Finite-size effects, pseudocritical quantities and signatures of the chiral critical endpoint of QCD

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We investigate finite-size effects on the phase diagram of strong interactions, and discuss their influence (and utility) on experimental signatures in high-energy heavy ion collisions. We calculate the modification of the pseudocritical transition line and isentropic trajectories, and discuss how this affects proposed signatures of the chiral critical endpoint. We argue that a finite-size scaling analysis may be crucial in the process of data analysis in the Beam Energy Scan program at RHIC and in future experiments at FAIR-GSI. We propose the use of extrapolations, full scaling plots and a chi-squared method as tools for searching the critical endpoint of QCD and determining its universality class.

I. INTRODUCTION

Although the process of phase conversion of hot hadronic matter that presumably happens in ultra-relativistic heavy-ion collision (HIC) experiments is often compared to the cosmological quark-hadron transition in the early universe, the relevant space-time scales differ by almost twenty orders of magnitude. In particular, while one would need temperatures $T \sim 10^8$ GeV to be subject to appreciable finite-size effects in the case of the early universe, which of course spares the primordial quark-hadron transition from these effects, this is not the case for the quark-gluon plasma formed in HICs [1, 2]. Therefore, in the context of HICs, descriptions of an equilibrium quark-gluon plasma in the thermodynamic limit are, in principle, missing non-negligible finite-size corrections.

Strictly speaking, from the statistical mechanics standpoint, there is no phase transition in a system of finite size, and no criticality can be defined. Singularities that would play the role of strong lighthouses in the search for criticality are rounded and become smooth. Actually, the originally critical quantities are also shifted in the $T - \mu$ plane according to volume variations, becoming pseudocritical, with some unavoidable ambiguity in their definition. This is the actual scenario in any experiment in HICs. In addition, the time scale involved in the collision process is also not large compared to the microscopic time scale to achieve equilibrium. Therefore, thermodynamic quantities directly inferred from data assuming an infinite system in equilibrium should not correspond to its true and unique value in the thermodynamic limit. Moreover, even neglecting dynamical non-equilibrium effects, all signatures of the second-order critical endpoint based on non-monotonic behaviour [3, 4] (or sign modifications [5]) of particle correlation fluctuations will probe a pseudocritical endpoint, shifted significantly from the genuine critical endpoint by finite-size corrections and boundary effects.

In this paper, we do not address non-equilibrium effects, but argue that finite-size modifications will play a crucial role in the search for the critical endpoint in HICs. On one hand, they restrict the access of the proposed particle correlation fluctuation signatures to (volume- and boundary-condition-dependent) pseudocritical quantities. On the other hand, the fact that the experimental data can be arranged as a set of systems of different sizes can actually help us extract information directly related to the thermodynamic limit of QCD, especially concerning its critical endpoint and the universality class of the transition.

First, we investigate finite-size effects on the phase diagram of strong interactions, presenting results for the modification of the pseudocritical line in the temperature-chemical potential phase diagram, as well as for isentropic trajectories. For this purpose, we employ the linear sigma model coupled to quarks with two flavors, $N_f = 2$ [6]. This effective theory has been widely used to describe different aspects of the chiral transition, such as thermodynamic properties [7, 8, 9, 10] and the nonequilibrium phase conversion process [11], as well as combined to other models in order to include effects from confinement [12]. We show that the volume-dependence of the QCD phase diagram in the regime of energy scales probed by current heavy ion experiments can be large.

Second, treating HIC data separated into slices of different impact parameter width as a realization of a set of thermodynamical systems of different sizes and temperatures, we propose the use of full scaling plots of cumulants of fluctuations of pions as a tool for searching the critical endpoint of QCD and determining its universality class. From
this point of view, HICs could be seen as the “experimental realization” of lattice simulations for systems of different sizes. In this picture, signatures of the second-order critical endpoint based on non-monotonic behaviour (or sign modifications) of particle correlation fluctuations will actually probe a set of pseudocritical endpoints, a feature which could contribute to the broadening of the experimental signal, helping to wash it out in the large thermal background. As in Monte Carlo simulations, the peculiarities of the finite system become relevant (technically, this corresponds to the need of inclusion of irrelevant operators in the formalism). In that case, one has either to use the knowledge of the peculiarities of the system or resort to finite-size scaling (FSS) techniques to extract indirect information about criticality.

