How to locate the QCD phase boundary by scanning observable in the phase plane

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For small volume of the quark-gluon plasma formed in heavy ion collisions, the observable near criticality must obey finite-size scaling. According to the finite-size scaling, there exists a fixed point at the critical temperature, where scaled susceptibility at different system sizes intersect. It also exists at the transitional temperature of a first order phase transition and can be generalized to the region of the crossover. In order to quantify the feature of the fixed point, we introduce the width of a set of points. When all points in the set are in their mean position within error, the width reaches its minimum, and all points merge into the fixed point. Using the observable produced by the Potts model, we demonstrate that the contour plot of the width defined in this study clearly indicates the exact values of the temperatures and exponent ratios of fixed point, which could correspond to the critical point, or the points on the transition line, or the crossover region. This method is therefore instructive to the determination of QCD phase boundary by beam energy scan in relativistic heavy ion collisions.

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I. INTRODUCTION

The phase transition from hadron gas to quark-gluon plasma (QGP) is one of the most fundamental properties of Quantum Chromodynamics (QCD). The QCD phase diagram is expected to be a first-order phase transition of Quantum Chromodynamics (QCD). The QCD phase plasma (QGP) is one of the most fundamental properties of the collisions (FAIR, and NICA [9, 11–13]. Varying the incident energy in progress at relativistic heavy-ion collisions (RHIC), the QGP is determined by either calculations of lattice QCD or experiment.

To map the QCD phase diagram from experiment, beam energy scan (BES) are suggested and in progress at relativistic heavy-ion collisions (RHIC), FAIR, and NICA [9,11,13]. Varying the incident energy of the collisions (√sNN), the T and μB of formed system change in the phase plane accordingly. At a given √sNN, the associated T and μB of freeze-out curve are usually estimated by the phenomenology of thermal models [14–16]. So the beam energy scan in fact tune the T and/or μB of formed system in the phase plane [11,14,15,17].

As we know, in the thermodynamic limit, i.e., an infinite number of particles and volume, the phase transition is characterized by singularity in the derivatives of the thermodynamic potential, e.g., the specific heat and susceptibility (χ2). Discontinuities in the first and second derivatives signal the first and second order phase transitions, respectively. The generalized susceptibilities (χi) are theoretically calculable by Lattice QCD [18,19]. Their corresponding cumulants of the conserved charges and correlations are experimentally measurable, and considered as the sensitive observable of the critical fluctuations [20,23].

The non-monotonic dependence of those cumulant on incident energy is considered as an indicator of the critical end point of QCD phase transition [24,25]. But they are not specific to the critical point, and may also appear at other points of the first-order phase transition line and the crossover region [26,27]. So non-monotonic fluctuations are not sufficient in concluding a critical end point.

Due to the small volume of the QGP formed in heavy ion collisions, a possible CEP will be blurred. Critical related fluctuations will be severely influenced by the finite volume. The singularities of χi are smeared into finite peaks with modified positions and widths [28,29]. With decrease of the volume size, the position of CEP shifts towards smaller temperatures and larger values of the chemical potential [30,32]. The peak position indicates the so called pseudo-critical point. For a restricted volume which is not very small, the CEP has to be determined by the finite-size scaling of the observable [14,15,26,33,34].

In statistical physics, the observable is usually the function of temperature and system size, such as the order parameter m(T, L). In the vicinity of the critical temperature TC, the order parameter follows the finite size scaling (FSS) [35,36],

\[ m(T, L) = L^{-\beta/\nu} f_m(tL^{1/\nu}), \]  

(cf., Fig. 1(a). Where t = (T − TC)/TC is reduced temperature. L is the system size. f_m is scaling function. tL^{1/\nu} is scaled variable. \( \beta \) is the scaling exponent of order parameter. \( \nu \) is the scaling exponent defined by the divergence of the correlation length \( \xi \propto |\tau|^{-\nu} \). The scaling exponents characterize the universal class of the phase transition. The exponent ratio \( \beta/\nu \) is usually a
fraction between the spatial dimension $d$ and zero.

