Lee-Yang zeros for the investigation of phase transition points by using OCTOPUS

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Abstract

As liquid water turns into solid ice or gaseous steam, phase transition phenomena exist in quantum chromodynamics (QCD). However, even basic questions such as phase transition points of QCD have not been revealed yet due to the strong coupling of QCD. This paper is devoted to report recent calculations of Lee-Yang zeros for investigation of phase transition points from the canonical approach in lattice QCD and a QCD effective theory by using a supercomputer, OCTOPUS.

1. Introduction

The role of Quantum Chromodynamics (QCD), the theory of the strong interaction, at finite temperature and density is getting more and more important as it provides basic inputs in the fundamental questions of the universe such as the matter generation in the early universe, formation of galaxies and stars, and mysterious stellar objects such as neutron stars and black-halls. Especially the latter objects are under active discussions due to the recent observation of gravitational waves [1, 2]. There temperatures and/or densities reach around 10^{10} times and/or 10^{15} times higher than those on the earth, respectively.

Experimentally, those problems are approached by the high energy experiments at such as J-PARC (KEK/JAEA), FAIR (GSI) and NICA (JINR), which will be expected to operate in the near future. Theoretically, lattice QCD is known as an ideal and almost unique method to perform first principle calculations of QCD.

However, lattice QCD suffers from the sign problem at finite density: the fermion determinant $\det D(\mu_q)$ at finite quark chemical potential is complex in general, $[\det D(\mu_q)]^* = \det D(-\mu_q^*)$, and consequently, it is impossible to apply the conventional Monte Carlo method. Many methods have been proposed toward avoiding the sign problem. Meanwhile, a method called the canonical approach [3] has been recently developed rapidly with multiple-precision arithmetic [4–11]. In this article, we introduce the canonical approach and show how the method provides a promising tool to solve the problems. In this research the use of high-performance supercomputer with good simulation code is indispensable. Supercomputer at RCNP provides such opportunities.

2. Canonical approach

The canonical approach takes advantage of the fact that the fermion determinant at pure imaginary chemical potential $\mu_q = i\mu_{qI}$ ($\mu_{qI} \in \mathbb{R}$) is real, $[\det D(i\mu_{qI})]^* = \det D(i\mu_{qI})$. Because we can calculate physical quantities without the sign problem at pure imaginary μ_q, information at physical real finite chemical potential is extracted by performing Fourier transforms.

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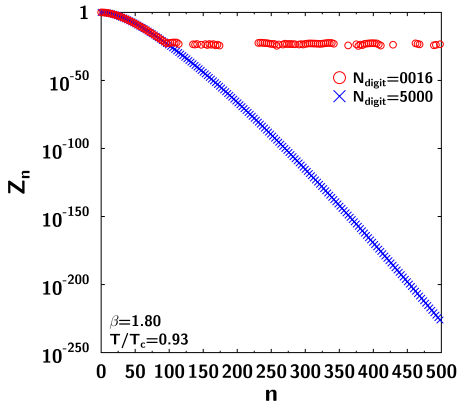

Figure 1: Quark number n dependence of the canonical partition function $Z_n = Z(n)/Z(0)$. Red circles and blue crosses are results in the double-precision and multiple-precision arithmetics, respectively. The cancellation of significant digits in Z_n is not seen in the simulation in 5,000 significant digits.

Let us begin with a brief review of the canonical approach. The grand canonical partition function $Z_{GC}(\mu_q, T, V)$ at μ_q, temperature T and volume of the system V can be written as

$$Z_{\rm GC}(\mu_q, T, V) \;=\; \sum_{n=-\infty}^{\infty} Z_C(n, T, V)\xi_q^n \;, \tag{1}$$

where ξ_q is the quark fugacity defined by $\xi_q = e^{\mu_q/T}$ and $Z_C(n, T, V)$ are the canonical partition functions. Applying Fourier transforms to Z_{GC} at the pure imaginary μ_q, we obtain the canonical partition functions,

$$Z_C(n, T, V) \;=\; \int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{-in\theta} Z_{\rm GC}(\mu_q = i\mu_{qI}, T, V) \;, \quad \theta = \mu_{qI}/T \;. \tag{2}$$

Since the $Z_{\rm GC}(i\mu_{qI}, T, V)$ can be calculated with the conventional Monte Carlo method free from the sign problem, we can obtain the $Z_{\rm GC}(\mu_q, T, V)$ at physical real μ_q though Z_C.

