the chiral and thermodynamic limits [100] while we find a negative region between two positive peaks in the fourth-order cumulant on a finite size lattice at large μ/T in the chiral limit; then the fourth-order cumulant shows oscillatory behavior due to the finite size effect [78, 133]. Our simulations are carried out at $LT \simeq 3 - 9$ [78], so the negative region or the oscillatory behavior of higher-order cumulants can be observed in experiments where $LT \simeq 2.4 - 3.6$ [147], when the mass effect is small enough and the regular part of the corresponding cumulant does not overcome the smeared singular part.

This thesis is organized as follows. In Chap. 2, we introduce the basic concepts of lattice QCD, including the strong coupling approach. We develop the strong coupling approach with the field fluctuations and give the QCD phase diagram in Chap. 3 based on Ref. [172]. Next, we investigate fluctuation observables of the net-baryon number in Chap. 4 based on Ref. [78]. We finally conclude this thesis in Chap. 5.

Chapter 2

Lattice QCD approaches for QCD phase diagram

Lattice QCD (LQCD) is a first-principles method and is one of the most useful tools to investigate properties of QCD. In this chapter, we review the lattice formulation of QCD in Sect. 2.1 and the strong coupling approach in Sect. 2.2 based on Refs. [1, 173, 174].

2.1 Lattice QCD

In order to study the non-perturbative dynamics such as the chiral and confinement-deconfinement phase transitions, one of the powerful tools is LQCD. The LQCD approach achieves great successes at zero chemical potential such as the hadron masses [175, 176], the string tension [177, 178], the nuclear force [179, 180], phase transition temperature [41, 41, 42, 42, 43] and order [39], and so on. Other achievements are found in Refs. [1, 42, 173], for example. We investigate the QCD phase diagram based on the LQCD action in this thesis. We here review the concept of LQCD based on Refs. [1, 173, 174].

Before introducing LQCD action, we consider the Euclidean partition function and action as $\int \mathcal{D}[\psi, \bar{\psi}, A] \exp[iS_{\text{QCD}}] \rightarrow \int \mathcal{D}[\psi, \bar{\psi}, A] \exp[-S_{\text{QCD}}^{\text{Eucl}}]$ under the rotation to Euclidean variables as $x^0 \rightarrow -ix_4, A^0 \rightarrow iA_4, \gamma_0 \rightarrow \gamma_4$, and $\gamma_i \rightarrow -i\gamma_i$ ($i = 1, 2, 3$) which satisfies $\gamma_\mu^\dagger = \gamma_\mu$ ($\mu = 1, \dots, 4$). In LQCD, we interpret the Boltzmann weight factor, $\exp[-S_{\text{QCD}}^{\text{Eucl}}]$, as the probability weight. At finite temperature, we impose the periodic boundary condition for bosons and anti-periodic boundary condition for fermions in the temporal direction.

In the lattice field theory, the Euclidean space-time is discretized on a lattice with a lattice spacing a and then the lattice field theory is regularized

by the ultraviolet cut-off $1/a$. The continuum theory should be realized in the continuum limit $a \rightarrow 0$ and LQCD rigorously defines the field theory, maintaining the gauge symmetry.

2.1.1 Lattice QCD action

The lattice action is constructed based on the gauge invariance and the correspondence to the continuum action in the continuum limit [25]. Here, we give a review based on Ref. [1, 173, 174]. First, we construct the gauge action. In order to maintain the gauge invariance, we introduce the Wilson line for convenience;

$$U(y, x) = \mathcal{P} \exp \left[ig \int_x^y dz_\mu A_\mu \right] = \mathcal{P} \exp \left[ig \int_0^1 ds \lambda_\mu A_\mu \right] , \quad (2.1)$$

where $z_\mu(s=1) = y_\mu, z_\mu(s=0) = x_\mu, \lambda_\mu = dz_\mu/ds$, and $\mathcal{P}$ is the path ordering operator here. The Wilson line is transformed as $U(y, x) \rightarrow g(y)U(y, x)g^\dagger(x)$ under the gauge transformation $\psi(x) \rightarrow g(x)\psi(x); \bar{\psi}(y)U(y, x)\psi(x)$ is gauge invariant. Then, we can define a link variable as

$$U_{x,\mu} = U(x, x + \hat{\mu}) , \quad U_{x,\mu}^\dagger = U_{x+\hat{\mu}, -\hat{\mu}} , \quad (2.2)$$

where x is the lattice coordinate and $\hat{\mu}$ is the direction. The link variables are transformed as $U_{x,\mu} \rightarrow g_x U_{x,\mu} g_{x+\hat{\mu}}^\dagger$, where $g_x \in \text{SU}(N_c)$ is the gauge transformation matrix. Then the trace product $\text{Tr} \prod_C U$ of the link variables along a closed path C is gauge invariant. Now, we can define the plaquette as $U_{\mu\nu}(x) = U_{x,\mu} U_{x+\mu,\nu} U_{x+\nu,\mu}^\dagger U_{x,\nu}^\dagger$, and write down the standard plaquette action,

$$S_G = \sum_{x,\mu < \nu} \beta \left[1 - \frac{1}{2N_c} \text{Tr} (U_{\mu\nu}(x) + U_{\mu\nu}(x)^\dagger) \right] , \quad (2.3)$$

where $\beta = 2N_c/g^2$. In the continuum limit, the continuum gauge action in Eq. (1.1) is restored as

$$\lim_{a \rightarrow 0} S_G = \sum_{n,\mu < \nu} \beta \left[a^4 \frac{g^2}{2N_c} \text{Tr} F_{\mu\nu}^2 \right] + \mathcal{O}(a^6) , \quad (2.4)$$

since $\text{Tr} U_{\mu\nu}(x) = \text{Tr} [1 - a^4 g^2/2 \times F_{\mu\nu}^2 + \dots]$ where we utilize the Baker-Campbell Hausdorff formula, $\exp X \exp Y = \exp(X + Y + [X, Y]/2 + \dots)$.

Second, we construct the fermion terms. We can discretize the fermion action,

$$S_F = a^4 \sum_x \bar{\psi}_x \left[\frac{1}{2a} \sum_{\mu} \gamma_{\mu} \left(U_{x,\mu} \psi_{x+\hat{\mu}} - U_{x-\hat{\mu},\mu}^{\dagger} \psi_{x-\hat{\mu}} \right) + m \psi_x \right] , \quad (2.5)$$

by preserving the gauge invariance [25, 173, 174]. This lattice fermion is referred to as the naive fermion.

In this naive fermion term, there is a famous problem called the (fermion) doubling problem [181, 182, 183, 184]. Suppose that the free field theory is realized for $U = 1$, the action in the momentum space is given as

$$S_F = \int \frac{d^4 p}{(2\pi)^4} \bar{\psi}(pa) (i\gamma_{\mu} \sin(p_{\mu}a) + ma) \psi(pa) , \quad (2.6)$$

so the propagator is described as $(-i\gamma_{\mu} \sin(p_{\mu}a) + ma)/(\sin^2(p_{\mu}a) + (ma)^2)$. From the pole contribution of the propagator, $\sin^2(p_{\mu}a) + (ma)^2 = 0$, one finds two poles per one dimension in the chiral limit, $p_{\mu} = 0$ and π/a . In the continuum limit, only one pole appears, $p_{\mu} = 0$ in the chiral limit. A mode at π/a is referred to as a doubler and is an extra degree of freedom. When we put a naive fermion on the lattice in four-dimension space-time ($d = 4$), one finds $2^d = 16$ particles; then we have unexpected degrees of freedom of fermions in the lattice field theory. This phenomenon is called the doubling problem. The Nielsen-Ninomiya theorem gives some insights into the fermion doubling problem [182, 183, 184]. One cannot remove doublers when all of the following conditions are satisfied: the translation invariance, the (exact) chiral symmetry, the hermiticity, the locality, and the fermion bilinear form. Therefore, we need to abandon at least one of the above conditions to evade the doubling problem.

There are several kinds of the fermion actions, where we can weaken the doubling problem; the Wilson fermion [181, 185], the staggered fermion [186, 187], the domain wall fermion [188], the overlap fermion [189], and so on. In the Wilson fermion action, we put some mass to the doubler and evade the unexpected zero poles, but there is no chiral symmetry due to the effective mass term (See, for example [173, 174]). In the staggered fermion formalism, we interpret doublers as the flavors of quarks. There is the remnant chiral symmetry, but it corresponds to four flavors in the continuum limit in the four space-time dimension after removing the four-fold degeneracy (See, for example [173, 174]). The overlap fermion and domain wall fermion satisfy the exact Ginsparg-Wilson relation [190], which ensures the chiral symmetry up to the order of the lattice spacing a . However, these fermions require relatively large computational costs.

In this thesis, we utilize the staggered fermion. The staggered fermion has a remnant chiral symmetry, then the chiral phase transition has been studied from early times of the lattice field theory studies [173, 174]. In addition, the numerical cost is low due to the reduced gamma matrix indices. We will review the staggered fermion studies in the context of the strong coupling approach in Sect. 2.2.

2.1.2 Monte Carlo simulation

In order to obtain observables by using computational calculations, we often apply the Monte Carlo (MC) technique. We give a review on MC based on Refs. [1, 173, 174].

We have large degrees of freedom in lattice QCD [173, 174]. We generate configurations of the link variables in the standard lattice QCD, and the link variables have the following degrees of freedom: the 4 space-time dimension, the lattice size, and $N_c^2 - 1 = 8$ degrees of freedom for SU(3). The total degrees of freedom of the link variables on a 12^4 lattice are roughly about 4×12^4 (lattice size) $\times 8 \sim 660,000$, so we must evaluate about 660,000 multiple integrations. For large multiple integrals, it is common to utilize the Monte Carlo (MC) technique.

The expectation values of the observables are given as

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi O(\Phi) \exp[-S(\Phi)]}{\int \mathcal{D}\Phi \exp[-S(\Phi)]}, \quad (2.7)$$

where Φ and $S(\Phi)$ denote field variables and the action, respectively. In the lattice formalism, the degrees of freedom are finite and we can evaluate path integral numerically. In MC, we commonly apply the importance sampling, where we generate MC configurations in accordance with the probability of the Boltzmann weight factor, $\exp[-S(\Phi)]$. We evaluate the statistical average by using these configurations and obtain an observable as

$$\langle O \rangle \simeq \frac{1}{N_{\text{config.}}} \sum_{i=1}^{N_{\text{config.}}} O(\Phi_i), \quad (2.8)$$

where $N_{\text{config.}}$ is the number of configurations.

In the actual calculation, we update configurations $\Phi \rightarrow \Phi'$ with a stochastic process [1, 173, 174]: $W'[\Phi'] = \sum_{\Phi} W[\Phi] P(\Phi \rightarrow \Phi')$. $P(\Phi \rightarrow \Phi')$ is the transition probability from the old configurations Φ to the new configurations Φ' . $W[\Phi]$ is the probability density, which is expected to be proportional to the Boltzmann weight factor in equilibrium. We often consider a

Markov process to produce new configurations, which satisfies the following all conditions: $\sum_{\Phi} P(\Phi \rightarrow \Phi') = 1$, $P(\Phi \rightarrow \Phi') > 0$, and $\sum_{\Phi} W[\Phi] = 1$ [1, 173, 174]. We here assume that there exists the equilibrium probability density $W_{\text{eq}}[\Phi]$, which is realized after sufficiently long computational time, $W_{\text{eq}}[\Phi'] = \sum_{\Phi} W[\Phi]_{\text{eq}} P(\Phi \rightarrow \Phi')$. When we impose the detailed balance, $W_{\text{eq}}[\Phi'] P(\Phi' \rightarrow \Phi) = W[\Phi]_{\text{eq}} P(\Phi \rightarrow \Phi')$, we can obtain the equilibrium distribution. One of the methods satisfying the detailed balance is the Metropolis method [191]. In the Metropolis method, the transition probability is given as $P(\Phi \rightarrow \Phi') \propto \min(1, \exp[-\{S[\Phi'] - S[\Phi]\}])$. In the case where $S[\Phi'] > S[\Phi]$, we obtain $P(\Phi \rightarrow \Phi') = P_0(\Phi \rightarrow \Phi')$ and $P(\Phi' \rightarrow \Phi) = P_0(\Phi' \rightarrow \Phi) \exp[-(S[\Phi] - S[\Phi'])]$, with the microreversible probability $P_0(\Phi \rightarrow \Phi') = P_0(\Phi' \rightarrow \Phi)$. Then, the detailed balance and the equilibrium distribution $W_{\text{eq}}[\Phi] \propto \exp[-(S[\Phi])]$ are satisfied. In the case where $S[\Phi'] < S[\Phi]$, we can confirm the realization of the detailed balance and the equilibrium distribution as the previous condition, $S[\Phi'] > S[\Phi]$. In this thesis, we use the Metropolis method to obtain configurations.

As previously introduced in Sect. 2.1.1, lattice QCD action contains the fermion part and the gauge (boson) part as $S_{\text{LQCD}} = S_{\text{F}} + S_{\text{G}}$. The fermion action is given by the Wilson fermion, staggered fermion, or other fermions. The gauge part corresponds to the action in Eq. (2.3) in the standard case. The partition function of lattice QCD reads

$$\begin{aligned} Z_{\text{LQCD}} &= \int \mathcal{D} [\bar{\psi}, \psi, U] \exp[-S_{\text{QCD}}] \\ &= \int \mathcal{D} [U] \det \mathfrak{D}(U) \exp[-S_{\text{G}}(U)] , \end{aligned} \quad (2.9)$$

where $\mathfrak{D}(U) = \not{D} + m_0 + \mu\gamma_4$. We integrate out Grassmann variables ψ analytically in the last line. We often generate link-variable configurations by using the weight, $\det \mathfrak{D}(U) \exp[-S_{\text{G}}(U)]$, in lattice QCD with the Monte Carlo technique.

In the actual calculations, we have some statistical error bars in results. Configurations obtained by a Markov process have the auto correlation, which indicates that the configuration set in each step is affected by that in the previous step. The jackknife (JK) method is one of the common methods to reduce the effect of the auto correlation to estimate error bars correctly [173, 174, 192]. When we have the configuration set $\{\Phi_k, (k = 1, \dots, N_{\text{config}})\}$, we divide the set into each bin as $\Phi_l^{(\text{bin})} = (\Phi_{(l-1)n+1}, \dots, \Phi_{nl})$, where l runs from 1 to N_{bin} for $N_{\text{config}} = nN_{\text{bin}}$ and N_{bin} is the number of bins, respectively. We here define a JK average for each bin by using configurations except for a specified bin as $\langle \mathcal{O} \rangle^b = \sum_{k \notin \Phi_b^{(\text{bin})}} \mathcal{O}_k / (N_{\text{config}} - n)$.

Then, the average and the estimated error of the observable ($F(\mathcal{O})$) in JK are given as

$$\langle F(\mathcal{O}) \rangle = \sum_{b=1}^{N_{\text{bin}}} F(\langle \mathcal{O} \rangle^b) / N_{\text{bin}} , \quad (2.10)$$

$$\delta \langle F(\mathcal{O}) \rangle = \sqrt{\frac{N_{\text{bin}} - 1}{N_{\text{bin}}} \sum_{b=1}^{N_{\text{bin}}} \left[F(\langle \mathcal{O} \rangle^b) - \langle F(\mathcal{O}) \rangle \right]^2} , \quad (2.11)$$

respectively. We utilize this JK method to deduce error bars in this thesis.

2.1.3 Sign problem in QCD

In lattice QCD, we interpret the factor, $\det \mathfrak{D}(U) \exp[-S_G(U)]$, as the probability weight which should be real and positive definite. The weight factor cannot be regarded as the probability weight at finite chemical potential ($\mu \neq 0$) since the weight factor is complex and its real part can be negative. This is problematic in the MC simulations and we need large number of configurations, which is proportional to $\exp(CV)$, where V denotes the volume and C is some factor [37]. This problem is called the sign problem (See Refs. [37, 193, 194, 195, 196] for example). We review it based on Refs. [37, 193, 194, 195, 196].

The fermion determinant has a property,

$$\begin{aligned} \det \mathfrak{D}(\mu) &= \det \gamma_5 \mathfrak{D}(\mu) \gamma_5 \\ &= [\det \mathfrak{D}(-\mu^*)]^* , \end{aligned} \quad (2.12)$$

where $\mathfrak{D}(\mu) = \gamma_\mu D_\mu(\mu = 0) + \gamma_4 \mu + m$. We here utilize $\{\gamma_5, \gamma_\mu\} = 0$, $\not{D}^\dagger = -\not{D}$, and

$$\begin{aligned} \gamma_5 [\gamma_\mu D_\mu(\mu = 0) + \gamma_4 \mu] \gamma_5 &= -\gamma_\mu D_\mu(\mu = 0) - \gamma_4 \mu \\ &= [\gamma_\mu D_\mu(\mu = 0) - \gamma_4 \mu^*]^\dagger . \end{aligned} \quad (2.13)$$

At zero chemical potential, the fermion determinant is real while it becomes complex at finite chemical potential.

We could confirm the sign problem from another point of view [196]. We first consider the eigen value of the Dirac operator as

$$(\gamma_\mu D_\mu(\mu = 0) + m)\psi_n = (i\lambda_n + m)\psi_n , \quad (2.14)$$

where ψ_n and λ_n are the eigen function and the eigen value of the Dirac operator, respectively. Here, the Dirac eigen values are pure imaginary at

zero chemical potential ($\lambda_n \in \mathbb{R}$) due to the anti-hermiticity of the Dirac operator, $\not{D}^\dagger = -\not{D}$. By using the chiral symmetry $\{\not{D}, \gamma_5\} = 0$, the eigen value of $\gamma_5 \psi_n$ reads

$$\begin{aligned} (\gamma_\mu D_\mu(\mu=0) + m) \gamma_5 \psi_n &= (-i\lambda_n + m) \gamma_5 \psi_n \\ &= (i\lambda_n + m)^* \gamma_5 \psi_n, \end{aligned} \quad (2.15)$$

where $\gamma_5 \gamma_\mu D_\mu(\mu=0) \psi_n = -\gamma_\mu D_\mu(\mu=0) \gamma_5 \psi_n = i\lambda_n \gamma_5 \psi_n$. Therefore, the fermion determinant at zero chemical potential becomes

$$\begin{aligned} \det(\gamma_\mu D_\mu(\mu_q=0) + m) &= m^{N_0} \prod_n (i\lambda_n + m)(i\lambda_n + m)^* \\ &= m^{N_0} \prod_n |i\lambda_n + m|^2 \geq 0, \end{aligned} \quad (2.16)$$

with the number of zero eigen modes N_0 , since non-zero eigen values appear as the pair of $\pm i\lambda_n + m$.

At finite chemical potential, the eigen value of $\gamma_5 \psi_n$ reads

$$[\gamma_\mu D_\mu(\mu=0) + \gamma_4 \mu] \gamma_5 \psi_n = -z_n \gamma_5 \psi_n, \quad (2.17)$$

where $\{\gamma_\mu D_\mu(\mu=0) + \mu\gamma_4, \gamma_5\} = 0$ [197] and $[\gamma_\mu D_\mu(\mu=0) + \mu\gamma_4] \psi_n = z_n \psi_n, z_n \in \mathbb{C}$ due to the non-hermitian property of $[\gamma_\mu D_\mu(\mu=0) + \mu\gamma_4]$. As a result, the fermion determinant becomes complex and we cannot apply the MC simulation. When we consider the pure imaginary chemical potential [198], color SU(2) [199], or the isospin chemical potential [200, 201, 202] cases, there is no sign problem.

Now, let us consider the effect of the sign problem on observables in terms of the reweighting method [203, 204, 205]. The expectation value of an observable O is expressed as

$$\begin{aligned} \langle O \rangle &= \frac{\int \mathcal{D}U O |\det \mathfrak{D}| e^{i\theta} e^{-S_G}}{\int \mathcal{D}U |\det \mathfrak{D}| e^{i\theta} e^{-S_G}} \\ &\equiv \frac{\langle O e^{i\theta} \rangle_{\text{pq}}}{\langle e^{i\theta} \rangle_{\text{pq}}}, \end{aligned} \quad (2.18)$$

where

$$\langle \mathcal{O} \rangle_{\text{pq}} = \frac{\int \mathcal{D}U |\det \mathfrak{D}| \mathcal{O} e^{-S_G}}{\int \mathcal{D}U |\det \mathfrak{D}| e^{-S_G}}, \quad (2.19)$$

and $\langle \cdots \rangle_{\text{pq}}$ denotes the expectation value by using the phase quenched weight, $|\det \mathfrak{D}| e^{-S_G}$ and θ is the complex phase. The denominator in Eq. (2.18) is

the average phase factor, which indicates the statistical weight cancellation. In the case where the average phase factor is unity, there is no sign problem. By comparison, the severe weight cancellation arises when the average phase factor is close to zero.

The average phase factor is related to the free energy density difference [37], which is defined as the free energy density of the original theory minus that of the phase quenched theory ($\Delta f = f_{\text{orig}} - f_{\text{pq}}$), as

$$\langle e^{i\theta} \rangle_{\text{pq}} = \frac{Z_{\text{orig}}}{Z_{\text{pq}}} = \exp \left[-\frac{V}{T} \Delta f \right], \quad (2.20)$$

where $Z_{\text{orig}} = \int \mathcal{D}U \det \mathfrak{D} e^{-S_G}$ and $Z_{\text{pq}} = \int \mathcal{D}U |\det \mathfrak{D}| e^{-S_G}$. In Eq. (2.20), we use a relation: $Z = \exp[-F/T] = \exp[-V/T \times f]$, where T is the temperature, V is the volume, F is the free energy, and f is the free energy density, respectively [37, 170]. According to Eq. (2.20), the average phase factor becomes zero for the sufficiently large volume when the real part of Δf is positive and finite.

There are many attempts to evade the sign problem: the reweighting method [94, 95, 206, 207], the Taylor expansion method [139, 208, 209], the analytic continuation from the imaginary chemical potential [198, 210], the canonical approach [207, 211, 212, 213, 214, 215], the fugacity expansion [216], the histogram method [217], the finite isospin chemical potential [201, 202, 217], the density of state method [218, 219], the complex Langevin method [220, 221], and so on. Nowadays, there are some breakthroughs regarding the sign problem: the complex Langevin method with gauge cooling [222] and the Lefschetz thimble method [223, 224, 225]. However, most of these methods are not yet reliable in the cold dense matter, where the first order phase transition may exist, so we need theoretical developments to investigate the finite chemical potential region.

2.2 Strong coupling lattice QCD

In this thesis, we utilize the strong coupling approach to investigate the QCD phase diagram. The strong coupling approach is an approximation method by using the lattice QCD action. We expand the partition function by $1/g^2$ in the plaquette terms, assuming that the coupling constant g in QCD is sufficiently large. In this framework, we can describe two non-perturbative features: the chiral symmetry breaking and the quark confinement. We review the strong coupling approach in this section based on Refs. [1, 173, 174].

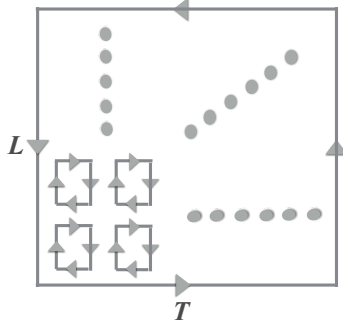


Figure 2.1: A schematic figure of the Wilson loop [25]. A small square shows a plaquette. The leading-order contribution to the Wilson loop is a planer-like diagram as in this figure.

2.2.1 Quark confinement at strong coupling

The quark confinement at strong coupling is firstly shown by Wilson in the pure Yang-Mills theory [25]. Now let us consider the following gauge-invariant Wilson loop

$$W(C) = \text{Tr} \left[\prod_{i \in C} U_i \right] , \quad (2.21)$$

where $C = L \times T$ for space L and time T lengths. The Wilson loop at $T \rightarrow \infty$ is given as

$$\langle W(C) \rangle = \frac{\int dU \exp[-S_G(U)] W(C)}{\int dU \exp[-S_G(U)]} \propto \exp[-V(L)T] , \quad (2.22)$$

where $V(L)$ is the static quark potential between a quark and an anti-quark, since the Wilson loop in this context can be interpreted as the following scenario. The heavy quark and anti-quark are produced at a distance L , the two heavy quarks propagate along the temporal axis, (staying at the same spatial points) and finally vanish at time T . The leading term of the strong coupling expansion contributing to the Wilson loop is given as the planar diagram as shown in Fig. 2.1;

$$\langle W(C) \rangle = N_c \exp \left[-TL \log(g^2 N_c) \right] , \quad (2.23)$$

and the static potential is expressed as $V(L) = L \log(g^2 N_c)$ by using $\text{SU}(N_c)$ group integral, $\int dU 1 = 1$, $\int dU U_{ab} = 0$, $\int dU U_{ab} U_{kl}^\dagger = \delta_{al} \delta_{bk} / N_c$, $\int dU U_{a_1, b_1}$

$\cdots U_{a_{N_c}, b_{N_c}} = \epsilon_{a_1, \dots, a_{N_c}} \epsilon_{b_1, \dots, b_{N_c}} / N_c!$ [226]. This linear potential implies the quark confinement since the potential is proportional to the distance between quarks¹.

Higher-order corrections to the strong coupling expansion are investigated [174, 227, 228, 229] and the convergence radius in the pure Yang-Mills theory is finite, so the quark confinement is realized at strong coupling [230]. As long as we apply the strong coupling expansion, the roughening phase transition occurs and the Wilson loop in the strong coupling region does not retain the confinement feature in the continuum limit (or scaling region) [174, 229]. By comparison, we consider that there is no phase transition by using MC simulation [177, 178]. Then, the confinement feature is kept even in the continuum limit in nature. With quark actions, one does not know whether the roughening phase transition occurs or not even when we utilize the strong coupling expansion method.

2.2.2 Chiral phase transition at strong coupling

When we consider lattice QCD with the fermions, we can describe the chiral phase transition. We review the chiral phase transition in the strong coupling lattice QCD based on Ref. [162]. Now let us consider one species of unrooted staggered fermion on isotropic lattice since it has a remnant chiral symmetry [186, 187]. We briefly introduce the description of the chiral phase transition in the mean field (MF) analysis. In the following, we take the lattice spacing as unity, $a = 1$.

In the strong coupling limit (SCL), the partition function and the action are given as

$$\begin{aligned} Z_{\text{SCL}} &= \int \mathcal{D}[\chi, \bar{\chi}, U_0, U_j] e^{-S_{\text{SCL}}} , \\ S_{\text{SCL}} &= \sum_x \frac{1}{2} \left[e^\mu \bar{\chi}_x U_{0,x} \chi_{x+\hat{0}} - e^{-\mu} \bar{\chi}_{x+\hat{0}} U_{0,x}^\dagger \chi_x \right] \\ &\quad + \sum_{x,j=1}^d \frac{\eta_{j,x}}{2} \left[\bar{\chi}_x U_{j,x} \chi_{x+\hat{j}} - \bar{\chi}_{x+\hat{j}} U_{j,x}^\dagger \chi_x \right] + \sum_x m_0 \bar{\chi}_x \chi_x , \end{aligned} \quad (2.24)$$

where $\eta_{j,x} = (-1)^{\sum_{i=1}^j x_{i-1}}$, χ is the staggered quark, μ is the quark chemical potential, d is the spatial dimension, and m_0 is the bare quark mass. The temporal- and spatial-link variables are given as U_0 and U_j , respectively. The above staggered fermion has a remnant chiral symmetry in the chiral

¹The expectation value of the Wilson loop in Eq. (2.23) is proportional to the exponential form of the area $L \times T$. This property is called the area law [1].

limit. The chiral transformation of the staggered fermion is defined as $\chi_x \rightarrow \chi'_x = e^{i\varepsilon_x v/2} \chi_x$ and $\bar{\chi}_x \rightarrow \bar{\chi}'_x = e^{i\varepsilon_x v/2} \bar{\chi}_x$, for an angle v and a factor $\varepsilon_x = (-1)^{x_0 + \dots + x_d}$ [173, 174].

From Eq. (2.24), the effective potential in MF in the leading order of the large dimensional expansion [231] is obtained as

$$F_{\text{eff}} = \frac{d}{4N_c} \sigma^2 - T \log \left[\frac{\sinh[(N_c + 1)E/T]}{\sinh[E/T]} + 2 \cosh(N_c \mu/T) \right], \quad (2.25)$$

where $E = \text{arcsinh}(m_{\text{eff}})$, $m_{\text{eff}} = m_0 + d\sigma/(2N_c)$, and $T = 1/N_\tau$ after we apply the bosonization technique. The detailed derivation of the effective potential in MF is given in Appendix A.1 under the isotropic condition, $\gamma = 1$ with an anisotropy factor γ . It should be noted that the pseudo-scalar (π) mode vanishes in MF.

According to Eq. (2.25), one finds that a quark can obtain the constituent quark mass when the chiral condensate $\sigma = -\langle \bar{\chi}\chi \rangle$ is finite; we can investigate the chiral phase transition in the framework of the strong coupling expansion with the quark action. In actual calculations, the equilibrium configuration is obtained by the effective potential analysis where the stationary condition is imposed $\partial F_{\text{eff}}/\partial \sigma = 0$.

2.2.3 QCD phase diagram at strong coupling

As we reviewed, the chiral phase transition and the confinement nature have been studied in the framework of the strong coupling lattice QCD (SC-LQCD). The history of the SC-LQCD are well summarized in Ref. [168] and the following brief historical review is based on Refs. [164, 168]. We also review properties of the QCD phase diagram in SC-LQCD here.