Based on the finite size scaling, the scaling behaviour of several observable in relativistic heavy ion collisions have been studied \[14, 15, 37, 40\]. In particular, the finite size scaling of emission source radii difference in Au+Au collisions at RHIC BES energies is shown to be valid at $T_{\text{CEP}} = 165$ MeV and $\mu_B^{\text{CEP}} = 95$ MeV, consistent with the CEP of deconfinement phase transition of 3D Ising model universality class \[37\].

Recently, the finite size scaling of intermittency analysis for transverse momentum in central A+A collisions from NA49 experiments restrict the CEP to the region $119$ MeV $\leq T_{\text{CEP}} \leq 162$ MeV, and $252$ MeV $\leq \mu_B^{\text{CEP}} \leq 258$ MeV \[40\].

Along the line, there are still a few questions left. Those analyses only check if the scaling law appears valid at a specific temperature and exponent \[37\], or a region \[40\]. The process of the observable approaching the critical point has not been demonstrated, and the precision of obtained temperature and exponent is difficult to assess. Moreover, if it is on the first order phase transition line, and what it would be in crossover region, have not been discussed.

It is known that the finite size scaling keeps valid on the first order phase transition line \[39\], cf., the bottom panels of Fig. 1, which is also obtained by the renormalization group transformations \[41, 43\]. Here the exponent ratio is usually an integer.

In contrast to the first and second order phase transitions, the fixed point disappears in the crossover region. The observable is system size independent \[43\]. All kinds of observable changes smoothly without singularity. If we still scale the observable in general scaling form, the exponent ratio is zero.

There are in fact two features in Eq. (1) of FSS, i.e., at critical temperature $T = T_c$, the double logarithm plot of order parameter versus system size is a straight line, and all curves of scaled observable $(m(T,L)L^{\beta/\nu})$ at different system sizes versus temperature ($T$), instead of scaled variable ($tL^{1/\nu}$), intersect to a fixed point \[44\], cf., Fig. 1(b). This is because the scaled variable is zero at the critical temperature, and the scaling function is a constant, independent of system size.

If we can quantitatively describe how the observable at different system sizes approach the fixed point with the change of temperature and scaling exponent, it will be possible to locate the critical point, the first order phase transition line, and crossover region precisely and systematically.

The fixed points corresponding to the second and first order phase transitions are shown in Fig. 1 (b) and (d). They come from the 2D Ising and 3D three-states Potts models, respectively \[29, 45, 48\]. Both of them show the feature of fixed point, i.e., all size curves intersect at critical (transition) temperature. Any deviation from the critical (transition) temperature, the points with different system sizes would go away from each other. So we can define the width of a set of points to quantify the feature of fixed point.

In this paper, we will demonstrate how to locate the fixed point by the contour plot of defined width. In Section II, we quantify the feature of fixed point by defining the width of a set of points. Then in Section III, using the 3D three-state Potts model, we produce the samples at three external fields, which correspond to the CEP, the first order phase transition, and crossover region, respectively. In section IV, we demonstrate how to find the position of the fixed point in a given sample. A brief summary and conclusions are presented in Section V.

**II. THE DESCRIPTION OF FIXED POINT**

In general, the finite-size scaling Eq. (1) is valid for the observable which is a phase transition related fluctuations. If we denote the observable as $Q(T,L)$, its finite-size scaling would be,

$$Q(T,L) = L^{\lambda/\nu} f_Q(tL^{1/\nu}).$$  \hspace{1cm} (2)

Here $\lambda$ is the scaling exponent of the observable $Q(T,L)$. $f_Q$ is scaling function with the scaled variable $tL^{1/\nu}$.

