

Lee-Yang zero analysis for the study of QCD phase structure

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We comment on the Lee-Yang zero analysis for the study of the phase structure of QCD at high temperature and baryon number density by Monte-Carlo simulations. We find that the sign problem for nonzero density QCD induces a serious problem in the finite volume scaling analysis of the Lee-Yang zeros for the investigation of the order of the phase transition. If the sign problem occurs at large volume, the Lee-Yang zeros will always approach the real axis of the complex parameter plane in the thermodynamic limit. This implies that a scaling behavior which would suggest a crossover transition will not be obtained. To clarify this problem, we discuss the Lee-Yang zero analysis for SU(3) pure gauge theory as a simple example without the sign problem, and then consider the case of nonzero density QCD. It is suggested that the distribution of the Lee-Yang zeros in the complex parameter space obtained by each simulation could be more important information for the investigation of the critical endpoint in the (T, μ_q) plane than the finite volume scaling behavior.

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I. INTRODUCTION

In the last few years, remarkable progress in exploring the QCD phase structure in the temperature (T) and quark chemical potential (μ_q) plane have been made in numerical studies of lattice QCD. The phase transition line, separating hadron phase and quark-gluon plasma phase, was investigated from $\mu_q = 0$ to finite μ_q [1–6], and the equation of state was also analyzed quantitatively at low density [4,7–9].

Among others, study of the endpoint of the first order phase transition line in the (T, μ_q) plane, whose existence is suggested by phenomenological studies [10,11], is particularly important both from the experimental and theoretical point of view. To locate the critical endpoint, Fodor and Katz [2,3] investigated the positions of the Lee-Yang zeros (to be explained more below) in the complex $\beta = 6/g^2$ plane using lattices with different spatial volumes, and examined the finite-volume scaling behavior of a Lee-Yang zero closest to the real axis. There are also studies in which the behavior of the critical endpoint as a function of the quark masses is examined by using the property that a critical endpoint exists at $\mu_q = 0$ in the very small quark mass region for QCD with three flavors having degenerate quark masses. For extrapolating the result to the case with physical quark masses, an approach on the basis of the Taylor expansion in terms of μ_q/T [12] and that of the imaginary chemical potential [13,14] have been developed. Moreover, a study of phase-quenched finite density QCD, i.e. simulations with an isospin chemical potential, has been discussed in Ref. [15]. The radius of convergence in the framework of the Taylor expansion of the grand canonical potential can establish a lower bound of the location of the critical endpoint [7,9,16]. Also, the Glasgow method [17] is an interesting approach for the study of QCD at nonzero baryon density.

In this paper, we focus our attention on the method of the Lee-Yang zero [18] applied to finite density QCD. The Lee-Yang zero analysis is a popular method that is used to investigate the order of phase transitions. In order to study the existence of singularities in the thermodynamic limit (infinite volume limit), Lee and Yang proposed the following approach: Because there are no thermodynamic singularities as long as the volume is finite, the partition function Z is always nonzero; it can develop zeros only in the infinite volume limit. However, if a real parameter of the model is extended into the complex parameter plane, a singularity, characterized by $Z = 0$, can appear in the complex parameter plane even in a finite volume. These zeros are called the Lee-Yang zeros. Therefore, one can find the position of a singularity by exploring the position of the Lee-Yang zero in the complex parameter plane as a function of volume, and extrapolating the position of the Lee-Yang zero in the thermodynamic limit. For a system with a first order phase transition, the position of the nearest Lee-Yang zero approaches to the real axis in inverse proportion to the volume. On the other hand, the Lee-Yang zeros do not reach the real axis for crossover transition, i.e. rapid change without any thermodynamic singularities. For QCD at nonzero baryon density, we expect a rapid crossover transition in the low density regime which changes into a first order phase transition beyond a critical value of the density.

As we mentioned, Fodor and Katz have investigated the finite volume dependence of the Lee-Yang zeros in the complex $\beta \equiv 6/g^2$ plane for various values of the chemical potential. To carry out such analysis, the reweighting method [19] is adopted, in which one performs simulations at $\mu_q = 0$, and then corrects for the modified Boltzmann weight in the measurement of observables. In this case a famous problem arises for large μ_q/T and large volume, which is called “sign problem.” The sign problem is

caused by complex phase fluctuations of the fermion determinant. In the region of small μ_q/T , the phase fluctuations are not large and the sign problem is not serious. However, if the sign of the modification factor changes frequently during subsequent Monte-Carlo steps for large μ_q/T , the statistical error becomes larger than the expectation values in general.

We find that the sign problem induces a serious problem in the finite-volume scaling analysis of the Lee-Yang zero, which is used by Fodor and Katz. For any nonzero μ_q the normalized partition function calculated on the real axis with necessarily limited statistics will numerically always be consistent with zero once the volumes grow large. This means that the scaling behavior suggesting a crossover transition will not be obtained for the case with the sign problem, which is in contrast with the usual expectation.

Before discussing the case of nonzero density QCD, we study in Sec. II, as a simple example, the Lee-Yang zeros in the complex β plane for SU(3) pure gauge theory by analyzing data from Monte-Carlo simulations. This model has a first order phase transition [20] and simulations are much easier than for QCD at nonzero baryon density. Moreover, the pure gauge theory does, of course, not have a sign problem. Hence it is a good example to demonstrate how the Lee-Yang analysis works in the complex β plane. In addition, it will become clear during this exercise that the complex phase fluctuations arising from the imaginary part of β near Lee-Yang zeros are quite similar to those coming from the quark determinant where the sign problem exists for nonzero density QCD. The problem of the complex measure is reviewed in Sec. III. There we also comment on the reweighting method for the study at nonzero baryon density. In Sec. IV, we discuss a problem which arises when we apply the Lee-Yang zero analysis for nonzero baryon density QCD by using the reweighting technique, and consider possible other approaches in the framework of the Lee-Yang zero analysis for the investigation of the critical endpoint. Conclusions and discussions are given in Sec. V.