One can describe the confinement nature in the pure Yang-Mills theory [25] and higher-order corrections are also investigated in Refs. [174, 227, 228, 229]. In addition, we find early works of the chiral symmetry breaking [158, 159, 231] at finite temperature [161, 232, 233] and at finite chemical potential [160, 161]. Finite coupling effects are also considered in Refs. [233, 234, 235, 236, 237, 238, 239, 240]. The QCD phase diagram is obtained in the strong coupling limit [162, 163], with the next-to-leading order (NLO) [164, 167] and next-to-next-to-leading order (NNLO) effects [165]. Fluctuation effects are recently included in monomer-dimer-polymer (MDP) simulations [169, 170, 171] based on Ref. [241] and an auxiliary field Monte Carlo (AFMC) method [172]. We can also find the finite coupling effects with fluctuation effects in MDP by using the reweighting method in Ref. [242]. In order to describe both chiral and confinement-deconfinement phase transitions, the Polyakov

loop effects are also investigated with a quark action [166, 168, 243, 244, 245] based on Refs. [66, 245].

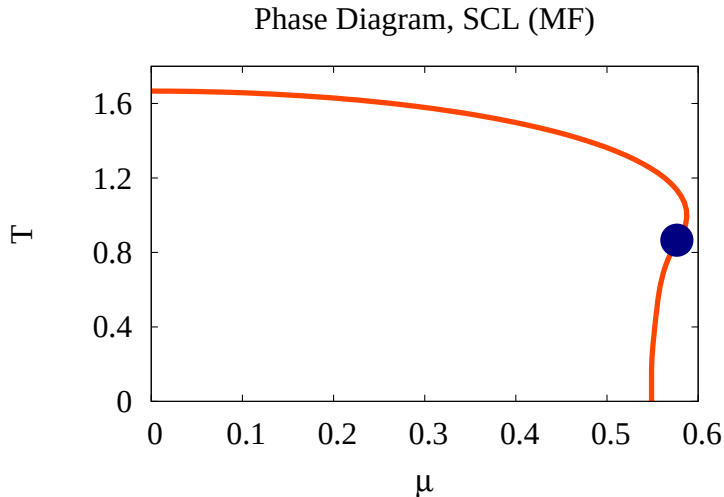


Figure 2.2: QCD phase diagram in the strong coupling and chiral limits in the mean field (MF) approximation [162, 163]. A dot is a tricritical point derived in Ref. [162]. This figure is obtained by numerical data calculated by A. Ohnishi based on Refs. [162, 163].

We review properties of the QCD phase diagram in SC-LQCD. In the strong coupling limit, the order of the chiral phase transition is the second (crossover) at low chemical potential and the first at high chemical potential in the chiral limit (at finite mass) in the mean field (MF) approximation as shown in Fig. 2.2 [162, 163]. We find that the critical temperature of the phase transition is suppressed by finite coupling effects [164, 165, 167]. In addition, the critical temperature is also reduced at small chemical potential by the Polyakov loop effects [168]. The suppressed critical temperature in the strong coupling limit is found in MDP [169, 171] and AFMC [172] methods compared with that in MF, when field fluctuation effects are taken into account. Both finite coupling and fluctuation effects reduce the critical temperature at low μ in MDP with the reweighting method [242] and in AFMC [246]. We expect that critical temperature at zero μ becomes closer to that in lattice QCD, when including the fluctuation, the finite coupling, and the Polyakov loop effects; the reliability of SC-LQCD approach would increase ².

²It should be noted that the QCD phase diagram in SC-LQCD without the Polyakov loop effects describes the confined phase [166, 168].

In Fig. 2.2, we find that $dT/d\mu > 0$ at high chemical potential. In the first order phase transition region, the Clausius-Clapeyron relation reads $dT/d\mu = -\Delta\rho/\Delta s$, where $\Delta\rho = \rho_W - \rho_{NG}$ and $\Delta s = s_W - s_{NG}$ [84]. The entropy density and the quark number density are denoted as $s_{W,NG}$ and $\rho_{W,NG}$ in the Wigner and Nambu-Goldstone phases, respectively. In the strong coupling limit, we find that $\Delta\rho > 0$ and $\Delta s < 0$, respectively [162] probably due to the lattice artifact. This is the opposite tendency compared with effective model calculations [35, 79, 84, 85]. When we include finite coupling effects, we find that $d\mu/dT$ tends to be close to zero [164, 165], supposing that $g \rightarrow 0$; then finite coupling effects are considered to be important.

As we reviewed, the first-principles method LQCD faces the sign problem at finite μ and cannot apply the high density region [37]; then SC-LQCD is an approach to study the QCD phase diagram based on lattice QCD action.

Chapter 3

QCD phase diagram in the strong coupling limit with fluctuations

Studying the QCD phase diagram is important to know features of QCD and has been an interesting subject. In the low temperature and chemical potential region, we observe hadrons in which quarks and gluons are confined. We can expect the quark-gluon plasma (QGP) at high temperature via crossover transition at finite mass [39, 40], in the heavy-ion collision experiments at Relativistic Heavy Ion collider (RHIC) [38] and Large Hadron collider (LHC) [247]. We may expect that there exists a first-order phase transition from hadron phase to quark matter at large μ and its phase transition line ends at CP according to some model calculations [30, 35].

The location of CP is a kind of cornerstone to understand the QCD phase structure, but the CP location has not been determined since the predicted CP location depends on models [30]. Then, the first-principles method, lattice QCD (LQCD), is required to pin down the CP location. However, one faces the notorious sign problem at large chemical potential in LQCD, so we have not yet obtained conclusive results [37].

The strong coupling lattice QCD (SC-LQCD) is one of the methods to study the QCD phase diagram and has some merits. SC-LQCD can be one of the methods to investigate the finite density region due to the milder sign problem [170] while the strong coupling limit is the opposite of the continuum limit. In SC-LQCD, we integrate link variables first. The integration for fermion fields is the next step; then the effective action is given in terms of the hadronic DOF. We could expect that the sign problem coming from the link variables can be milder. In fact, we have no sign problem in the mean field (MF) approximation [164, 165]. We could investigate the QCD

phase transition beyond the MF approximation at least in the strong coupling limit (SCL) by using the monomer-dimer-polymer (MDP) simulation [169, 170, 171] and the auxiliary field Monte Carlo (AFMC) method [172, 248, 249] with milder sign problem.

From a theoretical point of view, it is important to integrate field variables exactly. In SC-LQCD, the MDP simulation is one of the methods to include the field fluctuation effects beyond the MF approximation [169, 170, 171, 242]. The AFMC method is an alternative way to evaluate field fluctuation effects and is applied to various problems in physics [250, 251, 252]. The AFMC method has another merit for finite coupling effects, since we have the MF results [164, 165] and AFMC is a generalization of these mean-field approach.

In this chapter, we first develop the AFMC method in the strong coupling limit (SCL) in Sect. 3.1 and evaluate observables numerically in AFMC in Sects. 3.1 and 3.2. Next, we introduce a new method to obtain the appropriate chiral condensate on a finite-size lattice in the NG phase. We discuss the chiral transition and show the numerical data on the (T, μ) dependence of observables in Sect. 3.3. In Sect. 3.4, we give the QCD phase diagram in the chiral and strong coupling limits in AFMC. Finally, we discuss an origin of the sign problem in AFMC in Sect. 3.5.

Throughout this thesis, the spatial lattice spacing, the number of color, and the spacial dimension are taken to be $a = 1$, $N_c = 3$, and $d = 3$, respectively. The numbers shown in figures are in the lattice unit. This chapter is based on Ref. [172].

3.1 Strong coupling lattice QCD action

We first give the full lattice QCD action on an anisotropic lattice [173, 174]. We here use one species of unrooted staggered fermion [186, 187] since we could study the chiral phase transition due to the remnant chiral symmetry. The LQCD action is given as

$$\mathcal{Z}_{\text{LQCD}} = \int \mathcal{D}[\chi, \bar{\chi}, U_\nu] e^{-S_{\text{LQCD}}} , \quad S_{\text{LQCD}} = S_F + S_G , \quad (3.1)$$

$$\begin{aligned} S_F = & \frac{1}{2} \sum_x [V_x^+ - V_x^-] + \frac{1}{2} \sum_x \sum_{j=1}^d \eta_{j,x} [\bar{\chi}_x U_{j,x} \chi_{x+\hat{j}} \\ & - \bar{\chi}_{x+\hat{j}} U_{j,x}^\dagger \chi_x] + m_0 \sum_x M_x , \end{aligned} \quad (3.2)$$

$$S_G = \frac{2N_c \xi}{g_\tau^2(g_0, \xi)} \mathcal{P}_\tau + \frac{2N_c}{g_s^2(g_0, \xi) \xi} \mathcal{P}_s, \quad (3.3)$$

$$\mathcal{P}_i = \sum_{P_i} \left[1 - \frac{1}{2N_c} \text{Tr} \left(U_{P_i} + U_{P_i}^\dagger \right) \right] \quad (i = \tau, s), \quad (3.4)$$

where

$$V_x^+ = \gamma e^{\mu/f(\gamma)} \bar{\chi}_x U_{0,x} \chi_{x+\hat{0}}, \quad V_x^- = \gamma e^{-\mu/f(\gamma)} \bar{\chi}_{x+\hat{0}} U_{0,x}^\dagger \chi_x, \quad \text{and } M_x = \bar{\chi}_x \chi_x, \quad (3.5)$$

are mesonic composites. The staggered quark, quark chemical potential, and bare quark mass are denoted as χ, μ , and m_0 , respectively. The staggered sign factor is defined as $\eta_{0,x} = 1$ and $\eta_{j,x} = (-1)^{\sum_{i=0}^{j-1} x_i}$. We here adopt the convention, $x_0 = \tau$ as the temporal coordinate in the following chapters. g_τ and g_s are temporal and spatial coupling constants, which depend on the lattice spacing a . Anisotropy factors are denoted as γ and ξ . $\mathcal{P}_\tau$ and $\mathcal{P}_s$ represent temporal and spatial plaquette actions, respectively. Plaquette is given by U_{P_i} . The physical lattice spacing ratio of the spatial lattice spacing to the temporal lattice spacing is expressed as $f(\gamma) = a_s^{\text{phys}}/a_\tau^{\text{phys}}$, which appears with μ [173, 174].

In this thesis, we assume $f(\gamma) = \gamma^2$ in the strong coupling limit [170, 238, 239, 240]. The coupling constants become $g_\tau^2(g_0, 1) = g_s^2(g_0, 1) = g_0^2$ on an isotropic lattice: $\xi \rightarrow 1$ [173, 174]. We could expect that $f(\gamma) = \gamma = \xi$ when we construct the lattice spacing ratio as $a_s^{\text{phys}}/a_\tau^{\text{phys}} = \gamma$ in the continuum limit: $a \rightarrow 0$ and $g_0 \rightarrow 0$. In the strong coupling region, it may be more suitable to take $f(\gamma) = \gamma^2$ due to the quantum corrections [170, 238, 239, 240]. In the mean field approximation at $\mu = 0$, the phase transition temperature $T_c = 1/(N_\tau a_\tau^{\text{phys}}) = f(\gamma)/(N_\tau a_s^{\text{phys}})$ in $\text{SU}(N_c)$ leads to the critical anisotropic parameter as $\gamma_c^2 = N_\tau d(N_c + 1)(N_c + 2)/\{6(N_c + 3)\}$ in the strong coupling limit [170, 238, 239, 240]. Here we note that the phase transition temperature should not depend on the temporal lattice size N_τ . Once one sets $a_s^{\text{phys}} T_c = \gamma_c^2/N_\tau$, the transition temperature is independent of the temporal lattice size, which indicates $f(\gamma) = \gamma^2$. Furthermore, the critical chemical potential μ_c in the zero temperature limit ($N_\tau \rightarrow \infty$) does not depend on the anisotropic parameter γ for $\gamma \gg 1$ [170, 238] if we set $f(\gamma) = \gamma^2$. These results indicate that we can take the parametrization $f(\gamma) = \gamma^2$ in the strong coupling limit. (In Ref. [242], the authors have recently suggested an exponential type function.)

In the strong coupling limit (SCL), we can ignore plaquette terms. By integrating over spatial link variables, we obtain the effective action in the

leading order of the $1/d$ expansion as [231, 237, 253]

$$S_{\text{eff}} = \frac{1}{2} \sum_x [V_x^+ - V_x^-] - \frac{1}{4N_c} \sum_{x,j} M_x M_{x+\hat{j}} + m_0 \sum_x M_x . \quad (3.6)$$

It should be noted that we have no spatial baryonic hopping terms in Eq. (3.6) (see Appendix A.1).

3.2 Effective action with auxiliary field fluctuations for mesonic fields

In this section, we introduce an effective action with fluctuations in SCL based on Ref. [172].

We first apply the Fourier transformation to $M_x M_{x+\hat{j}}$ terms in Eq. (3.6);

$$\begin{aligned} -\frac{1}{4N_c} \sum_{x,j} M_x M_{x+\hat{j}} &= -\frac{L^3}{4N_c} \sum_{\mathbf{k},\tau} f(\mathbf{k}) M_{-\mathbf{k},\tau} M_{\mathbf{k},\tau} \\ &= -\frac{L^3}{4N_c} \sum_{\mathbf{k},\tau, f(\mathbf{k})>0} f(\mathbf{k}) (M_{\mathbf{k},\tau} M_{-\mathbf{k},\tau} - M_{\bar{\mathbf{k}},\tau} M_{-\bar{\mathbf{k}},\tau}) , \end{aligned} \quad (3.7)$$

where $M_{x=(\mathbf{x},\tau)} = \sum_{\mathbf{k}} M_{\mathbf{k},\tau} \exp[i\mathbf{k} \cdot \mathbf{x}]$, $f(\mathbf{k}) = \sum_{j=1}^d \cos k_j$, and we utilize a relation, $f(\bar{\mathbf{k}}) = -f(\mathbf{k})$ ($\bar{\mathbf{k}} = \mathbf{k} + (\pi, \pi, \pi)$) in the last line. According to Eq. (3.7), we have divided the four-Fermi terms into two parts with respect to the sign of the coefficient: the positive mode $f(\mathbf{k}) > 0$ and the negative mode $f(\mathbf{k}) < 0$. The zero mode $f(\mathbf{k}) = 0$ does not contribute to the action.

We here introduce the extended Hubbard-Stratonovich (eHS) transformation [164, 165, 167] as

$$\begin{aligned} e^{C_\alpha AB} &= \int d\varphi d\phi e^{-C_\alpha \{ [\varphi - (A+B)/2]^2 + [\phi - i(A-B)/2]^2 \} + C_\alpha AB} \\ &= \int d\varphi d\phi e^{-C_\alpha \{ \varphi^2 - (A+B)\varphi + \phi^2 - i(A-B)\phi \}} \\ &= \int d\psi d\psi^* e^{-C_\alpha \{ \psi^* \psi - A\psi - \psi^* B \}} , \end{aligned} \quad (3.8)$$

and

$$e^{-C_\alpha AB} = \int d\psi d\psi^* e^{-C_\alpha \{ \psi^* \psi - iA\psi - i\psi^* B \}} , \quad (3.9)$$

where $\psi = \varphi + i\phi$, $C_\alpha(> 0)$ is a coefficient. Field variables are expressed as A and B .

For the positive mode, we can bosonize the four-Fermi terms as

$$\begin{aligned}
& \exp \left\{ \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} C_\alpha f(\mathbf{k}) M_{-\mathbf{k}, \tau} M_{\mathbf{k}, \tau} \right\} \\
&= \int \mathcal{D}[\sigma] \exp \left\{ - \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} C_\alpha f(\mathbf{k}) \times [|\sigma_{\mathbf{k}, \tau}|^2 + \sigma_{\mathbf{k}, \tau}^* M_{\mathbf{k}, \tau} + M_{-\mathbf{k}, \tau} \sigma_{\mathbf{k}, \tau}] \right\} \\
&= \int \mathcal{D}[\sigma] \exp \left\{ - \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} C_\alpha f(\mathbf{k}) |\sigma_{\mathbf{k}, \tau}|^2 - \frac{1}{4N_c} \sum_{x, j} [\sigma_{x+\hat{j}} + \sigma_{x-\hat{j}}] M_x \right\},
\end{aligned} \tag{3.10}$$

where $C_\alpha = L^3/(4N_c)$, $\sigma_x = \sum_{\mathbf{k}, f(\mathbf{k}) > 0} e^{i\mathbf{k} \cdot \mathbf{x}} \sigma_{\mathbf{k}, \tau}$, and $\mathcal{D}[\sigma] = \prod_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} d\sigma_{\mathbf{k}, \tau} d\sigma_{\mathbf{k}, \tau}^*$. The field $\sigma_{\mathbf{k}, \tau}$ is the auxiliary fields of $M_{\mathbf{k}, \tau}$ and the lowest 4-momentum mode $\sigma_{\mathbf{k}=0, \omega=0}$ corresponds to the scalar mode, where $\sigma_{\mathbf{k}, \omega}$ is the sigma field after temporal Fourier transformation of $\sigma_{\mathbf{k}, \tau}$. The sigma modes in the spatial coordinate are real since they satisfy a relation $\sigma_{-\mathbf{k}, \tau} = \sigma_{\mathbf{k}, \tau}^*$.

We also obtain an equation for the negative modes,

$$\begin{aligned}
& \exp \left\{ - \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} C_\alpha f(\mathbf{k}) M_{-\bar{\mathbf{k}}, \tau} M_{\bar{\mathbf{k}}, \tau} \right\} \\
&= \int \mathcal{D}[\pi] \exp \left\{ - \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} C_\alpha f(\mathbf{k}) \times [|\pi_{\mathbf{k}, \tau}|^2 - i\pi_{\mathbf{k}, \tau}^* M_{\bar{\mathbf{k}}, \tau} - iM_{-\bar{\mathbf{k}}, \tau} \pi_{\mathbf{k}, \tau}] \right\} \\
&= \int \mathcal{D}[\pi] \exp \left\{ - \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} C_\alpha f(\mathbf{k}) |\pi_{\mathbf{k}, \tau}|^2 - \frac{1}{4N_c} \sum_{x, j} [(i\varepsilon\pi)_{x+\hat{j}} + (i\varepsilon\pi)_{x-\hat{j}}] M_x \right\},
\end{aligned} \tag{3.11}$$

where $\pi_x = \sum_{\mathbf{k}, f(\mathbf{k}) > 0} (-1)^\tau e^{i\mathbf{k} \cdot \mathbf{x}} \pi_{\mathbf{k}, \tau}$ and $\mathcal{D}[\pi] = \prod_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} d\pi_{\mathbf{k}, \tau} d\pi_{\mathbf{k}, \tau}^*$. A pre-factor $\varepsilon_x = (-1)^{x_0 + \dots + x_d}$ is related to γ_5 in the continuum limit. The pi fields, $\pi_{\mathbf{k}, \tau}$, are introduced as the auxiliary fields of $iM_{-\bar{\mathbf{k}}, \tau}$. The $\pi_{\mathbf{k}, \tau}$ fields contain the pseudoscalar mode and other higher 4-momentum modes. The pi modes are also real in the spatial coordinate : $\pi_{-\mathbf{k}, \tau} = \pi_{\mathbf{k}, \tau}^*$.

After combining Eqs. (3.10) and (3.11), the effective action is written as

$$S_{\text{eff}}^{\text{EHS}} = \frac{1}{2} \sum_x [V_x^+ - V_x^-] + \sum_x m_x M_x + \frac{L^3}{4N_c} \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} f(\mathbf{k}) [|\sigma_{\mathbf{k}, \tau}|^2 + |\pi_{\mathbf{k}, \tau}|^2] , \quad (3.12)$$

$$m_x = m_0 + \frac{1}{4N_c} \sum_j [(\sigma + i\varepsilon\pi)_{x+\hat{j}} + (\sigma + i\varepsilon\pi)_{x-\hat{j}}] . \quad (3.13)$$

We obtain the effective action of auxiliary fields by integrating out Grassmann variables and temporal-link variables as

$$\mathcal{Z}_{\text{AF}} = \int \mathcal{D}[\sigma_{\mathbf{k}, \tau}, \pi_{\mathbf{k}, \tau}] e^{-S_{\text{eff}}^{\text{AF}}} , \quad (3.14)$$

$$S_{\text{eff}}^{\text{AF}} = \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} \frac{L^3 f(\mathbf{k})}{4N_c} [|\sigma_{\mathbf{k}, \tau}|^2 + |\pi_{\mathbf{k}, \tau}|^2] - \sum_{\mathbf{x}} \log [X_{N_\tau}(\mathbf{x})^3 - 2X_{N_\tau}(\mathbf{x}) + 2 \cosh(3N_\tau \mu / \gamma^2)] , \quad (3.15)$$

where $\mathcal{D}[\sigma_{\mathbf{k}, \tau}, \pi_{\mathbf{k}, \tau}] = \prod_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} d\sigma_{\mathbf{k}, \tau} d\sigma_{\mathbf{k}, \tau}^* d\pi_{\mathbf{k}, \tau} d\pi_{\mathbf{k}, \tau}^*$ and $X_{N_\tau}(\mathbf{x})$ is a given function of $\sigma_{\mathbf{k}, \tau}$ and $\pi_{\mathbf{k}, \tau}$ [233, 238, 240] (See also Appendix B.1).

It should be noted that the auxiliary fields are introduced, maintaining $O(2)$ symmetry, as will be shown in Eq. (3.18). Another comment on the effective action is that there is the sign problem as discussed later in Sect. 3.5.

3.3 Order parameters and susceptibilities

From now on, we include mesonic fluctuation effects by using MC simulation to integrate over auxiliary fields $(\sigma_{\mathbf{k}, \tau}, \pi_{\mathbf{k}, \tau})$. This is called the auxiliary field Monte Carlo (AFMC) method [250, 251, 252].

In this section, we introduce a method to obtain an appropriate chiral condensate on a fixed size lattice (chiral angle fixing method) and show results of observables.

3.3.1 Chiral angle fixing method

On a finite lattice, the expectation value of the chiral condensate is zero in the chiral limit, because of the chiral symmetry. In order to evaluate the chiral condensate in the chiral limit, we put the mass which is an explicitly

symmetry breaking term. Next, we take the thermodynamic limit, and finally impose the chiral limit; for example,

$$\langle \sigma_0 \rangle = \lim_{m_0 \rightarrow 0} \lim_{V \rightarrow 0} \langle \sigma_0 \rangle_{(m_0, V)} . \quad (3.16)$$

In order to follow the above steps, lots of statistics are required with regard to various volume and mass parameters. In addition, we need many more configurations to obtain appropriate observables, when the sign problem exists (See Sect. 2.1.3). Alternatively, we introduce the chiral angle fixing (CAF) method at low simulation cost and obtain an appropriate chiral condensate on a fixed size lattice [172].

The lattice QCD action with one species of unrooted staggered fermion has the remnant chiral symmetry in the chiral limit under the chiral transformation:

$$\chi_x \rightarrow \chi'_x = e^{i\varepsilon_x v/2} \chi_x , \quad \bar{\chi}_x \rightarrow \bar{\chi}'_x = e^{i\varepsilon_x v/2} \bar{\chi}_x , \quad (3.17)$$

for an angle v [173, 174]. The effective action $S_{\text{eff}}^{\text{AF}}$ in Eq. (3.15) retains the chiral symmetry, and is invariant under the transformation,

$$\begin{pmatrix} \sigma_k \\ \pi_k \end{pmatrix} \rightarrow \begin{pmatrix} \sigma'_k \\ \pi'_k \end{pmatrix} = \begin{pmatrix} \cos v & -\sin v \\ \sin v & \cos v \end{pmatrix} \begin{pmatrix} \sigma_k \\ \pi_k \end{pmatrix} , \quad (3.18)$$

where

$$\sigma_{k=(\mathbf{k}, \omega)} = \frac{1}{N_\tau} \sum_{\tau} e^{-i\omega\tau} \sigma_{\mathbf{k}, \tau} , \quad (3.19)$$

$$\pi_{k=(\mathbf{k}, \omega)} = \frac{1}{N_\tau} \sum_{\tau} (-1)^\tau e^{-i\omega\tau} \pi_{\mathbf{k}, \tau} = \frac{1}{N_\tau L^3} \sum_x e^{-ik \cdot x} \pi_x . \quad (3.20)$$

Because of the chiral symmetry, the expectation value of the chiral condensate $\langle \sigma_0 \rangle$ vanishes on a finite lattice as shown in Fig. 3.1 (1). On a finite size lattice, the chiral condensate in the chiral limit is rewritten as

$$\begin{aligned} \langle \sigma_0 \rangle &= \frac{1}{\mathcal{Z}_{\text{AF}}} \int \mathcal{D}[\sigma_0, \pi_0] \prod_{(\mathbf{k}, \omega) \neq (0, 0)} \int \mathcal{D}[\sigma_{\mathbf{k}, \omega}, \pi_{\mathbf{k}, \omega}] \\ &\quad \times \sigma_0 \exp \left[-S(\sigma_{\mathbf{k}, \omega}, \pi_{\mathbf{k}, \omega}, \phi = \sqrt{\sigma_0^2 + \pi_0^2}, v) \right] \\ &= \frac{1}{\mathcal{Z}_{\text{AF}}} \int \mathcal{D}[\phi, v] \phi \cos v \prod_{(\mathbf{k}, \omega) \neq (0, 0)} \int \mathcal{D}[\sigma'_{\mathbf{k}, \omega}, \pi'_{\mathbf{k}, \omega}] \\ &\quad \times \exp \left[-S(\sigma'_{\mathbf{k}, \omega}, \pi'_{\mathbf{k}, \omega}, \phi, 0) \right] \\ &= 0 , \end{aligned} \quad (3.21)$$

where the chiral angle for the lowest four-momentum modes, $\sigma_{k=0}$ and $\pi_{k=0}$, is defined as $v = \arctan(\pi_0/\sigma_0)$. It should be noted that σ_0 and π_0 are the scalar mode and pseudo-scalar mode, respectively. We utilize the following relation to obtain the second line in Eq. (3.21): $S(\sigma_{\mathbf{k},\omega}, \pi_{\mathbf{k},\omega}, \phi, v) = S(\sigma'_{\mathbf{k},\omega}, \pi'_{\mathbf{k},\omega}, \phi, 0)$ for configurations $(\sigma'_{\mathbf{k},\omega}, \pi'_{\mathbf{k},\omega})$ rotated by an angle $(-v)$. This situation is similar to the magnetization [254]. In the magnetization under $Z(2)$ symmetry, the effective potential has two local minima in which one of the magnetization shows M_0 and the other of the magnetization is $-M_0$ at zero magnetic field; then the expectation value becomes zero.

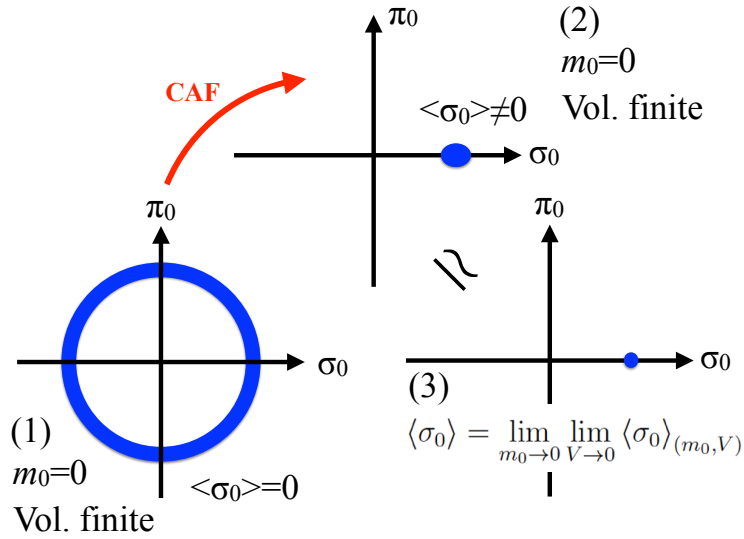


Figure 3.1: Schematic picture of chiral angle fixing (CAF) method in the symmetry breaking phase [172]. Before applying CAF, $\langle \sigma_0 \rangle$ is zero due to the chiral symmetry (1). In CAF, all configurations are rotated and then $\langle \sigma_0 \rangle \neq 0$ (2). The results in CAF are expected to mimic results (3) given by Eq. (3.16). This figure is basically taken from Ref. [172].

In the calculation of the magnetization, we often use the absolute value to obtain the expectation value of the magnetization as $\langle M_0 \rangle \rightarrow \langle |M_0| \rangle$ ($\neq 0$ in the symmetry broken phase) [254]. CAF is a generalization of taking the absolute value of magnetization $\langle |M_0| \rangle$ [172]. In CAF, all configurations are rotated by an angle $(-v)$ and the pseudo-scalar condensate is set to zero. This procedure corresponds to taking $|M_0|$ in the magnetization. When we calculate the expectation value in CAF, we utilize the chiral rotated configurations corresponding to $\langle |M_0| \rangle$ in the magnetization. After CAF, the chiral

condensate becomes finite as

$$\begin{aligned} \langle \sigma_0 \rangle &= \frac{1}{\mathcal{Z}_{\text{AF}}} \int \mathcal{D}[\sigma_0] \sigma_0 \prod_{(\mathbf{k}, \omega) \neq (0,0)} \int \mathcal{D}[\sigma'_{\mathbf{k}, \omega}, \pi'_{\mathbf{k}, \omega}] \exp[-S(\sigma'_{\mathbf{k}, \omega}, \pi'_{\mathbf{k}, \omega}, \phi = \sigma_0, 0)] \\ &\neq 0, \end{aligned} \quad (3.22)$$

in the NG phase as shown in Fig. 3.1 (2). When we obtain observables, we use the rotated configurations.

