Lee-Yang zero distribution of high temperature QCD and Roberge-Weiss phase transition

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Canonical partition functions and Lee-Yang zeros of QCD at finite density and high temperature are studied. We present analytic derivation of the canonical partition functions and Lee-Yang zeros based on the free energy in the Stefan-Boltzmann limit using a saddle point approximation. We also perform lattice QCD simulation in a canonical approach using the fugacity expansion of the fermion determinant, and carefully examine its reliability. By comparing the analytic and numerical results, we conclude that the canonical partition functions follow the Gaussian distribution of the baryon number, and the accumulation of Lee-Yang zeros of these canonical partition functions exhibit the first order Roberge-Weiss phase transition. We discuss the validity and applicable range of the result, and its implications both for theoretical and experimental studies.

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I. INTRODUCTION

Quantum chromodynamics (QCD) undergoes a phase transition from the hadronic phase to the quark gluon plasma (QGP) phase at high temperature. Recently, a beam energy scan (BES) program at Relativistic Heavy Ion Collider (RHIC) has reported valuable data for the longstanding issue of identifying the phase boundary in the QCD phase diagram by using heavy ion collisions with different collision energies, centralities, etc. [1–3]. There the probability distribution of conserved charges has been constructed by measuring them for each collision. Extensive efforts have been invested to understand event-by-event fluctuations of those charges, as they are expected to be useful observables for locating the critical endpoint [4–8].

The setup in BES experiments, where a part of fireballs is accessible for measurements, resembles a grand canonical ensemble in statistical mechanics [9–11], and this parallelism enables us to study the probability distribution of the net baryon number \( n_B \) theoretically: Consider a grand canonical ensemble for a single species of particle. The grand canonical partition function \( Z(\mu) \) is expanded in terms of the number of particles \( n \) as \( Z(\mu) = \sum_n Z_n e^{\mu n} / T \). Here \( Z_n \) is a canonical partition function, which depends on temperature \( T \) but not on the chemical potential \( \mu \). For given \( \mu \) and \( T \), \( Z_n e^{\mu n} / T \) is proportional to the probability of observing an \( n \)-particle state in the grand canonical system. The BES experiments have so far measured the net proton multiplicity and reported [2] that it closely follows the Skellam distribution for several collision energies and centralities. This observation is consistent with the hadron resonance gas (HRG) model, in which the net baryon multiplicity is approximately given by a Skellam distribution [9].

On the other hand, in lattice QCD simulations the canonical approach has been proposed as a tool to circumvent the sign problem associated with a finite chemical potential [12–22]. In previous studies [21–22], two of the authors (KN and AN) found that the canonical partition functions follow the Gaussian distribution of the baryon number at high temperatures, and that the Lee-Yang zeros obtained from the canonical partition functions of the Gaussian type exhibit a behavior consistent with a Roberge-Weiss (RW) phase transition [23]. This result has several implications: the connection between the Gaussian behavior of the net-baryon number distribution and the RW phase transition can be used as an experimental probe indicating the QGP phase, since the RW phase transition is a phenomenon specific to the QGP phase. The result is also interesting in the context of the Lee-Yang zero analysis [24–25], since the distribution of Lee-Yang zeros are known for some limited cases, e.g. [25–26].

Despite of the aforementioned importance, the determination of Lee-Yang zeros in Monte Carlo simulations is difficult task. Canonical partition functions suffer from a phase fluctuation for configuration by configuration due to the sign problem. This problem may be reduced by using sophisticated approaches proposed in e.g. [15–19]. However, the phase fluctuation becomes more severe as the baryon number increases, and the truncation of the fugacity polynomial at a certain order is inevitable. Such methodological artifacts might sensitively affect the thermodynamic behavior of the Lee-Yang zeros that are the roots of the truncated polynomial.

The purpose of the present work is to determine the canonical partition functions and Lee-Yang zeros in QCD at high temperatures, and to reexamine their relationships. To this end, we present an alternative analytical calculation and assess the reliability of the lattice results in the light of the former. Specifically, we first derive the canonical partition functions and Lee-Yang zeros at high temperature, by utilizing the fact that the free-energy is then given as a simple quartic function of the quark chemical potential. The canonical partition function is defined as a Fourier integral of the grand canoni-
cal partition function with pure imaginary chemical potential. At high temperature, this integral can be evaluated in a saddle point approximation, yielding the Gaussian function. Accordingly, the grand canonical partition function is expressed as a Jacobi theta function. Using the property of the zeros of the theta function, we show that the Lee-Yang zeros are located on the negative real axis on the complex plane of the baryon fugacity. Due to the RW periodicity, these zeros are aligned on three radial lines on the complex plane of the quark fugacity. This elucidates the close connection between the Gaussian behavior of the canonical partition functions and the RW phase transition.