II. LEE-YANG ZERO FOR SU(3) PURE GAUGE THEORY

A. General remarks

In this section, we apply the method of Lee-Yang zeros to the SU(3) pure gauge theory (quenched QCD).¹ The phase transition of the SU(3) pure gauge theory is known to be of first order [20], which is expected from the corresponding Z(3) spin models. The pure gauge theory is controlled by only one parameter $\beta = 6/g^2$ with the partition function,

$$Z = \int \mathcal{D}U e^{6\beta N_{\text{site}} P}, \quad (1)$$

where P is an averaged plaquette $P = (\sum_{x, \mu < \nu} W_{\mu\nu}^{1 \times 1}(x)) / (6N_{\text{site}})$, and $W_{\mu\nu}^{1 \times 1}$ is the 1×1 Wilson loop operator for the lattice size $N_{\text{site}} = N_\sigma^3 \times N_\tau$. Here, N_σ and N_τ are spatial and temporal extension of the lattice. We extend the real parameter β into the complex plane $(\beta_{\text{Re}}, \beta_{\text{Im}})$, and determine the position of Lee-Yang zeros, at which $Z(\beta_{\text{Re}}, \beta_{\text{Im}}) = 0$ is satisfied, by numerical simulations. We use standard Monte-Carlo techniques; configurations $\{U_\mu\}$ are generated with the probability of the Boltzmann weight. The expectation value of an operator $\mathcal{O}[U_\mu]$, $\langle \mathcal{O} \rangle$, is then calculated by taking an average over the configurations. We expect that the position of the Lee-Yang zero $(\beta_{\text{Re}}^0, \beta_{\text{Im}}^0)$ approaches the real β axis in the infinite volume limit; with $\beta_{\text{Im}}^0 \sim 1/V \equiv N_\sigma^{-3}$ for a first order phase transition.

In carrying out the above calculation two problems arise: One is that the Monte Carlo method is applicable only to the expectation values of physical quantities but not to the partition function itself. Another problem is that the measure is complex for a complex coupling β , and hence we cannot apply the Monte Carlo method directly, since the probabilities (Boltzmann weights) must be real and positive. To avoid these problems, we introduce the normalized partition function Z_{norm} together with the reweighting technique,

$$\begin{aligned} Z_{\text{norm}}(\beta_{\text{Re}}, \beta_{\text{Im}}) &\equiv \left| \frac{Z(\beta_{\text{Re}}, \beta_{\text{Im}})}{Z(\beta_{\text{Re}}, 0)} \right| \\ &= \left| \frac{\int \mathcal{D}U e^{6(\beta_{\text{Re}} + i\beta_{\text{Im}})N_{\text{site}}P}}{\int \mathcal{D}U e^{6\beta_{\text{Re}}N_{\text{site}}P}} \right| \\ &= \left| \left\langle e^{6i\beta_{\text{Im}}N_{\text{site}}P} \right\rangle_{(\beta_{\text{Re}}, 0)} \right| \\ &= \left| \left\langle e^{6i\beta_{\text{Im}}N_{\text{site}}\Delta P} \right\rangle_{(\beta_{\text{Re}}, 0)} \right|. \end{aligned} \quad (2)$$

Here $\Delta P = P - \langle P \rangle$ and $|\exp(6i\beta_{\text{Im}}N_{\text{site}}\langle P \rangle)| = 1$. Because the denominator $Z(\beta_{\text{Re}}, 0)$ is always finite for any finite volume, the position of $Z(\beta_{\text{Re}}, \beta_{\text{Im}}) = 0$ can be identified by analyzing Z_{norm} . Although the partition function is not zero for $\beta_{\text{Im}} = 0$, it can be zero at some points in the $(\beta_{\text{Re}}, \beta_{\text{Im}})$ plane, when the complex phase factor in Eq. (2) changes sign frequently on the generated configurations. For the determination of the critical point in the original theory, i.e. on the real β axis, the position of the nearest Lee-Yang zero should be investigated as a function of the volume $V = N_\sigma^3$.

The mechanism that leads the occurrence of a Lee-Yang zero in Eq. (2) is quite similar to that which limits the applicability of the reweighting method for QCD with finite chemical potential [4,22]. We will discuss this in more detail in Sec. III. At a point for which the width of the probability distribution of $6\beta_{\text{Im}}N_{\text{site}}P$ is smaller than

¹A pioneering study has been done for lattices with $N_\tau = 2$ in Ref. [21].

$O(\pi/2)$, the sign of the complex phase does not change. Therefore, the standard deviation of the plaquette distribution is required to be larger than $\pi/(12\beta_{\text{Im}}N_{\text{site}})$ in the region where Lee-Yang zeros exist. Moreover, because the square of standard deviation is in proportion to the value of the plaquette susceptibility, the position of its maximum must agree with the position where Z_{norm} becomes minimal as function of β_{Re} for fixed β_{Im} . Hence, the real part, β_{Re} , of the position of the nearest Lee-Yang zero must be consistent with the peak position of the plaquette susceptibility. The method to find a critical point from the location of Lee-Yang zeros thus is essentially the same as the method which determines a critical point through the location of the peak position of the susceptibility and its finite-volume scaling.