Because of the non-vanishing chiral condensate, we could expect that the chiral susceptibility has a peak around the phase transition. The chiral susceptibility expressed as $\chi_\sigma = \langle \sigma_0^2 \rangle - \langle \sigma_0 \rangle^2$ could be $\chi_\sigma = \langle \sigma_0^2 \rangle$ before CAF on a finite size lattice even in the NG phase. Therefore, the chiral susceptibility increases with decreasing temperature T before applying CAF. In CAF, the chiral susceptibility can have a peak due to the non-vanishing contribution of $\langle \sigma_0 \rangle$ in the NG phase with the chiral rotated configurations. It should be noted that the pseudo-scalar mode π_0 is absorbed into the scalar mode σ_0 , then the lowest mode is expected to be the $\pi_{\mathbf{k}, \omega}$ with the smallest non-zero momentum, $|\mathbf{k}| = 2\pi/L$ after CAF.

3.3.2 Observables in AFMC in the strong and chiral limits

Simulation details

We generate configuration sets of $(\sigma_{\mathbf{k}, \tau}, \pi_{\mathbf{k}, \tau})$ in AFMC [250, 251, 252] at finite T and μ . In one Metropolis step, a new configuration candidate is chosen for all spatial momenta $\mathbf{k}$ at each τ under the real field conditions: $\sigma_{-\mathbf{k}, \tau} = \sigma_{\mathbf{k}, \tau}^*$ and $\pi_{-\mathbf{k}, \tau} = \pi_{\mathbf{k}, \tau}^*$. As will be discussed in Sect. 3.5, we have the sign problem in AFMC, so we apply the reweighting method [203, 204, 205],

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} \exp(i\theta) \rangle_{\text{pq}}}{\langle \exp(i\theta) \rangle_{\text{pq}}}, \quad (3.23)$$

where $\theta = -\text{Im}(S_{\text{eff}}^{\text{AF}})$ and $\langle \cdots \rangle_{\text{pq}}$ is the phase quenched average. Error bars are estimated by the jackknife method [1, 173, 174].

We generate auxiliary field configurations by using $S_{\text{eff}}^{\text{AF}}$ in Eq. (3.15) in the Metropolis method. We start the Metropolis sampling from two initial conditions. Around the first order phase transition, configurations are located in a local minimum and sometimes do not jump to another local minimum since the potential barrier can be large compared with a MC step and our simulation has limitation of sampling time. Thus, we utilize the

MC simulation with two initial conditions: the Wigner phase initial condition $(\sigma_{\mathbf{0},\tau}, \pi_{\mathbf{0},\tau}) \sim \mathcal{O}(0.01, 0)$ and the Nambu-Goldstone (NG) phase initial condition $(\sigma_{\mathbf{0},\tau}, \pi_{\mathbf{0},\tau}) \sim \mathcal{O}(1, 0)$ in the lattice unit.

Order parameters

The chiral condensate and the quark number density are given as

$$\langle \sigma_0 \rangle = \frac{1}{L^3 N_\tau} \frac{\partial \log \mathcal{Z}_{\text{AF}}}{\partial m_0} = -\langle \bar{\chi} \chi \rangle = \phi, \quad (3.24)$$

$$\rho_q = \frac{T}{L^3} \frac{\partial \log \mathcal{Z}_{\text{AF}}}{\partial \mu}, \quad (3.25)$$

after CAF. In actual calculations, we simulate $\langle \sigma_0 \rangle = \langle \sum_\tau \sigma_{\mathbf{k}=\mathbf{0},\tau} / N_\tau \rangle$. In

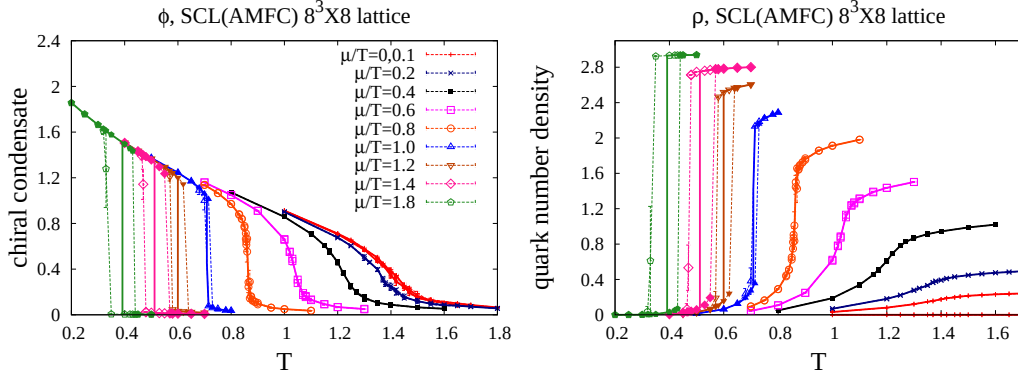


Figure 3.2: Chiral condensate (Quark number density) as a function of T on a $8^3 \times 8$ lattice in the left (right) panel [172]. Dotted lines show results with two initial conditions and lines show expected values in the realized phase, respectively. These figures are basically taken from Ref. [172].

Fig. 3.2, we show the chiral condensate and the quark number density as functions of temperature T at several μ/T . As we can see, both chiral condensate and quark number density show the phase transition behavior. The chiral condensate decreases and the quark number density increases with increasing temperature. The behaviors of order parameters are moderate at low μ/T and are prominent at high μ/T . At high μ/T , both order parameters show sudden jumps and the initial condition dependence appears as hysteresis. Thin dotted lines in Fig. 3.2 show results of the Wigner start and the NG start initial conditions. This is because MC configurations are localized around a local minimum until MC configurations overcome a potential barrier between two local minima, as expected for the first order phase transition. Then, we could expect the first-order phase transition at high μ/T . In

this thesis, we call this phase transition *would-be first order* transition as in Ref. [172]. At small μ/T , there seems to be no hysteresis behavior which indicates crossover or second-order phase transition. According to the Pisarski and Wilczek's work [11], the phase transition would be of the second order for the $O(2)$ symmetry, then this phase transition is referred to as *would-be second order* transition [172].

Finite size scaling analysis of chiral susceptibility

In order to deduce the phase transition order, we perform the finite size scaling analysis [39] for the chiral susceptibility $\chi_\sigma = \partial^2 \log \mathcal{Z}_{\text{AF}} / \partial m_0^2 / (L^3 N_\tau)$ at *would-be second order*, for $\mu/T = 0.0$ and 0.2 . The chiral susceptibility

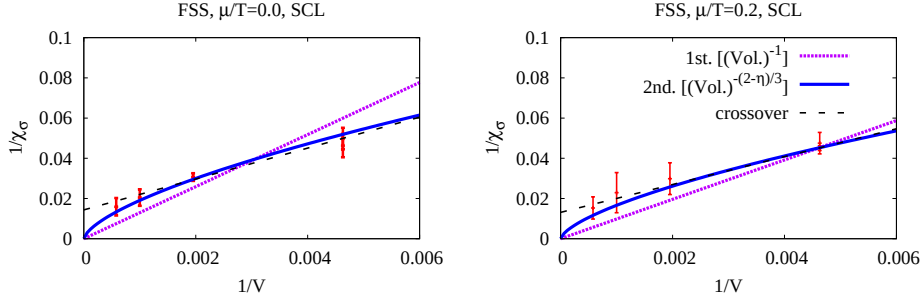


Figure 3.3: Finite size scaling analysis of the chiral susceptibility as a function of T at $\mu/T = 0.0$ (0.2) in the left (right) panel [172]. Solid, dotted, and thin dashed lines show the fitting lines by using the second, first, and crossover volume dependence, respectively. These figures are basically taken from Ref. [172].

does not diverge for crossover while we find $\chi_\sigma \propto V$ and $\chi_\sigma \propto V^{(2-\eta)/3}$ at the first-order and second-order phase transitions, respectively [39, 148, 255], where $V = L^3$ is the space volume and $\eta \simeq 0.0380(4)$ is a critical exponent of $O(2)$ [256]¹. In Fig. 3.3, we show $1/\chi_\sigma$ as a function of $1/V$ at $\mu/T = 0.0$ and 0.2 . We can rule out the first order phase transition, but we cannot

¹According to Refs. [148, 255], we can obtain an equation as

$$\frac{f_s}{T^4} = L^{-\beta(1+\delta)/\nu} f_L(\omega = tL^{1/\nu}, \omega_h = hL^{\beta\delta/\nu}), \quad (3.26)$$

where f_L is the scaling function and other notations are found in Appendix C. Then we can find the volume scaling as

$$\frac{\partial^2 (f_s/T^4)}{\partial h^2} = L^{2-\eta} \frac{\partial^2 f_L}{\partial \omega_h^2} \propto V^{(2-\eta)/d}, \quad (3.27)$$

conclude whether the phase transition order at small μ/T is of the second or crossover with the current statistics; χ^2/DOF ($\mu/T = 0$) $\simeq 0.477$ and 0.480 for the second and crossover, respectively, and χ^2/DOF ($\mu/T = 0.2$) $\simeq 0.331$ and 0.187 for the second and crossover, respectively.

3.4 QCD phase diagram in the strong coupling limit with mesonic fluctuations

In this section, we give results of the phase boundary and the QCD phase diagram in SCL.

3.4.1 Chiral susceptibility and effective potential analysis

In order to determine the phase boundary, we utilize the peak position of the chiral susceptibility: $\chi_\sigma = \partial^2 \log \mathcal{Z}_{\text{AF}} / \partial m_0^2 / (L^3 N_\tau)$ at *would-be second order* phase transition. In the left panel of Fig. 3.4, we show the chiral susceptibility

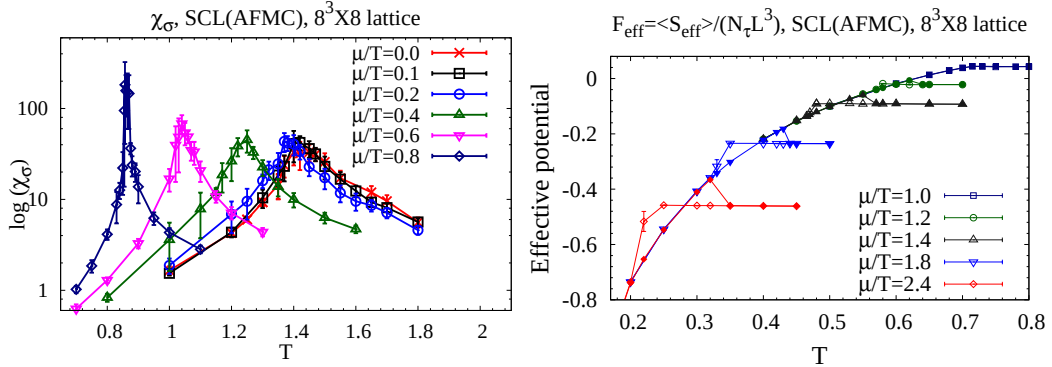


Figure 3.4: Logarithm of the chiral susceptibility (effective potential) as a function of T on a $8^3 \times 8$ lattice in the left (right) panel [172]. Dotted lines in the right panel show results with two initial conditions: the Wigner start and NG start initial conditions. These figures are basically taken from Ref. [172].

as a function of T . As we can see, the chiral susceptibility grows around the phase transition. In order to define the transition temperature, we fit the chiral susceptibility by a quadratic function and error bars contain not only

for the second-order phase transition, using the scaling and the hyper-scaling relations [257].

statistical error bars but also systematic errors by varying the fitting range [172].

We determine the first order phase boundary by using the effective potential. At the *would-be first order* phase transition, it is not easy to deduce the phase boundary due to the hysteresis behavior; the order parameters depend on the initial conditions (Wigner phase and NG phase initial conditions), so there are ambiguities in the critical temperature. We here adopt the effective potential F_{eff} analysis, by assuming that effective potential is given as $F_{\text{eff}} = \langle S_{\text{eff}} \rangle / (N_\tau L^3)$. In the right panel of Fig. 3.4, we show the results of the effective potential as a function of temperature at $\mu/T \geq 1.0$. Around the phase transition, we find the initial condition dependence of the effective potential as in the order parameters; then we determine the phase boundary at the *would-be first order* phase transition as a point where the two values of F_{eff} with two initial conditions match.

3.4.2 QCD phase diagram in the strong coupling and chiral limits with fluctuations

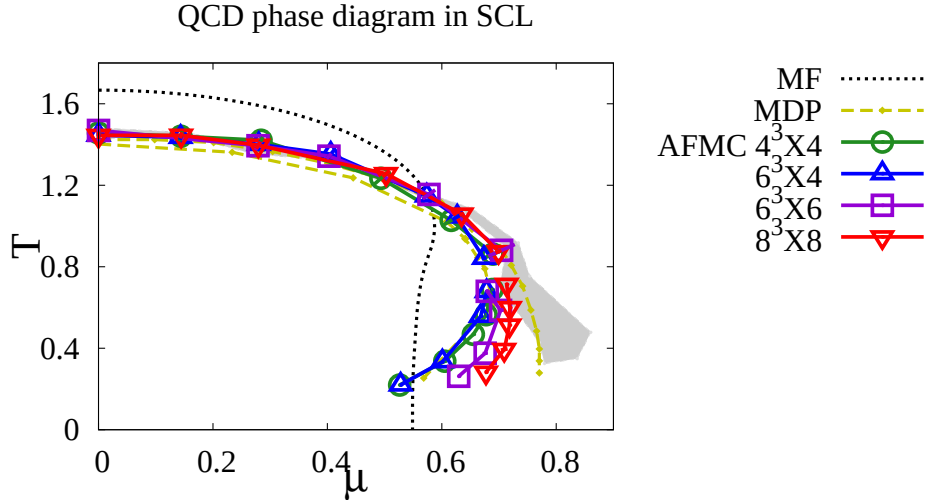


Figure 3.5: QCD phase diagram in SCL [172]. The dotted, dash-dotted, and solid lines with symbols are MF [162], MDP [169, 170, 171], and AFMC results on various size lattices [172], respectively. A line in MDP at smaller (larger) μ denotes results on a $N_\tau = 4$ lattice (with $N_\tau \rightarrow \infty$) [169, 170, 171]. The shaded area indicates $N_\tau \rightarrow \infty$ extrapolation in AFMC. This figure is basically taken from Ref. [172].

In Fig. 3.5, we show the QCD phase diagram. The phase boundary is determined by the chiral susceptibility analysis in the *would-be second order* phase transition region and the effective potential analysis in the *would-be first order* phase transition region.

In the low chemical potential region, the critical temperature is suppressed compared with the mean field results due to the fluctuation effects. There seems to be almost no lattice size dependence in AFMC around the would-be second order phase transition. In the would-be first order phase transition region, the phase boundary in AFMC is broaden to higher chemical potential direction than that in MF. One sees that the phase boundary depends on the temporal lattice size in the would-be first order phase transition region. One also finds that the phase boundary in AFMC agrees well with that in MDP [169, 170, 171].

The phase boundary shows $d\mu/dT > 0$ in the high chemical potential region except for infinitely large temporal lattice size in MDP [169, 171]. The Clausius Clapeyron relation on the first-order phase-transition line tells as $d\mu/dT = -(s_S - s_B)/(\rho_S - \rho_B)$, where $s_{S,B}$ and $\rho_{S,B}$ indicate the entropy density and number density in the symmetric (S) and broken (B) phases, respectively [84]. The entropy density in the broken (NG) phase should be larger than in the symmetric (Wigner) phase $s_S - s_B < 0$, since $\rho_S - \rho_B > 0$ as shown in Fig. 3.2. This is the similar situation in the mean-field approximation [162, 163]. Then finite coupling effects might be important [164, 165, 167] to reduce the lattice artifact toward $d\mu/dT \geq 0$.

Here are some comments on effective model calculations. Fluctuation effects are also studied in the framework of the functional renormalization group (FRG) method [91, 258] in chiral effective models. The phase boundary and the CP (or TCP) location can be shifted due to the fluctuation effects [90, 92, 259] as studied in SC-LQCD. Next, the contribution of the baryon number density plays key role at finite density [86, 87, 88], and the baryon number susceptibility is an important observable around CP or TCP [79]; thus properties of the baryon number are investigated in FRG [260]. It is also desirable explicitly to consider the fluctuation effects on baryon number in SC-LQCD. DOF of the quark (baryon) number density are given by auxiliary fields of the temporal next-to-leading order (NLO) terms in the strong coupling expansion and the critical temperature is found to be reduced with NLO auxiliary fields in MF [164]. We can expect that the fluctuations of the baryon number density can be explicitly investigated by improving AFMC method to NLO corrections of the strong coupling expansion [246, 261]. In fact, we find that the reduced critical temperature with NLO terms [246] as studied in MF [164]. Finally, the size dependence of the phase boundary can be an interesting topic to obtain deep insights into the QCD phase diagram

by comparing with other studies as in Refs. [152, 153], for example.

3.5 Sign problem in AFMC

In AFMC, there is a sign problem due to complex phases with π fields. We first show results on the average phase factor, $\langle \exp[i\theta] \rangle_{\text{pq}}$, as a function of T on several μ/T lines. The average phase factor indicates the severity of the statistical weight cancellation. When $\langle \exp[i\theta] \rangle_{\text{pq}} \sim 0$, the average phase factor shows the severe statistical weight cancellation. Especially, we cannot simulate observables by using the reweighting method for $\langle \exp[i\theta] \rangle_{\text{pq}} = 0$.

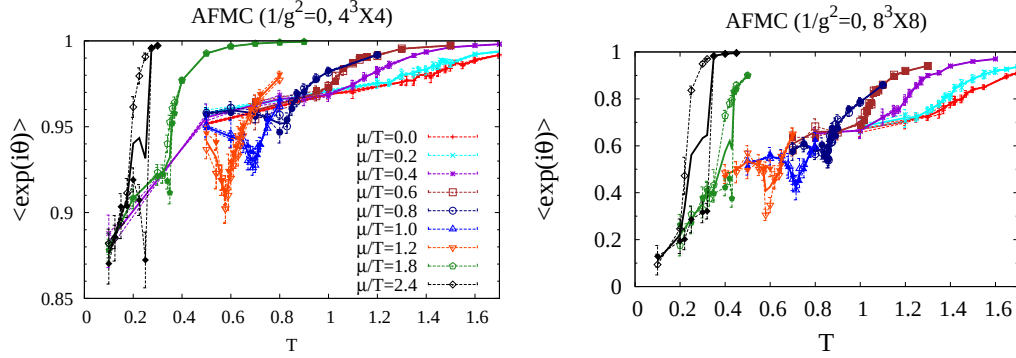


Figure 3.6: Average phase factor as a function of T on a $4^3 \times 4$ ($8^3 \times 8$) lattice in the left (right) panel [172]. Dotted lines show results with two initial conditions: the Wigner start and the NG start. These figures are basically taken from Ref. [172].

As indicated in Fig. 3.6, the average phase factor at small μ/T for a given T is smaller than that at large μ/T . This trend is opposite compared with the standard lattice QCD. The complex phase comes from $X_\tau(\mathbf{x})$ in Eq. (3.15) in the strong coupling limit, and does not come from the chemical potential term, $2 \cosh(3\mu/T)$. The effect of the complex phase becomes subordinate when the chemical potential term, $2 \cosh(3\mu/T)$, is dominant. Then, the average phase factor at high μ/T for a given T is larger than that at low μ/T .

The average phase factor is small when the temperature is low and shows sudden decrease around the phase transition temperature, $\langle \exp[i\theta] \rangle_{\text{pq}} \gtrsim 0.85$ on the $4^3 \times 4$ lattice and $\langle \exp[i\theta] \rangle_{\text{pq}} \gtrsim 0.1$ on the $8^3 \times 8$ lattice. The statistical weight cancellation is not severe on the $4^3 \times 4$ lattice but is severer on the

$8^3 \times 8$ lattice. Therefore, we need more configurations on the $8^3 \times 8$ lattice than those on the $4^3 \times 4$ lattice.

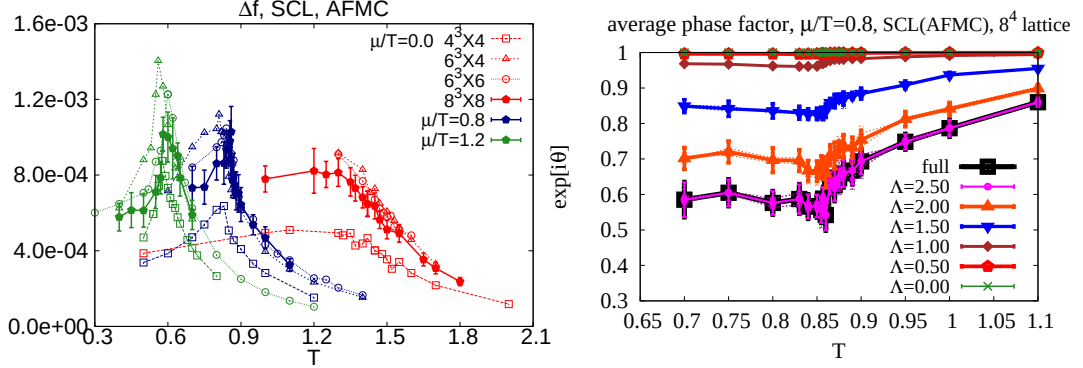


Figure 3.7: The free energy density as a function of T on $4^3 \times 4$ (square), $6^3 \times 4$ (triangle), $6^3 \times 6$ (circle), and $8^3 \times 8$ (pentagon) lattices in the left panel [172]. The cut-off parameter dependence of the average phase factor as a function of T on a $8^3 \times 8$ lattice in the right panel with the cut-off parameters: $\Lambda = 3$ (square), 2.5 (big circle), 2 (triangle), 1.5 (upside-down triangle), 1 (diamond), 0.5 (pentagon), and 0 (small circle), respectively [172]. These figures are basically taken from Ref. [172].

In order to quantify the severity of the sign problem, we show the free energy density difference between the original theory and the phase quenched theory, $\Delta f = f_{\text{orig}} - f_{\text{pq}}$ as a function of T in the left panel of Fig. 3.7. One finds that Δf shows almost the same values on large lattices so we can expect that Δf does not change drastically even on larger lattices. Compared with MDP results at similar T and μ [170], the value of Δf in AFMC is about twice larger than that in MDP, which means that the sign problem in AFMC is severer than that in MDP. This fact indicates that we may need further developments to evade the sign problem in AFMC when, for example, we include finite coupling effects.

We anticipate that the high-momentum modes of auxiliary fields contribute to the sign problem in AFMC. In the mean field analyses [162, 163, 164, 165, 167], there is no sign problem. In our calculation, we have the sign problem from the bosonization procedure. We need to decompose the composite products of the different mesonic fields in the eHS transformation to integrate out Grassmann variables [164, 165, 167]. An imaginary number is introduced in the eHS transformation and appears with the π fields with

the sign factor, $\epsilon_x = (-1)^{x_1 + \dots + x_d}$. Provided that π fields are constant, a π field on one site (i.e. π_c) has an opposite contribution to the nearest neighbor π fields (i.e. $-\pi_c$). We could expect that a complex phase on one site is tend to be eliminated from the nearest neighbor contributions.

In order to examine the above consideration, we apply the momentum cut-off method. We first introduce the cut-off parameter Λ and remove contributions of modes that satisfies $\sum_j \sin^2 k_j > \Lambda$. When we set the value of the cut-off parameter $\Lambda = 3(= d)$, all configurations are included. For $\Lambda = 0$, only the lowest modes of auxiliary fields are considered. In the right panel of Fig. 3.7, we show the momentum cut-off dependence of the average phase factor as a function of T . The average phase factor becomes larger and finally takes unity, which indicates the effects of statistical weight cancellation become weaker. In conclusion, the high auxiliary momentum modes do contribute to the sign problem in AFMC.

3.6 Short summary

We have derived the auxiliary field action in the leading order of the strong coupling and large dimensional expansions. When we evaluate partition function, we apply the auxiliary field Monte Carlo (AFMC) method. In AFMC, we can include mesonic field fluctuation effects by using the Monte Carol (MC) technique.

We introduce the chiral angle fixing (CAF) method in this chapter. Because of the chiral symmetry, the expectation value of the chiral condensate is zero in finite volume. In CAF, all configurations are rotated by the minus chiral angle ($-v$) and we obtain an appropriate order parameter by using the chiral rotated new configurations even in the NG phase.

We show the order parameters as functions of temperature: the chiral condensate and quark number density. At low density, the order parameters evolve moderately around the phase transition, where we call the phase transition order the *would-be second*. The behaviors of the order parameters at high density depend on the initial conditions and show hysteresis, which implies that the phase transition is of the first order. We call it the *would-be first*.

In order to deduce the phase boundary, we use two observables; the chiral susceptibility and the effective potential. The critical temperature is determined by the peak position of the chiral susceptibility at *would-be second order* phase transition. We apply the effective potential analysis at *would-be first order* phase transition. We determine the phase boundary as an intersection point of the effective potentials with two initial conditions in the

would-be first order phase transition region.

Obtained QCD phase diagram in AFMC is consistent with that in monomer-dimer-polymer (MDP) simulation [169, 170, 171]. At small μ , the critical temperature is lower than that in the mean field analysis and the phase boundary has weak lattice size dependence. The hadron phase is extended to high chemical potential direction at large μ . The phase boundary has strong temporal lattice size dependence.

In AFMC, we have the sign problem from the fermion determinant, but the appearance of the sign problem is not in the same way as that in the standard lattice QCD simulations at a given T ; the average phase factor is larger with larger μ/T . By using the momentum cut-off method, we investigate the mechanism of the sign problem in AFMC. We find that high momentum modes lead to the statistical weight cancellation.

With higher-order corrections in the strong coupling expansion, we expect that the sign problem may become severer. The bosonized action contains large number of auxiliary fields coupled with an imaginary number in the eHS transformation. We may need to develop some methods to reduce the sign problem. In fact, we find the severe sign problem when we naively introduce auxiliary fields for the next-to-leading order (NLO) contributions in the strong coupling approach [261]. In the would-be second-order phase-transition region, we can investigate the QCD phase diagram with auxiliary fields for the NLO effects by shifting the integration path [246].

Chapter 4

Cumulant ratios in the strong coupling limit at finite density with/without mesonic field fluctuations

The location of the QCD critical point (CP) [35] provides important information to deduce the QCD phase structure. For massless two flavors, the second-order phase transition [11] may be connected with the first-order phase transition at the tricritical point (TCP) [35]. At finite mass, the second-order phase transition in the chiral limit turns into crossover [39, 40] and its pseudo-critical phase boundary is expected to be connected with the first-order phase boundary at $Z(2)$ CP [35]. One can infer the QCD phase structure once we identify the CP location. The CP location, however, has not been determined because of large model dependences [30] and the sign problem in lattice QCD [37].

In order to pin down the position of CP, the Beam Energy Scan (BES) program has been performed at relativistic heavy-ion collider (RHIC) where higher-order cumulants are investigated as promising observables [38]: the higher-order cumulants of the net-proton number as a proxy for the net-baryon number [44, 45, 114], for example. They are expected to remain sensitive to the critical phenomena when the system passes around CP while the expected divergent behavior of the higher-order cumulants can be milder due to the finite volume realized at RHIC experiments [98]. The sign flips of the higher-order cumulants around the phase transition are also useful tools to deduce the CP location or critical phenomena [97, 99, 100].

Once the singular behavior around the phase transition is masked by finite volume and/or finite mass effects [100, 133], the contribution of the singu-

lar part governed by criticality is masked by the regular part contribution, and then we need explicit calculations to see how much critical behavior is realized in more realistic cases. In addition, the higher-order cumulants are fluctuation observables and the critical phenomena are characterized by the critical exponents, so it is desirable to include the field fluctuation effects in the calculations beyond the mean field analysis.

The first-principles method, lattice QCD (LQCD), is a suitable method to investigate higher-order cumulants with field fluctuations mainly at zero μ (See, for example [262, 263, 264, 265]). There are some attempts to study them at finite density in LQCD, but cumulants in LQCD currently have large errors due to the sign problem [142, 143, 144, 145]; then we need other ways to investigate cumulants at finite density, including field fluctuation effects.

In the strong coupling lattice QCD (SC-LQCD), we can investigate field fluctuation effects based on the lattice QCD action at finite density even in the large μ/T region around CP or TCP [170, 171, 172]. To the best of our knowledge, the study in this chapter would be a first systematic attempt to investigate the higher-order cumulants of the net-baryon number at sufficiently small mass on various size lattices based on a lattice QCD action, including the large chemical potential region: i.e. around TCP.

We can also find the finite volume effect in SC-LQCD. The finite size effect is expected to be given as the order of $1/(LT)$ with a finite system length, L . In BES, the system size is evaluated as $LT \simeq 2.4 - 3.6$ through kinematic cuts of the phase space [147], and we anticipate that higher-order cumulants' behavior would be affected by the finite size effect as reviewed in Sect. 1.2.4 [133, 147, 154, 156]. We here focus on the finite volume effect by performing AFMC simulations in the chiral limit. In the chiral limit, we can ignore the finite mass effect and the divergent behavior of cumulants is smeared only by the finite size effect. In fact, we find the oscillatory behavior of third- and fourth-order cumulants around the phase transition and their negative region at $LT \simeq 3 - 9$. These results indicate that the negative region or the oscillatory behavior of higher-order cumulants could be found in BES program at RHIC [133] while the boundary condition might be different from each other.

Once we investigate higher-order cumulants, our study might be of great help for constructing the scaling function of the net-baryon number cumulants with regard to the finite size in the strong coupling limit. In addition, we can see explicitly the region where the underlying universality emerges in the QCD phase diagram by using our calculations.