Finally, we also propose a chi-squared method for searching the critical endpoint of QCD and determining its universality class that could be useful in the process of data analysis in HIC experiments, in particular in the Beam Energy Scan program at RHIC-BNL and at FAIR-GSI.

**II. FINITE-SIZE CORRECTIONS TO THE PHASE DIAGRAM OF QCD**

Finite-size effects in the study of phase transitions via lattice simulations, seen as an inevitable drawback of the method, and the necessary extrapolation to the thermodynamic limit have been thoroughly studied for decades [13], the ultimate answer to the problem being given by the method of FSS [14]. Systematic calculations of finite-volume corrections can then be computed not only near the criticality of continuous (second-order) transitions, but also for first-order phase transitions [15], so that the thermodynamic limit can be taken in the calculation of properties of phase diagram.

However, for natural systems that are truly small, one should study the modifications caused by its finitude in the phase diagram before comparing to experimental observables. This is the situation in the study of the chiral transition in HICs. Contrasting to the large number of studies in the computation of the chiral condensate and related quantities within chiral perturbation theory (see e.g. [16] and references therein), this issue is often overlooked in the case of the quark-gluon plasma. Among the exceptions, there is a lattice estimate of finite-size effects in the process of formation within chiral perturbation theory (see e.g. [16] and references therein), this issue is often overlooked in the case of the in HICs. Contrasting to the large number of studies in the computation of the chiral condensate and related quantities within chiral perturbation theory (see e.g. [16] and references therein), this issue is often overlooked in the case of the quark-gluon plasma. Among the exceptions, there is a lattice estimate of finite-size effects in the process of formation within chiral perturbation theory (see e.g. [16] and references therein), this issue is often overlooked in the case of the quark-gluon plasma.

To describe the chiral phase structure of strong interactions at finite temperature and baryon density, we adopt the linear sigma model

\[
\mathcal{L} = \overline{\psi}_f \left[i\gamma^\mu \partial_\mu + \mu \gamma^0 - g \sigma \right] \psi_f + \frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - V(\sigma, \pi),
\]

where \( \mu \) is the quark chemical potential,

\[
V(\sigma, \pi) = \frac{\lambda}{4} (\sigma^2 - v^2)^2 - h \sigma
\]

is the self-interaction potential for the mesons, exhibiting both spontaneous and explicit breaking of chiral symmetry. We dropped the pion terms for simplicity [32]. The \( N_f = 2 \) massive fermion fields \( \psi_f \) represent the up and down constituent-quark fields \( \psi = (u, d) \). The scalar field \( \sigma \) plays the role of an approximate order parameter for the chiral transition, being an exact order parameter for massless quarks and pions. Quarks constitute a thermalized fluid that provides a background in which the long wavelength modes of the chiral condensate evolve. We incorporate quark thermal fluctuations in the effective potential for \( \sigma \), i.e. we integrate over quarks to one loop. The parameters of the lagrangian are chosen such that the effective model reproduces correctly the phenomenology of QCD at low energies and in the vacuum. So, we impose that the chiral SU(2) \( \otimes \) SU(2) symmetry is spontaneously broken in the vacuum, and the expectation values of the condensates are given by \( \langle \sigma \rangle = f_\pi \) and \( \langle \pi \rangle = 0 \), where \( f_\pi = 93 \text{ MeV} \) is the pion decay constant. The explicit symmetry breaking term is determined by the PCAC relation which gives \( h = f_\pi m_\pi^2 \), where \( m_\pi \approx 138 \text{ MeV} \) is the pion mass. This yields \( v^2 = f_\pi^2 - m_\pi^2 / \lambda \). The value of \( \lambda = 20 \) leads to a \( \sigma \)-mass, \( m_\sigma^2 = 2 \lambda f_\pi^2 + m_\pi^2 \), equal to 600 MeV. The choice \( g = 3.3 \), which yields a reasonable mass for the constituent quarks in the vacuum, \( M_q = gf_\pi \), leads to a crossover at finite temperature, \( T \), and vanishing chemical potential, so that the first-order transition line that starts at vanishing temperature and nonzero chemical potential stops at a critical endpoint.