Here, it is instructive to introduce a probability distribution function for the plaquette, $w(P)$, which is defined by

$$w(P') = \frac{1}{Z} \int \mathcal{D}U \delta(P' - P) e^{6\beta_{\text{Re}}N_{\text{site}}P}, \quad (3)$$

where $\delta(x)$ is the delta function. Then, Eq. (2) can be rewritten as

$$Z_{\text{norm}}(\beta) = \left| \int dP e^{6i\beta_{\text{Im}}N_{\text{site}}\Delta P} w(P) \right|. \quad (4)$$

This means that the partition function Z_{norm} as a function of $6\beta_{\text{Im}}N_{\text{site}}$ is obtained through a Fourier transformation of $w(P)$.

Using this equation, the relation between the scaling behavior of the Lee-Yang zeros in the infinite volume limit and the distribution function of the plaquette becomes clearer. In Monte-Carlo simulations, configurations with probabilities proportional to their Boltzmann weight are generated by a computer, and we obtain a distribution function of the plaquette from the histogram of the plaquette. The histogram has usually a Gaussian shape at a normal, noncritical point, but it deviates from the Gaussian form near a critical point, and attains a double peak shape at a first order transition point, corresponding to the coexistence of two phases.

For the case of a nonsingular point of β_{Re} or a crossover pseudocritical point, where the distribution is expected to be a Gaussian function, the point of $Z_{\text{norm}} = 0$ does not exist except in the limit of $\beta_{\text{Im}}N_{\text{site}} \rightarrow \infty$ or $-\infty$, because the function which is obtained through a Fourier transformation of a Gaussian function again is a Gaussian function. Of course, results of numerical simulations have statistical errors, hence Z_{norm} can become zero "within errors," if the expectation value and the error become of the same order. However, in this case, the point at which $Z_{\text{norm}} = 0$ appears at random in terms of $\beta_{\text{Im}} \times N_{\text{site}}$. Therefore, the volume dependence of the position of the Lee-Yang zero ($\beta_{\text{Re}}^0, \beta_{\text{Im}}^0$) does not necessary to be $\beta_{\text{Im}}^0 \sim 1/V (\equiv N_{\sigma}^{-3})$ for fixed N_{τ} .

On the other hand, in the case of a first order phase transition, we expect that the plaquette histogram has two peaks having the same peak height at the transition point. Performing the Fourier transformation of such a double peaked function leads to a function which has zeros periodically. For example, a distribution function $w(P)$ having two Gaussian peaks at $\Delta P = \pm A$ leads to a normalized partition function Z_{norm} which has zeros at

$$\beta_{\text{Im}}^0 = \frac{\pi(2n+1)}{12N_{\text{site}}A}, \quad (n = 0, 1, 2, 3, \dots). \quad (5)$$

This is mathematically the same as that for the interference experiment using a laser and a double-slit. The Lee-Yang zeros correspond to dark lines (destructive interference) and they appear periodically as given in Eq. (5). Moreover, for a first order phase transition the difference of plaquette values in cold and hot phases, $2A$, is related to the latent heat $\Delta\varepsilon$, i.e. the energy difference between the hot and cold phases,

$$\frac{\Delta\varepsilon}{T^4} \approx -12AN_{\tau}^4 a \frac{d\beta}{da}, \quad (6)$$

where a is the lattice spacing. Since $\Delta\varepsilon$ is nonzero, A does not vanish in the infinite volume limit ($N_{\sigma}^3 \rightarrow \infty$). Therefore, we find that in the infinite volume limit the nearest Lee-Yang zero approaches the real β axis like $\beta_{\text{Im}}^0 \sim 1/V$, which is consistent with the general argument on the Lee-Yang zero for a first order phase transition. We also emphasize that the isolated Lee-Yang zeros appear periodically. The distances to these points from the real axis are 1, 3, 5, \dots in units of the distance to the first Lee-Yang zero. This is also an important property, which is not observed for a crossover transition.

In addition, the discussion given for the plaquette distribution function can be extended to the analysis of fourth order Binder cumulants,

$$B_4 \equiv \frac{\langle \Delta P^4 \rangle}{\langle \Delta P^2 \rangle^2}, \quad (7)$$

which is an alternative to the method of Lee-Yang zeros often used to identify the order of a phase transition. The value of the Binder cumulant at the critical point depends on the universality class. In the case of a first order phase transition, assuming the plaquette distribution is a double peaked function, the Binder cumulants are estimated as

$$B_4 = \frac{\int dP \Delta P^4 w(P)}{(\int dP \Delta P^2 w(P))^2} \approx \frac{A^4}{(A^2)^2} \approx 1, \quad (8)$$

where the distance between two peaks is $2A$ and is wider than the width of each peak. On the other hand, when the distribution function can be modeled by a Gaussian function for a crossover transition, the Binder cumulants are given by

$$\begin{aligned}
B_4 &\approx \frac{\sqrt{x/\pi} \int dP \Delta P^4 e^{-x\Delta P^2}}{(\sqrt{x/\pi} \int dP \Delta P^2 e^{-x\Delta P^2})^2} \\
&= \left(\frac{\sqrt{x}}{\pi} \frac{d^2 \sqrt{\pi/x}}{dx^2} \right) / \left(-\sqrt{\frac{x}{\pi}} \frac{d\sqrt{\pi/x}}{dx} \right)^2 = 3. \quad (9)
\end{aligned}$$

In a region where a first order phase transition changes to a crossover, the Binder cumulant changes rapidly from one to three. We expect to find such a region for full QCD at high temperature and density. The value of the Binder cumulant at the endpoint of the first order transition line, which is of second order, is determined by the universality class. Hence, the plaquette distribution function plays an important role for both methods to identify the order of a phase transition.