Multiplying $L^{-\lambda/\nu}$, Eq. (2) becomes,

$$f_Q(tL^{1/\nu}) = Q(T,L)L^{-\lambda/\nu}. \hspace{1cm} (3)$$

It implies a scaling plot, scaled observable $Q(T,L)L^{-\lambda/\nu}$ versus scaled variable $tL^{1/\nu}$, where all curves at different system sizes overlap into a single curve nearby the critical temperature, as illustrated in Fig. 1(a).
At critical temperature \( T = T_C \), the scaled variable \( tL^{1/\nu} = 0 \), independent of system size \( L \), and the scaling function becomes a constant, i.e.,

\[
f_Q(0) = Q(T_C, L)L^{-\lambda/\nu}. \tag{4}\]

It implies the existence of a fixed point in the plot of \( Q(T, L)L^{-\lambda/\nu} \) versus the temperature \( T \), instead of scaled variable \( tL^{1/\nu} \). The curves of different system sizes are intersected to a fixed point at \( T_C \), and separated from each other when \( T \) deviates from \( T_C \), as shown in Fig. 1(b).

In Fig. 1(b), at a given temperature, the collection of the points of different system can be defined as a set. When \( T \) approaching \( T_C \), all points in the set becomes closer and closer to each other. The trend of all points going close to each other is necessary for forming a unique intersect point. In order to quantify the relative distance between the points in the set, we define the width of all points to their mean position, i.e.,

\[
D(T, a) = \sqrt{\frac{\sum_{i=1}^{N_L} [Q(T, L_i)L_i^a - \langle Q(T, L)L^a \rangle]^2}{\omega_i^2}}. \tag{5}\]

It is the function of temperature \( T \) and exponent ratio \( a = -\lambda/\nu \), which is usually unknown and varies with observable. \( N_L \) is the number of sizes, \( N_L - 1 \) is the degree of freedom. Where \( \chi^2_{Q(T, L)L^a} \) is the error weighted variance of all size points, i.e.,

\[
\chi^2_{Q(T, L)L^a} = \sum_{i=1}^{N_L} \frac{[Q(T, L_i)L_i^a - \langle Q(T, L)L^a \rangle]^2}{\omega_i^2}. \tag{6}\]

\( \omega_i = \delta [Q(T, L_i)L_i^a] \) is the error of \( Q(T, L_i)L_i^a \). \( \langle Q(T, L)L^a \rangle \) is the weighted mean,

\[
\langle Q(T, L)L^a \rangle = \frac{\sum_{i=1}^{N_L} Q(T, L_i)L_i^a}{\sum_{i=1}^{N_L} 1/\omega_i^2}. \tag{7}\]

Here, the definition of \( \chi^2 \) is similar to that in curve-fitting. For the curve-fitting, the variance is the difference of measured value to that given by the curve, rather than the mean position of all points \( \langle Q(T, L)L^a \rangle \). So the minimum \( \chi^2 \) of curve-fitting means all measured points have a best fitting to a given curve.

At critical temperature and exponent ratio, all points are coincident to their mean position within error, i.e., they are in fact an identical point in an experimental sense. \( D(T, a) \) reaches its minimum, around unity. When the temperature deviates from the critical one, the points of different system sizes go away from each other, and the width become larger. So the width \( D(T, a) \) presents the relative distance of all points to their mean position.

In real experiments, due to the error of the observable and related uncertainties, the fixed point may not converge to an ideal point, and \( D(T, a) \) may be larger than unity. Nevertheless, if there is a fixed point in \( T \) and a

FIG. 2. (Color line) \( D(T, a) \) nearby the temperatures of the first (I), and the second (II) order phase transitions, and crossover region (III).

plane, the \( D(T, a) \) will change with \( T \) and \( a \) and converge to a minimum. This is essential for forming a fixed point.

At three different regions of phase boundary, the change of \( D(T, a) \) with \( T \) and \( a \) are expected to be the cases of I, II and III, respectively, as showed in Fig. 2.