The idea of the canonical approach was already introduced by Hasenfratz and Toussaint in 1992 [3]. However, due to high frequencies of $e^{-in\theta}$ at large n in Fourier transforms, Z_C cannot be evaluated with accuracy. Apparently, there is no the sign problem in the canonical approach, but is the problem for high frequencies, so the problem was recognized as the residual sign problem. Therefore, it was considered that the canonical approach was not practical for use.

In 2016, it was discovered that the problem is not in the sign problem but in the cancellation of significant digits [4]. Although simulations are usually performed in double-precision arithmetic, i.e. 16 significant digits in decimal notation, the cancellation of significant digits occurs frequently in the Fourier transforms such as

$$1.234567890123456 - 1.234567890123455 \;=\; 1 \times 10^{-15} \;. \tag{3}$$

In this example, we no longer trust only the results within one significant digit. On the contrary, multiple-precision arithmetic makes the cancellation of significant digits suppress:

$$1.23456789012345612345678 - 1.23456789012345501234567 \;=\; 1.11111111 \times 10^{-15} \;, \tag{4}$$

where the example is in 24 significant digits in decimal notation.

In 2017, the integration method [6] was proposed as a useful method to extract Z_C for further large n. It is well known that the imaginary number density n_{qI} defined by $n_q = in_{qI}$ can be approximated by a Fourier series,

$$\frac{n_{qI}}{T^3}(\theta) = \sum_{k=1}^{N_{\rm sin}} f_k \sin(k\theta) \ , \tag{5}$$

with a small $N_{\rm sin}$ [13, 14]. Fitting the Fourier series to n_{qI}, we can evaluate Z_{GC} at the pure imaginary μ_q in good approximation from

$$Z_{\rm GC}(i\mu_{qI}, T, V) = C \exp\left\{ -V \int_0^\theta d\theta' \, n_{qI}(\theta') \right\} \ , \tag{6}$$

where C is an integration constant.

We use the integration method and perform the Fourier transforms in 5,000 significant digits in decimal notation with multiple-precision arithmetic. As shown in Fig. 1, the cancellation of significant digits in $Z_n = Z(n)/Z(0)$ is not seen in the simulation in 5,000 significant digits, although the cancellation occurs above $n = 100$ in the simulation with double-precision arithmetic. Considering the fact that Z_n is only evaluated up to $n = 10$ in the canonical approach without the integration method with double-precision arithmetic, the developed canonical approach can be a promising method for the investigation of phase transition points at finite density.

3. Lee-Yang zeros

In numerical calculations, the fugacity expansion of the grand canonical partition function in Eq. (1) is truncated with a finite value $N_{\rm max}$ as

$$Z_{\rm GC}(\mu_q, T, V) = \sum_{n=-N_{\rm max}}^{N_{\rm max}} Z_C(n, T, V) \xi_q^n \ . \tag{7}$$

Since $N_{\rm max}$ means the maximal value of the net-quark number in the system, DOF of the system are limited by a finite $N_{\rm max}$. Therefore, we need to take the limit $N_{\rm max} \to \infty$ so that a system with the finite DOF never has a phase transition in the real finite chemical potential.

The theorems of Yang and Lee [15, 16] are of universal and powerful use to investigate phase structures for a system with the finite DOF. The so-called Lee-Yang zeros (LYZs), which are zeros of grand canonical partition functions in complex fugacity plane provide us various information of phase transitions. In case of Eq. (7), LYZs are given as roots of the polynomial equation of degree of $2N_{\rm max}$,

$$\sum_{n=-N_{\rm max}}^{N_{\rm max}} Z_C(n, T, V) \xi_q^{n+N_{\rm max}} = 0 \ , \tag{8}$$

in the complex ξ_q plane. As DOF increases, a distribution of LYZs becomes to form one-dimensional curves in the complex ξ_q plane. If there is a point that LYZs accumulate and are stable for increasing DOF, the point represents a phase transition point. Therefore, we investigate the DOF dependence of distributions of LYZs near the positive real axis of ξ_q.