B. Numerical results

We calculate the normalized partition function for SU(3) pure gauge theory to find Lee-Yang zeros in the complex β plane, using data for plaquettes obtained by QCDPAX in Ref. [23]. There are five data sets measured at the transition point for $N_\tau = 4$ and 6. The spatial lattice sizes are $24^2 \times 36 \times 4$, $12^2 \times 24 \times 4$, $36^2 \times 48 \times 6$, $24^3 \times 6$, and $20^3 \times 6$. $O(10^6)$ configurations are available for the analysis of each data set. The reweighting technique is also used for the real β direction to analyze the Lee-Yang zeros in the complex β plane for a data set obtained at only one β point $(\beta_{\text{Re}}, \beta_{\text{Im}}) = (\beta_0, 0)$. The normalized partition function is given by

$$Z_{\text{norm}}(\beta_{\text{Re}}, \beta_{\text{Im}}) = \left| \frac{\langle e^{6i\beta_{\text{Im}} N_{\text{site}} \Delta P} e^{6\beta_{\text{Re}} N_{\text{site}} \Delta P} \rangle_{(\beta_0, 0)}}{\langle e^{6\beta_{\text{Re}} N_{\text{site}} \Delta P} \rangle_{(\beta_0, 0)}} \right|. \quad (10)$$

Figure 1 shows the contour plot of Z_{norm} for the $24^2 \times 36 \times 4$ lattice. The simulation point is $\beta_0 = 5.692$. In this definition, Z_{norm} is normalized to be one on the real β axis. Circles at $(\beta_{\text{Re}}^0, \beta_{\text{Im}}^0) \approx (5.6925, 0.0021)$ and $(5.6931, 0.0056)$ are Lee-Yang zeros. Since the SU(3) pure gauge theory has a first order phase transition, Lee-Yang zeros appear periodically. For this data, two clear peaks are visible in the plaquette histogram [23]. The distance between these two peaks is $2A \approx 0.003$. The positions of the Lee-Yang zeros are consistent with $\beta_{\text{Im}}^0 \sim \pi/(12N_{\text{site}}A) \approx 0.002$ and $3\pi/(12N_{\text{site}}A) \approx 0.006$, as given in Eq. (5).

The above property is not seen so clearly for lattices having small N_σ and large N_τ . The position of the next-to-leading zero points of Z_{norm} appear at random for the other data sets relative to the nearest zero point. The positions of Lee-Yang zeros are shown in Table I. We could not obtain clearly isolated Lee-Yang zeros for the lattices $24^3 \times 6$ and $20^3 \times 6$. The second nearest Lee-Yang zero to the real axis could be measured only for the $24^2 \times 36 \times 4$ lattice. The result on the $36^2 \times 48 \times 6$ lattice ($\beta_0 = 5.8936$) is also shown in Fig. 2. Only the nearest Lee-Yang zero is obtained

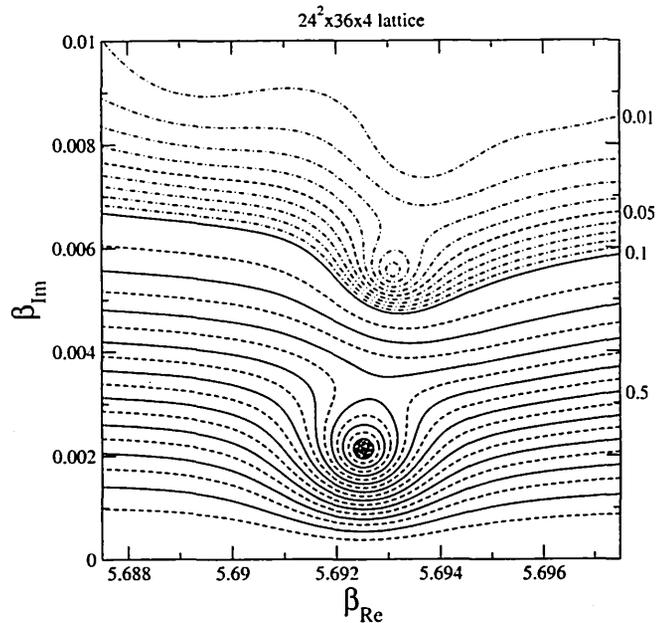


FIG. 1. Contour plot of the normalized partition function Z_{norm} in the $(\beta_{\text{Re}}, \beta_{\text{Im}})$ plane measured on the $24^2 \times 36 \times 4$ lattice. Values in the right edge are Z_{norm} . The simulation point is $\beta_0 = 5.6925$.

clearly. The Lee-Yang zero becomes less clear as N_τ increases and N_σ decreases, hence simulations on lattices having large N_σ/N_τ seem to be necessary for the study of Lee-Yang zeros.