In the case of a finite system of linear size \( L \), the momentum integral from the one-loop quark contribution to the effective potential is substituted by a sum

\[
\frac{V_q}{T^3} = \frac{N_f N_c}{(LT)^3} \sum_k \left[ \log \left( 1 + e^{-(E_k - \mu)/T} \right) + \log \left( 1 + e^{-(E_k + \mu)/T} \right) \right],
\]
where \( E_k = \sqrt{k^2 + m_{eff}^2} \), and \( m_{eff} = |g| \sigma | \) is the effective mass of the quarks. It is clear that finite-size effects in a quantum field theory are, in a way, very similar to thermal effects with \( 1/L \) playing the role of the temperature. However, in the latter boundary conditions are determined by the spin-statistics theorem, whereas in the former there is no clear guidance (see, e.g., discussions in Refs. [18, 22]). Choosing periodic boundary conditions (PBC) are useful to focus on bulk properties of the model undisturbed by surface effects [21, 23, 24], but one is always free to choose anti-periodic boundary conditions (APC) or any other, instead. Depending on the physical situation of interest, a boundary condition may be more realistic than others. To illustrate the dependence of the pseudocritical phase diagram on the boundary conditions, we show results for PBC and APC. For PBC, e.g., the components of the momentum assume the discretized values \( k_i = 2\pi \ell_i/L \), \( \ell_i \) being integers, and there is a zero mode (absent for APC, for which \( k_i = \pi (2\ell_i + 1)/L \)). At zero temperature, this zero mode in the case with PBC will modify the classical potential, generating size-dependent effective couplings and masses.

In what follows, we analyze systems of sizes between 10 fm and 2 fm which relate to the typical linear dimensions involved in central and most peripheral collisions of \( Au \) or \( Pb \) ions at RHIC and LHC, respectively. Figure 1 displays the shift of the pseudocritical transition lines and their respective endpoints as the size of the system is decreased. The transition lines represent pseudo-first-order transitions, characterized by a discontinuity in the approximate order parameter, the chiral condensate \( \sigma \), and the production of latent heat through the process of phase conversion. We find that those lines are displaced to the region of higher \( \mu \) and shrunk by finite-size corrections. The former effect is sensibly larger when PBC are considered, indicating that the presence of the spatial zero mode tends to shift the transition region to the regime of larger chemical potentials. Both boundary conditions reproduce the infinite-volume limit for \( L \gtrsim 10 \) fm. Figure 2 shows the corresponding displacement of the pseudocritical endpoint, comparing PBC and APC: both coordinates of the critical point are significantly modified, and \( \mu_{CEP} \) is about 30% larger for PBC. For \( \mu = 0 \), the crossover transition is also affected by finite-size corrections, increasing as the system decreases, as shown in Figure 3. Again, PBC generate larger effects: up to \( \sim 80\% \) increase in the crossover transition temperature at \( \mu = 0 \) when \( L = 2 \) fm.

FIG. 1: Pseudocritical transition lines and endpoints for different system sizes within the linear \( \sigma \) model with periodic (left) and antiperiodic (right) boundary conditions.

FIG. 2: Displacement of the pseudocritical endpoint in the \( T - \mu \) plane as the system size is decreased for different boundary conditions.