In the case of I, the temperature is low. \( D(T, a) \) has a minimum at phase transition temperature, where the ratio \( a \) is around \((n - 1)d\), an integer. \( n \) is the order of susceptibility. It characterizes the fixed point of the first order phase transition.

In the case of II, the temperature is in the middle. \( D(T, a) \) has also a minimum at the critical temperature, and ratio \( a \) is a fraction, in contrast to the case of I. It indicates the fixed point of the second order phase transition, i.e., the CEP.

In the case of III, the temperature is high. \( D(T, a) \) keeps in the same minimum at all temperature, and ratio \( a \) is around zero. This implies \( D(T, a) \) is a constant, independent of the temperature. The observable is the system size independent. It is the feature of crossover region.

In the following, it is interesting to display the defined width in a given sample, where the first and second order phase transitions, and crossover region are passed over, respectively. We will see how its minimum locate the fixed point in the samples.

III. THREE SPECIAL SAMPLES GENERATED BY THE POTTs MODEL

The 3D three-state Potts model is one of the standard paradigms of lattice QCD \[49–52\]. It is a pure gauge QCD effective model, and shares the same \( Z(3) \) global symmetry as that of QCD with finite temperature and infinite quark mass. Where external magnetic field plays the role of the quark mass of the finite temperature QCD. At vanishing external field, the temperature-driven phase transition has proved to be of the first-order \[53, 54\]. With increase of the external field, the
The new couplings are given by,

\[ H = \beta E - h M. \]  

The partition function is,

\[ Z(\beta, h) = \sum_{\{s_i\}} e^{-\beta E - h M}. \]  

The order parameter in terms of \( \tilde{\xi} \) and \( \tilde{\tau} \) is,

\[ m(T, h) = \frac{1}{L^3} [\tilde{M}(T, h) - \langle \tilde{M}(T_c, h_c) \rangle]. \]  

Here \( r \) and \( s \) are the mixing parameters and have been determined in ref. [55] by,

\[ r^{-1} = \left( \frac{d\beta_c(h)}{dh} \right)_{h=h_c}, \quad \text{and} \quad (\delta \tilde{M} \cdot \delta \tilde{E}) = 0, \]  

with \( \delta \tilde{X} = \tilde{X} - \langle \tilde{X} \rangle \) for \( X = M, \) or \( E. \)

The order parameter in terms of \( \tau \) and \( \xi \) is,

\[ m(\tau, \xi) = \frac{1}{L^3} [\tilde{M}(\tau, \xi) - \langle \tilde{M}(\tau_c, \xi_c) \rangle]. \]  

It is the most sensitive observable to the phase transition. According to Eq. (15) and (16), it can be written in terms of \( T \) and \( h \) as,

\[ m(T, h) = \frac{1}{L^3} [\tilde{M}(T, h) - \langle \tilde{M}(T_c, h_c) \rangle]. \]  

IV. LOCATING THE FIXED POINT BY DEFINED WIDTH

Now, suppose that we have three samples. In each of them, only the mean of the order parameter for different temperatures and system sizes are presented. All other information is unknown. Let’s apply only these known information to calculate the width \( D(T, a) \) and see if we can find the position of temperature and exponent ratio corresponding to the first and second order phase transitions and crossover region.

According to defined width \( D(T, a) \) in Eq. (5), the corresponding width of the mean of order parameter at a given temperature \( T \) and exponent ratio \( a \) is,

\[ D(T, a) = \sqrt{\frac{\chi^2}{N_L - 1}}. \]  

Where the 3D three-state Potts model is described in terms of spin variable \( s_i \in \{1, 2, 3\} \), which is located at sites \( i \) of a cubic lattice of size \( V = L^3 \). The Hamiltonian of the model is defined by \[ H = \beta E - h M. \]  

The partition function is,

\[ Z(\beta, h) = \sum_{\{s_i\}} e^{-\beta E - h M}. \]  

The order parameter of the system is defined as,

\[ m(\tau, \xi) = \frac{1}{L^3} [\tilde{M}(\tau, \xi) - \langle \tilde{M}(\tau_c, \xi_c) \rangle]. \]  

For fixed external field \( h \), it is the function of temperature and system size, i.e., \( m(T, L) \).