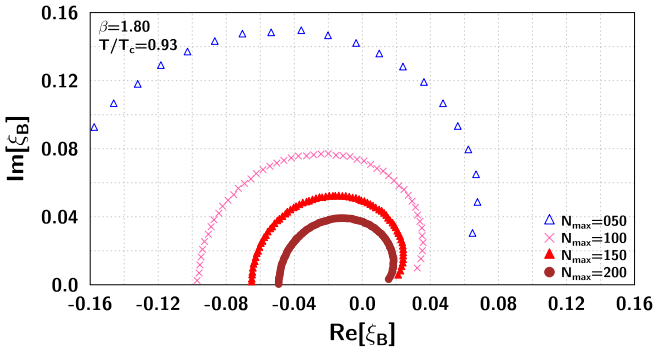

Figure 2: The $N_{\max}$ dependences of LYZs at $T/T_c = 0.93$ in the complex ξ_B plane.

4. Lattice QCD simulations

We report results of LYZs of lattice QCD simulations in this section. We generate the gauge field configurations in full QCD by using the hybrid Monte Carlo method. Simulations are carried out on a spacial lattice size $N_s = 16$ and a temporal lattice size $N_t = 4$ at temperatures $T/T_c = 0.84$-1.35 with the mass ratio of pion and ρ meson, $m_\pi/m_\rho = 0.80$. T_c is the pseudo-critical temperature at zero chemical potential.

The numerical calculations were partially carried out on a GPU supercomputer, OCTOPUS at RCNP/CMC of Osaka University. Because GPUs are good at a massively parallel computing, our GPU program is constructed to be computed on $16^3 \times 4$ (=16,384) parallels. In order to calculate the Fourier transforms and LYZs without the cancelation of the significant digits, we implement a multiple-precision arithmetic package, FMLIB [17]. Calculations of LYZs are mainly performed on the general CPU job class in OCTOPUS, which memory size is limited to 192 [GByte]. However, calculations of LYZs at high $N_{\max}$ such as $N_{\max} = 2048$, which results are not reported in this paper though, need more memory. The large-scale shared-memory job class, which memory size is limited to 6 [TByte], is enable us to calculate LYZs at high $N_{\max}$.

Figure 2 shows the $N_{\max}$ dependence of LYZs at $T/T_c = 0.93$ in the complex $\xi_B (= \xi_q^3)$ plane. Because we concern about phase transition points at the real chemical potential, we focus the behavior of the right edge of LYZs, which is defined by a LYZ to be $\min(\mathrm{Im}[\xi_B])$ in the first quadrant. As $N_{\max}$ increases, the right edges of LYZs approach to the positive real axis. To extrapolate linear or quadratic functions, we can roughly estimate that a phase transition point exists around $\mu_B/T \sim$ 5-6 at $T/T_c = 0.93$. Here, we use the charge-parity invariant, $Z(n) = Z(-n)$: if $\xi_B = \alpha$ is a LYZ, $\xi_B = \alpha^{-1}$ is also a LYZ.

5. Simulations in the NJL model

Although the phase transition points have been estimated from distributions of LYZs from lattice QCD, a problem of extrapolation procedure to physical situations of infinite DOF remains as a matter to be discussed. QCD effective theories are superior to lattice QCD in investigation of the problem because phase transition structures at the real chemical potential have been already discovered in some of the QCD effective theories. Phase structures of the Nambu-Jona-Lasinio (NJL) model [18, 19], which is a typical one of the effective theories of QCD, are also investigated by many studies. Therefore, the NJL model is very useful to check the extrapolation procedure of simulations. In this section, we would like to search the exploration procedure of LYZs from finite DOF to infinite DOF in the canonical approach of the NJL model.

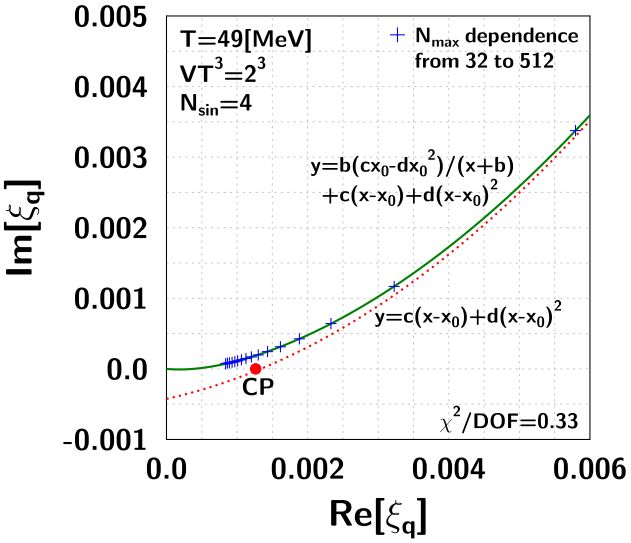

Figure 3: The $N_{\max}$ dependence of LYZs at $T = 49$ [MeV] in the complex ξ_q plane. The blue crosses stand for the right edges of LYZs. The red filled circle corresponds to the expected critical point (CP) calculated at the real finite chemical potential.