In this chapter, we show results on cumulant ratios in the strong coupling limit (SCL) based on Ref. [78]. We first show the mean field (MF) results at finite mass in Sect. 4.1 and the AFMC results in the chiral limit in Sect. 4.2.

We here concentrate on the region $\mu/T < (\mu/T)_{\text{TCP}}$, where the second-order phase transition is expected.

4.1 Net-baryon number cumulants in the mean field approximation

First, we show results of cumulant ratios in the mean field (MF) approximation in the strong coupling limit. Formulae to calculate cumulant ratios of the net-baryon number are given in Appendix A. It should be noted that we can set $\pi = 0$ in the MF approximation.

In this subsection, we show the following cumulant ratios in MF as

$$R_{3,2}^B = c_B^{(3)}/c_B^{(2)}, \quad R_{4,2}^B = c_B^{(4)}/c_B^{(2)}, \quad (4.1)$$

where $c_B^{(n)} = \partial^n(-F/T^4)/\partial\hat{\mu}^n$ and F is the effective free energy density in MF as given in Appendix A.3. In the chiral limit, singular parts of the third- and fourth-order cumulants diverge around the phase transition. When we put finite mass, the divergent behavior is smeared and milder peaks emerge. We here analyze the smearing effect of the finite mass in MF.

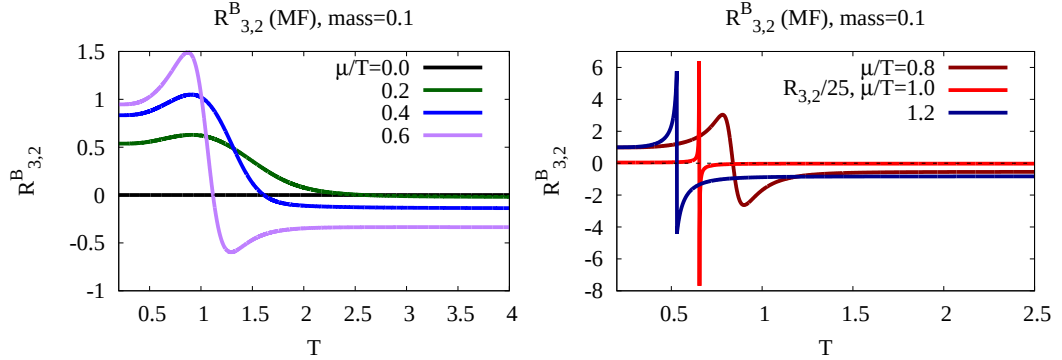


Figure 4.1: Cumulant ratio of third to second at $m_0 = 0.1$ and $\mu/T = 0.0 - 0.6$ (left panel) or $\mu/T = 0.8 - 1.2$ (right panel). At $\mu/T = 1.0$, the value of $R_{3,2}^B$ is divided by a factor 25.

In Fig. 4.1, we show $R_{3,2}^B$ at $m = 0.1$ as a function of T . At zero chemical potential, odd-order cumulants vanish, so $R_{3,2}^B = 0$. At small μ/T , $R_{3,2}^B$ takes finite positive values and there is a broad peak. Above the phase transition, it decreases toward some small value. When μ/T increases and it becomes

close to CP, $\mu/T \sim 1.0$, one finds that a negative valley appears. Magnitudes of a negative valley and a positive peak are enhanced. The peak and valley widths have tendencies to decrease with increasing μ/T .

In Fig. 4.2, we show $R_{4,2}^B$ at $m = 0.1$ as a function of T . One can

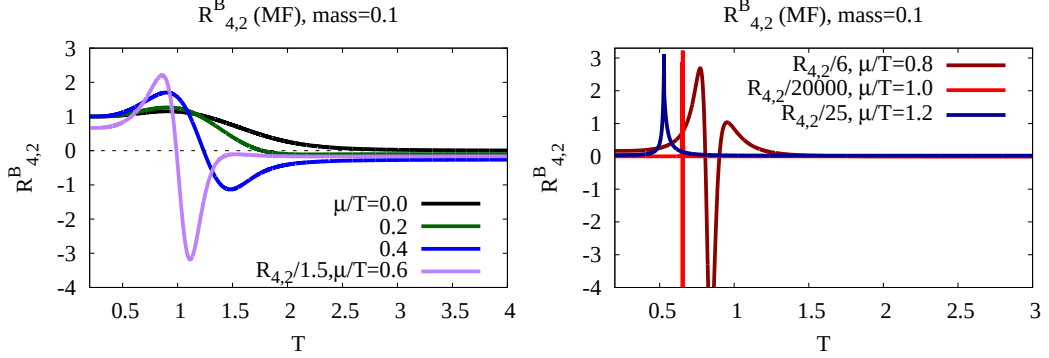


Figure 4.2: Cumulant ratio of fourth to second at $m_0 = 0.1$ and $\mu/T = 0.0 - 0.6$ (left panel) or $\mu/T = 0.8 - 1.2$ (right panel). The value of $R_{4,2}^B$ is divided by a factor 1.5, 6, 20'000, and 25 at $\mu/T = 0.6, 0.8, 1.0$ and 1.2 , respectively.

confirm that $R_{4,2}^B$ becomes unity at low temperature and zero μ/T , which indicates that the baryon number is carried by baryons rather than quarks [90, 124, 266, 267, 268]. $R_{4,2}^B$ has a broad positive peak as $R_{3,2}^B$ at small μ/T . At large μ/T , it has a negative valley and two positive peaks. These peak and valley widths are shrinking when μ/T is close to $(\mu/T)_{\text{CP}}$ as in $R_{3,2}^B$. The cumulant ratio of fourth to second $R_{4,2}^B$ becomes small at high temperature, depending on μ/T .

In short, we find the oscillatory behavior of $R_{3,2}^B$ and $R_{4,2}^B$ in MF due to the finite mass effect. These behaviors can be understood as reviewed in Sect. 1.2.4 due to the smeared singular part of the corresponding cumulants by the mass effect [100]. The finite volume effect is also expected to mask the singular behavior of cumulants; then we investigate the finite volume effect in Sect. 4.2.

It should be noted that the high temperature behavior of $R_{4,2}^B$ and $R_{3,2}^B$ does not correspond to the ideal gas limit, where $R_{4,2}^B \rightarrow 2/(\hat{\mu}^2 + 3\pi^2)$ and $R_{3,2}^B \rightarrow 2\hat{\mu}/(\hat{\mu}^2 + 3\pi^2)$ (See, for example [140, 269]). This is probably because all quarks are confined [166, 168] and there is no spatial baryonic hopping terms [162] (See also Appendix A.1) in the current treatment. Then, we focus on cumulant ratios around the phase transition in the next section.

We also show $R_{3,2}^B$ and $R_{4,2}^B$ in the QCD phase diagram in the MF approximation in Sect. A.3 as references.

4.2 Net-baryon number cumulants with mesonic field fluctuations

In this section, we show results of cumulant ratios $R_{4,2}^B$ and $R_{3,2}^B$ of the net-baryon number with mesonic fluctuations in the chiral limit, $m_0 \rightarrow 0$. These ratios are defined as

$$R_{3,2}^B = c_B^{(3)}/c_B^{(2)}, \quad R_{4,2}^B = c_B^{(4)}/c_B^{(2)}, \quad (4.2)$$

where

$$c_B^{(n)} = \frac{1}{VT^3} \frac{\partial^n \log \mathcal{Z}_{AF}}{\partial \hat{\mu}^n}. \quad (4.3)$$

$c_B^{(n)}$ is the n -th order cumulant of the net-baryon number, $\hat{\mu} = N_c \mu/T$, and $\mathcal{Z}_{AF}$ is the partition function of the auxiliary fields given in Eq. (3.14). The formulae of the third- and fourth-order cumulants are given in Appendix B.2.

We here mainly focus on the finite size effect on cumulants. As reviewed in Sect. 1.2.4, we anticipate that both finite mass and finite size effects mask the singular behavior of cumulants; then there is a possibility that we can observe the negative region or significant decrease of higher-order cumulants around the phase transition due to the finite size effect [133]. In the chiral limit, we investigate the finite size effect on cumulants. In addition, the smeared singular part of higher-order cumulants in the chiral limit would be larger than that at finite mass on the same lattice size; then our results may show the upper limits of the oscillatory behavior because of the finite size effect.

4.2.1 Simulation details

We calculate cumulant ratios in the strong coupling limit (SCL) on $4^3 \times 4$, $6^3 \times 4$, and $6^3 \times 6$ lattices at $\mu/T \leq 0.8$, in the second-order phase transition region [172]. Results on a $8^3 \times 8$ lattice are found in Ref. [270]. We utilize configurations used in Chap. 3, and we add new configurations to reduce statistical error bars. It should be noted that there is no hysteresis behavior in the second-order phase transition region, so we do not have to distinguish results with the Wigner phase start from those with the NG phase start; then

we apply an initial condition between the NG phase start and the Wigner phase start in new configurations, $(\sigma_{\mathbf{k},\tau}, \pi_{\mathbf{k},\tau}) \sim \mathcal{O}(0.01, 0) - \mathcal{O}(1, 0)$.

We find the finite size effect on cumulants and this analysis can imply its effect on higher-order cumulants realized in experiments [133]. Our simulations are carried out on a lattice: $4^3 \times 4 - 6^3 \times 6$. Thus $LT \simeq 3 - 9$ in the second-order phase transition region and this condition could provide insights into experimental data: $LT \simeq 2.4 - 3.6$ [147]. We note that the boundary condition might not be the same in experiments and lattice calculations, but we could expect that qualitative feature is not different.

As we mentioned in previous sections, error bars tend to be large due to the sign problem and the error propagation. In order to estimate error bars more appropriately, we apply a jackknife (JK) method [174]. For example, let us consider error estimations for $c_B^{(4)}$, where $c_B^{(4)}$ is obtained as a combination of various averages, $c_B^{(4)} \equiv \langle A \rangle = \langle a \rangle + \langle b \rangle \langle c \rangle + \dots$; explicit forms of $a, b, \dots$, are found in Appendix B.2. If we evaluate error propagation from the averages $(\langle a \rangle, \langle b \rangle, \dots)$, the total error (*i.e.* the error of $\langle A \rangle$) becomes too large. In the JK method [174, 271], first, we evaluate JK averages for each observable (*i.e.* $\langle a \rangle_{\text{bin}}, \langle b \rangle_{\text{bin}}, \langle c \rangle_{\text{bin}}, \dots$). Next, we obtain the JK average for $\langle A \rangle_{\text{bin}}$. Finally, we guess the error bar of $\langle A \rangle = c_B^{(4)}$ by using $\langle A \rangle_{\text{bin}}$. We apply the same technique to $R_{4,2}^B$ and $R_{3,2}^B$ since they are given by cumulant ratios.

In AFMC, we have the sign problem, then observables have an imaginary part even if the observables are real in principle. Therefore, we take a real part of expectation values. We also check the magnitude of the imaginary part. For instance, the real part of a maximum amplitude of $R_{4,2}^B$ is about 720 on a $6^3 \times 6$ lattice for $\mu/T = 0.8$, while the imaginary part of a maximum amplitude of $R_{4,2}^B$ is about 70 for the same condition and is small enough compared with the real part around the phase transition. We are interested in the critical phenomena around phase transition, so we can study higher-order cumulant ratios even when we face the sign problem in AFMC.

4.2.2 (T, μ) dependence of $R_{3,2}^B$ and $R_{4,2}^B$

First, we show T, μ dependence of $R_{3,2}^B$ and $R_{4,2}^B$ on a $6^3 \times 6$ lattice as functions of T/T_c in the chiral limit in Fig. 4.3, where T_c is the critical temperature at $\mu/T = 0$ on a $6^3 \times 6$ lattice. It should be noted that the tricritical point would exist between $\mu/T = 0.8$ and $\mu/T = 1.0$, so the results shown here are in the *would-be second order* transition region.

We find the similar tendency of $R_{4,2}^B$ and $R_{3,2}^B$ as in MF analysis at finite mass in Sect. 4.1. Both $R_{4,2}^B$ and $R_{3,2}^B$ exhibit a positive and broad peak at

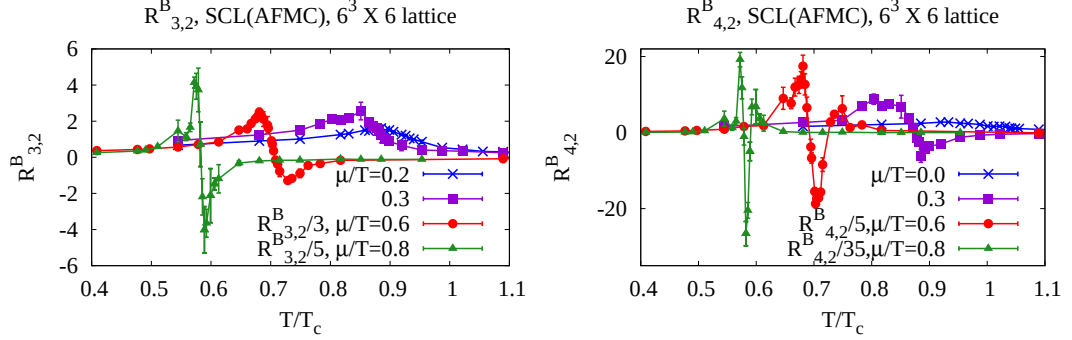


Figure 4.3: $R^B_{3,2}$ (left panel) and $R^B_{4,2}$ (right panel) along fixed μ/T lines on a $6^3 \times 6$ lattice [78]. We rescale $R^B_{3,2}$ by factors 3 and 5 for $\mu/T = 0.6$ and 0.8, respectively. We also rescale $R^B_{4,2}$ by factors 5 and 35 for $\mu/T = 0.6$ and 0.8, respectively. These figures are basically taken from Ref. [78].

small μ/T around the phase boundary. A negative valley appears at large μ/T ; there are a(two) positive peak(s) and a negative valley for $R^B_{3,2}$ ($R^B_{4,2}$). In addition, (a) peak heights (height) and a valley depth of $R^B_{4,2}$ ($R^B_{3,2}$) become large toward TCP. Therefore, we conclude that both effects, *i.e.* the finite volume and the finite mass effects, mask the singular part of the free energy density; then we can find oscillatory behavior at large μ/T around the phase transition as reviewed in Sect. 1.2.4 [100, 133]. The detailed discussion will be given in Sect. 4.2.4.

4.2.3 Lattice size dependence of $R^B_{3,2}$ and $R^B_{4,2}$

Next, we show the lattice size dependence of $R^B_{3,2}$ and $R^B_{4,2}$ in Figs. 4.4 and 4.5 as functions of the reduced temperature $(T - T_c)/T_c$, where T_c is defined as the critical temperature with the corresponding conditions: the lattice size and μ/T . At small μ/T , cumulant ratios on each lattice have a moderate peak and their heights are somewhat larger compared with results of smaller lattices. At large μ/T , magnitudes of peak heights and a valley depth are much larger and their widths are smaller on larger lattices. The detailed discussion will be given in Sect. 4.2.4.

In Appendix B.3, we show numerical results on cumulants for completeness.

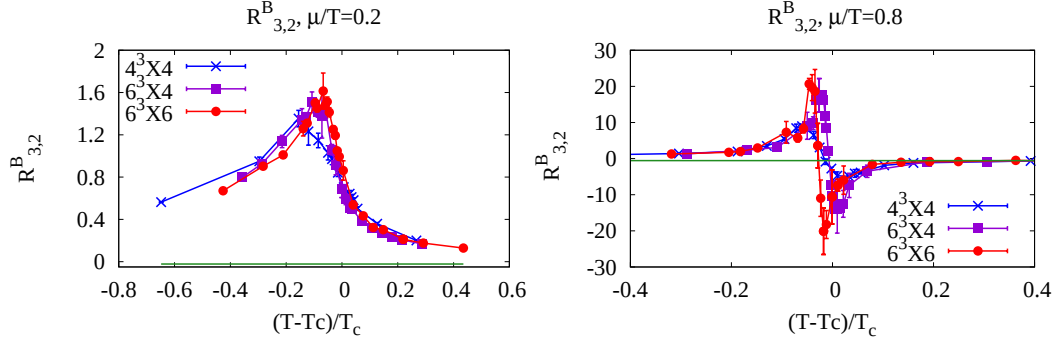


Figure 4.4: $R_{3,2}^B$ at $\mu/T = 0.2$ (left panel) and $\mu/T = 0.8$ (right panel) on various size lattices. The horizontal line shows the asymptotic value at high T in the MF analysis. These figures are basically taken from Ref. [78].

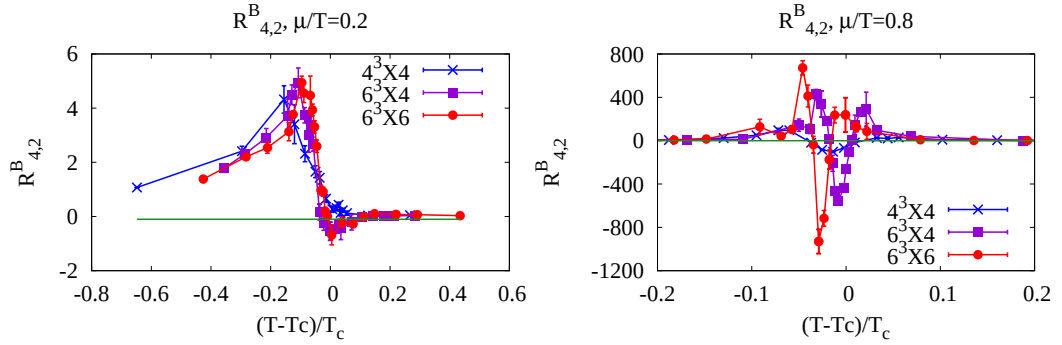


Figure 4.5: $R_{4,2}^B$ at $\mu/T = 0.2$ (left panel) and $\mu/T = 0.8$ (right panel) on $4^3 \times 4$, $6^3 \times 4$, and $6^3 \times 6$ lattices. The horizontal line shows the asymptotic value at high T in the MF analysis. These figures are basically taken from Ref. [78].

4.2.4 Discussion of cumulants in AMFC

The $O(N)$ scaling function analysis is of great help to understand the behavior of cumulants in the current study. We discuss the relation between cumulant ratios obtained here and $O(N)$ ($N=2,4$) scaling function of the net-baryon number around the second-order phase transition [100]. As given in Appendix C, the free energy density can be divided into two parts: the singular (divergent) part and the regular part. Higher-order cumulants also have the corresponding two parts: derivatives of the singular part and the regular part, respectively. The leading contribution of the divergent term in the chiral and thermodynamic limits is governed by the critical exponents as

$$c_B^{(n)} \sim \begin{cases} -(2\kappa_q)^{n/2} |t|^{(2-\alpha-n/2)} f_{\pm}^{(n/2)}(z) & \text{for } \hat{\mu}_q = 0, \text{ even } n \\ -(2\kappa_q)^n \hat{\mu}_q^n |t|^{(2-\alpha-n)} f_{\pm}^{(n)}(z) & \text{for } \hat{\mu}_q > 0, \end{cases} \quad (4.4)$$

where

$$f_{\pm}^{(n)}(z) = \lim_{z \rightarrow \pm\infty} |z|^{-(2-\alpha-n)} f_f^{(n)}(z), \quad \frac{f_s(T, \mu_q, h)}{T^4} = Ah^{1+1/\delta} f_f(z), \quad (4.5)$$

$z = t/h^{1/(\beta\delta)}$, t is a reduced temperature, h is a dimensionless external field, A is a normalization parameter, and f_s is the singular part of the free energy density. α, β , and δ are critical exponents of the specific heat, the order parameter, and the order parameter with the external field as $C \sim |t|^{-\alpha}$, $\sigma \sim |t|^{\beta}(T < T_c)$, and $\sigma \sim |h|^{1/\delta}(T = T_c)$, respectively. We find a brief review of $O(N)$ scaling function in Appendix C.

We can anticipate that the qualitative behaviors of cumulants are the same in the $O(4)$ universality class and the $O(2)$ universality class. For instance, if the critical exponent α is negative, the first divergent cumulant of the net-baryon number is $c_B^{(6)}$ at zero chemical potential; this is the case for $O(2)$ and $O(4)$ symmetries, whose critical exponents are $\alpha \simeq -0.0147$ [256] and $\alpha \simeq -0.21$ [257], respectively. Then we expect that the qualitative behavior is the same in $O(2)$ and $O(4)$. It should be noted that the critical exponent α is positive for $Z(2)$ symmetry [125]; the first divergence is realized in $c_B^{(4)}$ [100, 125]. We also note that the effective action in AFMC (Eq. (3.18)) belongs to $O(2)$.

The oscillatory behavior of $c_B^{(3)}$ and $c_B^{(4)}$ is considered to be the finite size effect as reviewed in Sect. 1.2.4 [133]. In the thermodynamic and chiral limits, both cumulants diverge according to $O(N)$ scaling function [100] while we find the oscillatory behavior in the chiral limit on a lattice [133]. Then the reason for the oscillatory behavior is the smeared singular part due to the finite size effect; we can expect that we observe the divergent behavior of

these cumulants when we apply the finite size scaling analysis [100, 148, 150, 155, 255]. One of the evidences is the increasing tendency of the peak height and valley depth. Especially at $\mu/T = 0.2$, we observe no negative valley of $R_{4,2}^B$ on a $4^3 \times 4$ lattice. By comparison with the smallest lattice data, we find the negative region on $6^3 \times 4$ and $6^3 \times 6$ lattices. This is probably because the smeared singular part becomes larger on larger lattices and it overcomes the regular part contribution; then the negative valley emerges on larger lattices. We can expect that the singular part becomes much larger toward the thermodynamic limit and finally the singular behavior would be observed. Second one is the decreasing tendency of the width. We can anticipate that a negative valley of $R_{4,2}^B$ will vanish in the thermodynamic limit as expected in the scaling function analysis [100, 148, 255]. Hence, we can conclude that the appearance of the negative valley of $R_{4,2}^B$ in the chiral limit is a evidence of the smearing effect by finite size effect [133].

The singular part of higher-order cumulants at small μ/T is tend to be more suppressed than that at large μ/T . This is because the most singular part at finite chemical potential are proportional to $-(2\kappa_q\hat{\mu})^n$ in Eq. (4.4). Above discussions agree with the present results on cumulant ratios in AFMC. At small μ/T , the smeared singular part is subordinated to the regular part, and we do not observe the oscillatory behavior. Around the expected TCP ($\mu/T \sim 0.8 - 1.0$), the singular part grows and overtakes the regular part; then we can observe the oscillatory behavior at large μ/T . In conclusion, μ/T dependence of $R_{3,2}^B$ and $R_{4,2}^B$ is consistent with the scaling function analysis [100].

Higher-order cumulants and their ratios at sufficiently large chemical potential with field fluctuation effects are also studied in effective models [90, 100, 272] and lattice QCD calculations [142, 143, 144, 145]. As for the lattice QCD approach [142, 143, 144, 145], we find some negative values of $c_B^{(4)}$ [142, 144, 145], but it is difficult to conclude the existence of the negative $c_B^{(4)}$ region at physical mass due to large errors and a small number of data points. According to the effective model analyses with field fluctuations [90, 100, 272], we find the oscillatory behavior of higher-order cumulants at large μ/T around the phase transition as we studied in this chapter in Figs. 4.3, 4.4, and 4.5. We note that these studies [90, 100] are carried out in the thermodynamic limit; then the oscillatory behavior of $c_B^{(3)}$ and $c_B^{(4)}$ should originate from the finite mass effect [100]. The finite size effect on higher-order cumulants is also investigated by using the scaling function, specific models, and cutting off the momentum scale [133, 147, 148, 150, 151, 152, 154, 155, 156, 272]. As we anticipated, the behavior of cumulants are affected by the finite size effect as previous studies

[133, 147, 148, 150, 151, 152, 154, 155, 156, 272]. In fact, we observe the oscillatory behavior with a negative valley of $c_B^{(3)}$ and $c_B^{(4)}$ in the chiral limit because of the finite size effect as in Ref. [133] in comparison with $O(N)$ scaling function analysis [100].

The present study may be of help for constructing the scaling function with the system size, $f_s(T, \mu_q, m_q, L)$; the SC-LQCD analysis in this thesis is a concrete example of the scaling behavior. In addition, both finite mass and volume effects mask the singular contribution to cumulants, but the quantitative behavior should be different from each other. Then theoretical studies of the scaling function for the finite volume effects are demanded to understand each contribution to cumulants [133, 148].

According to our analysis, we expect that we can confirm the regions characterized by critical exponents from the underlying universality: critical exponents in $O(2)$ universality due to the staggered fermion at small chemical potential and mean field critical exponents around TCP in the chiral limit, for example. As a result, we can think that we explicitly find the critical region when field fluctuations are taken into account.

Calculations in this chapter are performed under a condition, $LT \simeq 3 - 9$ around the phase transition. In experiments, the finite system is characterized by $LT \simeq 2.4 - 3.6$ [147]; thus the negative $c_B^{(4)}$ region can emerge at RHIC experiments because of the finite size effect, provided that the finite mass effect is not so large that the regular part is minor contribution.

The results obtained here may show the upper limits of their negative valley depths on a fixed size lattice since the simulations are carried out in the chiral limit. The negative region of cumulants would remain at finite mass even in the thermodynamic limit, supposing that the finite mass effect does not suppress the singular part significantly. The finite mass effect should be included to see the explicit behavior of higher-order cumulants toward more realistic case in the thermodynamic limit or in a finite volume.

4.2.5 $R_{4,2}^B$ in the QCD phase diagram in the strong coupling limit

We here show the negative region of $R_{4,2}^B$ with AFMC in the QCD phase diagram in both strong coupling and chiral limits in Fig. 4.6. The phase boundary is determined in the same way as the previous chapter. We here define the negative region where $R_{4,2}^B$ is smaller than both zero and the high temperature value of MF¹. We do not consider error bars to define the neg-

¹The high temperature behavior should be an artifact of the large dimensional expansion [78].

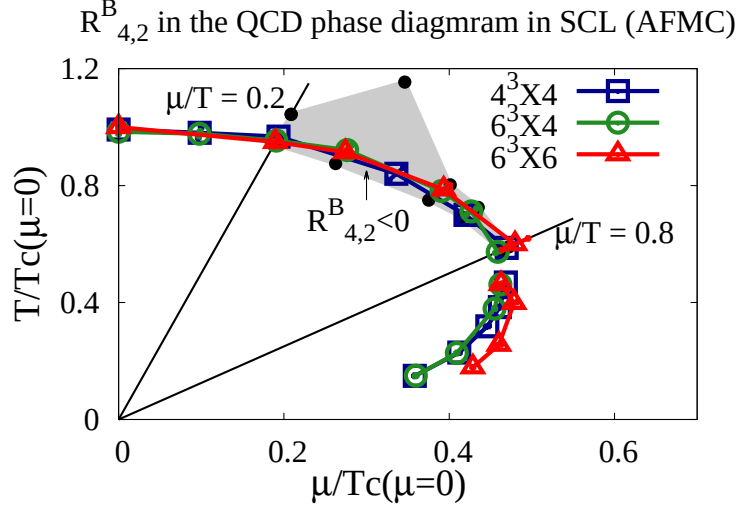


Figure 4.6: $R_{4,2}^B$ in the QCD phase diagram in the chiral and strong coupling limits [78]. The vertical and horizontal lines are the temperature and chemical potential divided by the critical temperature at $\mu/T = 0$ on a $6^3 \times 6$ lattice, respectively. The shaded area shows the negative $R_{4,2}^B$ region, where $R_{4,2}^B$ is also smaller than the asymptotic value at high T in MF. Black dots are the boundary points and the shaded area is obtained by connecting the black dots. This figure is basically taken from Ref. [78].

ative region. Black points denote the phase boundary of the negative $R_{4,2}^B$ region and the shaded area is given by lines connecting the black points.

The negative region of $R_{4,2}^B$ can be a signal of the critical phenomena. We find that the negative region appears from about $\mu/T \sim 0.2$. Probably due to the suppression factor, $(\kappa_q \hat{\mu})^n$ in Eq. (4.4), the singular part gets to overtake the regular part at sufficiently large $\hat{\mu}$. One finds the largest region at $\mu/T = 0.3$, and the negative region shrinks toward TCP above $\mu/T \sim 0.3$. The location of the phase boundary is consistent with the negative region.

As discussed in Sects. 4.2.3 and 4.2.4, the negative region will shrink on larger lattices, and will vanish in the thermodynamic and chiral limits according to the $O(N)$ scaling function analysis [100]. There is the possibility that the negative region exists in hot matter formed in heavy-ion collisions due to the finite mass and size effect [100, 133].

4.3 Short summary

We have investigated the net-baryon number cumulant ratios in the strong coupling limit. In MF, the higher-order cumulants' behavior becomes moderate at finite mass. We find the oscillatory behavior of them at large μ/T due to the finite mass effect [100]. In the auxiliary field Monte Carlo (AFMC) method, mesonic fluctuation effects are taken into account. $R_{3,2}^B$ and $R_{4,2}^B$ also exhibit moderate behavior on a finite size lattice in AFMC and the higher-order cumulants oscillate around the phase transition at large μ/T in the chiral limit because of the finite size effect [133].

We find that $R_{3,2}^B$ and $R_{4,2}^B$ in AFMC has a small peak at small μ/T while they have a negative region near the phase boundary for large μ/T . $R_{3,2}^B$ ($R_{4,2}^B$) has a (two) positive peak(s) and a negative valley at large μ/T and their widths become narrower on large lattices. The scaling function analysis indicates that $R_{4,2}^B$ positively diverges in the thermodynamic and chiral limits [100] then a negative valley of $R_{4,2}^B$ between two positive peaks appears due to the finite size effect [133]. The shrinking behavior of the cumulants' widths on larger lattices are consistent with the scaling function analysis [100].