We performed simulations at three fixed external fields, \( h = 0.0005, 0.000775, 0.002 \) and 18 \( T \)-values starting from \( T_0 = 1.8180 \) with \( \Delta T = 0.0001 \), which covers the points on the first order phase transition line, the CEP, and crossover region, respectively. The temperature and exponent ratio at three special points are listed in the bracket of Table I. The sample is generated for four system sizes \( L = 30, 40, 50, 60 \). The \( m(T, L) \) at different temperatures and system sizes are obtained in total 100,000 configurations.
Diverges to a minimum at a specified temperature (1.82023372) and ratio (0.564) from the original sample.

The exponent ratio is -0.054, which is almost the same close to zero as that from the original one 1.8188763. The smallest minimum is the red line with exponent ratio 1 for all system sizes, and another minimum is the red line with exponent ratio -0.0541. Then turn to the sample for the external field \( h = 0.0005 \), its contour plot is showed in Fig. 3(b). Here, it shows again that \( D(T, a) \) gradually converges to a minimum red area. This means that all curves of scaled observable at different system sizes are more and more close to each other with the change of \( T \) and \( a \). The minimum red area corresponds to the ranges of temperature and exponent ratio 1.81885 ± 0.047. Here

| Table I | The parameters at \( D_{\text{min}}(T_c, a_c) \) and in the Potts model (inside brackets) for three samples. |
|---------|-------------------------------------------------------------------------------------------------|
| Sample  | \( D_{\text{min}}(T_c, a_c) \) | \( T_c \) | \( a_c \) |
| 2nd order PT | 1.0291±0.2946 (1.82023372) | 1.82023 (1.82023372) | 0.583 (0.564) |
| 1st order PT | 1.5287±0.5591 (1.8188763) | 1.81887 (1.8188763) | -0.047 (-0.0541) |
| crossover | \( \sim 1 \) for all \( T \) | 1.82585039 | -0.1 ~ 0.1 |

From the projection along the direction of temperature as showed in Fig. 4(c), for a given ratio \( a \), there is also a minimum \( D(T, a) \). Among them, the smallest minimum is the red line which corresponds to the same critical temperature and exponent ratio as those from Fig. 4(a).

These features of \( D(T, a) \) are consistent with those of the critical point as showed in the case II of Fig. 2. The contour plot of \( D(T, a) \) demonstrate how all curves of the mean of absolute order parameter at different system sizes intersect at the critical temperature and exponent ratio.

To amplify the fine structure and minimum nearby the red area, we project \( D(T, a) \) to \( T \) and \( a \) axis, respectively, as showed in Fig. 4(a) and 4(c). In Fig. 4(a), for a given \( T \), there is an \( a \) which makes the \( D(T, a) \) minimum. Among these lines, the minimum is the red one with \( D_{\text{min}} = 1.0291 \pm 0.2946 \), and corresponding \( T = 1.82023 \) and \( a = 0.583 \). They are very close to the original critical temperature (1.82023372) and ratio (0.564) from the given sample.
the order parameter can be considered as the first order of susceptibility. So the exponent ratio is zero at the first order phase transition line, the same as that for the crossover region.

The projection along the direction of ratio \(a\) is showed in Fig. 4(d), for a given ratio \(a\), there is also a minimum \(D(T, a)\). The minimum gives the same critical temperature and exponent ratio as those along the direction of \(T\) in Fig. 4(b). So \(D(T, a)\) again demonstrates the features of fixed point at the first order phase transition line, as those showed in the case I of Fig. 2.