In reexamine the results from the lattice QCD simulation, some of which have been already presented in [22], we address the issue of the convergence of the fugacity polynomial and Lee-Yang zeros, and perform a bootstrap analysis for their distribution. We find that the Lee-Yang zeros related to the RW phase transition are not sensitive to the truncated part of the fugacity polynomial. We also find an agreement between the lattice data and analytic calculation.

This work is organized as follows. In the next section, we start by introducing the concept of the canonical approach and Lee-Yang zero theorem. In section III we derive the canonical partition functions from the free-energy in the Stefan-Boltzmann limit, and Lee-Yang zeros from the canonical partition functions. In section IV we compute the canonical partition functions and Lee-Yang zeros in lattice QCD simulation. In section V we summarize our findings and discuss their implications and reliability.

II. CANONICAL APPROACH AND LEE-YANG ZEROS

In this section, we explain the canonical approach and Lee-Yang zero theorem. The grand canonical partition function is defined by

\[ Z(\mu) = \text{tr} e^{-\beta (\hat{H} - \mu \hat{N})}, \]

(1)

where \( \hat{H} \) and \( \hat{N} \) denote the Hamiltonian and the quark number operator in QCD, and \( T \) and \( \mu \) the temperature and the quark chemical potential. Using the eigenstates of the number operator, \( Z(\mu) \) can be expanded in powers of fugacity \( \xi = e^{\mu/T} \)

\[ Z(\mu) = \lim_{N \to \infty} \sum_{n=-N}^{N} Z_n \xi^n. \]

(2)

Here \( Z_n = \text{tr}(e^{-\beta \hat{H}/T} \delta_{\hat{N}, n}) \) is the canonical partition functions at a fixed quark number \( n \), which is the eigenvalue of \( \hat{N} \). In the next section, we will show that only the triality sector \( (n \equiv 0 \mod 3) \) contributes to \( Z(\mu) \) due to the RW periodicity. For the triality we refer the reader to [23]. By definition, \( Z_n \) is real and positive for any \( n \), and satisfies \( Z_n = Z_{-n} \). \( N \) is the maximum number of quarks that can be supported on the system. It is finite on the lattice and diverges in the thermodynamic limit.

For real \( \mu \) (i.e. real and positive \( \xi \)), \( Z(\mu) \) has no zero since its coefficient \( Z_n \) is real and positive for any \( n \). However, \( Z(\mu) \) can have zeros for complex \( \mu \). Using the roots \( \xi_i \) of \( Z(\mu) \) in the complex \( \xi \) plane, called Lee-Yang zeros, it is expressed in a factorized form

\[ Z(\mu) = \lim_{N \to \infty} Z_{-N}^{-N} \prod_{i=1}^{2N} (1 - \frac{\xi}{\xi_i}). \]

(3)

Due to the symmetry \( Z_0 = Z_{-n} \), any root \( \xi_i \) inside the unit circle is accompanied by another root \( 1/\xi_i \) outside. Although Lee-Yang zeros are generally complex, they can approach the positive real axis on the complex \( \xi \) plane in the thermodynamic limit \( V \to \infty \), which causes a thermodynamic singularity [24, 25].

III. LEE-YANG ZEROS IN QCD AT HIGH TEMPERATURE

The free energy density of QCD, \( f(\mu) = -(T/V) \ln Z(\mu) \), can be expanded in even powers of chemical potential \( \mu \). At high temperature, \( f \) approaches that of the free gas of quarks and gluons, where Taylor coefficients vanish for \( n \geq 6 \)

\[ f(\mu) = c_0 + c_2 \left( \frac{\mu}{T} \right)^2 + c_4 \left( \frac{\mu}{T} \right)^4. \]

(4)

The minus sign in the l.h.s is introduced according to the convention. Although Eq. (4) is obtained for massless quarks, it holds true even in the case of nonzero quark mass in lattice QCD simulations.