We also show the negative $R_{4,2}^B$ region in the QCD phase diagram. The negative $R_{4,2}^B$ region clearly signals the phase transition even in finite volume [133]. The region is the largest at $\mu/T \sim 0.3$ and shrinks toward TCP. This result may be suggestive for the finite volume effect in both theoretical and experimental works while the meaning of the finite volume effect in our study might not be the same as that in experiments: e.g. boundary condition [133]. This is because our simulations are carried out where $LT \simeq 3 - 9$ while the realized system in heavy-ion collisions is consider to be $LT \simeq 2.4 - 3.6$ [147].

It would be interesting to investigate critical exponents in AFMC. Critical exponents can be well described by MF value around TCP [79] while critical exponents would be well characterized by O(2) universality at second order phase transition in the chiral limit [100]. The finite size scaling analysis is also important to find the behavior of the singular part of the net-baryon number cumulants in the chiral limit with the finite size scaling; our analysis would suggest the properties of the scaling function [148, 150]. The finite-mass effect is another important subject. We expect that the negative region remains even in the thermodynamic limit due to the finite mass effect when the regular part does not overcome the singular part [100]. Both finite mass and volume effects contribute to the behavior of cumulants in experiments; then we need to perform simulations with finite mass [100, 133]. In addition, it is desirable to include higher-order corrections of the large dimensional expansion to take account of spatial baryonic hopping terms.

Chapter 5

Summary and outlook

In this thesis, we have discussed the role of fluctuations in two ways; auxiliary (mesonic) field fluctuations to obtain observables beyond the mean-field approximation and net-baryon number fluctuations to detect the criticality.

We review common concepts of the QCD and its phase diagram in Chap. 1. We also review the theoretical approaches of lattice QCD and the strong coupling lattice QCD in Chap. 2. We give our studies of the QCD phase diagram with fluctuation effects in the strong coupling limit (SCL) in Chap. 3 and of the net-baryon number cumulants in SCL in Chap. 4.

First, we have investigated the QCD phase diagram in SCL and chiral limit ($m_0 \rightarrow 0$) with the auxiliary field Monte Carlo (AFMC) method. In order to obtain the effective action, we start from the lattice QCD action with one species of unrooted staggered fermion [173, 174, 186, 187] to investigate the chiral phase transition. We apply the large dimensional ($1/d$) expansion method [231, 237, 253] and integrate out spatial-link variables analytically. We bosonize four-Fermi like terms to integrate over staggered quark fields, applying the extended Hubbard-Stratonovich (eHS) transformation [164, 165, 167] and temporal-link variables are integrated out analytically [233, 238, 240]. The obtained effective action is given as a function of auxiliary fields $(\sigma_{\mathbf{k},\tau}, \pi_{\mathbf{k},\tau})$, which include the scalar mode in $\sigma_{\mathbf{k},\tau}$, the pseudo-scalar mode in $\pi_{\mathbf{k},\tau}$, and higher momentum modes. In order to take mesonic field fluctuation effects into account, we apply the AFMC method by using Monte Carlo (MC) technique and obtain configurations of $\sigma_{\mathbf{k},\tau}$ and $\pi_{\mathbf{k},\tau}$.

When we derive observables, we introduce the chiral angle fixing (CAF) method since the expectation value of the chiral condensate is canceled to be zero in finite volume due to the chiral symmetry. In CAF where we can investigate the spontaneous symmetry breaking on a fixed size lattice, all configurations are rotated by the negative chiral angle to set the chiral angle and pseudo-scalar mode zero. Thus we have finite value of the chiral conden-

sate in the symmetry breaking phase. This procedure is inspired by the $Z(2)$ magnetization M_0 where we often take the expectation value of $|M_0|$ [254]. By using rotated configurations, we observe order parameters: the chiral condensate and quark number density, which indicate the phase transition. As for the chiral condensate, the chiral symmetry is spontaneously broken and the chiral condensate is finite at low temperature while the condensate is almost absent at high temperature where the chiral symmetry is restored. The quark number density is consistent with zero at low temperature and takes a finite value at high temperature. Both order parameters at small μ/T show moderate changes from the Wigner phase to Nambu-Goldstone (NG) phase with decreasing T , which show the second order or crossover phase transition named as the *would-be second order* phase transition. In the large μ/T region, we find discontinuous jumps of the order parameters and the initial condition dependences (*hysteresis*) of the MC simulation: Wigner initial condition $(\sigma_{\mathbf{0},\tau}, \pi_{\mathbf{0},\tau}) \sim \mathcal{O}(0.01, 0)$, $(\sigma_{\mathbf{k}\neq\mathbf{0},\tau}, \pi_{\mathbf{k}\neq\mathbf{0},\tau}) = (0, 0)$ and NG initial condition $(\sigma_{\mathbf{0},\tau}, \pi_{\mathbf{0},\tau}) \sim \mathcal{O}(1, 0)$, $(\sigma_{\mathbf{k}\neq\mathbf{0},\tau}, \pi_{\mathbf{k}\neq\mathbf{0},\tau}) = (0, 0)$. This hysteresis indicates the first order phase transition since the MC configurations cannot overcome the potential barrier between two local minima related to the NG and Wigner phase. We named this phase transition as the *would-be first order* phase transition. We here deduce that the tricritical point (TCP) in SCL would exist between $\mu/T = 0.8$ and 1.0 .

The chiral phase boundary is determined by the peak point of the chiral susceptibility at would be second order phase transition and by the effective potential analysis at would be first order phase transition. We find that the pseudo-critical temperature T_c is lower than the mean-field result on an isotropic lattice at small chemical potential, and the NG phase is broaden to higher chemical potential direction at large μ . We also confirm that T_c is not sensitive to the spatial lattice size as in the monomer-dimer-polymer simulations (MDP) [169, 170, 171]. The phase boundary at would-be first order phase transition strongly depends on the temporal lattice size, which is also consistent with MDP [171].

We apply the finite size scaling analysis for the chiral susceptibility to determine the phase transition order at the would-be second phase transition. We can exclude the possibility of the first-order phase transition, but we cannot identify the phase transition order due to the few statistics, so we need more statistics to determine the phase transition order at the would-be second order phase transition.

In AFMC, we have the sign problem since we must introduce imaginary numbers in the eHS transformation [164, 165, 167]. These imaginary numbers are coupled with $\pi_{\mathbf{k},\tau}$ modes, which appear in the fermion determinant; the fermion determinant has an imaginary part and the sign problem appears.

In order to find the origin of the sign problem in the current treatment, we apply the momentum cut-off method to the configurations of auxiliary fields. Supposing that the high-momentum modes of auxiliary fields are cut off, the average phase factor tends to take a larger value; then the severe statistical weight cancellation is found to originate from the high-momentum modes of auxiliary fields. This can be understood as follows. Because of the staggered sign factor ϵ_x coupled with $\pi_{\mathbf{k},\tau}$, the complex phase on a site and that on the nearest neighbor sites contribute oppositely and they cancel each other, provided that the low-momentum modes dominate. When we only consider the lowest modes of the auxiliary fields, the average phase factor is about unity and the weight cancellation is almost absent, where we have no sign problem. We also analyze the severity of the sign problem in AFMC and find that the problem is severer than that in MDP [170], but the statistical weight cancellation is manageable in the current analyses as shown in Sect. 3.3.

Next, we have investigated the higher-order cumulant ratios with regard to the net-baryon number in the strong coupling and chiral limits. We show the cumulant ratios in the mean field approximation at finite mass. We find a moderate peak for both $R_{3,2}^B$ and $R_{4,2}^B$ at small μ/T and the oscillatory behavior at large μ/T .

We have discussed results of $R_{3,2}^B$ and $R_{4,2}^B$ in AFMC in the chiral limit. We find that the cumulant ratios have a broad positive peak at small μ/T and show oscillatory behavior around the phase transition as the μ/T value approaches that at expected TCP ($\mu/T \sim 0.8$); $R_{3,2}^B$ ($R_{4,2}^B$) has a (two) positive peak(s) and a negative valley at large μ/T . This is probably because the smeared singular part overcomes the regular part of $c_B^{(n)}$ at large μ/T [100]. The peak heights and the valley depth increase and their widths shrink on larger lattices. In the thermodynamic limit, one positive and one negative divergences are anticipated for $R_{3,2}^B$ while the negative valley would disappear and two positive peaks merge into one positive divergence for $R_{4,2}^B$ [100]; then the lattice size dependence of the higher-order cumulant ratios does not contradict the $O(N)$ scaling function analysis [100]. We can conclude that the oscillatory behavior and the negative region of $R_{3,2}^B$ and $R_{4,2}^B$ emerges because of the finite size effect [100, 133]. In addition, there is a possibility that such a negative region can be found in heavy-ion experiments where $LT \simeq 2.4 - 3.6$ [147] since our analysis is carried out under a condition $LT \simeq 3 - 9$.

There are several directions of study as extensions of this work. The finite coupling effects of the strong coupling approach are important to know criticality in QCD phase transition. By using the AFMC method, we can take account of finite coupling effects [164, 165, 167] and generate AFMC configurations at finite μ and T [246, 261]. Applying the naive eHS transfor-

mation, the sign problem is so severe that the average phase factor collapses with next-to-leading order (NLO) effects even on a small lattice [261] while we could investigate the QCD phase diagram by shifting the integration path [273, 274] at would-be second order phase transition [246]. At would-be first order phase transition [246], it is not easy to determine the shifted path due to the existence of two local minima in the effective potential. Possible methods to evade the above problem are the configuration-dependent shifted path by using a method given in Refs. [273, 274] and the complex Langevin method [220, 221, 222], for example. It is also important to take account of higher-order contributions of the large dimensional ($1/d$) expansion [241]. In the leading order in the $1/d$ expansion method, there is no baryon hopping terms. Thus, we need to include higher-order effects of the $1/d$ expansion, which may affect the phase boundary at large μ and cumulants of the net-baryon number as discussed in Chap. 4.

As for cumulants, the finite mass effect is one of the important ingredients for the next study. Another important ingredient is to find the critical region and the finite size scaling function with finite size effect in the QCD phase diagram [79]. In the chiral limit, critical behavior is expected to be governed by the critical exponents of $O(2)$ (or $O(4)$ in two massless flavor case) at low chemical potential [100] and by those of MF around TCP [79]. At finite mass, the chiral phase transition may be characterized by the remnant effect of $O(2)$ ($O(4)$) at small $\hat{\mu}$ [100] and $Z(2)$ symmetry around CP [99]. Then, one of the interesting studies is to see a region between $O(2)$ -type phase transition and MF- ($Z(2)$ -) type phase transition in the chiral limit (with finite mass). If we could construct the scaling function with respect to the finite size effect [100, 148] in the chiral limit, we have deeper understanding about the scaling behavior with mass and volume scalings.

Acknowledgement

The author would like to show my greatest appreciation to his supervisor, Prof. Akira Ohnishi for useful discussion and advice on this thesis. The author is also grateful to collaborators, Dr. Takashi Z. Nakano and Dr. Kenji Morita for useful discussion and comment on his works. He would like to offer his special thanks to Frithjof Karsch, Swagato Mukherjee, and Hiroshi Ohno for guiding him to interesting topics and discussion on them. He would like to thank Takatoshi Ichikawa, Hideaki Iida, Sinya Aoki, Yu Maezawa, and Keitaro Nagata for advice on numerical simulations. My appreciation also goes to Wolfgang Unger, Shuntaro Sakai, Takahiro Sasaki, and Philippe de Forcrand for useful discussion. In addition, he is grateful to the members of

the Nuclear Theory Group at Kyoto University for useful discussion. The author is a Research Fellow of Japan Society for the Promotion of Science (JSPS) and is supported by the Grant-in-Aid for JSPS Fellows (No.25-2059). He is grateful for the support from JSPS.

Appendix A

Mean field formulae at strong coupling

A.1 Effective action in the mean field analysis

Following derivations are mainly based on Ref. [162]. The one species of unrooted staggered fermion action in the strong coupling limit is give as

$$\begin{aligned}
S_{\text{SCL}} &= a_s^2 a_\tau m_0 a_s \sum_x \bar{\chi}_x \chi_x \\
&+ a_s^2 a_\tau \frac{a_s}{a_\tau} \frac{1}{2} \sum_x \eta_0(x) \left[\bar{\chi}_x e^{\mu a_\tau} U_{0,x} \chi_{x+\hat{0}} - \bar{\chi}_{x+\hat{0}} e^{-\mu a_\tau} U_{0,x}^\dagger \chi_x \right] \\
&+ a_s^2 a_\tau \frac{1}{2} \sum_{x,j} \eta_j(x) \left[\bar{\chi}_x U_{j,x} \chi_{x+\hat{j}} - \bar{\chi}_{x+\hat{j}} U_{j,x}^\dagger \chi_x \right] \\
&= a_s^2 a_\tau (m_0 a_s) \sum_x \bar{\chi}_x \chi_x \\
&+ a_s^2 a_\tau \gamma \frac{1}{2} \sum_x \eta_0(x) \left[\bar{\chi}_x e^{\mu a_\tau} U_{0,x} \chi_{x+\hat{0}} - \bar{\chi}_{x+\hat{0}} e^{-\mu a_\tau} U_{0,x}^\dagger \chi_x \right] \\
&+ a_s^2 a_\tau \frac{1}{2} \sum_{x,j} \eta_j(x) \left[\bar{\chi}_x U_{j,x} \chi_{x+\hat{j}} - \bar{\chi}_{x+\hat{j}} U_{j,x}^\dagger \chi_x \right] \\
&\equiv a_s^2 a_\tau (m_0 a_s) \sum_x \bar{\chi}_x \chi_x + S_0 + S_j , \tag{A.1}
\end{aligned}$$

where a_τ and a_s are lattice spacing for temporal and spatial directions, respectively. S_0 and S_j denote temporal and spatial action, respectively. First, we apply the large dimensional ($1/d$) expansion [231] and bosonization technique

(Hubbard-Stratonovich transformation) [231, 237, 253], $\exp[C_o M^2] = \int \mathcal{D}\sigma \exp[-(C_o \sigma^2 + 2C_o \sigma M)]$, as follows

$$\begin{aligned} \int \mathcal{D}U_j e^{-S_j} &= 1 + (a_s^2 a_\tau)^2 \frac{1}{8N_c} \sum \bar{\chi}_x \chi_x \bar{\chi}_{x+\hat{j}} \chi_{x+\hat{j}} + \cdots \\ &= \int \mathcal{D}\sigma e^{-(a_s^2 a_\tau)^2 \frac{1}{2} b_\sigma \sum_{x,y} [\sigma(x) V_{x,y} \sigma(y) + 2\sigma(x) V_{x,y} M_y]} , \end{aligned} \quad (\text{A.2})$$

where $M_x = \bar{\chi}_x \chi_x$, $V_{x,y} = \sum_j (\delta_{x+\hat{j},y} + \delta_{x-\hat{j},y})/2d$, and $b_\sigma = d/2N_c$ [162, 164, 167]. In Eq. (A.2), we only consider the leading order of the $1/d$ expansion [231].

Now let us consider the order counting of the $1/d$ expansion¹. In the leading term of the large dimensional expansion, we only consider the 2-body mesonic interactions for $N_c > 2$. The sum $\sum_{j,x}$ is the order of the spatial dimension d : $\mathcal{O}(d)$. Supposing that $\sum_j M_x M_{x+\hat{j}} \sim \mathcal{O}(1)$ in large d , χ and $\bar{\chi}$ become the order of $\mathcal{O}(1/d^{1/4})$. The order of the other mesonic hopping terms and the baryonic hopping terms for $N_c \geq 3$ are as follows: $\sum_j (M_x M_{x+\hat{j}})^2 \sim \mathcal{O}(1/d)$, $\sum_j (M_x M_{x+\hat{j}})^3 \sim \mathcal{O}(1/d^2)$, and $\sum_j \bar{B}_x B_{x+\hat{j}} \sim \mathcal{O}(1/d^{N_c/2-1})$, so the above hopping terms are suppressed with large d . This expansion is one of the schematic methods to include many-body interactions. In the leading order of the $1/d$ expansion for $N_c \geq 3$, we have no spatial baryonic hopping terms. By comparison, one can take account of temporal baryonic hopping terms; we exactly integrate over the temporal-link variables [161, 162, 232]. It should be noted that the spatial-baryonic hopping terms are the same order as the 2-body mesonic interactions for $N_c = 2$ [162, 277, 278].

In the following analysis, we can assign the scalar and pseudo-scalar modes as $\sigma(x) = \sigma + i\epsilon_x \pi$ for $\epsilon_x = (-1)^{x_0 + \cdots + x_d}$ [158, 162, 231, 237, 253].

$$\begin{aligned} S &= (a_s^2 a_\tau)^2 \frac{1}{2} b_\sigma \sum_x (\sigma^2 + \pi^2) + a_s^2 a_\tau \sum_x \{(m_0 a_s) + b_\sigma (\sigma - i\epsilon_x \pi)\} M_x \\ &\quad + (a_s^2 a_\tau)^2 \gamma \frac{1}{2} \sum_x \eta_0(x) \left[\bar{\chi}_x e^{\mu a_\tau} U_{0,x} \chi_{x+\hat{0}} - \bar{\chi}_{x+\hat{0}} e^{-\mu a_\tau} U_{0,x}^\dagger \chi_x \right] . \end{aligned}$$

We here apply the Polyakov gauge $U_0(\tau, \mathbf{x}) = \text{diag}[e^{i\phi_1(\mathbf{x})/N_\tau}, \dots, e^{i\phi_1(\mathbf{x})/N_\tau}]$ with a condition $\sum_a^{N_c} \phi_a(\mathbf{x}) = 0$ [161, 232]. In order to respect anti-periodic boundary conditions to include the temperature effect, we first apply the following Fourier transformation to staggered quarks $\chi(\tau, \mathbf{x}) = \sum_{n=1}^{N_\tau} e^{ik_n \tau a_\tau}$

¹We can integrate out spatial-link variables analytically in the strong coupling limit. Higher-order corrections in the $1/d$ expansion are found in Refs. [174, 241, 275, 276], for example.

$\chi(n, \mathbf{x})/\sqrt{N_\tau}$ for $k_n = 2\pi(n-1/2)/(a_\tau N_\tau)$ [162]. After integrating out Grassmann variables, a fermion determinant is given by

$$\begin{aligned} & \prod_{\mathbf{x}} \prod_{a=1}^{N_c} \prod_{n=1}^{N_\tau/2} [\gamma^2 \sin^2 \bar{k}_n a_\tau + M^2 + (a_s^2 a_\tau b_\sigma \pi)^2] , \\ & \equiv \prod_{\mathbf{x}} \prod_{a=1}^{N_c} \prod_{n=1}^{N_\tau/2} [\gamma^2 \sin^2 \bar{k}_n a_\tau + \lambda^2] \end{aligned} \quad (\text{A.3})$$

where $M = m_0 a_s + a_s^2 a_\tau b_\sigma \sigma$, $\bar{k}_n a_\tau = 2\pi(n-1/2)/N_\tau + \phi/N_\tau - i\mu a_\tau$ and $\lambda^2 = M^2 + (a_s^2 a_\tau b_\sigma \pi)^2$. In Eq. (A.3), we assume that the lattice spacing ratio is given as $f(\gamma) = \gamma^2$ [170, 238, 239, 240]. Here, we also take account of Matsubara frequency as in Sect. A.2. Then, we can perform U_0 integration in the Polyakov gauge as

$$\begin{aligned} & \int \mathcal{D}U_0 \prod_{\mathbf{x}} \prod_{a=1}^{N_c} \{2 \cosh[N_\tau E a_\tau] + 2 \cos[\phi_a(\mathbf{x}) - N_\tau \mu a_\tau]\} \\ & = \prod_{\mathbf{x}} \left[2 \cosh(N_c a_\tau \mu N_\tau) + \frac{\sinh[(N_c + 1) E a_\tau N_\tau]}{\sinh[E a_\tau N_\tau]} \right] \\ & \equiv \prod_x \mathcal{R} , \end{aligned} \quad (\text{A.4})$$

where $E = \text{arcsinh}[\lambda/\gamma]$. Therefore, the effective free energy is given as

$$\begin{aligned} F & = -\log Z / \left(\sum_x \right) = -\log Z / (N_s^3 N_\tau a_s^3 a_\tau) \\ & = \left\{ a_s^2 a_\tau \sum_x \left[\frac{1}{2} b_\sigma (\sigma^2 + \pi^2) a_s^2 a_\tau \right] - \sum_x \log[\mathcal{R}] \right\} / (N_s^3 N_\tau a_s^3 a_\tau) \\ & = \frac{1}{2} \underbrace{(\sigma^2 + \pi^2) a_s a_\tau}_{[(a_s^2 a_\tau)^2]^{-1}} - \underbrace{\frac{1}{N_\tau a_\tau} \log[\mathcal{R}] \frac{1}{a_s^3}}_{[a_s^3 a_\tau]^{-1}} . \end{aligned} \quad (\text{A.5})$$

As a result, $a_s^3 a_\tau F$ is a dimensionless quantity.

A.2 Matsubara frequency

We here consider the effect of Matsubara frequency [162], assuming that the lattice spacing ratio is given as $f(\gamma) = \gamma^2$ [170, 238, 239, 240]. In the

lattice formulation, a formula for the Matsubara frequency is slightly different compared with continuum theory. Now, let us define I as

$$I \equiv \prod_{a=1}^{N_\tau/2} [\gamma^2 \sin^2 \bar{k}_n a_\tau + \lambda^2] = \prod_{a=1}^{N_\tau} [\gamma^2 \sin^2 \bar{k}_n a_\tau + \lambda^2]^{1/2}, \quad (\text{A.6})$$

where $\lambda^2 = M^2 + (a_s^2 a_\tau b_\sigma \pi)^2$, $\bar{k}_n a_\tau = 2\pi(n - 1/2)/N_\tau + \phi/N_\tau - i\mu a_\tau$ and $M = m_0 a_s + a_s^2 a_\tau b_\sigma \sigma$. Next, we differentiate Eq. (A.6) with respect to λ as

$$\frac{\partial}{\partial \lambda} \log I = \frac{1}{\Omega} \left[\oint \frac{dz}{2\pi i} \frac{\lambda}{\gamma^2 \sin^2(z + \phi/N_\tau - i\mu a_\tau)} \frac{-iN_\tau a_\tau}{1 + e^{1N_\tau z}} \right. \\ \left. \sum_z \frac{\lambda}{\gamma^2 2 \sin(\bar{z} + \phi/N_\tau - i\mu a_\tau) \cos(\bar{z} + \phi/N_\tau - i\mu a_\tau)} \frac{-iN_\tau a_\tau}{1 + e^{1N_\tau z}} \right], \quad (\text{A.7})$$

where Ω is a degeneracy factor. In (A.7), the first term vanishes and $\bar{z}$ satisfies

$$\gamma^2 \sin^2(\bar{z} + \phi/N_\tau - i\mu a_\tau) + \lambda^2 = 0, \quad (\text{A.8})$$

which leads

$$\bar{z} + \phi/N_\tau - i\mu a_\tau = \begin{cases} \pm iEa_\tau + 2\pi n \\ \pm iEa_\tau + 2\pi n + \pi \end{cases}, \quad (\text{A.9})$$

with $Ea_\tau = \text{arcsinh}[\lambda/\gamma]$. In order to obtain the expression for I , we calculate the above equation further more as

$$\frac{\partial}{\partial \lambda} \log I = \frac{1}{\Omega} \sum_{n=-\infty}^{\infty} \frac{1}{\gamma \cosh Ea_\tau} \left[\frac{N_\tau a_\tau}{1 + e^{-N_\tau a_\tau E - i\phi - N_\tau \mu a_\tau}} - \frac{N_\tau a_\tau}{1 + e^{N_\tau a_\tau E - i\phi - N_\tau \mu a_\tau}} \right] \\ = \frac{\partial E}{\partial \lambda} \left[\frac{N_\tau a_\tau}{1 + e^{-N_\tau a_\tau E - i\phi - N_\tau \mu a_\tau}} - \frac{N_\tau a_\tau}{1 + e^{N_\tau a_\tau E - i\phi - N_\tau \mu a_\tau}} \right] \\ = \frac{\partial}{\partial \lambda} [\log\{e^{N_\tau Ea_\tau} + e^{-i\phi - N_\tau \mu a_\tau}\} + \log\{e^{-N_\tau Ea_\tau} + e^{-i\phi - N_\tau \mu a_\tau}\}] \\ = \frac{\partial}{\partial \lambda} (-i\phi - N_\tau \mu a_\tau + \log\{2 \cosh[N_\tau Ea_\tau] + 2 \cos[\phi - iN_\tau \mu a_\tau]\}). \quad (\text{A.10})$$

After λ integration, we obtain I as

$$I = 2 \cosh[N_\tau Ea_\tau] + 2 \cos[\phi - iN_\tau \mu a_\tau], \quad (\text{A.11})$$

for $Ea_\tau = \text{arcsinh}[\lambda/\gamma]$.

A.3 Some formulae for cumulants in MF analysis

We show the expression for higher derivatives of $\hat{\mu} = N_c \mu / T$, for the quark chemical potential μ . In the following, we consider isotropic lattice $\gamma = 1$. We here summarize the effective potential as

$$\begin{aligned} F &= \frac{1}{2} b_\sigma \sigma^2 - T \log R[\sigma, \hat{\mu}] , \\ R[\sigma, \hat{\mu}] &= X_n[\sigma]^3 - 2X_n[\sigma] + 2 \cosh[\hat{\mu}] , \\ X_n[\sigma] &= 2 \cosh[E[\sigma]/T] , \\ E[\sigma] &= \operatorname{arcsinh}[m_0 + b_\sigma \sigma] , \end{aligned} \quad (\text{A.12})$$

for $b_\sigma = d/2N_c$ [162]. In order to obtain higher derivatives of $\hat{\mu}$, we should note a realign, $\frac{d}{d\hat{\mu}} = \frac{\partial}{\partial \hat{\mu}} + \frac{\partial \sigma(T, \hat{\mu})}{\partial \hat{\mu}} \frac{\partial}{\partial \sigma}$, due to the μ dependence of σ field. Applying the stationary condition, $\partial F / \partial \sigma = 0$, the derivatives of σ read

$$\frac{d\sigma}{d\hat{\mu}} = - \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} / \frac{\partial^2 F}{\partial \sigma^2} \right) , \quad (\text{A.13})$$

$$\begin{aligned} \frac{d^2 \sigma}{d\hat{\mu}^2} &= \left[- \frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 + 2 \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} - \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^2 \frac{\partial^3 F}{\partial \sigma^3} \right] \\ &\quad / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^3 , \end{aligned} \quad (\text{A.14})$$

$$\begin{aligned} \frac{d^3 \sigma}{d\hat{\mu}^3} &= \left[- \frac{\partial^4 F}{\partial \sigma \partial \hat{\mu}^3} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^3 + \left[3 \left(\frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} - \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) \right. \right. \\ &\quad \left. \left\{ \frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \left(-2 \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) \right\} \right] / \frac{\partial^2 F}{\partial \sigma^2} \\ &\quad + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \left\{ 3 \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 \frac{\partial^4 F}{\partial \sigma^2 \partial \hat{\mu}^2} - 3 \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^4 F}{\partial \sigma^3 \partial \hat{\mu}} + \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^2 \frac{\partial^4 F}{\partial \sigma^4} \right\} \\ &\quad / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^4 , \end{aligned} \quad (\text{A.15})$$

$$\begin{aligned}
\frac{d^4\sigma}{d\hat{\mu}^4} = & - \left\langle \left[\frac{\partial^5 F}{\partial\sigma\partial\hat{\mu}^4} - \left(4 \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \frac{\partial^5 F}{\partial\sigma^2\partial\hat{\mu}^3} \right) / \frac{\partial^2 F}{\partial\sigma^2} \right. \right. \\
& - \left[6 \frac{\partial^4 F}{\partial\sigma^2\partial\hat{\mu}^2} \left\{ \frac{\partial^3 F}{\partial\sigma\partial\hat{\mu}^2} \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^2 + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \left(-2 \frac{\partial^2 F}{\partial\sigma^2} \frac{\partial^3 F}{\partial\sigma^2\partial\hat{\mu}} + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \frac{\partial^3 F}{\partial\sigma^3} \right) \right\} \right] \\
& \left. / \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^3 \right. \\
& + \left[3 \frac{\partial^3 F}{\partial\sigma^3} \left\{ \frac{\partial^3 F}{\partial\sigma\partial\hat{\mu}^2} \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^2 + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \left(-2 \frac{\partial^2 F}{\partial\sigma^2} \frac{\partial^3 F}{\partial\sigma^2\partial\hat{\mu}} + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \frac{\partial^3 F}{\partial\sigma^3} \right) \right\}^2 \right] \\
& \left. / \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^6 \right. \\
& + \left[12 \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \left\{ \frac{\partial^3 F}{\partial\sigma\partial\hat{\mu}^2} \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^2 + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \left(-2 \frac{\partial^2 F}{\partial\sigma^2} \frac{\partial^3 F}{\partial\sigma^2\partial\hat{\mu}} + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \frac{\partial^3 F}{\partial\sigma^3} \right) \right\} \frac{\partial^4 F}{\partial\sigma^3\partial\hat{\mu}} \right] \\
& \left. / \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^4 \right. \\
& + \left\{ 6 \left(\frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \right)^2 \frac{\partial^5 F}{\partial\sigma^3\partial\hat{\mu}^2} \right\} / \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^2 \\
& - \left[6 \left(\frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \right)^2 \left\{ \frac{\partial^3 F}{\partial\sigma\partial\hat{\mu}^2} \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^2 \right. \right. \\
& \left. \left. + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \left(-2 \frac{\partial^2 F}{\partial\sigma^2} \frac{\partial^3 F}{\partial\sigma^2\partial\hat{\mu}} + \frac{\partial^2 F}{\partial\sigma\partial\hat{\mu}} \frac{\partial^3 F}{\partial\sigma^3} \right) \right\} \frac{\partial^4 F}{\partial\sigma^4} \right] / \left(\frac{\partial^2 F}{\partial\sigma^2} \right)^5
\end{aligned}$$

$$\begin{aligned}
& + \left\{ \left\{ 4 \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} - \left(4 \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) / \frac{\partial^2 F}{\partial \sigma^2} \right\} \left(- \frac{\partial^4 F}{\partial \sigma \partial \hat{\mu}^3} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^3 \right. \right. \\
& + \left[3 \left(\frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} - \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) \right. \\
& \left. \left. \left\{ \frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \left(-2 \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) \right\} \right] / \frac{\partial^2 F}{\partial \sigma^2} \right. \\
& + \left. \left. \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \left\{ 3 \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 \frac{\partial^4 F}{\partial \sigma^2 \partial \hat{\mu}^2} - 3 \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^4 F}{\partial \sigma^3 \partial \hat{\mu}} + \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^2 \frac{\partial^4 F}{\partial \sigma^4} \right\} \right) \right\} \\
& \quad / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^4 \\
& - 4 \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^3 \frac{\partial^5 F}{\partial \sigma^4 \partial \hat{\mu}} / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^3 + \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^4 \frac{\partial^5 F}{\partial \sigma^5} / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^4 \left. \right] / \frac{\partial^2 F}{\partial \sigma^2} \Bigg\rangle .
\end{aligned} \tag{A.16}$$