The values for $\beta_{\text{Im}}^0 V$ on $24^2 \times 36 \times 4$ and $12^2 \times 24 \times 4$ lattices are 43.9(5) and 42.0(6), respectively. These are roughly constant and suggest the scaling behavior of $\beta_{\text{Im}}^0 \sim 1/V$ for a first order phase transition. Also, in the previous study for lattices with $N_\tau = 2$ [21], the $1/V$ scaling behavior has been confirmed for $N_\sigma = 6, 8, 10$, and 12. However, for a more precise quantitative investigation that takes into account the errors, the spatial lattice size $12^2 \times 24$ may not be large enough to check the $1/V$ scaling for $N_\tau = 4$, since the difference of $\beta_{\text{Im}}^0 V$ is larger than the statistical error. We should fit the data obtained on more than two lattices by a curved function of $1/V$, to confirm through a $1/V$ scaling analysis that the phase transition of the SU(3) pure gauge theory is first order. E.g. for the study of the SU(2) gauge-Higgs model [24], the following fitting functions have been used, $\text{Im}\kappa_0(V) = \kappa_0^c + CV^{-\nu}$ and $\text{Im}\kappa_0(V) = \kappa_0^c + CV^{-1} + DV^{-2}$ for a

TABLE I. Positions of Lee-Yang zeros for the SU(3) pure gauge theory.

Lattice size		β_{Re}	β_{Im}
$12^2 \times 24 \times 4$	1st zero	5.691 78(23)	0.012 16(17)
$24^2 \times 36 \times 4$	1st zero	5.692 52(5)	0.002 12(2)
$24^2 \times 36 \times 4$	2nd zero	5.693 09(7)	0.005 56(7)
$36^2 \times 48 \times 6$	1st zero	5.894 11(10)	0.004 34(8)

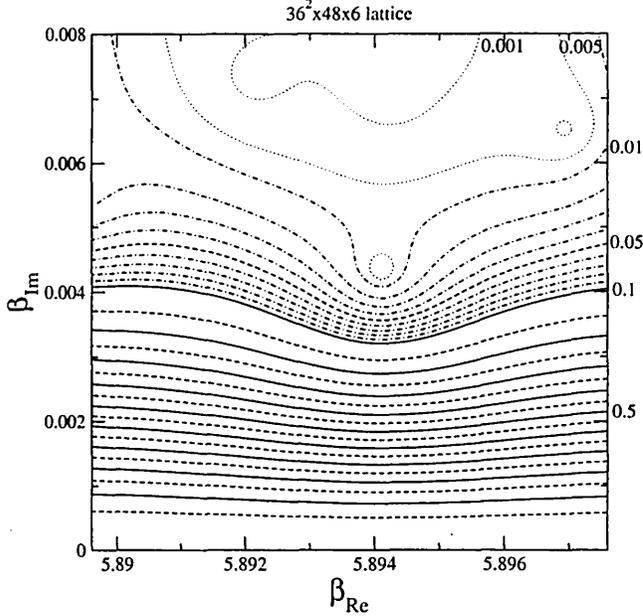


FIG. 2. Contour plot of the normalized partition function Z_{norm} for the $36^2 \times 48 \times 6$ lattice. The simulation point is $\beta_0 = 5.8936$.

complex parameter κ in the model with fitting parameters κ_0^c , C , D , and ν .

III. COMPLEX PHASE FLUCTUATION AND SIGN PROBLEM

As seen in the previous section, the investigation of Lee-Yang zeros in the complex β plane seems to be useful to identify the order of phase transition. However, if we try to extend this analysis to full QCD at nonzero baryon density, a serious problem arises. This problem is closely related to the sign problem for finite density QCD, since the normalized partition function can be zero in the complex β plane due to fluctuations of the complex phase related to β_{Im} and also due to the complex phase from the quark determinant that causes the sign problem. Before discussing the Lee-Yang zero analysis for finite density QCD, we would like to review the sign problem briefly.

The main difficulty for studies at finite baryon density is that the Boltzmann weight is complex if the chemical potential is nonzero. In this case the Monte-Carlo method is not applicable directly, since configurations cannot be generated with a complex probability. One approach to avoid this problem is the reweighting method. We perform simulations at $\mu = 0$, and incorporate the remaining part of the correct Boltzmann weight for finite μ in the calculation of expectation values. Expectation values $\langle \mathcal{O} \rangle$ at (β, μ) are thus computed by a simulation at $(\beta, 0)$ using the following identity,

$$\langle \mathcal{O} \rangle_{(\beta, \mu)} = \frac{\langle \mathcal{O} e^{N_f(\text{Indet}M(\mu) - \text{Indet}M(0))} \rangle_{(\beta, 0)}}{\langle e^{N_f(\text{Indet}M(\mu) - \text{Indet}M(0))} \rangle_{(\beta, 0)}}, \quad (11)$$

where M is the quark matrix and N_f is the number of flavors ($N_f/4$ for staggered type quarks instead of N_f); μ is a quark chemical potential in lattice units, i.e. $\mu \equiv \mu_q a = \mu_q / (N_\tau T)$, and μ_q is the quark chemical potential in physical units. This is the basic formula of the reweighting method. However, because $\text{Indet}M(\mu)$ is complex, the calculations of the numerator and denominator in Eq. (11) becomes in practice increasingly more difficult for larger μ . We define the phase of the quark determinant θ by $(\det M(\mu))^{N_f/4} \equiv |\det M(\mu)|^{N_f/4} e^{i\theta}$ for staggered type quarks. If the typical value of θ becomes larger than $\pi/2$, the real part of $e^{i\theta}$ ($= \cos\theta$) changes its sign frequently. Eventually both the numerator and denominator of Eq. (11) become smaller than their statistical errors and Eq. (11) can no longer be evaluated. We call it the “sign problem.”