FIG. 3: Normalized crossover temperature at \( \mu = 0 \) as a function of the inverse size \( 1/L \) for the cases with PBC and APC.
Results for the isentropic trajectories are shown in Figure 4 comparing the infinite-volume limit with the finite system with $L = 2$ fm in the cases with PBC and APC. For sufficiently high temperatures, the isentropic lines in the thermodynamic limit are reproduced, while large discrepancies are found around and below the transition region. The remarkable variations at low temperatures are due to the shift of the pseudocritical line and, for PBC, to the zero-mode-induced modifications of the vacuum properties, especially the vacuum constituent quark mass. Although there is no strong focusing effect around the critical endpoint (as observed previously for this chiral model [8] and similar ones [26]), it is clear that the density of isentropic trajectories around the pseudocritical endpoint is sensibly higher than in the thermodynamic limit.

![Diagram of isentropic trajectories](image)

**FIG. 4:** Isentropic trajectories, labeled by the respective value of entropy per baryon number, in the thermodynamic limit (solid, red lines) and for $L = 2$ fm with PBC (left) and APC (right). The red dot is the genuine critical endpoint, while the square is pseudocritical one.

## III. SCALING PLOTS AND THE UNIVERSALITY CLASS OF QCD

The close neighborhood of critical points exhibit strong and peculiar scaling behavior that can be used as signals of its presence [13, 14]. This fact has been recognized long ago as a possible means of detecting experimentally the critical endpoint of QCD by using event-by-event analysis in HIC experiments [3]. In fact, higher moments of fluctuations of particle multiplicities diverge with increasing powers of the correlation length [4]. As discussed in the introduction and shown quantitatively for the chiral phase diagram in the last section, finite-size corrections are relevant in the context of HICs, not only smoothening those singularities but also generating shifted peaks and pseudocritical observables. Based on the analysis of the last section, the amount of displacement of the pseudocritical transition parameters that are probed at each experimental event should present a significant centrality (size) dependence. Therefore, when considering data from a centrality window, there is an average between different peaks which should broaden even further the non-monotonic signal of the pseudocritical endpoint. Furthermore, if the transition line is indeed strongly shrinked and shifted to higher chemical potentials, the current experiments may not be able to probe this regime of pseudocritical peaks and no non-monotonic behaviour would be found in the data. Finally, if this is not the case, to obtain, within this method, experimental information about the genuine QCD critical endpoint, one would need to gather a set of pseudocritical endpoint measurements for different system sizes and apply a procedure of extrapolation to the thermodynamic limit, namely a FSS analysis.

Recently, it was proposed that a FSS analysis on top of the critical point would be a more efficient way of searching [27], and, as mentioned previously, FSS was also used before in the context of the dynamics of a first-order transition in QCD in a finite-volume quark-gluon plasma [1, 2]. The caveat of the aforementioned method for searching experimentally the critical endpoint of QCD is the assumption that one is essentially on top of the criticality. This condition will be hardly met in HIC experiments, at least with enough statistics to stand out of the background. Even if one is very close, or on top, of the critical point, a system that is as small as the quark-gluon plasma created under these conditions, where all relevant length scales are close [2], will be strongly affected by finite-size effects. Namely, all singularities will be rounded and spread, something that can provide misleading artifact “signals” even in a FSS analysis when restricted to the assumption of being on top of the critical point.

The alternative is simply making use of the full power of FSS, which is a method that is valid also when one is not so close to the critical point [35], provided that we use full scaling plots. This technique is predictive even for tiny systems in statistical mechanics (see, e.g., Ref. [28]), and, since it can be used in various different regions of the phase diagram not far from the critical point, it can in principle provide enough statistics for data analysis. We propose the
use of this method to search for the critical point of QCD and determine its universality class, making profit out of the fact that we can build out of heavy ion data a set of systems of different sizes.