We can find cumulant ratios as

$$-c_B^{(1)} T^4 \equiv \frac{dF}{d\hat{\mu}} = \frac{\partial F}{\partial \hat{\mu}} , \tag{A.17}$$

$$-c_B^{(2)} T^4 = \frac{\partial^2 F}{\partial \hat{\mu}^2} - \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^2 / \frac{\partial^2 F}{\partial \sigma^2} , \tag{A.18}$$

$$\begin{aligned}
-c_B^{(3)} T^4 &= \frac{\partial^3 F}{\partial \hat{\mu}^3} \\
&- \left[\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \left\{ 3 \frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 \right. \right. \\
&+ \left. \left. \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \left(-3 \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) \right\} \right] / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^3
\end{aligned} \tag{A.19}$$

$$\begin{aligned}
-c_B^{(4)} T^4 = & \left[-3 \left(\frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} \right)^2 \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^4 \right. \\
& - 4 \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^4 F}{\partial \sigma \partial \hat{\mu}^3} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^4 + \frac{\partial^4 F}{\partial \hat{\mu}^4} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^5 \\
& + 6 \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^2 \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 \left\{ -2 \left(\frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} \right)^2 + \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^4 F}{\partial \sigma^2 \partial \hat{\mu}^2} \right\} \\
& - 6 \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^2 \left(-2 \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} + \frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} \right) \\
& - 4 \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^3 \frac{\partial^2 F}{\partial \sigma^2} \left\{ -3 \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} \frac{\partial^3 F}{\partial \sigma^3} + \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^4 F}{\partial \sigma^3 \partial \hat{\mu}} \right\} \\
& \left. + \left(\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} \right)^4 \left\{ -3 \left(\frac{\partial^3 F}{\partial \sigma^3} \right)^2 + \frac{\partial^2 F}{\partial \sigma^2} \frac{\partial^4 F}{\partial \sigma^4} \right\} \right] / \left(\frac{\partial^2 F}{\partial \sigma^2} \right)^5 \quad (\text{A.20})
\end{aligned}$$

The derivatives of the free energy are obtained as

$$\frac{\partial F}{\partial \sigma} = b_\sigma \sigma - \left(T \frac{\partial R}{\partial \sigma} \right) / R \quad (\text{A.21})$$

$$\frac{\partial F}{\partial \hat{\mu}} = -T \frac{\partial R}{\partial \hat{\mu}} / R \quad (\text{A.22})$$

$$\frac{\partial^2 F}{\partial \sigma \partial \hat{\mu}} = T \frac{\partial R}{\partial \hat{\mu}} \frac{\partial R}{\partial \sigma} / R^2 - T \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} / R \quad (\text{A.23})$$

$$\frac{\partial^2 F}{\partial \sigma^2} = b_\sigma - T \left[- \left(\frac{\partial R^2}{\partial \sigma} / R^2 \right) + \frac{\partial^2 R}{\partial \sigma^2} / R \right] \quad (\text{A.24})$$

$$\frac{\partial^2 F}{\partial \hat{\mu}^2} = - \left[T \left(- \frac{\partial R^2}{\partial \hat{\mu}} / R^2 + \frac{\partial^2 R}{\partial \hat{\mu}^2} / R \right) \right], \quad (\text{A.25})$$

$$\frac{\partial^3 F}{\partial \sigma^3} = -T \left\{ 2 \frac{\partial R^3}{\partial \sigma} / R^3 - \left(3 \frac{\partial R}{\partial \sigma} \frac{\partial^2 R}{\partial \sigma^2} \right) / R^2 + \frac{\partial^3 R}{\partial \sigma^3} / R \right\} , \quad (\text{A.26})$$

$$\begin{aligned} \frac{\partial^3 F}{\partial \sigma^2 \partial \hat{\mu}} = -T & \left\{ 2 \frac{\partial R}{\partial \hat{\mu}} \left(\frac{\partial R}{\partial \sigma} \right)^2 / R^3 - 2 \frac{\partial R}{\partial \sigma} \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} / R^2 \right. \\ & \left. - \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^2 R}{\partial \sigma^2} / R^2 + \frac{\partial^3 R}{\partial \sigma^2 \partial \hat{\mu}} / R \right\} \end{aligned} \quad (\text{A.27})$$

$$\begin{aligned} \frac{\partial^3 F}{\partial \sigma \partial \hat{\mu}^2} = -T & \left[\left\{ 2 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^2 / R^3 - \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^2 \right\} \frac{\partial R}{\partial \sigma} \right. \\ & \left. - 2 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} / R^2 + \frac{\partial^3 R}{\partial \sigma \partial \hat{\mu}^2} / R \right] , \end{aligned} \quad (\text{A.28})$$

$$\frac{\partial^3 F}{\partial \hat{\mu}^3} = -T \left\{ 2 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^3 / R^3 - 3 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^2 + \frac{\partial^3 R}{\partial \hat{\mu}^3} / R \right\} , \quad (\text{A.29})$$

$$\begin{aligned} \frac{\partial^4 F}{\partial \sigma^4} = -T & \left\{ -6 \left(\frac{\partial R}{\partial \sigma} \right)^4 / R^4 + 12 \left(\frac{\partial R}{\partial \sigma} \right)^2 \frac{\partial^2 R}{\partial \sigma^2} / R^3 \right. \\ & \left. - 3 \left(\frac{\partial^2 R}{\partial \sigma^2} \right)^2 / R^2 - 4 \frac{\partial R}{\partial \sigma} \frac{\partial^3 R}{\partial \sigma^3} / R^2 + \frac{\partial^4 R}{\partial \sigma^4} / R \right\} , \end{aligned} \quad (\text{A.30})$$

$$\begin{aligned} \frac{\partial^4 F}{\partial \sigma^3 \partial \hat{\mu}} = -T & \left\{ -6 \frac{\partial R}{\partial \hat{\mu}} \left(\frac{\partial R}{\partial \sigma} \right)^3 / R^4 + 6 \left(\frac{\partial R}{\partial \sigma} \right)^2 \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} / R^3 \right. \\ & + 6 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial R}{\partial \sigma} \frac{\partial^2 R}{\partial \sigma^2} / R^3 - 3 \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} \frac{\partial^2 R}{\partial \sigma^2} / R^2 \\ & \left. - 3 \frac{\partial R}{\partial \sigma} \frac{\partial^3 R}{\partial \sigma^2 \partial \hat{\mu}} / R^2 - \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^3 R}{\partial \sigma^3} / R^2 + \frac{\partial^4 R}{\partial \sigma^3 \partial \hat{\mu}} / R \right\} , \end{aligned} \quad (\text{A.31})$$

$$\begin{aligned} \frac{\partial^4 F}{\partial \sigma^2 \partial \hat{\mu}^2} = -T & \left[\left\{ -6 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^2 / R^4 + 2 \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^3 \right\} \left(\frac{\partial R}{\partial \sigma} \right)^2 \right. \\ & + 8 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial R}{\partial \sigma} \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} / R^3 - \left(2 \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}}^2 + 2 \frac{\partial R}{\partial \sigma} \frac{\partial^3 R}{\partial \sigma \partial \hat{\mu}^2} \right) / R^2 \\ & + \left\{ \left(2 \frac{\partial R}{\partial \hat{\mu}} \right)^2 / R^3 - \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^2 \right\} \frac{\partial^2 R}{\partial \sigma^2} \\ & \left. - 2 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^3 R}{\partial \sigma^2 \partial \hat{\mu}} / R^2 + \frac{\partial^4 R}{\partial \sigma^2 \partial \hat{\mu}^2} / R \right] , \end{aligned} \quad (\text{A.32})$$

$$\begin{aligned}
\frac{\partial^4 F}{\partial \sigma \partial \hat{\mu}^3} = & -T \left[\left\{ -6 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^3 / R^4 + 6 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^3 - \frac{\partial^3 R}{\partial \hat{\mu}^3} / R^2 \right\} \frac{\partial R}{\partial \sigma} \right. \\
& + 3 \left\{ 2 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^2 / R^3 - \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^2 \right\} \frac{\partial^2 R}{\partial \sigma \partial \hat{\mu}} \\
& \left. - 3 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^3 R}{\partial \sigma \partial \hat{\mu}^2} / R^2 + \frac{\partial^4 R}{\partial \sigma \partial \hat{\mu}^3} / R \right] , \tag{A.33}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial^4 F}{\partial \hat{\mu}^4} = & -T \left[-6 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^4 / R^4 + 12 \left(\frac{\partial R}{\partial \hat{\mu}} \right)^2 \frac{\partial^2 R}{\partial \hat{\mu}^2} / R^3 - 3 \left(\frac{\partial^2 R}{\partial \hat{\mu}^2} \right)^2 / R^2 \right. \\
& \left. - 4 \frac{\partial R}{\partial \hat{\mu}} \frac{\partial^3 R}{\partial \hat{\mu}^3} / R^2 + \frac{\partial^4 R}{\partial \hat{\mu}^4} / R \right] \tag{A.34}
\end{aligned}$$

The derivatives of R are obtained as

$$\frac{\partial R}{\partial \hat{\mu}} = 2 \sinh[\hat{\mu}] , \tag{A.35}$$

$$\frac{\partial R}{\partial \sigma} = -2 \frac{\partial X_n[\sigma]}{\partial \sigma} + 3 X_n[\sigma]^2 \frac{\partial X_n[\sigma]}{\partial \sigma} , \tag{A.36}$$

$$\frac{\partial^2 R}{\partial \hat{\mu}^2} = 2 \cosh[\hat{\mu}] , \tag{A.37}$$

$$\frac{\partial^2 R}{\partial \sigma^2} = 6 X_n[\sigma] \left(\frac{\partial X_n[\sigma]}{\partial \sigma} \right)^2 - 2 \frac{\partial^2 X_n[\sigma]}{\partial \sigma^2} + 3 X_n[\sigma]^2 \frac{\partial^2 X_n[\sigma]}{\partial \sigma^2} \tag{A.38}$$

$$\frac{\partial^3 R}{\partial \hat{\mu}^3} = 2 \sinh[\hat{\mu}] \tag{A.39}$$

$$\begin{aligned}
\frac{\partial^3 R}{\partial \sigma^3} = & 6 \left(\frac{\partial X_n[\sigma]}{\partial \sigma} \right)^3 + 18 X_n[\sigma] \frac{\partial X_n[\sigma]}{\partial \sigma} \frac{\partial^2 X_n[\sigma]}{\partial \sigma^2} \\
& - 2 \frac{\partial^3 X_n[\sigma]}{\partial \sigma^3} + 3 X_n[\sigma]^2 \frac{\partial^3 X_n[\sigma]}{\partial \sigma^3} \tag{A.40}
\end{aligned}$$

$$\frac{\partial^4 R}{\partial \hat{\mu}^4} = 2 \cosh[\hat{\mu}] \tag{A.41}$$

$$\begin{aligned}
\frac{\partial^4 R}{\partial \sigma^4} = & 36 \left(\frac{\partial X_n[\sigma]}{\partial \sigma} \right)^2 \frac{\partial^2 X_n[\sigma]}{\partial \sigma^2} + 18 X_n[\sigma] \left(\frac{\partial^2 X_n[\sigma]}{\partial \sigma^2} \right)^2 \\
& + 24 X_n[\sigma] \frac{\partial X_n[\sigma]}{\partial \sigma} \frac{\partial^3 X_n[\sigma]}{\partial \sigma^3} - 2 \frac{\partial^4 X_n[\sigma]}{\partial \sigma^4} + 3 X_n[\sigma]^2 \frac{\partial^4 X_n[\sigma]}{\partial \sigma^4} , \tag{A.42}
\end{aligned}$$

and other derivatives are equal to zero in the current analyses. Derivatives of a matrix for X_n are given as

$$\frac{\partial X_n}{\partial \sigma} = \left(2 \sinh[E[\sigma]/T] \frac{\partial E}{\partial \sigma} \right) / T , \quad (\text{A.43})$$

$$\frac{\partial^2 X_n}{\partial \sigma^2} = 2 \left[\cosh[E[\sigma]/T] \left(\frac{\partial E}{\partial \sigma} \right)^2 / T^2 + \sinh[E[\sigma]/T] \frac{\partial^2 E}{\partial \sigma^2} / T \right] , \quad (\text{A.44})$$

$$\begin{aligned} \frac{\partial^3 X_n}{\partial \sigma^3} = 2 & \left[\sinh[E[\sigma]/T] \left(\frac{\partial E}{\partial \sigma} \right)^3 / T^3 + 3 \cosh[E[\sigma]/T] \frac{\partial E}{\partial \sigma} \frac{\partial^2 E}{\partial \sigma^2} / T^2 \right. \\ & \left. + \sinh[E[\sigma]/T] \frac{\partial^3 E}{\partial \sigma^3} / T \right] , \end{aligned} \quad (\text{A.45})$$

$$\begin{aligned} \frac{\partial^4 X_n}{\partial \sigma^4} = 2 & \left(\cosh[E[\sigma]/T] \left(\frac{\partial E}{\partial \sigma} \right)^4 / T^4 + 6 \sinh[E[\sigma]/T] \left(\frac{\partial E}{\partial \sigma} \right)^2 \frac{\partial^2 E}{\partial \sigma^2} / T^3 \right. \\ & + 3 \cosh[E[\sigma]/T] \left(\frac{\partial^2 E}{\partial \sigma^2} \right)^2 / T^2 + 4 \cosh[E[\sigma]/T] \frac{\partial E}{\partial \sigma} \frac{\partial^3 E}{\partial \sigma^3} / T^2 \\ & \left. + \sinh[E[\sigma]/T] \frac{\partial^4 E}{\partial \sigma^4} / T \right) , \end{aligned} \quad (\text{A.46})$$

and derivatives for E are obtained as

$$\frac{\partial E}{\partial \sigma} = b_\sigma / \sqrt{1 + (m_0 + b_\sigma \sigma)^2} , \quad (\text{A.47})$$

$$\frac{\partial^2 E}{\partial \sigma^2} = -b_\sigma^2 (m_0 + b_\sigma \sigma) / (1 + (m_0 + b_\sigma \sigma)^2)^{3/2} , \quad (\text{A.48})$$

$$\frac{\partial^3 E}{\partial \sigma^3} = (3b_\sigma^3 (m_0 + b_\sigma \sigma)^2) / (1 + (m_0 + b_\sigma \sigma)^2)^{5/2} - b_\sigma^3 / (1 + (m_0 + b_\sigma \sigma)^2)^{3/2} , \quad (\text{A.49})$$

$$\begin{aligned} \frac{\partial^4 E}{\partial \sigma^4} = & (-15b_\sigma^4 (m_0 + b_\sigma \sigma)^3) / (1 + (m_0 + b_\sigma \sigma)^2)^{7/2} \\ & + (9b_\sigma^4 (m_0 + b_\sigma \sigma)) / (1 + (m_0 + b_\sigma \sigma)^2)^{5/2} . \end{aligned} \quad (\text{A.50})$$

If we consider the anisotropic lattice case, the energy reads $E[\sigma] = \text{arcsinh}[(m_0 + b_\sigma \sigma)/\gamma] = \log \left[(m_0 + b_\sigma \sigma)/\gamma + \sqrt{1 + (m_0 + b_\sigma \sigma)^2/\gamma^2} \right]$; then higher deriva-

tives of E are given by

$$\frac{\partial E}{\partial \sigma} = \frac{b_\sigma}{\gamma} \frac{1}{\sqrt{1 + (m_0 + b_\sigma \sigma)^2 / \gamma^2}}, \quad (\text{A.51})$$

$$\frac{\partial^2 E}{\partial \sigma^2} = -\frac{b_\sigma^2}{\gamma^2} \frac{(m_0 + b_\sigma \sigma) / \gamma}{(1 + (m_0 + b_\sigma \sigma)^2 / \gamma^2)^{3/2}}, \quad (\text{A.52})$$

$$\frac{\partial^3 E}{\partial \sigma^3} = \frac{b_\sigma^3}{\gamma^3} \frac{(m_0 + b_\sigma \sigma)^2 / \gamma^2}{(1 + (m_0 + b_\sigma \sigma)^2 / \gamma^2)^{5/2}} - \frac{b_\sigma^3}{\gamma^3} \frac{1}{(1 + (m_0 + b_\sigma \sigma)^2 / \gamma^2)^{3/2}}, \quad (\text{A.53})$$

$$\frac{\partial^4 E}{\partial \sigma^4} = -\frac{b_\sigma^4}{\gamma^4} \frac{15(m_0 + b_\sigma \sigma)^3 / \gamma^3}{(1 + (m_0 + b_\sigma \sigma)^2 / \gamma^2)^{7/2}} + \frac{b_\sigma^4}{\gamma^4} \frac{9(m_0 + b_\sigma \sigma) / \gamma}{(1 + (m_0 + b_\sigma \sigma)^2 / \gamma^2)^{5/2}}.$$

We evaluate cumulant ratios as

$$R_{3,2}^B = \frac{c_B^{(3)}}{c_B^{(2)}}, \quad R_{4,2}^B = \frac{c_B^{(4)}}{c_B^{(2)}}, \quad (\text{A.54})$$

in Sect. 4.1.

We now show the cumulant ratios in the QCD phase diagram in MF with various mass parameter in Figs. A.1, A.2, and A.3. The phase boundary is determined by the peak position of the chiral susceptibility. At small μ/T , the phase transition is considered to be crossover and its pseudo-critical line is connected with the first-order phase-transition line at a critical point (CP) since the bare quark mass is finite [35, 162]. We here determine the CP position as a location at which the peak height of the chiral susceptibility is the largest on the phase transition line.

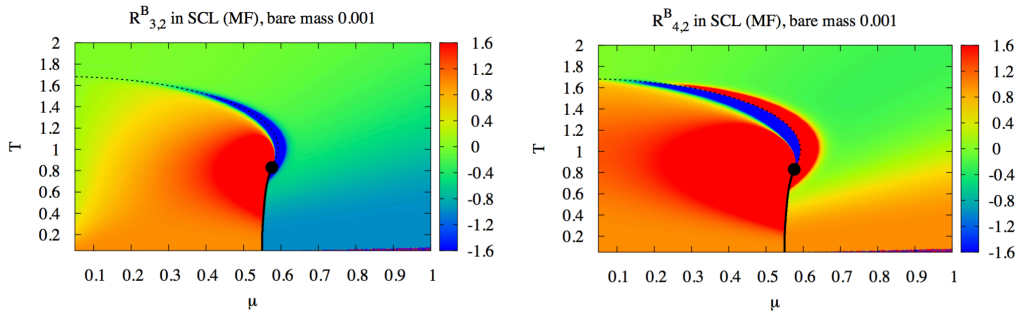


Figure A.1: $R_{3,2}^B$ and $R_{4,2}^B$ in the QCD phase diagram at $m_0 = 0.001$. A dash line (solid line) represents the crossover (first-order) phase transition. A circle shows the CP location.

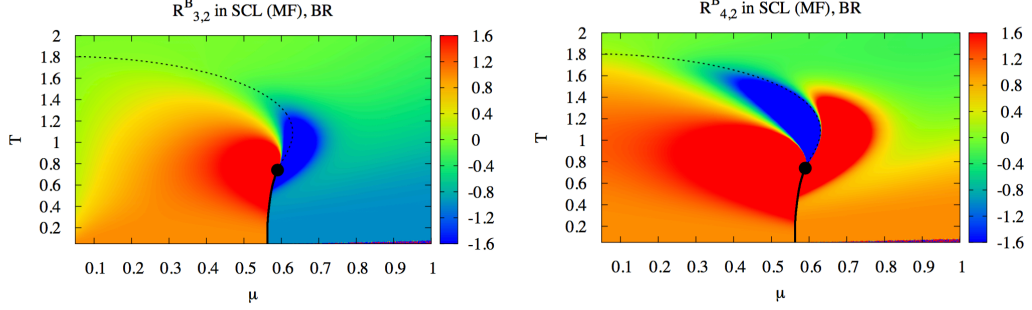


Figure A.2: $R_{3,2}^B$ and $R_{4,2}^B$ in the QCD phase diagram at $m_0 \simeq 0.019$ by using parameters, $a^{-1} = 497$ MeV and $m_0 = 9.5$ MeV in Ref. [279]. A dash line (solid line) represents the crossover (first-order) phase transition. A circle shows the CP location.

In Fig. A.2, we use a bare-quark mass value as $m_0 a \simeq 0.019$ since we find that $a^{-1} = 497$ MeV and $m_0 = 9.5$ MeV when we fit hadron masses in the strong coupling limit [279]. As you can see in Figs. A.1, A.2, and A.3,

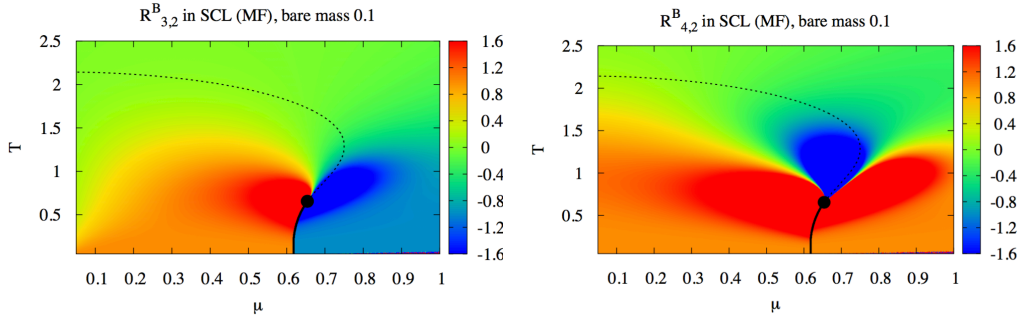


Figure A.3: $R_{3,2}^B$ and $R_{4,2}^B$ in the QCD phase diagram at $m_0 = 0.1$. A dash line (solid line) represents the crossover (first-order) phase transition. A circle shows the CP location.

the negative region of cumulant ratios are almost consistent with the phase boundary.

Appendix B

Formulae with fluctuation effects

We review some formulae in AFMC based on Refs. [78, 172]

B.1 Fermion determinant with fluctuations

Here, we introduce recursion formulae to evaluate X_{N_τ} in the fermion determinant and its derivatives based on Refs. [172, 233, 238, 240].

B.1.1 Fermion determinant and recursion formulae

When we obtain the analytic expression for the fermion determinant, we introduce a matrix B_{N_τ} as [233, 238, 240]

$$B_{N_\tau}(I_1, \dots, I_{N_\tau}) = \begin{vmatrix} I_1 & e^{\mu/f(\gamma)} & 0 & \dots & 0 \\ -e^{-\mu/f(\gamma)} & I_2 & e^{\mu/f(\gamma)} & & \vdots \\ 0 & -e^{-\mu/f(\gamma)} & I_3 & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & I_{N_\tau-1} & e^{\mu/f(\gamma)} \\ 0 & \dots & 0 & -e^{-\mu/f(\gamma)} & I_{N_\tau} \end{vmatrix}, \quad (\text{B.1})$$

where $I_k = 2m_{\mathbf{x},k}/\gamma$ is related to the effective mass terms and $f(\gamma) = \gamma^2$. B_k is obtained by a recursion formula [233, 238, 240] as

$$B_k(I_1, \dots, I_k) = I_k B_{k-1}(I_1, \dots, I_{k-1}) + B_{k-2}(I_1, \dots, I_{k-2}), \quad (\text{B.2})$$

for $B_1 = I_1$, $B_2 = I_1 I_2 + 1$. As for a matrix X_{N_τ} in Eq. (3.15), we utilize a following recursion formula as

$$X_k(I_1, \dots, I_k) = B_k(I_1, \dots, I_k) + B_{k-2}(I_2, \dots, I_{k-1}) ; \quad (\text{B.3})$$

then we evaluate the fermion determinant from the above recursion formulae.

It should be noted that the mean-field calculations are realized, supposing that $I_k = \text{const.}$ for any k . I_k takes a different value at each space-time when fluctuation effects are included; $I_k \neq I_l$ for $k \neq l$.