Here, the denominator of Eq. (11), or simply $\langle \cos\theta \rangle$, is a good indicator for the occurrence of the sign problem. If this indicator is zero within statistical errors, Eq. (11) cannot be computed. In the following we give an estimate for the value of the complex phase. Since the direct calculation of the quark determinant is difficult except for calculations on small lattices, we expand $\text{Indet}M(\mu)$ in a Taylor series,

$$\text{Indet}M(\mu) - \text{Indet}M(0) = \sum_{n=1}^{\infty} \left[\frac{\partial^n (\text{Indet}M)}{\partial \mu^n} \right] \frac{\mu^n}{n!}. \quad (12)$$

Then, we can easily separate it into real and imaginary parts because the even derivatives of $\text{Indet}M(\mu)$ are real and the odd derivatives are purely imaginary [4]. The complex phase θ is given by

$$\theta = \frac{N_f}{4} \sum_{n=1}^{\infty} \text{Im} \frac{\partial^{2n-1} (\text{Indet}M)}{\partial \mu^{2n-1}} \frac{\mu^{2n-1}}{(2n-1)!}, \quad (13)$$

for staggered type quarks at small μ . The Taylor expansion coefficients are rather easy to calculate by using the stochastic noise method. The comparison between the value of θ with this approximation and the exact value has been done in Ref. [25], and the reliability and the application range have been discussed.

We use data for the Taylor expansion coefficients obtained in Ref. [9]. The data were generated by using Symanzik-improved gauge and p4-improved staggered fermion actions. Coefficients up to $O(\mu^5)$ have been calculated. Figure 3 shows the indicator $\langle \cos\theta \rangle$ measured at $\beta = \{3.60, 3.65, \text{ and } 3.68\}$, for $ma = 0.1$, corresponding to $T/T_c = 0.90, 1.00, \text{ and } 1.07$, respectively, on a $16^3 \times 4$ lattice.² We also estimate the values of $\mu_q/T \equiv N_\tau \mu$ at

²As mentioned in Ref. [4], in the calculation using the stochastic noise method, the error due to the finite number of noise vector (N_{noise}) is large for the calculation of $\langle \cos\theta \rangle$ with $N_{\text{noise}} = 10$. For the purpose of this study we increased the number of noise vector to $N_{\text{noise}} = 100$. We checked that the difference between the results with $N_{\text{noise}} = 50$ and $N_{\text{noise}} = 100$ is about 10% for the calculation of the position at which $\langle \cos\theta \rangle = 0.1$.

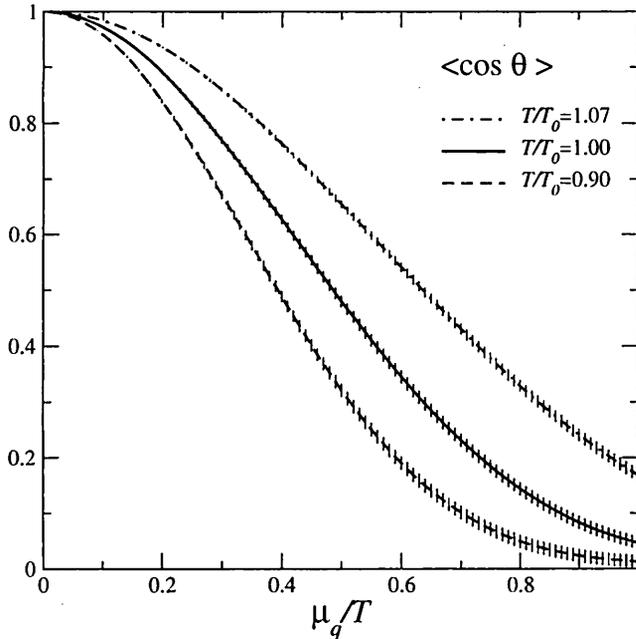


FIG. 3. The expectation value of the complex phase $\langle \cos \theta \rangle$ for QCD with two flavors of p4-improved staggered quarks at $ma = 0.1$.

which $\langle \cos \theta \rangle = 0.1, 0.01$ and 0.0 . Results are given in Table II. The situation now is quite similar to the non-singular case of the normalized partition function in the

$$\begin{aligned} Z_{\text{norm}}(\beta_{\text{Re}}, \beta_{\text{Im}}, \mu) &\equiv \left| \frac{Z(\beta_{\text{Re}}, \beta_{\text{Im}}, \mu)}{Z(\beta_{\text{Re}}, 0, 0)} \right| \\ &= \left| \left\langle e^{6i\beta_{\text{Im}}N_{\text{site}}\Delta P} e^{i\theta} \middle| e^{(N_f/4)(\text{Indet}M(\mu) - \text{Indet}M(0))} \right\rangle_{(\beta_{\text{Re}}, 0, 0)} \right| \end{aligned} \quad (14)$$

or

$$Z_{\text{norm}}(\beta_{\text{Re}}, \beta_{\text{Im}}, \mu) \equiv \left| \frac{Z(\beta_{\text{Re}}, \beta_{\text{Im}}, \mu)}{Z(\beta_{\text{Re}}, 0, \mu)} \right| = \left| \frac{\langle e^{6i\beta_{\text{Im}}N_{\text{site}}\Delta P} e^{i\theta} | e^{(N_f/4)(\text{Indet}M(\mu) - \text{Indet}M(0))} \rangle_{(\beta_{\text{Re}}, 0, 0)}}{\langle e^{i\theta} | e^{(N_f/4)(\text{Indet}M(\mu) - \text{Indet}M(0))} \rangle_{(\beta_{\text{Re}}, 0, 0)}} \right| \quad (15)$$

for staggered type quarks. θ is the complex phase of $\exp[(N_f/4)(\text{Indet}M(\mu) - \text{Indet}M(0))]$. Since the numerator of Eq. (15), which is the same as Z_{norm} in Eq. (14), is

TABLE II. Values of $\mu_q/T \equiv N_\tau \mu$ at which $\langle \cos \theta \rangle = 0.1, 0.01$, and 0.0 $N_{\text{site}} = 16^3 \times 4$.