The canonical partition function \( Z_n \) can be extracted from Eqs. (2) and (4) by Fourier transformation. This requires to extend \( \mu \) to pure imaginary \( \mu = i \mu_1, \mu_1 \in \mathbb{R} \). The free energy \( \mu_1 \) is obtained in the absence of the background gauge field, which is valid only for the angular domain \( i \mu_1/T \in [\pi/3, \pi/3] \). For other domains, the Polyakov loop \( P \) acquires a nonzero value,

\[ P = \frac{1}{i} \text{tr} \int \exp(i g A_\mu d\tau) = e^{i \omega} \left( \pm 2\pi/3 \right), \]

where \( \theta = \mu_1/T \). Using the RW periodicity [23], this reads

\[ Z_n = \int_{-\pi/3}^{\pi/3} e^{-Vf/\theta} e^{i n \theta} d\theta \]

\[ = \int_{-\pi/3}^{\pi/3} e^{-Vf/\theta} e^{i n \theta} d\theta. \]

(5)

This ensures \( Z_n = 0 \) for \( n \neq 0 \mod 3 \). Eq. (5) is expressed as

\[ Z_n = \frac{3}{2\pi} \int_{-\pi/3}^{\pi/3} d\theta e^{3Vg(\theta) + in \theta} \left( \pm \frac{2\pi/3}{\pi} \right). \]

(6)
where \( g(\theta) = c_0 - c_2 \theta^2 + c_4 \theta^4 \). The function \( g(\theta) \) has one maximum at \( \theta = 0 \) and two minima at \( \theta = \pm \sqrt{c_2/(2c_4)} \). In the Stefan-Boltzmann limit, these minima are located at \( \sqrt{c_2/(2c_4)} = \sqrt{2} \pi \), outside of the integral domain. \( g(\theta) \) is a concave function for \( \theta \in [-\pi/3,\pi/3] \) with the maximum at \( \theta = 0 \). It has a sharper peak for larger volume, and the integral Eq. (7) is dominated by \( \theta = 0 \) for large \( V \). This allows for the use of the saddle point approximation to Eq. (7), so that \( Z_n \) is reduced to

\[
Z_n = C e^{-n^2/(4T^3 V c_2)} \quad (n \equiv 0 \mod 3),
\]

where \( C = \frac{3}{\pi^2} \sqrt{\frac{\pi}{T^3 V c_2}} \). In transition from Eq. (7) to (8), we approximated an incomplete Gamma function by a complete counterpart (see Appendix A). The validity of our approximation is estimated by the condition \( c_2 (\mu/T)^2 \gg c_4 (\mu/T)^4 \) so that the free energy is dominated by the second order term. To evaluate the applicable range of Eq. (9), we have plotted \( (f(\mu) - f(0))/T^4 \) for the saddle point approximation and original one in Fig. 1. It indicates that the saddle point approximation is valid for small \( \mu/T \lesssim 0.5 \).

![Graph showing comparison between exact and saddle point approximation](image)

FIG. 1: Comparison of the saddle point approximation and exact result for the free energy density. We use values of \( c_2, c_4 \) and \( V/T^3 \) used in our simulations in the next section (\( c_2 = 2.20, c_4 = 0.27 \)).

Assuming the validity of Eq. (8), \( Z(\mu) \) is reconstructed as

\[
Z(\mu) = C \sum_{n_B = -\infty}^{\infty} e^{-9n_B^2/(4T^3 V c_2) + 3n_B \mu/T}.
\]

The zeros of the grand canonical partition function are readily obtained by recognizing that Eq. (8) is equal to the Jacobi theta function

\[
\vartheta(z, \tau) = \sum_{n=-\infty}^{\infty} e^{\pi i n^2 \tau + 2 \pi i n z},
\]

where \( z \) and \( \tau \) are given by

\[
2 \pi i z = \frac{\mu}{T}, \quad \pi i \tau = -\frac{9}{4T^3 V c_2}.
\]

Thus the Lee-Yang zeros of Eq. (9) are given by the zeros of \( \vartheta(z, \tau) \) located at

\[
\frac{\mu}{T} = \frac{(2k + 1)\pi i}{3} - \frac{3(2\ell + 1)}{4T^3 V c_2},
\]

where \( k \) and \( \ell \) take all integer values as a consequence of the pseudo double periodicity of the theta function.