First, we calculate the imaginary number density in the NJL model as it was done in the lattice QCD simulations. By using the integration method and performing the Fourier transforms with multiple-precision arithmetic, we obtain the canonical partition functions. After that, we can show the $N_{\max}$ dependence of LYZs, see Fig. 3. Only the right edges of LYZs are plotted for each $N_{\max}$. We find that the right edges of LYZs pass over the expected critical point (CP) calculated at the real chemical potential and go to the origin as $N_{\max}$ increases. The reason why the right edges approach not the CP but the origin in large-$N_{\max}$ limit is that the imaginary number density is approximated by a Fourier series in Eq. (5). In this case, phase transitions do not occur in the real chemical potential.

To gain more insight, we try to fit the right edges of LYZs by the smooth curve,

$$y = \frac{b\left(cx_0 - dx_0^2\right)}{x+b} + c\left(x - x_0\right) + d\left(x - x_0\right)^2 \ , \tag{9}$$

where $y = \mathrm{Im}[\xi_q]$, $x = \mathrm{Re}[\xi_q]$ and b, c, d and x_0 are fitting parameters. The fitting function is basically constructed from the quadratic function like a Taylor expansion at $x = x_0$. If there is a phase transition point at x_0 in the system, it is anticipated that the right edges of LYZs cross the real axis at x_0 at large-$N_{\max}$ limit. However, since there is no phase transition in the system due to the approximation in Eq. (5), the fitting function needs a correction term to be through the origin. Therefore, we choose the correction term as the first term, which may be interpreted as a finite $N_{\sin}$ effect. In Fig. 3, the fitting function is represented by the solid curve. As if to prove that the first term is the finite $N_{\sin}$ effect, the curve subtracting the first term, which is represented by the dotted curve, crosses the real axis at $x_0 = 1.33(14) \times 10^{-3}$. The result is consistent with the value of expected CP, $\xi_{\mathrm{CP}} = 1.26 \times 10^{-3}$. Therefore, we can conclude that the extrapolation procedure of LYZs is reasonable to extract the correct transition points from the canonical approach.

6. Summary

We have investigated phase transition points from LYZs calculated from the canonical approach of lattice QCD and the NJL model. As one of the results of the lattice QCD simulations, we have estimated that a phase transition point exists around $\mu_B/T \sim$ 5-6 at $T/T_c = 0.93$.

However, a problem of extrapolation procedure to physical situations of infinite DOF remains as a matter to be discussed. Therefore, we have searched the problem with the NJL model. Because phase transition structures at real μ_q of the NJL model have been already well known, we can check whether the extrapolation procedure works well or not. As a result of the NJL model, we have then succeeded in subtracting a term associated with approximation effect in the integration method from fitted function of LYZs. We have found that the curve after subtracting the term from the fitted function nicely reproduces the expected critical point in the NJL model. The method can be applicable to lattice QCD simulations for better understanding of nature of the QCD critical points.

Now, more realistic simulations on a spacial lattice size $N_s = 24$ with $m_\pi/m_\rho = 0.48$ are ongoing on OCTOPUS. It will enable us to reveal realistic phase transitions around T_c with the extrapolation procedure for LYZs. Moreover, in Ref.[20], it was demonstrated to extract the canonical partition functions, $Z(n)$, from the RHIC experimental data. By comparing $Z(n)$ of experiments with ones of lattice simulations, we can extract a temperature and chemical potential of matter created in experiments, see also Ref. [9].

In addition, we aim to search phase structures at $T/T_c \sim 0.2$ with lattice QCD in the near future. Although computational resources for $T/T_c \sim 0.2$ is roughly 5 times larger than ones for $T = T_c$, the lattice QCD simulations must be able to approach to mysterious stellar physics such as the neutron star.

Acknowledgments

The author would like to thank V. G. Borynakov, D. L. Boyda, V. A. Goy, H. Iida, A. V. Molochkov, A. Nakamura, V. I. Zakharov and A. Hosaka for their collaborations. This work was supported by "Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures" in Japan (ID: EX18705). The calculations were partially carried out on OCTOPUS at RCNP/CMC, Osaka University.

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