T/T_0	$\langle \cos \theta \rangle = 0.1$	$\langle \cos \theta \rangle = 0.01$	$\langle \cos \theta \rangle = 0.0$
0.90	0.70(2)	1.0(2)	1.2(2)
0.96	0.80(2)	1.1(1)	1.1(1)
1.00	0.87(2)	1.9(2)	2.3(4)
1.02	0.96(3)	2.2(12)	2.3(1)
1.07	1.13(3)	1.8(4)	2.0(2)

complex β plane discussed in the previous section. This becomes even more apparent if we consider for simplicity only the first term in the expansion of θ which is proportional to μ . Then $\langle \cos \theta \rangle$, μ and $\text{Im}[\partial(\text{Indet}M)/\partial\mu]$ correspond to the normalized partition function, β_{Im} and plaquette, respectively.

Because the distribution of the complex phase θ is almost of Gaussian shape, the indicator, $\langle \cos \theta \rangle$, decreases exponentially as μ increases, and it may cross zero at a point where the expectation value becomes smaller than the statistical error. Therefore, the points of $\langle \cos \theta \rangle = 0$ appear accidentally and the results given in Table II are unstable. Moreover, $\partial(\text{Indet}M)/\partial\mu$ becomes larger as the volume increases, hence the indicator for the sign problem vanishes in the infinite volume limit for any nonzero μ , which means that the range of applicability for the reweighting method approaches $\mu = 0$ in the infinite volume limit.

IV. LEE-YANG ZERO ANALYSIS FOR FINITE DENSITY QCD

The Lee-Yang zero analysis for finite density QCD has been performed by Fodor and Katz [2,3]. They measured the normalized partition function Z_{norm} using the reweighting method, and determined the points where $Z_{\text{norm}} = 0$ as a function of spatial volume. The normalized partition function is defined by

required to be zero at a zero point of Z_{norm} in Eq. (15), we consider Eq. (14) as an indicator for the Lee-Yang zero.

Here, we notice that for $\beta_{\text{Im}} = 0$ this normalized partition function is exactly the same as the indicator for the sign problem, i.e. the denominator of Eq. (11). As discussed in the previous section, in any practical simulation this indicator will be consistent with zero within errors for large values of μ . Moreover, the region where the indicator is nonzero becomes narrower as the volume increases, and this region vanishes in the infinite volume limit. Hence, the Lee-Yang zeros always approach the $\beta_{\text{Im}} = 0$ axis in the infinite volume limit for any finite μ . This means that the scaling behavior for crossover will not be obtained for the case with the sign problem. This is clearly different from

the usual expectation for the QCD phase diagram in the (T, μ) plane. Most model calculations suggest that the transition is crossover in the low density region. This might be a problem of the definition of the normalized partition function, Eq. (14). The normalized partition function on the real β axis is exactly one for $\mu = 0$, but it vanishes for finite μ in the infinite volume limit. Therefore, it is very difficult to distinguish the first order transition and crossover by investigating the position of Lee-Yang zeros as a function of spatial volume. This is the most important difference between the definitions for the pure gauge theory in Sec. II and QCD at nonzero density.

The critical endpoint is shown to be located at $\mu_B = 3\mu_q = 725(35)$ MeV in Ref. [2] and $360(40)$ MeV in Ref. [3], which is inconsistent with the above argument. This may be a problem of the fitting function. In Refs. [2,3] the position of Lee-Yang zeros has been fitted by $\beta_{\text{Im}}^0 = A(1/V) + \beta_{\text{Im}}^\infty$, where A and β_{Im}^∞ are fitting parameters. The first order transition and crossover have then been distinguished by the value of β_{Im}^∞ . As we discussed in Sec. II, this fitting function is too simple to fit the data of Lee-Yang zeros obtained on lattices as small as those used in Refs. [2,3], i.e. $V \leq 12^3$. In fact, if one assumes a curved extrapolation function, all data in Table 1 of Ref. [3] seems to approach $\beta_{\text{Im}} = 0$ in the $1/V \rightarrow 0$ limit.

In our argument, the statistical error of Z_{norm} , which is controlled by the number of configurations in the Monte-Carlo simulation, plays an important role. If the statistical error of Z_{norm} becomes much smaller than the mean value of Z_{norm} by increasing the statistics for each simulation, the method in Refs. [2,3] would be applicable. However, one cannot satisfy this condition in general simply because we are looking for the Lee-Yang zero which gives $Z_{\text{norm}} = 0$. Namely, statistical error cannot be smaller than 0. Moreover, if the error of Z_{norm} is sizeable, there appear fake Lee-Yang zeros which are located even closer to the real β axis than the true zero in the region where the mean value of Z_{norm} is smaller than the error. Since we adopt the closest zero as the Lee-Yang zero in the actual scaling analysis, we may thus misidentify the true zero by the fake one.