B.1.2 Order parameters and Susceptibilities

We introduce formulae for order parameters and their susceptibilities [172, 233]. First, we show the chiral condensate $\langle \sigma_0 \rangle$ and the chiral susceptibility χ_σ as

$$\begin{aligned} \langle \sigma_0 \rangle &= -\frac{1}{L^3 N_\tau} \frac{\partial \ln \mathcal{Z}_{\text{AF}}}{\partial m_0} = -\frac{1}{L^3 N_\tau} \frac{1}{\mathcal{Z}_{\text{AF}}} \int \mathcal{D}[\sigma, \pi] \left(-\frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \right) e^{-S_{\text{eff}}^{\text{AF}}} , \\ &= \frac{1}{L^3 N_\tau} \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \right\rangle , \end{aligned} \quad (\text{B.4})$$

$$\begin{aligned} \chi_\sigma &= \frac{1}{L^3 N_\tau} \frac{\partial^2 \ln \mathcal{Z}_{\text{AF}}}{\partial m_0^2} = \frac{1}{L^3 N_\tau} \left[\left\langle \left(\frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \right)^2 \right\rangle - \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \right\rangle^2 - \left\langle \frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial m_0^2} \right\rangle \right] \\ &= \frac{1}{L^3 N_\tau} \left[\left\langle \left(\frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} - \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \right\rangle \right)^2 \right\rangle - \left\langle \frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial m_0^2} \right\rangle \right] , \end{aligned} \quad (\text{B.5})$$

where $\mathcal{Z}_{\text{AF}} = \int \mathcal{D}[\sigma, \pi] \exp(-S_{\text{eff}}^{\text{AF}})$. Derivatives of the effective action with respect to quark mass m_0 in Eqs. (B.4) and (B.5) are obtained as

$$\begin{aligned} \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} &= -\sum_{\mathbf{x}} \frac{\partial \ln R(\mathbf{x})}{\partial m_0} = -\sum_{\mathbf{x}} \frac{1}{R(\mathbf{x})} \frac{\partial I_x}{\partial m_0} \frac{\partial X_{N_\tau}(\mathbf{x})}{\partial I_x} \frac{\partial R(\mathbf{x})}{\partial X_{N_\tau}(\mathbf{x})} \\ &= -\sum_{\mathbf{x}} \frac{1}{R(\mathbf{x})} \frac{2}{\gamma} \sum_t B_{N_\tau-1}(I_{t+1}, \dots, I_{N_\tau}, I_1, \dots, I_{t-1}) (3X_{N_\tau}(\mathbf{x})^2 - 2) , \end{aligned} \quad (\text{B.6})$$

$$\begin{aligned}
\frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial m_0^2} = & \sum_{\mathbf{x}} \left[\frac{1}{R(\mathbf{x})^2} \left(\frac{2}{\gamma} \sum_t B_{N_\tau-1}(I_{t+1}, \dots, I_{N_\tau}, I_1, \dots, I_{t-1}) (3X_{N_\tau}(\mathbf{x})^2 - 2) \right)^2 \right. \\
& - \frac{1}{R(\mathbf{x})} \left(\frac{2}{\gamma} \right)^2 \sum_{t, t'} \times \\
& \left\{ \sum_{t > t'} B_{N-t+t'-1}(I_{t+1}, \dots, I_N, I_1, \dots, I_{t'-1}) B_{t-t'-1}(I_{t'+1}, \dots, I_{t-1}) \right. \\
& + \sum_{t < t'} B_{t'-t-1}(I_{t+1}, \dots, I_{t'-1}) B_{N-t'+t-1}(I_{t'+1}, \dots, I_N, I_1, \dots, I_{t-1}) \left. \right\} \\
& (3X_{N_\tau}(\mathbf{x})^2 - 2) \\
& \left. - \frac{1}{R(\mathbf{x})} \frac{24}{\gamma^2} X_{N_\tau}(\mathbf{x}) \left(\sum_t B_{N_\tau-1}(I_{t+1}, \dots, I_{N_\tau}, I_1, \dots, I_{t-1}) \right)^2 \right] , \tag{B.7}
\end{aligned}$$

where $R(\mathbf{x}) = X_{N_\tau}(\mathbf{x})^3 - 2X_{N_\tau}(\mathbf{x}) + 2 \cosh(3N_\tau\mu/\gamma^2)$. Next, the quark number density ρ_q and quark number susceptibility $\chi_{\mu, \mu}$ are evaluated as

$$\rho_q = -\frac{T}{L^3} \frac{\partial \ln Z}{\partial \mu} = \frac{T}{L^3} \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial \mu} \right\rangle , \tag{B.8}$$

$$\chi_{\mu, \mu} = \frac{1}{L^3 N_\tau} \frac{\partial^2 \ln Z}{\partial \mu^2} = \frac{1}{L^3 N_\tau} \left[\left\langle \left(\frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial \mu} - \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial \mu} \right\rangle \right)^2 \right\rangle - \left\langle \frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial \mu^2} \right\rangle \right] , \tag{B.9}$$

where

$$\frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial \mu} = - \sum_{\mathbf{x}} \frac{\partial \ln R(\mathbf{x})}{\partial \mu} = - \sum_{\mathbf{x}} \frac{1}{R(\mathbf{x})} \frac{2 \cdot 3N_\tau}{\gamma^2} \sinh \left(\frac{3N_\tau\mu}{\gamma^2} \right) , \tag{B.10}$$

$$\begin{aligned}
\frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial \mu^2} = & \sum_{\mathbf{x}} \left[\frac{1}{R(\mathbf{x})^2} \left(\frac{2 \cdot 3N_\tau}{\gamma^2} \sinh \left(\frac{3N_\tau\mu}{\gamma^2} \right) \right)^2 \right. \\
& \left. - \frac{2}{R(\mathbf{x})} \left(\frac{3N_\tau}{\gamma^2} \right)^2 \cosh \left(\frac{3N_\tau\mu}{\gamma^2} \right) \right] . \tag{B.11}
\end{aligned}$$

We can also obtain the mixed susceptibility $\chi_{m_0, \mu}$ as

$$\begin{aligned}\chi_{m_0, \mu} &= \frac{1}{L^3 N_\tau} \frac{\partial^2 \ln Z}{\partial \mu \partial m_0} \\ &= \frac{1}{L^3 N_\tau} \left[\left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \cdot \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial \mu} \right\rangle - \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial m_0} \right\rangle \left\langle \frac{\partial S_{\text{eff}}^{\text{AF}}}{\partial \mu} \right\rangle - \left\langle \frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial m_0 \partial \mu} \right\rangle \right],\end{aligned}\tag{B.12}$$

where

$$\begin{aligned}\frac{\partial^2 S_{\text{eff}}^{\text{AF}}}{\partial m_0 \partial \mu} &= \sum_{\mathbf{x}} \frac{1}{R(\mathbf{x})^2} \frac{2 \cdot 3 N_\tau}{\gamma^2} \sinh \left(\frac{3 N_\tau \mu}{\gamma^2} \right) \left(\frac{2}{\gamma} \right) \\ &\quad \times \sum_t B_{N_\tau-1}(I_{t+1}, \dots, I_{N_\tau}, I_1, \dots, I_{t-1}) (3 X_{N_\tau}(\mathbf{x})^2 - 2) .\end{aligned}\tag{B.13}$$

B.2 Higher order derivatives of the baryon chemical potential in the auxiliary field Monte Carlo method

Higher-order derivatives with respect to dimensionless chemical potential $\hat{\mu}(= N_c \mu / T)$ are given in this appendix based on Ref. [78]. Fields Φ, Z and S denote all auxiliary fields, the partition function, and the action in AFMC in the strong coupling limit, respectively. Cumulants up to 4th order are given as

$$c_{\text{B}}^{(1)} = \frac{1}{VT^3} \frac{\partial(\log Z)}{\partial \hat{\mu}} = \frac{1}{VT^3} \left[\frac{1}{Z} \int \mathcal{D}\Phi \left(-\frac{\partial S}{\partial \hat{\mu}} \right) e^{-S} \right] = \frac{1}{VT^3} \left\langle -\frac{\partial S}{\partial \hat{\mu}} \right\rangle ,\tag{B.14}$$

$$c_{\text{B}}^{(2)} = \frac{1}{VT^3} \frac{\partial^2(\log Z)}{\partial \hat{\mu}^2} = \frac{1}{VT^3} \left[\left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right)^2 \right\rangle - \left\langle \frac{\partial^2 S}{\partial \hat{\mu}^2} \right\rangle \right] ,\tag{B.15}$$

$$\begin{aligned}c_{\text{B}}^{(3)} &= \frac{1}{VT^3} \frac{\partial^3(\log Z)}{\partial \hat{\mu}^3} \\ &= \frac{1}{VT^3} \left[- \left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right)^3 \right\rangle - \left\langle \frac{\partial^3 S}{\partial \hat{\mu}^3} \right\rangle \right. \\ &\quad \left. + 3 \left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right) \left(\frac{\partial^2 S}{\partial \hat{\mu}^2} - \left\langle \frac{\partial^2 S}{\partial \hat{\mu}^2} \right\rangle \right) \right\rangle \right] ,\end{aligned}\tag{B.16}$$

$$\begin{aligned}
c_B^{(4)} &= \frac{1}{VT^3} \frac{\partial^4(\log Z)}{\partial \hat{\mu}^4} \\
&= \frac{1}{VT^3} \left[\left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right)^4 \right\rangle - 3 \left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right)^2 \right\rangle^2 \right. \\
&\quad + 3 \left\langle \left(\frac{\partial^2 S}{\partial \hat{\mu}^2} - \left\langle \frac{\partial^2 S}{\partial \hat{\mu}^2} \right\rangle \right)^2 \right\rangle \\
&\quad - 6 \left\langle \left\{ \left(\frac{\partial S}{\partial \hat{\mu}} \right)^2 - \left\langle \left(\frac{\partial S}{\partial \hat{\mu}} \right)^2 \right\rangle \right\} \left(\frac{\partial^2 S}{\partial \hat{\mu}^2} - \left\langle \frac{\partial^2 S}{\partial \hat{\mu}^2} \right\rangle \right) \right\rangle \\
&\quad + 4 \left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right) \left(\frac{\partial^3 S}{\partial \hat{\mu}^3} - \left\langle \frac{\partial^3 S}{\partial \hat{\mu}^3} \right\rangle \right) \right\rangle \\
&\quad \left. + 12 \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \left\langle \left(\frac{\partial S}{\partial \hat{\mu}} - \left\langle \frac{\partial S}{\partial \hat{\mu}} \right\rangle \right) \left(\frac{\partial^2 S}{\partial \hat{\mu}^2} - \left\langle \frac{\partial^2 S}{\partial \hat{\mu}^2} \right\rangle \right) \right\rangle - \left\langle \frac{\partial^4 S}{\partial \hat{\mu}^4} \right\rangle \right] , \tag{B.17}
\end{aligned}$$

where $S = \sum_{\mathbf{k}, \tau, f > 0} \frac{L^3}{4N_c} f(\mathbf{k}) [|\sigma_{\mathbf{k}, \tau}|^2 + |\pi_{\mathbf{k}, \tau}|^2] - \sum_{\mathbf{x}} \log R(\mathbf{x})$ and $R(\mathbf{x}) = X_N^3(\mathbf{x}) - 2X_N(\mathbf{x}) + 2 \cosh \hat{\mu}$. The above expressions contain the derivatives of the action and they read

$$\frac{\partial S}{\partial \hat{\mu}} = - \sum_{\mathbf{x}} \frac{1}{R(\mathbf{x})} 2 \sinh \hat{\mu} , \tag{B.18}$$

$$\frac{\partial^2 S}{\partial \hat{\mu}^2} = \sum_{\mathbf{x}} \left[\frac{1}{R(\mathbf{x})^2} (2 \sinh \hat{\mu})^2 - \frac{1}{R(\mathbf{x})} 2 \cosh \hat{\mu} \right] , \tag{B.19}$$

$$\frac{\partial^3 S}{\partial \hat{\mu}^3} = \sum_{\mathbf{x}} \left[-\frac{2}{R(\mathbf{x})^3} (2 \sinh \hat{\mu})^3 + \frac{3}{R(\mathbf{x})^2} (2 \sinh \hat{\mu}) (2 \cosh \hat{\mu}) - \frac{1}{R(\mathbf{x})} 2 \sinh \hat{\mu} \right] , \tag{B.20}$$

$$\begin{aligned}
\frac{\partial^4 S}{\partial \hat{\mu}^4} &= \sum_{\mathbf{x}} \left[\frac{6}{R(\mathbf{x})^4} (2 \sinh \hat{\mu})^4 - \frac{12}{R(\mathbf{x})^3} (2 \sinh \hat{\mu})^2 2 \cosh \hat{\mu} \right. \\
&\quad \left. + \frac{3}{R(\mathbf{x})^2} (2 \cosh \hat{\mu})^2 + \frac{4}{R(\mathbf{x})^2} (2 \sinh \hat{\mu})^2 - \frac{1}{R(\mathbf{x})} 2 \cosh \hat{\mu} \right] . \tag{B.21}
\end{aligned}$$

When we simulate higher-order cumulants, we use these formulae in Sect. 4.

B.3 Cumulants in AMFC

We here show cumulants at $\mu/T = 0.2$ and 0.8 for completeness. First, we show cumulants at $\mu/T = 0.2$ as a function of the reduced temperature $(T - T_c)/T_c$ in Figs. B.1 and B.2. T_c is defined as the critical temperature with the corresponding conditions: the lattice size and μ/T .

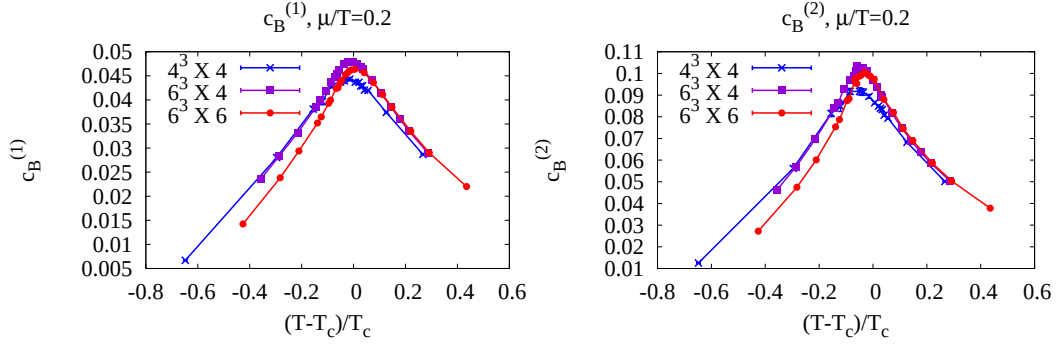


Figure B.1: The first (left panel) and second (right panel) order cumulants at $\mu/T = 0.2$ on $4^3 \times 4$, $6^3 \times 4$, and $6^3 \times 6$ lattices.

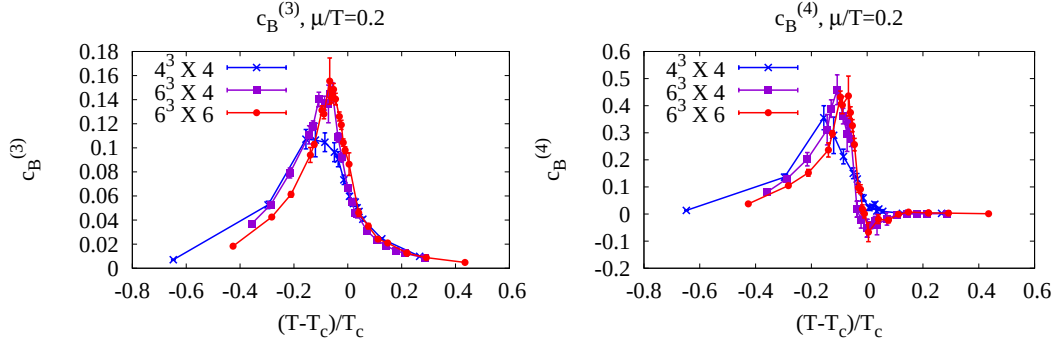


Figure B.2: The third (left panel) and fourth (right panel) order cumulants at $\mu/T = 0.2$ on $4^3 \times 4$, $6^3 \times 4$, and $6^3 \times 6$ lattices.

Next, we show cumulants at $\mu/T = 0.8$ as a function of the reduced temperature $(T - T_c)/T_c$ in Figs. B.3 and B.4.

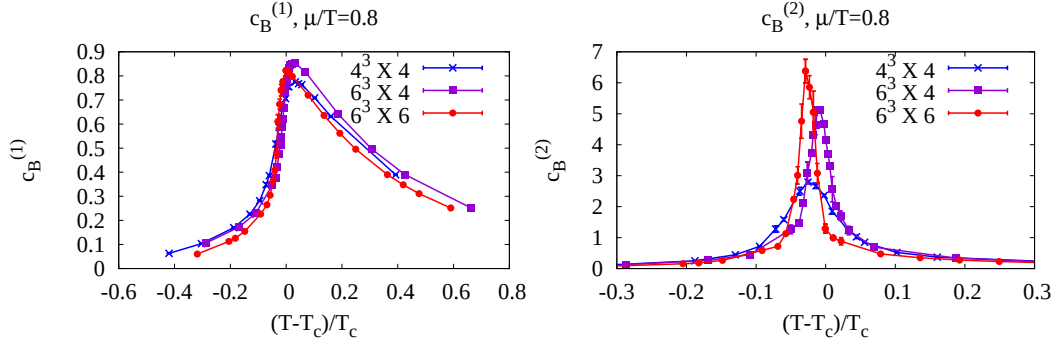


Figure B.3: The first (left panel) and second (right panel) order cumulants at $\mu/T = 0.8$ on $4^3 \times 4$, $6^3 \times 4$, and $6^3 \times 6$ lattices.

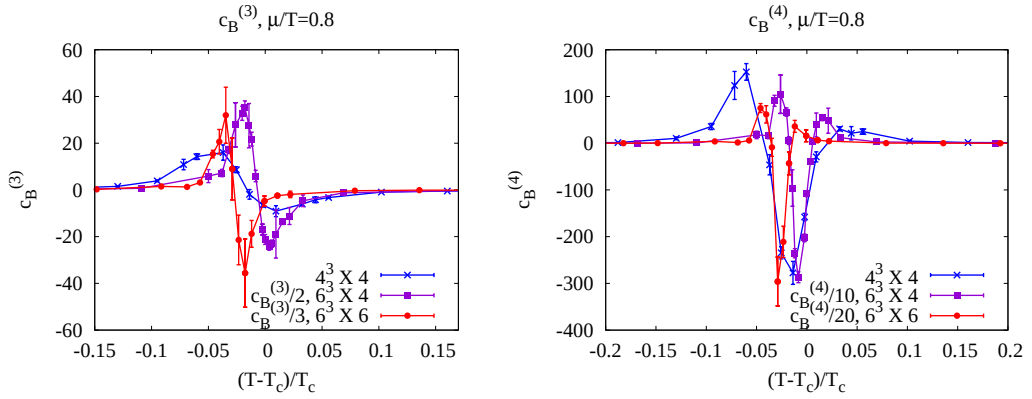


Figure B.4: The third (left panel) and fourth (right panel) order cumulants at $\mu/T = 0.8$ on $4^3 \times 4$, $6^3 \times 4$, and $6^3 \times 6$ lattices. The third order cumulants on $6^3 \times 4$ and $6^3 \times 6$ lattices are divided by 2 and 3, respectively. The fourth order cumulants on $6^3 \times 4$ and $6^3 \times 6$ lattices are divided by 10 and 20, respectively.

Appendix C

Review of $O(N)$ ($N=2,4$) scaling function

We review $O(4)$ scaling functions with respect to the net-baryon number fluctuations based on Ref. [100]. The order of the phase transition is the second order in the two flavor massless case due to the $O(4)$ criticality and the remnant effect of the $O(4)$ criticality may affect the critical phenomena at finite mass. In the following, α, β and δ are critical exponents.

The free energy density can be divided into two parts: the singular part f_s and the regular part f_r as $f(T, \mu_q, m_q) = f_s(T, \mu_q, m_q) + f_r(T, \mu_q, m_q)$ where these free energy densities depend on the temperature (T), the quark chemical potential (μ_q), and the quark mass (m_q). Around the chiral phase transition, the singular part dominates when there are no smeared effects such as finite mass or volume effects. The singular part f_s may read [100]

$$\frac{f_s(T, \mu_q, h)}{T^4} = Ah^{1+1/\delta} f_f(z) , \quad (\text{C.1})$$

where

$$\begin{aligned} z &= t/h^{1/\Delta} , \\ t &= \frac{1}{t_0} \left(\frac{T - T_c}{T_c} + \kappa_q (\mu_q/T)^2 \right) , \\ h &= \frac{1}{h_0} \frac{m_q}{T_c} , \end{aligned} \quad (\text{C.2})$$

for $\Delta = \beta\delta$. It should be noted that the reduced temperature t is expanded by the quark chemical potential with the phase transition curvature κ_q around the (pseudo-)critical temperature T_c [100]. The parameters t_0 and h_0 are non-universal scales and A in Eq. (C.1) is the amplitude.

The net-baryon number cumulants read

$$c_B^{(n)} = -\frac{\partial^n f/T^4}{\partial(3\hat{\mu}_q)^n}, \quad (\text{C.3})$$

for $\hat{\mu}_q = \mu_q/T$. According to the reduced temperature in Eq. (C.2), the derivatives of the singular part of the free energy density with respect to $\hat{\mu}_q$ is

$$\frac{\partial}{\partial \hat{\mu}_q} = \frac{\partial t}{\partial \hat{\mu}_q} \frac{\partial}{\partial t} \sim 2\kappa_q \hat{\mu}_q \frac{\partial}{\partial t}, \quad (\text{C.4})$$

so the odd number order derivatives of the net-baryon number at $\mu_q = 0$ will vanish. When the order of the derivatives is an even number, the n -th order derivative reads

$$\frac{\partial^n}{\partial \hat{\mu}_q^n} \sim (2\kappa_q)^{n/2} \frac{\partial^{(n/2)}}{\partial t^{(n/2)}}, \quad (\text{C.5})$$

at $\mu_q = 0$. By comparison, the highest order of the derivative of the free energy density at finite chemical potential is expressed as

$$\frac{\partial^n}{\partial \hat{\mu}_q^n} \sim (2\kappa_q)^n \frac{\partial^n}{\partial t^n}. \quad (\text{C.6})$$

As a result, the net-baryon number cumulants with the explicit symmetry breaking term are given as

$$\begin{aligned} c_B^{(n)} &\sim -\frac{\partial^n}{\partial \hat{\mu}_q^n} [h^{1+1/\delta} f_f(z)] \\ &= \begin{cases} -(2\kappa_q)^{n/2} h^{(2-\alpha-n/2)/\Delta} f_f^{(n/2)}(z), & \text{for } \hat{\mu}_q = 0, \text{ even } n \\ -(2\kappa_q)^n \hat{\mu}_q^n h^{(2-\alpha-n)/\Delta} f_f^{(n)}(z), & \text{for } \hat{\mu}_q > 0, \end{cases} \end{aligned} \quad (\text{C.7})$$

with $2 - \alpha = \Delta(1 + 1/\delta)$ and $\Delta = \beta\delta$. In the chiral limit, the net-baryon number cumulants are obtained as

$$c_B^{(n)} \sim \begin{cases} -(2\kappa_q)^{n/2} |t|^{(2-\alpha-n/2)} f_{\pm}^{(n/2)}(z) & , \text{for } \hat{\mu}_q = 0, \text{ even } n \\ -(2\kappa_q)^n \hat{\mu}_q^n |t|^{(2-\alpha-n)} f_{\pm}^{(n)}(z) & , \text{for } \hat{\mu}_q > 0, \end{cases} \quad (\text{C.8})$$

where

$$f_{\pm}^{(n)}(z) = \lim_{z \rightarrow \pm\infty} |z|^{-(2-\alpha-n)} f_f^{(n)}(z). \quad (\text{C.9})$$

In the cases where the critical exponent α is negative such as O(2) and O(4) universality cases [256, 257], the first divergent cumulant is the same. By comparison, it is different in the Z(2) universality case since the critical exponent α is positive [125]. For example, the first divergent cumulant is $c_B^{(6)}$ at vanishing chemical potential for O(2) and O(4) while it is $c_B^{(4)}$ for Z(2) according to the scaling function [100, 125]. At finite chemical potential, the first divergent cumulant is $c_B^{(3)}$ for O(2) and O(4) [100].

Bibliography

- [1] K. Yagi, T. Hatsuda, and Y. Miake, *Quark-gluon plasma: From big bang to little bang* Vol. 23 (Cambridge University Press, Cambridge, 2005), references therein.
- [2] K. Fukushima and T. Hatsuda, Rept. Prog. Phys. **74**, 014001 (2011), arXiv:1005.4814, references therein.
- [3] K. Fukushima and C. Sasaki, Prog. Part. Nucl. Phys. **72**, 99 (2013), arXiv:1301.6377, references therein.
- [4] M. Y. Han and Y. Nambu, Phys. Rev. **139**, B1006 (1965).
- [5] S. Godfrey and N. Isgur, Phys. Rev. **D32**, 189 (1985).
- [6] N. Isgur and G. Karl, Phys. Rev. **D18**, 4187 (1978).
- [7] C.-N. Yang and R. L. Mills, Phys. Rev. **96**, 191 (1954).
- [8] Reinhold A. Bertlmann, *Anomalies in Quantum Field Theory* (Oxford University Press, Oxford, 2000), references therein.
- [9] K. Fujikawa, Phys. Rev. **D21**, 2848 (1980), [Erratum: Phys. Rev.D22,1499(1980)].
- [10] M. Kobayashi and T. Maskawa, Prog. Theor. Phys. **44**, 1422 (1970).
- [11] R. D. Pisarski and F. Wilczek, Phys. Rev. **D29**, 338 (1984).
- [12] G. 't Hooft, Phys. Rept. **142**, 357 (1986).
- [13] K. Rajagopal and F. Wilczek, (2000), arXiv:hep-ph/0011333.
- [14] M. G. Alford, A. Schmitt, K. Rajagopal, and T. Schäfer, Rev. Mod. Phys. **80**, 1455 (2008), arXiv:0709.4635.
- [15] D. J. Gross and F. Wilczek, Phys. Rev. Lett. **30**, 1343 (1973).

- [16] H. D. Politzer, Phys. Rev. Lett. **30**, 1346 (1973).
- [17] G. 't Hooft, Nucl. Phys. **B254**, 11 (1985).
- [18] J. I. Kapusta and C. Gale, *Finite-Temperature Field Theory* (Cambridge University Press, Cambridge, 2006).
- [19] Y. Nambu, Phys. Rev. Lett. **4**, 380 (1960).
- [20] Y. Nambu and G. Jona-Lasinio, Phys. Rev. **122**, 345 (1961).
- [21] Y. Nambu and G. Jona-Lasinio, Phys. Rev. **124**, 246 (1961).
- [22] J. Goldstone, Nuovo Cim. **19**, 154 (1961).
- [23] J. Goldstone, A. Salam, and S. Weinberg, Phys. Rev. **127**, 965 (1962).
- [24] Particle Data Group, J. Beringer *et al.*, Phys. Rev. **D86**, 010001 (2012).
- [25] K. G. Wilson, Phys. Rev. **D10**, 2445 (1974).
- [26] E. Eichten *et al.*, Phys. Rev. Lett. **34**, 369 (1975).
- [27] G. S. Bali, Phys. Rept. **343**, 1 (2001), arXiv:hep-ph/0001312.
- [28] T. T. Takahashi, H. Matsufuru, Y. Nemoto, and H. Suganuma, Phys. Rev. Lett. **86**, 18 (2001), arXiv:hep-lat/0006005.
- [29] T. T. Takahashi, H. Suganuma, Y. Nemoto, and H. Matsufuru, Phys. Rev. **D65**, 114509 (2002), arXiv:hep-lat/0204011.
- [30] M. A. Stephanov, PoS **LAT2006**, 024 (2006), arXiv:hep-lat/0701002, references therein.
- [31] V. Koch, Hadronic Fluctuations and Correlations, in *Chapter of the book "Relativistic Heavy Ion Physics", R. Stock (Ed.), Springer, Heidelberg, 2010, p. 626-652. (Landolt-Boernstein New Series I, v. 23). (ISBN: 978-3-642-01538-0, 978-3-642-01539-7 (eBook))*, pp. 626–652, 2010, arXiv:0810.2520.
- [32] F. Karsch and E. Laermann, (2003), arXiv:hep-lat/0305025.
- [33] S. Jeon and V. Koch, (2003), arXiv:hep-ph/0304012.
- [34] P. Braun-Munzinger, K. Redlich, and J. Stachel, *Quark-gluon plasma. Vol. 3* (River Edge, USA: World Scientific (2004) 777 p, 2004).

- [35] M. Asakawa and K. Yazaki, Nucl. Phys. **A504**, 668 (1989).
- [36] K. Fukushima, Phys. Rev. **D77**, 114028 (2008), arXiv:0803.3318, [Erratum: Phys. Rev.D78,039902(2008)].
- [37] P. de Forcrand, PoS **LAT2009**, 010 (2009), arXiv:1005.0539.
- [38] STAR Collaboration, STAR Notes SN0598, <https://drupal.star.bnl.gov/STAR/starnotes/public/sn0598> (2014), references therein.
- [39] Y. Aoki, G. Endrődi, Z. Fodor, S. D. Katz, and K. K. Szabó, Nature **443**, 675 (2006), arXiv:hep-lat/0611014.
- [40] G. Endrődi, Z. Fodor, S. D. Katz, and K. K. Szabó, JHEP **04**, 001 (2011), arXiv:1102.1356.
- [41] F. Karsch, E. Laermann, and A. Peikert, Nucl. Phys. **B605**, 579 (2001), arXiv:hep-lat/0012023.
- [42] F. Karsch, Lect. Notes Phys. **583**, 209 (2002), arXiv:hep-lat/0106019, references therein.
- [43] CP-PACS, A. Ali Khan *et al.*, Phys. Rev. **D63**, 034502 (2001), arXiv:hep-lat/0008011.
- [44] STAR, M. M. Aggarwal *et al.*, Phys. Rev. Lett. **105**, 022302 (2010), arXiv:1004.4959.
- [45] STAR, X. Luo, PoS **CPOD2014**, 019 (2015), arXiv:1503.02558.
- [46] R. Hagedorn, Nuovo Cim. Suppl. **3**, 147 (1965).
- [47] F. Karsch, E. Laermann, and A. Peikert, Phys. Lett. **B478**, 447 (2000), arXiv:hep-lat/0002003.
- [48] E. V. Shuryak, Sov. Phys. JETP **47**, 212 (1978), [Zh. Eksp. Teor. Fiz.74,408(1978)].
- [49] J. I. Kapusta, Nucl. Phys. **B148**, 461 (1979).
- [50] P. B. Arnold and C.-x. Zhai, Phys. Rev. **D51**, 1906 (1995), arXiv:hep-ph/9410360.
- [51] C.-x. Zhai and B. M. Kastening, Phys. Rev. **D52**, 7232 (1995), arXiv:hep-ph/9507380.

- [52] E. Braaten and A. Nieto, Phys. Rev. **D53**, 3421 (1996), arXiv:hep-ph/9510408.
- [53] K. Kajantie, M. Laine, K. Rummukainen, and Y. Schroder, Phys. Rev. **D67**, 105008 (2003), arXiv:hep-ph/0211321.
- [54] A. M. Polyakov, Phys. Lett. **B72**, 477 (1978).
- [55] B. Svetitsky, Phys. Rept. **132**, 1 (1986).
- [56] B. Svetitsky and L. G. Yaffe, Nucl. Phys. **B210**, 423 (1982).
- [57] L. D. McLerran and B. Svetitsky, Phys. Rev. **D24**, 450 (1981).
- [58] S. Nadkarni, Phys. Rev. **D33**, 3738 (1986).
- [59] S. Nadkarni, Phys. Rev. **D34**, 3904 (1986).
- [60] L. G. Yaffe and B. Svetitsky, Phys. Rev. **D26**, 963 (1982).
- [61] M. Fukugita, M. Okawa, and A. Ukawa, Phys. Rev. Lett. **63**, 1768 (1989).
- [62] M. Fukugita, M. Okawa, and A. Ukawa, Nucl. Phys. **B337**, 181 (1990).
- [63] J. Kuti, J. Polonyi, and K. Szlachanyi, Phys. Lett. **B98**, 199 (1981).
- [64] L. D. McLerran and B. Svetitsky, Phys. Lett. **B98**, 195 (1981).
- [65] J. Engels, F. Karsch, H. Satz, and I. Montvay, Phys. Lett. **B101**, 89 (1981).
- [66] K. Fukushima, Phys. Lett. **B591**, 277 (2004), arXiv:hep-ph/0310121.
- [67] F. R. Brown *et al.*, Phys. Rev. Lett. **65**, 2491 (1990).
- [68] U. M. Heller, PoS **LAT2006**, 011 (2006), arXiv:hep-lat/0610114.
- [69] H. Satz, (2009), arXiv:0903.2778, references therein.
- [70] P. de Forcrand and O. Philipsen, Journal of High Energy Physics **2007**, 077 (2007), arXiv:hep-lat/0607017.
- [71] S. Ejiri *et al.*, Phys. Rev. **D80**, 094505 (2009), arXiv:0909.5122.
- [72] Y. Nakayama and T. Ohtsuki, Phys. Rev. **D91**, 021901 (2015), arXiv:1407.6195.