On the complex plane of the baryon fugacity \( \xi_B = \xi^3 \), all zeros in Eq. (12) are located on the negative real axis. On the complex \( \xi \) plane, Eq. (12) lie on three radial lines at arguments \( \arg \xi = \text{Im}[\mu/T] = \pi/3, \pi, \) and \( 5\pi/3 \). The RW phase transition occurs at the points \( (\text{Re}[\mu/T], \text{Im}[\mu/T]) = (0, (2k + 1)\pi/3) \) \([23]\). The Lee-Yang zeros closest to these points are given by

\[
\frac{\mu}{T} = \frac{(2k + 1)\pi i}{3} \pm \frac{3}{4T^3 V c_2}.
\]

Each of them approaches the corresponding RW phase transition point in thermodynamic limit as \( 1/V \). This explains the first-order nature of the RW phase transition according to the Lee-Yang zero theorem. In addition, Eq. (12) also indicates that the RW phase transition occurs at \( \mu/T = \pi/3 \) even for \( \text{Re}[\mu/T] \neq 0 \), as long as the saddle point approximation is valid. We note that it is possible to obtain the Lee-Yang zeros Eq. (13) directly from the free energy by using a method in \([24]\).

IV. LATTICE QCD SIMULATIONS

A. Method and setup

In this section, we reexamine the data of our previous lattice QCD simulations, in which three quantities, the RW phase transition \([30]\), Taylor coefficients of the free energy \([31]\), canonical partition functions and Lee-Yang zeros \([21, 22]\), were calculated in the same lattice setup. Below we recapitulate the calculation of \( Z_n \) and Lee-Yang zeros on the lattice, and summarize the setup of the simulations to make the paper self-contained.

The grand canonical partition function of lattice QCD is given by

\[
Z(\mu) = \int D U (\det \Delta(\mu))^N_T e^{-S_g},
\]

where \( U, \Delta(\mu) \), and \( S_g \) denote link variables, fermion matrix, and gauge action, respectively. We employ a clover-improved Wilson fermion action with \( N_f = 2 \) and renormalization-group improved gauge action \([32]\).

We calculate \( Z_n \) using a Glasgow method \([13, 14]\). We expand the fermion determinant in powers of \( \xi \) using a reduction formula of the Wilson fermion determinant \([14, 33, 37]\):

\[
(\det \Delta(\mu))^{N_f} = \sum_{n=-\infty}^{\infty} d_n \xi^n,
\]

which provides the fugacity expansion of \( Z(\mu) \). Since \( d_n \) is complex, it is not possible to use \( d_n \) as a measure for Monte Carlo simulations. Instead we use Ferrenberg-Swendsen reweighting for the fermion determinant: \( \det \Delta(\mu) = (\det \Delta(\mu)/\det \Delta(0)) \det \Delta(0) \), and express \( Z(\mu) \) as an expectation value of the operator \( \det \Delta(\mu)/\det \Delta(0) \) averaged.
over gauge configurations generated at $\mu = 0$. Then $Z_n$ is given by
\[ Z_n = \int \mathcal{D}U \frac{d_n}{(\det \Delta(0))^N} e^{-S_u}, \]
\[ = Z_0 \left\langle \frac{d_n}{(\det \Delta(0))^N} \right\rangle_0, \]  
(16)
where $Z_0 = \int \mathcal{D}U (\det \Delta(0))^{N_f} e^{-S_u}$, and $\left\langle \cdots \right\rangle_0$ denotes the expectation value obtained from gauge configurations generated at $\mu = 0$ with reweighting.

The simulation was performed in the following setup: The lattice volumes were $N_s^3 \times N_t = 8^3 \times 4$ and $10^3 \times 4$ with spatial and temporal lattice sizes $N_s$ and $N_t$. The simulation was performed along the line of constant physics with $m_\pi/m_\rho = 0.8$ [38]. We considered two temperatures $T/T_c = 0.99$ ($\beta = 1.85$) and $1.20$ (1.95), where $\beta = 6/g^2$ is the bare lattice coupling constant and $T_c$ is the pseudo critical temperature at $\mu = 0$. The RW phase transition point was estimated to be at $\beta_c = 1.92$ [30]. 11,000 HMC trajectories were simulated for each parameter set. The observables were calculated using 400 configurations with 20-trajectory intervals after removing the initial 3000 trajectories for thermalization.