The above point can be seen explicitly for the second Lee-Yang zero of the SU(3) gauge theory with $N_\tau = 6$ shown in Fig. 2. Theoretically, we expect the second Lee-Yang zero exists around $\beta_{\text{Im}} \approx 0.013$, i.e. 3 times larger than that of the first Lee-Yang zero as shown in Fig. 1. However, we find several β which give $Z_{\text{norm}} = 0$ in the region of $\beta_{\text{Im}} > 0.006$, and they distribute randomly. If we identify the second nearest point as the second Lee-Yang zero, the resulting β_{Im} is much smaller than the theoretical expectation. This problem is caused by the existence of the region in the complex β -plane where the statistical error of Z_{norm} is larger than the mean value as discussed above. As the statistics is increased for fixed V , such a region should become smaller and fake Lee-Yang zeros should disappear.

Now we discuss how the above situation changes by increasing the volume V . Fortunately, in the SU(3) gauge theory, the location of Lee-Yang zero can be determined better also as the volume increases as shown in Sec. II. In this case, the validity of the scaling assumption becomes better as the volume increases. On the other hand, for the case with the sign problem, the error normalized by the mean value grows exponentially as a function of volume. Then the size of the region having fake Lee-Yang zeros cannot be made smaller unless one has exponentially large statistics. This leads to the conclusion that the quality of the scaling analysis is not improved by increasing the volume, and any reliable information about Lee-Yang zeros in the infinite volume limit cannot be obtained. This is the reason why the serious problem of identifying the critical endpoint is intimately related to the sign problem.

This discussion suggests that the finite-volume scaling analysis suffers serious damage through the unsolved sign problem, and it is very difficult to apply the criterion used by Fodor and Katz for the investigation of the critical endpoint in practice. However, the property of the second nearest Lee-Yang zero characteristic for a first order transition in Fig. 1, i.e. the fact that the distance to the second Lee-Yang zero from the real axis is 3 times larger than that of the first Lee-Yang zero, could be investigated on a finite lattice. This study is possible for small μ without taking the infinite volume limit. On the other hand, we do not expect any isolated Lee-Yang zero for a crossover transition, hence we may be able to determine the order of phase transition by investigating the distribution of Lee-Yang zeros in the complex β plane. Although the measurements of the second Lee-Yang zero may require large lattice sizes and high statistics, as seen for the case of pure SU(3) gauge theory, it may be possible to find the region of the first order phase transition, if the critical endpoint exists in the low density region.

V. CONCLUSIONS

We commented on the Lee-Yang zero analysis for the study of the critical endpoint in the (T, μ_q) phase diagram. It is found that the Lee-Yang zero analysis at nonzero baryon density encounters a serious problem. The complex phases of the quark determinant and the complex β are mixed at nonzero chemical potential. In this case, in practical simulations with limited statistics the normalized partition function can develop zeros even on the real β axis for large μ_q in finite volumes. Moreover, in the infinite volume the normalized partition function is always zero except for $\mu_q = 0$. This means that the nearest Lee-Yang zero always approaches the real β axis in the infinite volume limit. The scaling behavior suggesting a crossover transition thus will not be obtained. This is clearly different from usual expectations for the QCD phase diagram. To avoid this problem, the sign problem must be removed by careful treatments increasing the number of configurations

exponentially as the volume or μ_q/T increases, otherwise the finite-volume scaling behavior for the position of Lee-Yang zeros, which has been analyzed by Fodor and Katz [2,3], does not provide an appropriate criterion for the investigation of the order of the phase transition.

To make the underlying problem more transparent, we applied the Lee-Yang zero analysis to the SU(3) pure gauge theory, which does not have a sign problem and for which the simulations are much easier. Lee-Yang zeros are found in the complex β plane. They appear periodically as expected by the discussion using a plaquette distribution function for a first order phase transition. The positions of the first Lee-Yang zero on two lattices having different volume sizes are roughly consistent with the finite size scaling behavior for a first order phase transition, i.e. $\beta_{\text{lm}}^0 \sim 1/V$. However, for quantitative analysis it is necessary to fit data from more than two different lattice sizes by a curved function to study the order of the phase transition. It is found, in this analysis, that complex phase fluctuations arising from the imaginary part of β play an important role, and the mechanism that leads to the appearance of the Lee-Yang zeros is quite similar to the situation in QCD where the sign problem is present.

The property of a first order phase transition that isolated Lee-Yang zeros appear periodically at $\beta_{\text{lm}} \sim C(2n + 1)$, where C is the distance to the nearest Lee-Yang zero and n is an integer, is free from the problems that arise in the infinite volume limit. Therefore, to investigate the pattern of the appearance of Lee-Yang zeros in the $(\beta_{\text{Re}}, \beta_{\text{Im}})$ plane is important. For this calculation, the simulations

by using high statistics data and large lattice size are indispensable. Further studies are clearly important to find the endpoint of the first order phase transition line in the (T, μ_q) plane.

Recently, a close relation between the strength of the sign problem and the position of the phase transition line for pion condensation in phase-quenched QCD has been discussed in Ref. [26]. There it has been found that the endpoints of the first order transition line determined in Refs. [2,3] are located near the phase transition line of pion condensation. These results may relate to our discussion given here.

Moreover, the pathologies in the Glasgow method have been discussed in Ref. [17]. Similar problems arise also in the Glasgow method. It would be interesting to consider the relation between the pathologies in the Glasgow method and those in the Lee-Yang zero analysis.

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