The FSS hypothesis \[13, 14, 29\], that can be derived applying the renormalization group to critical phenomena \[24, 30\], states that an observable \( X \) in a finite system at temperature \( T \) can be written, in the neighborhood of criticality, in the form \[24\]
\[
X(t, g; \ell; L) = L^{\gamma_x/\nu} f_x(t L^{1/\nu}) \tag{4}
\]
where \( t = (T - T_c)/T_c \) is the reduced temperature (\( T_c \) being the temperature associated with the critical point), \( \gamma_x \) is the bulk (dimension) exponent of \( X \), \( g \) the dimensionless coupling constant, \( \ell \) a length to fix the renormalization procedure, and \( \nu \) the critical exponent of the correlation length that diverges as \( \xi \sim t^{-\nu} \) at criticality. The function \( f_x(y) \) is universal up to scales fixing, and the critical exponents are sensitive essentially to dimensionality and internal symmetry, which will give rise to the different universality classes \[13, 30\].

The critical contribution to experimental observables such as moments of fluctuations of particle multiplicities near the critical point \[3, 4\] will suffer sizable corrections from the function \( f_x(y \neq 0) \) that can be computed within a model. One should note that the observables satisfying the scaling relation \( (4) \) are the ones directly related to correlation function of the order parameter of the transition, such as fluctuations of the multiplicity of soft pions, as discussed in Ref. \[3\]. Therefore, a careful investigation of how the evolution of the system in the hadronic phase and the large background of thermal correlations might affect or even hide the scaling behaviour of a given experimental observable is demanded. Looking for the collapse of points representing different sizes of the system at \( t = 0 \) \[27\] can be dangerously misleading when there is not enough statistics as in HICs \[37\].

Plotting observables such as cumulants of fluctuations of soft pions properly normalized \[38\] and as a function of the full scaling variable \( t L^{1/\nu} \) can be an efficient method for searching the critical endpoint of QCD and determining its universality class. The critical temperature and chemical potential (the coordinates of the critical endpoint) as well as the critical exponents would be parameters in a fit (scaling plot), in the same manner as is done in statistical mechanics simulations. In HICs, one can arrange the data as representing systems of different sizes by using centrality bins, or by directly using the number of participants in the collision, instead of \( L \), in the scaling plot \[37\], or each system of a given size, and also a given center-of-mass energy \( \sqrt{s} \), one can estimate the temperature and chemical potential employing thermal models in the chemical freeze-out, or use directly \( \delta s \equiv (\sqrt{s} - \sqrt{s_c})/\sqrt{s_c} \), \( \sqrt{s_c} \) substituting \( (T_c, \mu_c) \) as the free parameter associated with the position of the genuine critical endpoint. When one plots \( X L^{-\gamma_x/\nu} \) as a function of, e.g., \( T \) (not a scaling plot), one finds scattered curves that cross in the critical point. In a full scaling plot, though, that uses the correct scaling variable, all these curves collapse, provided that the system is not far from the critical point, as a consequence of scaling and universality. By finding the correct critical exponents in the case of the QCD phase transition in HICs, one would determine its universality class.