Lee-Yang zeros are obtained by using a method based on the Cauchy integral theorem with a Divide and Conquer algorithm and a multi-precision arithmetic [22, 39]. According to the RW periodicity, zeros are first obtained for the polynomial of the baryon fugacity ($\xi_B = \xi^3$), then they are translated into zeros for quark fugacity. For further detail, see [21, 22, 31].

B. Canonical Partition Functions

\[ f(\mu) \]  approaches the quartic function of $\mu$ as expected in [4]. We also observe that the coefficients $c_2$ and $c_4$ are insensitive to the lattice volume. Thus, the conditions used in the saddle point approximation are satisfied at $T/T_c = 1.20$ or higher temperature.

FIG. 2: Second and fourth order coefficients of Taylor expansion of the free energy, $c_2$ and $c_4$, for $N_s = 8$, and 16. The data for $N_s = 8$ and 16 are taken from [31] and [38], respectively.

The $T$- and $V$-dependences of Taylor coefficients $c_2$ and $c_4$ are plotted in Fig. 2. At $T/T_c = 0.99$, $c_2$ and $c_4$ are comparable in magnitude, while $c_2$ is several times larger than $c_4$ at $T/T_c = 1.20$. We observed in [31] that higher order coefficients $c_6$, $c_8$, and $c_{10}$ are consistent with zero at $T/T_c = 1.20$, so that $f(\mu)$ approaches the quartic function of $\mu$ as expected in [4].

FIG. 3: Canonical partition function as a function of the baryon number for $T/T_c = 0.99$ (top) and 1.20 (bottom). The data are obtained from the canonical formalism, while the solid curves are obtained from the saddle point approximation. Note that only positive $Z_n$ are shown.

We plot the canonical partition functions $Z_{n_B}$ ($n = 3n_B$) in Fig. 3. The squares and circles indicate the values obtained from the canonical approach, Eq. (16). Since the average of $Z_n$ can be negative for large $n$ due to the overlap problem, we plot the values of $Z_{n_B}$ up to $\pm n_B$ below which the partition functions are all positive. The solid curves represent the Gaussian functions [8] with $c_2$ obtained from the lattice simulation. We observe that $Z_{n_B}$ with relatively small $n_B$ follows the Gaussian function at $T/T_c = 1.20$ as expected, while they fail to match at $T/T_c = 0.99$.

In order to quantify the consistency, we plot the relative difference between the lattice data and Gaussian fit in Fig. 4. The data and Gaussian functions show better agreement for higher temperature and larger volume. However, the Gaussian function systematically deviates from the data for large $n$ even at high $T$. This deviation is partly caused by the smallness of the lattice volume, as a better agreement is observed for larger volume. It is likely that the deviation may originate from the
breakdown of the saddle point approximation, as its validity is limited to small $\mu/T$. Below we shall examine how the deviation affects the distribution of Lee-Yang zeros.

C. Lee-Yang Zeros

In this work we calculate Lee-Yang zeros for $T/T_c = 1.20$. Before proceeding to numerical results, we remark on the numerical instability of the canonical partition functions at large $n$. The fugacity coefficients $d_n$ take complex values for each configuration. The phase of $d_n$ fluctuates more rapidly for larger $n$, because its modulus is exponentially suppressed as $n$ is increased. Beyond a certain value of $n$, $Z_n$ becomes negative, and the inclusion of such $Z_n$ would yield unphysical zeros of $Z(\mu)$ and cause unphysical non-analyticity for the free energy, even in a finite volume. Accordingly we are obliged to truncate the fugacity polynomial at $|n_{1b}| = n_0$ so that all $Z_{n_0}$ are positive for $|n_{1b}| \leq n_0$. (a) For a larger spatial lattice of size $N_s = 10$, it is natural to take the maximal permissible value $n_0 = 37$ as seen from Fig. 4. For a smaller spatial lattice $N_s = 8$, we try the following two alternatives: (b) maximal permissible value $n_0 = 32$ as seen from Fig. 5 and (c) $n_0 = 19 \approx 37 \times (8/10)^3$ so that the truncation order is proportional to the lattice volume as compared to the case with $N_s = 10$. Below we examine the convergence of the fugacity polynomial by comparing these two choices. Fig. 5 shows the distributions of the Lee-Yang zeros on the complex plane of the quark fugacity $\xi$, corresponding to the cases (a) [red], (b) [green], and (c) [blue], respectively. The distributions on the baryon fugacity plane is readily obtained by using the relation $\xi_B = \xi^3$. Near the unit circle, the Lee-Yang zeros are located on three radial lines with arguments $\arg \xi = \pi/3$, $\pi$ and $5\pi/3$. This behavior is qualitatively consistent with the prediction in Eq. (12). As approaching the origin, each line branches to two curves. The zeros near the unit circle ($0.6 < |\xi| < 1$) are stable as $n_0$ is increased from 19 to 32 for $N_s = 8$, which indicates the convergence of the fugacity polynomial. On the other hand, the increment of $n_0$ affects the location of the zeros for large chemical potential (small $\xi$). We also observe that under a shift of $n_0$ as proportional to the volume ($n_0 = 19$ for $N_s = 8$ and $n_0 = 37$ for $N_s = 10$), the Lee-Yang zeros are located on the common trajectories, and the density of the zeros are doubled.