The contour plot of the sample for the external field \(h = 0.002\) is shown in Fig. 3(c). In contrast to Fig. 3(a) and 3(b), the \(D(T, a)\) in Fig. 3(c) are band lines parallel to the \(T\)-axis. This implies that \(D(T, a)\) is independent of temperature, and its value is determined by the ratio \(a\) only. The red band is close to zero. This is the same characteristics as the crossover region showed in the case III of Fig. 2.

So the contour plot of defined width \(D(T, a)\) beautifully quantifies the features of the fixed point. When all curves of the scaled the mean of the order parameter at different system sizes intersect to a fixed point, \(D(T, a)\) indeed converges to an expected unity.

Although it should be noticed that due to the error of the observable and uncertainties of related parameters in real experimental settings, the minimum of \(D(T, a)\) may be larger than the unity and vary with experiments, what’s more important for the formation of a fixed point is the trend that the contour plot of \(D(T, a)\) converges to a minimum area.

Here, we present three samples of observable which just pass two specified fixed points and the crossover region, respectively. The contour plot of defined width displays the regular regions, as the isolines indicated in Fig 3(a), (b) and (c), respectively. If the sample of observable does not pass the phase boundary, the plot would vary with its covered phase plane. If it is far away from the phase boundary, the observable are independent either of temperature or system size [20]. The plot keeps at its minimum. If it approaches to the phase boundary, or the transition temperature, the plot may show some contour regions which are a part of fig. 3(a), or (b), or (c). Therefore, the contour plot of defined width is helpful for exploring the phase boundary.

In relativistic heavy ion collisions, we measure the critical related fluctuations, such as, the cumulants of conserved charges at different incident energy and collision centrality. They are observable, similar to the mean of baryon chemical potential. The relation between them is currently given by thermal model [14] [19]. The size of formed matter is roughly estimated by the radii of Hambury Brown Twiss (HBT) interferometry [37–39, 56–58]. When all these relations are reliably set up, the defined width would be directly applicable to the data analysis at RHIC BES.

It should also mention the fact that Eq. (2) may not exactly hold for some critical related observable, such as energy density, and specific heat [59]. For this kind of observable, additional scaling violating terms are not negligible [60] [61]. They are usually the function of system size and temperature. So the fixed point will not appear in the plot of the scaled variable versus temperature. Its behaviour may vary with the observable and associated system [60] [61]. The suggested contour plot would not converge to a minimum as those showed in Fig. 3, and change with observable and associated system as well. Therefore, to determine the QCD phase structure from RHIC BES, it is necessary to measure as much as possible related observable, and exam their corresponding contour plots respectively.

V. SUMMARY AND CONCLUSIONS

If the volume of QGP formed in heavy ion collisions is not very small, the fluctuations near criticality should follow the finite-size scaling. Based on the finite-size scaling, the CEP corresponds to a fixed point, where all scaled observable at different system sizes intersect. It also exists on the first order phase transition line and can be generalized to the crossover like transition. Their corresponding exponent ratios are respectively fraction, integer and zero. So the phase boundary can be well identified by the corresponding fixed point in the phase plane.

To quantify the feature of the fixed point, at a given
temperature, we define the width of a set of points with different system sizes. It is the square root of the variance of scaled observable. When all points in the set are in their mean position within error, the defined width reaches its minimum, and all points are overlapped in an experimental sense, i.e., fixed point. So the minimum of the width corresponds to the position of the fixed point.

Then using the 3D three-state Potts model, we produce the samples at three external fields, which correspond to the CEP, the first order phase transition, and crossover, respectively. The temperature range of each sample covers the whole phase plane. We demonstrate that the minimum of the contour plot of defined width precisely indicates the temperature and scaling exponent ratio of fixed point presented in three samples, respectively.

Therefore, the contour plot of defined width well quantifies how the observable approaches the temperature and exponent ratio of phase transition. It provides an exact and systematic way to locate the critical point, the first order phase boundary, and the crossover region by scanning the related observable in the phase plane. When the relation between incident energy and the temperature of formed matter is well settled down, and system size of formed matter can be reliably estimated, the application of the method would be straightforward.

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