- [73] J. B. Kogut and M. A. Stephanov, *The phases of quantum chromodynamics: From confinement to extreme environments* Vol. 21 (Cambridge University Press, Cambridge, 2004), references therein.
- [74] P. Chomaz, (2004), arXiv:nucl-ex/0410024.
- [75] M. Kitazawa, T. Koide, T. Kunihiro, and Y. Nemoto, Prog. Theor. Phys. **108**, 929 (2002), arXiv:hep-ph/0207255.
- [76] T. Hatsuda, M. Tachibana, N. Yamamoto, and G. Baym, Phys. Rev. Lett. **97**, 122001 (2006), arXiv:hep-ph/0605018.
- [77] N. Yamamoto, M. Tachibana, T. Hatsuda, and G. Baym, Phys. Rev. **D76**, 074001 (2007), arXiv:0704.2654.
- [78] T. Ichihara, K. Morita, and A. Ohnishi, Prog. Theor. Exp. Phys. **2015**, 113D01 (2015), arXiv:1507.04527.
- [79] Y. Hatta and T. Ikeda, Phys. Rev. **D67**, 014028 (2003), arXiv:hep-ph/0210284.
- [80] O. Kaczmarek *et al.*, Phys. Rev. **D83**, 014504 (2011), arXiv:1011.3130.
- [81] R. Falcone, E. Laermann, and M. P. Lombardo, PoS **LATTICE2010**, 183 (2010), arXiv:1012.4694.
- [82] C. Bonati *et al.*, Phys. Rev. **D90**, 114025 (2014), arXiv:1410.5758.
- [83] P. Cea, L. Cosmai, and A. Papa, Phys. Rev. **D89**, 074512 (2014), arXiv:1403.0821.
- [84] A. M. Halasz, A. D. Jackson, R. E. Shrock, M. A. Stephanov, and J. J. M. Verbaarschot, Phys. Rev. **D58**, 096007 (1998), arXiv:hep-ph/9804290.
- [85] S. Roessner, C. Ratti, and W. Weise, Phys. Rev. **D75**, 034007 (2007), arXiv:hep-ph/0609281.
- [86] H. Fujii, Phys. Rev. **D67**, 094018 (2003), arXiv:hep-ph/0302167.
- [87] H. Fujii and M. Ohtani, Prog. Theor. Phys. Suppl. **153**, 157 (2004), arXiv:hep-ph/0401028.
- [88] H. Fujii and M. Ohtani, Phys. Rev. **D70**, 014016 (2004), arXiv:hep-ph/0402263.

- [89] D. T. Son and M. A. Stephanov, Phys. Rev. **D70**, 056001 (2004), arXiv:hep-ph/0401052.
- [90] V. Skokov, B. Friman, and K. Redlich, Phys. Rev. **C83**, 054904 (2011), arXiv:1008.4570.
- [91] B.-J. Schaefer and J. Wambach, Nucl. Phys. **A757**, 479 (2005), arXiv:nucl-th/0403039.
- [92] B.-J. Schaefer and J. Wambach, Phys. Rev. **D75**, 085015 (2007), arXiv:hep-ph/0603256.
- [93] Z. Fodor and S. D. Katz, Phys. Lett. **B534**, 87 (2002), arXiv:hep-lat/0104001.
- [94] Z. Fodor and S. D. Katz, JHEP **03**, 014 (2002), arXiv:hep-lat/0106002.
- [95] Z. Fodor and S. D. Katz, JHEP **04**, 050 (2004), arXiv:hep-lat/0402006.
- [96] S. Ejiri, Phys. Rev. **D73**, 054502 (2006), arXiv:hep-lat/0506023.
- [97] M. Asakawa, S. Ejiri, and M. Kitazawa, Phys. Rev. Lett. **103**, 262301 (2009), arXiv:0904.2089.
- [98] M. A. Stephanov, Phys. Rev. Lett. **102**, 032301 (2009).
- [99] M. A. Stephanov, Phys. Rev. Lett. **107**, 052301 (2011), arXiv:1104.1627.
- [100] B. Friman, F. Karsch, K. Redlich, and V. Skokov, Eur. Phys. J. **C71**, 1694 (2011), arXiv:1103.3511.
- [101] B. Berdnikov and K. Rajagopal, Phys. Rev. **D61**, 105017 (2000), arXiv:hep-ph/9912274.
- [102] C. Nonaka and M. Asakawa, Phys. Rev. **C71**, 044904 (2005), arXiv:nucl-th/0410078.
- [103] X.-N. Wang and M. Gyulassy, Phys. Rev. Lett. **68**, 1480 (1992).
- [104] STAR, C. Adler *et al.*, Phys. Rev. Lett. **90**, 082302 (2003), arXiv:nucl-ex/0210033.
- [105] STAR, J. Adams *et al.*, Phys. Rev. Lett. **91**, 072304 (2003), arXiv:nucl-ex/0306024.

- [106] PHENIX, K. Adcox *et al.*, Phys. Rev. Lett. **88**, 022301 (2002), arXiv:nucl-ex/0109003.
- [107] STAR, J. Adams *et al.*, Phys. Rev. Lett. **91**, 172302 (2003), arXiv:nucl-ex/0305015.
- [108] PHENIX, S. S. Adler *et al.*, Phys. Rev. Lett. **91**, 072301 (2003), arXiv:nucl-ex/0304022.
- [109] D. Molnár and S. A. Voloshin, Phys. Rev. Lett. **91**, 092301 (2003), arXiv:nucl-th/0302014.
- [110] R. J. Fries, B. Müller, C. Nonaka, and S. A. Bass, Phys. Rev. **C68**, 044902 (2003), arXiv:nucl-th/0306027.
- [111] STAR, J. Adams *et al.*, Phys. Rev. Lett. **92**, 052302 (2004), arXiv:nucl-ex/0306007.
- [112] PHENIX, S. S. Adler *et al.*, Phys. Rev. Lett. **91**, 182301 (2003), arXiv:nucl-ex/0305013.
- [113] A. Andronic, P. Braun-Munzinger, and J. Stachel, Phys. Lett. **B673**, 142 (2009), arXiv:0812.1186, [Erratum: Phys. Lett. **B678**, 516 (2009)].
- [114] STAR, L. Adamczyk *et al.*, Phys. Rev. Lett. **112**, 032302 (2014), arXiv:1309.5681.
- [115] STAR, L. Adamczyk *et al.*, Phys. Rev. Lett. **113**, 092301 (2014), arXiv:1402.1558.
- [116] M. Kitazawa and M. Asakawa, Phys. Rev. **C85**, 021901 (2012), arXiv:1107.2755.
- [117] M. Kitazawa and M. Asakawa, Phys. Rev. **C86**, 024904 (2012), arXiv:1205.3292, [Erratum: Phys. Rev. **C86**, 069902 (2012)].
- [118] H. Ono, M. Asakawa, and M. Kitazawa, Phys. Rev. **C87**, 041901 (2013), arXiv:1303.3338.
- [119] M. Kitazawa, M. Asakawa, and H. Ono, Phys. Lett. **B728**, 386 (2014), arXiv:1307.2978.
- [120] M. A. Stephanov, K. Rajagopal, and E. V. Shuryak, Phys. Rev. Lett. **81**, 4816 (1998), arXiv:hep-ph/9806219.

- [121] M. A. Stephanov, K. Rajagopal, and E. V. Shuryak, Phys. Rev. **D60**, 114028 (1999), arXiv:hep-ph/9903292.
- [122] M. Asakawa, U. W. Heinz, and B. Müller, Phys. Rev. Lett. **85**, 2072 (2000), arXiv:hep-ph/0003169.
- [123] S. Jeon and V. Koch, Phys. Rev. Lett. **85**, 2076 (2000), arXiv:hep-ph/0003168.
- [124] M. Asakawa and M. Kitazawa, (2015), arXiv:1512.05038.
- [125] K. Morita, V. Skokov, B. Friman, and K. Redlich, Eur. Phys. J. **C74**, 2706 (2014), arXiv:1211.4703.
- [126] C. Sasaki, B. Friman, and K. Redlich, Phys. Rev. **D75**, 054026 (2007), arXiv:hep-ph/0611143.
- [127] C. Sasaki, B. Friman, and K. Redlich, Phys. Rev. **D75**, 074013 (2007), arXiv:hep-ph/0611147.
- [128] F. Karsch, K. Redlich, and A. Tawfik, Phys. Lett. **B571**, 67 (2003), arXiv:hep-ph/0306208.
- [129] F. Karsch, K. Redlich, and A. Tawfik, Eur. Phys. J. **C29**, 549 (2003), arXiv:hep-ph/0303108.
- [130] E. Beth and G. Uhlenbeck, Physica **4**, 915 (1937).
- [131] R. Dashen, S.-k. Ma, and H. J. Bernstein, Phys. Rev. **187**, 345 (1969).
- [132] R. Venugopalan and M. Prakash, Nucl. Phys. **A546**, 718 (1992).
- [133] X. Pan, L. Chen, X. S. Chen, and Y. Wu, Nucl. Phys. **A913**, 206 (2013).
- [134] B.-J. Schaefer and M. Wagner, Phys. Rev. **D85**, 034027 (2012), arXiv:1111.6871.
- [135] V. Skokov, presented at Quark Matter 2012.
- [136] J.-W. Chen, J. Deng, H. Kohyama, and L. Labun, (2015), arXiv:1509.04968.
- [137] V. Vovchenko, D. V. Anchishkin, M. I. Gorenstein, and R. V. Poberezhnyuk, Phys. Rev. **C92**, 054901 (2015), arXiv:1506.05763.

- [138] S. Mukherjee, R. Venugopalan, and Y. Yin, Phys. Rev. **C92**, 034912 (2015), arXiv:1506.00645.
- [139] S. Ejiri *et al.*, Prog. Theor. Phys. Suppl. **153**, 118 (2004), arXiv:hep-lat/0312006.
- [140] C. R. Allton *et al.*, Phys. Rev. **D71**, 054508 (2005), arXiv:hep-lat/0501030.
- [141] C. DeTar *et al.*, Phys. Rev. **D81**, 114504 (2010), arXiv:1003.5682.
- [142] C. Gatttringer and H.-P. Schadler, Phys. Rev. **D91**, 074511 (2015), arXiv:1411.5133.
- [143] C. Schmidt, Prog. Theor. Phys. Suppl. **186**, 563 (2010), arXiv:1007.5164.
- [144] R. V. Gavai and S. Gupta, Phys. Lett. **B696**, 459 (2011), arXiv:1001.3796.
- [145] X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, Phys. Rev. **D88**, 094508 (2013), arXiv:1307.7205.
- [146] R. Bellwied *et al.*, Towards the QCD phase diagram from analytical continuation, in *25th International Conference on Ultra-Relativistic Nucleus-Nucleus Collisions (Quark Matter 2015) Kobe, Japan, September 27-October 3, 2015*, 2016, arXiv:1601.00466.
- [147] F. Karsch, K. Morita, and K. Redlich, (2015), arXiv:1508.02614.
- [148] J. Engels, S. Holtmann, T. Mendes, and T. Schulze, Phys. Lett. **B514**, 299 (2001), arXiv:hep-lat/0105028.
- [149] M. Cristoforetti, T. Hell, B. Klein, and W. Weise, Phys. Rev. **D81**, 114017 (2010), arXiv:1002.2336.
- [150] J. Braun and B. Klein, Eur. Phys. J. **C63**, 443 (2009), arXiv:0810.0857.
- [151] J. Braun, B. Klein, and P. Piasecki, Eur. Phys. J. **C71**, 1576 (2011), arXiv:1008.2155.
- [152] J. Braun, B. Klein, and B.-J. Schaefer, Phys. Lett. **B713**, 216 (2012), arXiv:1110.0849.
- [153] R.-A. Tripolt, J. Braun, B. Klein, and B.-J. Schaefer, Phys. Rev. **D90**, 054012 (2014), arXiv:1308.0164.

- [154] A. Bhattacharyya, R. Ray, and S. Sur, Phys. Rev. **D91**, 051501 (2015), arXiv:1412.8316.
- [155] P. Springer and B. Klein, Eur. Phys. J. **C75**, 468 (2015), arXiv:1506.00909.
- [156] A. Bhattacharyya, S. K. Ghosh, R. Ray, K. Saha, and S. Upadhaya, (2015), arXiv:1507.08795.
- [157] P. Braun-Munzinger, K. Redlich, and J. Stachel, "*PARTICLE PRODUCTION IN HEAVY ION COLLISIONS*" in the book "*Quark-Gluon Plasma 3*" (World Scientific Publishing, Singapore, 2004), references therein.
- [158] N. Kawamoto and J. Smit, Nucl. Phys. **B192**, 100 (1981).
- [159] H. Kluberg-Stern, A. Morel, O. Napoly, and B. Petersson, Nucl. Phys. **B190**, 504 (1981).
- [160] P. H. Damgaard, D. Hochberg, and N. Kawamoto, Phys. Lett. **B158**, 239 (1985).
- [161] P. H. Damgaard, N. Kawamoto, and K. Shigemoto, Nucl. Phys. **B264**, 1 (1986).
- [162] Y. Nishida, Phys. Rev. **D69**, 094501 (2004), arXiv:hep-ph/0312371.
- [163] K. Fukushima, Prog. Theor. Phys. Suppl. **153**, 204 (2004), arXiv:hep-ph/0312057.
- [164] K. Miura, T. Z. Nakano, A. Ohnishi, and N. Kawamoto, Phys. Rev. **D80**, 074034 (2009), arXiv:0907.4245.
- [165] T. Z. Nakano, K. Miura, and A. Ohnishi, Prog. Theor. Phys. **123**, 825 (2010), arXiv:0911.3453.
- [166] K. Miura, T. Z. Nakano, A. Ohnishi, and N. Kawamoto, (2011), arXiv:1106.1219.
- [167] K. Miura, T. Z. Nakano, and A. Ohnishi, Prog. Theor. Phys. **122**, 1045 (2009), arXiv:0806.3357.
- [168] T. Z. Nakano, K. Miura, and A. Ohnishi, Phys. Rev. **D83**, 016014 (2011), arXiv:1009.1518.

- [169] P. de Forcrand and M. Fromm, Phys. Rev. Lett. **104**, 112005 (2010), arXiv:0907.1915.
- [170] M. Fromm, *Lattice QCD at strong coupling: thermodynamics and nuclear physics*, PhD thesis, ETH, Zürich, 2010, Eidgenössische Technische Hochschule ETH Zürich, 2010.
- [171] W. Unger and P. de Forcrand, J. Phys. **G38**, 124190 (2011), arXiv:1107.1553.
- [172] T. Ichihara, A. Ohnishi, and T. Z. Nakano, Prog. Theor. Exp. Phys. **2014**, 123D02 (2014), arXiv:1401.4647.
- [173] H. J. Rothe, World Sci. Lect. Notes Phys. **43**, 1 (1992), [World Sci. Lect. Notes Phys.82,1(2012)].
- [174] I. Montvay and G. Münster, *Quantum Fields on a Lattice* (Cambridge University Press, Cambridge New York, 1994), references therein.
- [175] CP-PACS, S. Aoki *et al.*, Phys. Rev. Lett. **84**, 238 (2000), arXiv:hep-lat/9904012.
- [176] PACS-CS, S. Aoki *et al.*, Phys. Rev. **D79**, 034503 (2009), arXiv:0807.1661.
- [177] M. Creutz, Phys. Rev. Lett. **45**, 313 (1980).
- [178] M. Creutz and K. J. M. Moriarty, Phys. Rev. **D26**, 2166 (1982).
- [179] HAL QCD, T. Inoue *et al.*, Phys. Rev. Lett. **106**, 162002 (2011), arXiv:1012.5928.
- [180] HAL QCD, T. Inoue *et al.*, Nucl. Phys. **A881**, 28 (2012), arXiv:1112.5926.
- [181] K. G. Wilson, Quarks and strings on a lattice, in *New phenomena in subnuclear physics*, pp. 69–142, Springer, 1977.
- [182] H. B. Nielsen and M. Ninomiya, Nucl. Phys. **B185**, 20 (1981), [Erratum: Nucl. Phys.B195,541(1982)].
- [183] H. B. Nielsen and M. Ninomiya, Phys. Lett. **B105**, 219 (1981).
- [184] H. B. Nielsen and M. Ninomiya, Nucl. Phys. **B193**, 173 (1981).

- [185] K. G. Wilson, Quarks and Strings on a Lattice, in *Boston Conf. 1975:99, Erice Subnucl.Phys.1975:0069*, p. 99, 1975, [,0069(1975)].
- [186] L. Susskind, Phys. Rev. **D16**, 3031 (1977).
- [187] H. S. Sharatchandra, H. J. Thun, and P. Weisz, Nucl. Phys. **B192**, 205 (1981).
- [188] D. B. Kaplan, Phys. Lett. **B288**, 342 (1992), arXiv:hep-lat/9206013.
- [189] H. Neuberger, Phys. Lett. **B427**, 353 (1998), arXiv:hep-lat/9801031.
- [190] P. H. Ginsparg and K. G. Wilson, Phys. Rev. **D25**, 2649 (1982).
- [191] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, The Journal of Chemical Physics **21** (1953).
- [192] B. Efron, Siam Review **21**, 460 (1979).
- [193] S. Muroya, A. Nakamura, C. Nonaka, and T. Takaishi, Prog. Theor. Phys. **110**, 615 (2003), arXiv:hep-lat/0306031.
- [194] M.-P. Lombardo, Prog. Theor. Phys. Suppl. **153**, 26 (2004), arXiv:hep-lat/0401021.
- [195] S. Aoki, Int. J. Mod. Phys. **A21**, 682 (2006), arXiv:hep-lat/0509068.
- [196] K. Fukushima and Y. Hidaka, Phys. Rev. **D75**, 036002 (2007), arXiv:hep-ph/0610323.
- [197] G. Akemann, J. C. Osborn, K. Splittorff, and J. J. M. Verbaarschot, Nucl. Phys. **B712**, 287 (2005), arXiv:hep-th/0411030.
- [198] P. de Forcrand and O. Philipsen, Nucl. Phys. **B642**, 290 (2002), arXiv:hep-lat/0205016.
- [199] J. B. Kogut, M. A. Stephanov, and D. Toublan, Phys. Lett. **B464**, 183 (1999), arXiv:hep-ph/9906346.
- [200] D. T. Son and M. A. Stephanov, Phys. Rev. Lett. **86**, 592 (2001), arXiv:hep-ph/0005225.
- [201] J. B. Kogut and D. K. Sinclair, Phys. Rev. **D70**, 094501 (2004), arXiv:hep-lat/0407027.
- [202] P. de Forcrand, M. A. Stephanov, and U. Wenger, PoS **LAT2007**, 237 (2007), arXiv:0711.0023.

- [203] Z. W. Salsburg, J. D. Jacobson, W. Fickett, and W. W. Wood, The Journal of Chemical Physics **30** (1959).
- [204] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).
- [205] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **63**, 1195 (1989).
- [206] I. M. Barbour and A. J. Bell, Nucl. Phys. **B372**, 385 (1992).
- [207] A. Hasenfratz and D. Toussaint, Nucl. Phys. **B371**, 539 (1992).
- [208] S. Choe *et al.*, Phys. Rev. **D65**, 054501 (2002).
- [209] C. R. Allton *et al.*, Phys. Rev. **D66**, 074507 (2002), arXiv:hep-lat/0204010.
- [210] M. D’Elia and M.-P. Lombardo, Phys. Rev. **D67**, 014505 (2003), arXiv:hep-lat/0209146.
- [211] D. E. Miller and K. Redlich, Phys. Rev. **D35**, 2524 (1987).
- [212] J. Engels, O. Kaczmarek, F. Karsch, and E. Laermann, Nucl. Phys. **B558**, 307 (1999), arXiv:hep-lat/9903030.
- [213] P. de Forcrand and S. Kratochvila, Nucl. Phys. Proc. Suppl. **153**, 62 (2006), arXiv:hep-lat/0602024, [,62(2006)].
- [214] S. Ejiri, Phys. Rev. **D78**, 074507 (2008), arXiv:0804.3227.
- [215] A. Li, A. Alexandru, and K.-F. Liu, Phys. Rev. **D84**, 071503 (2011), arXiv:1103.3045.
- [216] K. Nagata and A. Nakamura, Phys. Rev. **D82**, 094027 (2010), arXiv:1009.2149.
- [217] WHOT-QCD, H. Saito *et al.*, Phys. Rev. **D84**, 054502 (2011), arXiv:1106.0974, [Erratum: Phys. Rev.D85,079902(2012)].
- [218] A. Gocksch, Phys. Rev. Lett. **61**, 2054 (1988).
- [219] Z. Fodor, S. D. Katz, and C. Schmidt, JHEP **03**, 121 (2007), arXiv:hep-lat/0701022.
- [220] G. Parisi, Phys. Lett. **B131**, 393 (1983).

- [221] J. R. Klauder, *Recent Developments in High-Energy Physics* (Springer Vienna, Vienna, 1983), chap. Stochastic Quantization, pp. 251–281.
- [222] E. Seiler, D. Sexty, and I.-O. Stamatescu, Phys. Lett. **B723**, 213 (2013), arXiv:1211.3709.
- [223] F. Pham, Proc. Symp. Pure Math. **40**, 319 (1983).
- [224] E. Witten, AMS/IP Stud. Adv. Math. **50**, 347 (2011), arXiv:1001.2933.
- [225] E. Witten, (2010), arXiv:1009.6032.
- [226] M. Creutz, J. Math. Phys. **19**, 2043 (1978).
- [227] J.-M. Drouffe and J.-B. Zuber, Phys. Rept. **102**, 1 (1983).
- [228] R. Balian, J. M. Drouffe, and C. Itzykson, Phys. Rev. **D11**, 2104 (1975), [Erratum: Phys. Rev.D19,2514(1979)].
- [229] G. Münster, Nucl. Phys. **B180**, 23 (1981).
- [230] E. Seiler, Lect. Notes Phys. **159**, 1 (1982).
- [231] H. Kluberg-Stern, A. Morel, and B. Petersson, Nucl. Phys. **B215**, 527 (1983).
- [232] P. H. Damgaard, N. Kawamoto, and K. Shigemoto, Phys. Rev. Lett. **53**, 2211 (1984).
- [233] G. Fäldt and B. Petersson, Nucl. Phys. **B265**, 197 (1986).
- [234] I. Ichinose, Phys. Lett. **B135**, 148 (1984).
- [235] I. Ichinose, Phys. Lett. **B147**, 449 (1984).
- [236] I. Ichinose, Nucl. Phys. **B249**, 715 (1985).
- [237] T. Jolicœur, H. Kluberg-Stern, A. Morel, M. Lev, and B. Petersson, Nucl. Phys. **B235**, 455 (1984).
- [238] N. Bilić, K. Demeterfi, and B. Petersson, Nucl. Phys. **B377**, 651 (1992).
- [239] N. Bilić, F. Karsch, and K. Redlich, Phys. Rev. **D45**, 3228 (1992).
- [240] N. Bilić and J. Cleymans, Phys. Lett. **B355**, 266 (1995), arXiv:hep-lat/9501019.

- [241] F. Karsch and K.-H. Mütter, Nucl. Phys. **B313**, 541 (1989).
- [242] P. de Forcrand, J. Langelage, O. Philipsen, and W. Unger, Phys. Rev. Lett. **113**, 152002 (2014), arXiv:1406.4397.
- [243] A. Gocksch and M. Ogilvie, Phys. Rev. **D31**, 877 (1985).
- [244] E.-M. Ilgenfritz and J. Kripfganz, Z. Phys. **C29**, 79 (1985), [I.57(1984)].
- [245] K. Fukushima, Phys. Rev. **D68**, 045004 (2003), arXiv:hep-ph/0303225.
- [246] A. Ohnishi and T. Ichihara, Preweighting method in Monte-Carlo sampling with complex action —Strong-Coupling Lattice QCD with $1/g^2$ corrections, as an example —, to appear in PoS **LATTICE2015**.
- [247] ALICE, B. Abelev *et al.*, Phys. Rev. **C88**, 044910 (2013), arXiv:1303.0737.
- [248] A. Ohnishi, T. Ichihara, and T. Z. Nakano, PoS **LATTICE2012**, 088 (2012), arXiv:1211.2282.
- [249] T. Ichihara, T. Z. Nakano, and A. Ohnishi, PoS **LATTICE2013**, 143 (2014), arXiv:1311.5352.
- [250] M. Honma, T. Mizusaki, and T. Otsuka, Phys. Rev. Lett. **75**, 1284 (1995).
- [251] T. Abe and R. Seki, Phys. Rev. **C79**, 054002 (2009), arXiv:0708.2523.
- [252] J. Carlson, S. Gandolfi, and A. Gezerlis, Prog. Theor. Exp. Phys. **2012**, 01A209 (2012), arXiv:1210.6659.
- [253] H. Kluberg-Stern, A. Morel, O. Napoly, and B. Petersson, Nucl. Phys. **B220**, 447 (1983).
- [254] Kurt Binder and Dieter W. Heermann, *Monte Carlo simulation in statistical physics: an introduction* (Springer Verlag, Berlin, 2010), references therein.
- [255] J. Engels and F. Karsch, Phys. Rev. **D90**, 014501 (2014), arXiv:1402.5302.
- [256] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. **B63**, 214503 (2001), arXiv:cond-mat/0010360.

- [257] J. Engels and F. Karsch, Phys. Rev. **D85**, 094506 (2012), arXiv:1105.0584.
- [258] C. Wetterich, Phys. Lett. **B301**, 90 (1993).
- [259] K. Kamikado, N. Strodthoff, L. von Smekal, and J. Wambach, Phys. Lett. **B718**, 1044 (2013), arXiv:1207.0400.
- [260] K. Kamikado, T. Kunihiro, K. Morita, and A. Ohnishi, Prog. Theor. Exp. Phys. **2013**, 053D01 (2013), arXiv:1210.8347.
- [261] T. Ichihara and A. Ohnishi, PoS **LATTICE2014**, 188 (2014), arXiv:1503.07049.
- [262] S. Borsányi *et al.*, JHEP **01**, 138 (2012), arXiv:1112.4416.
- [263] HotQCD, A. Bazavov *et al.*, Phys. Rev. **D86**, 034509 (2012), arXiv:1203.0784.
- [264] A. Bazavov *et al.*, Phys. Rev. Lett. **111**, 082301 (2013), arXiv:1304.7220.
- [265] R. Bellwied *et al.*, Phys. Rev. **D92**, 114505 (2015), arXiv:1507.04627.
- [266] F. Karsch and K. Redlich, Phys. Lett. **B695**, 136 (2011), arXiv:1007.2581.
- [267] S. Ejiri, F. Karsch, and K. Redlich, Phys. Lett. **B633**, 275 (2006), arXiv:hep-ph/0509051.
- [268] B. Stokić, B. Friman, and K. Redlich, Phys. Lett. **B673**, 192 (2009), arXiv:0809.3129.
- [269] M. Cheng *et al.*, Phys. Rev. **D79**, 074505 (2009), arXiv:0811.1006.
- [270] T. Ichihara, A. Ohnishi, and K. Morita, Higher order net baryon number cumulants in the strong coupling lattice QCD, to appear in PoS **LATTICE2015**.
- [271] S. Aoki, Y. Maezawa, and A. Ohnishi, private communication.
- [272] K. Morita and K. Redlich, Progress of Theoretical and Experimental Physics **2015**, 043D03 (2015), arXiv:1409.8001.
- [273] S. A. Baurle, R. Martoňák, and M. Parrinello, The Journal of Chemical Physics **117** (2002).

- [274] S. A. Baurle, Phys. Rev. Lett. **89**, 080602 (2002).
- [275] P. Rossi and U. Wolff, Nucl. Phys. **B248**, 105 (1984).
- [276] U. Wolff, Phys. Lett. **B153**, 92 (1985).
- [277] Y. Nishida, K. Fukushima, and T. Hatsuda, Phys. Rept. **398**, 281 (2004), arXiv:hep-ph/0306066.
- [278] Y. Nishida, Prog. Theor. Phys. Suppl. **153**, 325 (2004), arXiv:hep-ph/0310160.
- [279] A. Ohnishi, N. Kawamoto, and K. Miura, Mod. Phys. Lett. **A23**, 2459 (2008), arXiv:0803.0255.

Copyrights for repository

Chapter. 3 is based on

Auxiliary field Monte Carlo simulation of strong-coupling lattice QCD for QCD phase diagram

Terukazu Ichihara, Akira Ohnishi, and Takashi Z. Nakano

Progress of Theoretical and Experimental Physics **2014**, 123D02 (2014).

doi: 10.1093/ptep/ptu154

url: <http://ptep.oxfordjournals.org/content/2014/12/123D02>

©The Author(s) 2014. Published by Oxford University Press on behalf of the Physical Society of Japan. This is an Open Access article distributed under the terms of the Creative Commons Attribution License

(<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted reuse, distribution, and reproduction in any medium, provided the original work is properly cited.

Chapter. 4 is based on

Net-baryon number fluctuations across the chiral phase transition at finite density in strong-coupling lattice QCD

Terukazu Ichihara, Kenji Morita, and Akira Ohnishi

Progress of Theoretical and Experimental Physics **2015**, 113D01 (2015).

doi: 10.1093/ptep/ptv141

url: <http://ptep.oxfordjournals.org/content/2015/11/113D01>

©The Author(s) 2015. Published by Oxford University Press on behalf of the Physical Society of Japan. This is an Open Access article distributed under the terms of the Creative Commons Attribution License

(<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted reuse, distribution, and reproduction in any medium, provided the original work is properly cited.