In order to make quantitative comparison between lattice and analytic results, in Fig. 6 we plot $|\text{Re} \xi|$ (top) and $|\text{Re} \xi|^{1/\ell}$ (bottom) for several Lee-Yang zeros near the unit circle on the negative real axis. Statistical errors of the Lee-Yang zeros in the plot are estimated with a bootstrap method as follows: For each bootstrap sample, we calculate $Z_{n_0}$ up to $n_0$ and locate the Lee-Yang zeros. Since we are interested in the zeros relevant to the RW phase transition, we pick up some zeros near the unit circle and label them as $\ell = 1, 2, \ldots$ in the order of modulus. For each label $\ell$, statistical errors are estimated as the variance over 1000 bootstrap samples. Note that the zeros at $|\xi| \approx 1$ shown in Fig. 6 indicate no fluctuation in the imaginary part, while the zeros with smaller $|\xi| < 0.6$ fluctuate both in their real and imaginary parts. We observe that each Lee-Yang zero calculated in the simulation is systematically smaller in magnitude than the zero of the corre-
FIG. 6: Top: $|\text{Re} \xi|$ for zeros on the negative real axis near the unit circle. The curves represent predictions from the Jacobi theta function $\exp(-3(2\ell + 1)/(4T^3Vc_2))$ for $N_s = 10$ (red) and $N_s = 8$ (blue). Bottom: Volume-independent combination $|\text{Re} \xi|^{V/2}$. The curve represents $\exp(-3(2\ell + 1)/(4c_2))$.

responding order predicted in the saddle point approximation. In principle there could be two possible origins for this deviation: slow convergence of the fugacity expansion and/or deviation of the canonical partition functions from the Gaussian function. As there is no systematic difference between the two choices of the truncation order $\ell_0 = 19$ and 32, we can exclude the former origin and safely conclude that the deviation is caused by the deviation of $Z_n$ in the large-$n$ sector from the Gaussian function. Despite of this systematic deviation, the saddle point approximation well explains the features of the lattice data, such as trajectory of zeros, spacing between zeros and volume dependence.

V. DISCUSSIONS AND SUMMARY

Our result have several implications for theoretical and experimental studies. The connection between the Gaussian type of the canonical partition functions and the RW phase transition is worth emphasizing; the former can be extracted from an experimentally measurable quantity and the latter is a phenomenon specific to the QGP phase. Although there have been many studies on QCD at the imaginary chemical potential and the RW phase transition \cite{28,42}, we are not aware of any literature presenting a way to observe the RW phase transition experimentally. We predict that the canonical partition functions obtained from the probability distribution of the net baryon number, inferred from the multiplicity of baryons (or three-quark states) created at high temperature, be well approximated by the Gaussian function and associate the RW phase transition. (Such measurements, however, may be difficult at this moment because observed hadrons in heavy ion collisions are generated at the freeze-out temperature.) This observation, together with HRG, might serve as a basis to interpret experimental data obtained in BES experiments and help to distinguish deviations driven by the critical endpoint.

The distribution of the Lee-Yang zeros indicates that the RW phase transition persists at $\mu I/T = \pi/3$ even in the presence of the real part of the quark chemical potential. An analytic form of the canonical partition the Lee-Yang zero distribution obtained in this work can be used as a reference for future finite density QCD studies.

Recently STAR Collaboration reported \cite{2} that the net proton multiplicity closely follows the Skellam distribution for several collision energies and centralities. The multiplicity of the net baryon number is also approximately given by a Skellam distribution in the HRG model \cite{9}. In \cite{22} we applied the Lee-Yang zero theorem to the net proton multiplicity data in BES experiments, and found that they did not imply the RW phase transition. This suggests that the freeze-out temperature is lower than the temperature at which the RW phase transition takes place. However, there may be several controversies in deriving the above conclusion, namely the assumption of the equilibrium, the use of the net proton multiplicity as a substitute for net baryon multiplicity \cite{3,41}. In addition, the probability distribution has so far been measured for a limited range of the net proton number.

One of the interesting topics is an endpoint of the RW phase transition \cite{43,45}. The RW-like behavior appears when the free energy approaches the quartic function at high temperature, while it does not at $T \approx T_c$. In this sense, the RW phase transition is likely an indication of the completion of the deconfinement transition. It may be interesting to examine the relation between the RW end point and canonical partition functions, which may provide us with a possibility to study the latter experimentally. We leave this problem for future study.

The present work is also indicative in the viewpoint of the Lee-Yang zero theorem. Lee and Yang showed that zeros in Ising models are located on the unit circle on the complex activity plane ($e^{h/T}$) \cite{25}. As we have discussed, if the canonical partition function is Gaussian, then zeros are located on the negative real axis (for the baryon fugacity). Thus theories with the Gaussian type of the canonical partition functions, such as a gas of free fermions at small chemical potential, are exceptional cases of Lee-Yang zero circle theorem (Fig.7). QCD is expected to be an exceptional case of the Lee-Yang zero circle theorem if it undergoes a phase transition at $\text{Re} \mu \neq 0$. This can be trivially proved for the case with even number of flavors: Then the Boltzmann weight is real and positive on the unit circle on the complex fugacity plane, and zeros cannot
exist on the unit circle. A concrete example of the Lee-Yang zeros provided in the present work would help to deepen our understanding of the Lee-Yang zero theorem.

Admittedly we need to clarify the subtleties involved in numerical evaluation of canonical partition functions and Lee-Yang zeros. The present QCD simulation inevitably contains several lattice artifacts originated from coarse lattices, large quark masses, and small lattice volumes. However, we consider that the present results is robust and is likely to hold for other lattice setups in general, since the RW-like behavior is based only on a few assumptions, namely on the quartic form of the free-energy.

We obtained the Lee-Yang zeros as the roots of the fugacity polynomial. An alternative method is to calculate zeros of the grand partition function with a reweighting method. However, the validity of the latter case is controversial because Lee-Yang zeros appear when the average of a reweighting factor vanishes. This seems to imply the breakdown of the reweighting method. Moreover this problem tends to be more severe for large volume, which makes it difficult to distinguish physical zeros from the contamination of the sign problem [46]. The same problem does indeed occur even in the canonical approach: The sign problem sometimes makes $Z_n$ negative, which allows $Z(\mu)$ to vanish for real quark chemical potentials even in a finite volume. Such zeros are unphysical ones as a consequence of the sign problem. In this work, we have circumvented this problem by the truncation of the fugacity polynomial so that all $Z_n$ are positive. Although the truncated large-$n$ part of the canonical partition functions includes the severe sign problem, we confirmed that the zeros relevant to the RW phase transitions are insensitive to the truncated terms.

A further question still arises as to how the infinite sum of the truncated terms affects the location of Lee-Yang zeros. One of the main results of this work is that Lee-Yang zeros near the unit circle are robust and is likely to hold for a simple case where $Z_n$ is well approximated by a Gaussian function $Z_n^{(Gauss)}$ up to $N$, namely $\delta_n = Z_n - Z_n^{(Gauss)} \ll 1$ for $|n| < N$, and $\delta_n$ is not negligible for $|n| \geq N$. Denoting $Z = \sum_n Z_n \xi^n$, and $G = \sum_n Z_n^{(Gauss)} \xi^n$, the deviation is given by $Z - G \simeq \sum_{|n| \geq N} (Z_n - Z_n^{(Gauss)}) \xi^n$. For $\xi$ real and negative, $\xi^n$ is positive for even $n$ and negative for odd $n$.

Our lattice data exhibited in Fig. 4 suggests that $\delta_n$ is dominated by $Z_n$, which decreases monotonously as long as there is no phase transition at high temperature. Then the individual deviation $\delta_n$ monotonously decreases as $n$ increases, so that the overall deviation is bounded as $|Z - G| \leq \delta_N |\xi|^N$ due to the cancellation between even and odd terms. The point is that the sum of the truncated terms is bounded by the deviation at $n = N$, and does not increase as $N$ is increased.

Our numerical results suggest the deviation of of the Lee-Yang zeros from the RW-like behavior at large $\mu$, under which circumstance analytic calculation also breaks down. We do not understand if this deviation is physical or not as it lies beyond the applicable range of the present work. Since one ordinarily expects that there is no phase transition for the quark chemical potential in the QGP phase, we conjecture that the behavior smoothly changes from RW-like one to the $c_4$ dominance. It may be interesting to investigate whether there is a nontrivial Lee-Yang zero structure at large $\mu$.

In summary, we studied the canonical partition functions and Lee-Yang zeros in QCD at high temperature. We analytically derived them from the free energy in the Stefan-Boltzmann limit using the saddle point approximation. The canonical partition functions in QCD follow the Gaussian function at high temperature and at small chemical potential. We pointed out that the grand canonical partition function is approximately expressed as a Jacobi theta function, which enables us to determine all Lee-Yang zeros analytically. These Lee-Yang zeros are located on the negative real axis on the complex plane of the baryon fugacity. They are translated into three radial lines on the complex plane of the quark fugacity owing to the RW periodicity. The zeros exhibit the first order RW phase transition. We also performed lattice QCD simulations. To remove numerical subtleties, we examined the convergence of the fugacity polynomial, and perform the bootstrap analysis of the distribution of Lee-Yang zeros. The analytic calculations well explain the results obtained from the lattice QCD simulations.

Some of the numerical results presented in this work can be found in our previous studies, and in studies by other authors as well. The distribution of Lee-Yang zeros was studied by Barbour et al. in an early study of finite density lattice QCD [13]. They already obtained the Lee-Yang zeros located...
on lines near the unit circle. Specifically they found the zeros on the twelve radial lines on the $e^{it}$ plane, which are likely consequences of the RW phase transition. Kratochvila and de Forcrand showed the agreement of the free energy obtained from the canonical approach and Taylor expansion using a staggered fermion action \cite{16, 27}. Novelties of the present study are the analytic solution of the canonical partition functions and Lee-Yang zeros, examination of the convergence of the fugacity polynomial, and bootstrap analysis for the distribution of Lee-Yang zeros. Additionally we pointed out that the gas of free fermions provides an exceptional case of the Lee-Yang zero circle theorem.

We leave some problems for future studies: namely the confirmation of nontrivial behavior of Lee-Yang zeros observed at large quark chemical potentials, and the determination of the RW endpoint in the canonical approach are worth pursuing.

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Appendix A: Fourier Integral

A simple way to verify Eq. (8) is to expand the Fourier integral for $Z_n$ as

$$Z_n \propto \int_{-\pi/3}^{\pi/3} d\theta e^{-a\theta^2} \cos n\theta = \sum_{k=0}^{\infty} \frac{(-1)^k n^{2k}}{(2k)!} I_k. \quad (A1)$$

Here $a = V T^3 c_2$, and $I_k$ is defined by

$$I_k = \int_{-\pi/3}^{\pi/3} d\theta e^{-a\theta^2} \theta^{2k}, \quad (A2)$$

which is expressed in terms of complete and incomplete Gamma functions as

$$I_k = \frac{1}{a^{k+1/2}} \left( \Gamma(k + 1/2) - \Gamma(k + 1/2, a\pi^2/9) \right). \quad (A3)$$

Since the incomplete Gamma function $\Gamma(z, p) = \int_p^\infty e^{-t} t^{z-1} dt$ exponentially approaches zero as $p \propto V \to \infty$, $I_k$ is expressed solely as a complete Gamma function. By using an identity

$$\frac{\Gamma(k + 1/2)}{(2k)!} = \frac{\sqrt{\pi}}{4^k k!}, \quad (A4)$$

Eq. (A1) sums up to the exponential in Eq. (8).

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