One can search for this full scaling behavior in different cumulants of fluctuations and in different parts of the phase diagram, increasing dramatically the statistics. Still, realistically, the thermal background of particle production could, in principle, hide the critical contribution inside the error bars and the process of finding the correct value of the critical exponent could be difficult. Therefore, to put in practice the idea of scaling-plot fits described above, we may introduce the following chi-squared method. Once an ensemble of experimental results for the properly normalized observable is obtained, one can find the best scaling fit via the minimization of the quadratic deviation among them. For example, let
\[
Q \left( \sqrt{s}, \sqrt{N_{\text{part}}}, \nu \right) = X \ N_{\text{part}}^{-\gamma_x/2\nu}, \tag{5}
\]
for the observables \( X \) (say, cumulants of soft pion fluctuations). Then we may define the following \( \chi^2 \) function
\[
\chi^2(\nu, \sqrt{s_c}; y) = \sum_{N_{\text{part}}^{\nu/2}} \delta s = y \left( \frac{Q \left( \sqrt{s}, \sqrt{N_{\text{part}}}, \nu \right)}{Q \left( \sqrt{s_0}, \sqrt{N_{\text{part},0}}, \nu \right)} - 1 \right)^2 \tag{6}
\]
where the sums are taken over all pairs of \( \left( \sqrt{s}, \sqrt{N_{\text{part}}} \right) \) keeping the scaling variable \( y \) constant, with
\[
N_{\text{part},0}^{\nu/2} \delta s_0 = y.
\]
If all of \( X \) values for different \( \left( \sqrt{s}, \sqrt{N_{\text{part}}} \right) \) obey the finite size scaling, then the above \( \chi^2 \) should vanish at the correct value of \( \nu \) and \( \sqrt{s_c} \) for any \( y \). For energies to which the observables attain values close to the critical point, then we should have a very week \( y \)-dependence of \( \nu \) and \( \sqrt{s_c} \) and also the value of \( \chi^2 \) at the minimum, only coming from the statistical errors. In practice, we plot \( \chi^2 \) for a given \( y \) (or various combinations of \( \left( \sqrt{s_0}, \sqrt{N_{\text{part},0}} \right) \)) and localize the minimum in \( \nu \) and \( \sqrt{s_c} \).
Thus, by studying the energy dependence of the minimum of the above quantity, we may identify the energy value which passes close to the critical point with the free variational parameters being the critical exponent $\nu$ and the critical center-of-mass energy $\sqrt{s_c}$ (and $\gamma_x$ in the general case).

IV. FINAL REMARKS

In this paper, we have discussed different aspects of finite-size effects that render crucial features in various proposed signatures of the QCD critical endpoint in HICs. On one hand, in addition to the usual smoothening and broadening of singularities, the finiteness of the physical system under a phase conversion process shifts pseudocritical observables associated with pseudocritical parameters with respect to the genuine criticality, in the thermodynamic limit. We have shown that those displacements in the case of the chiral transition can be large for energy scales typically encountered in current experiments, shrinking the $T$-$\mu$ domain where discontinuities of the chiral condensate are found and pushing the pseudocritical lines further into the high chemical potential region. These findings should affect all signatures of the critical endpoint based on non-monotonic behaviours or sign changes in particle correlation fluctuations, probably contributing to the broadening of the signal within a not sufficiently small centrality window.

Based on these considerations we proposed the use of the full power of the FSS hypothesis as a tool to detect and locate the genuine chiral critical endpoint of QCD, and determine its corresponding universality class, using HICs experiments. We also described a chi-squared method that can be applied to data in a systematic manner to investigate the presence of the scaling phenomenon in the Beam Energy Scan project at RHIC and in future observations at FAIR.

Finally, to address the question of the viability of these different proposed signatures of the QCD critical endpoint when immersed in a large hadronic thermal background, as the one expected in the case of HICs, an interesting test to make would be the comparison of Monte Carlo simulations of thermal ensembles with and without a small fraction of critically correlated soft pions.

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(31) For simplicity, we completely ignore the dynamics of the phase conversion. Nevertheless, it was shown in Ref. [2] that finite-size effects will play a relevant role in the case of HICs.
(32) The pion directions play no major role in the process of phase conversion [4], so we focus on the sigma direction. However, the coupling of pions to the quark fields might be quantitatively important in the computation of the fermionic determinant inhomogeneity corrections [10].
(33) In general, the effects of finite size are not fully accounted for by the replacement of continuum integrals by discrete sums over momentum states. In certain cases, the importance of inhomogeneities can be enhanced in a small system, especially near its surface. For simplicity, we neglect these effects here.
(34) Lattice studies [25] of the pure-gauge SU(3) deconfining transition in a box with wall-type boundary conditions show sensibly larger effects as compared to the analogous case with PBC. We also do not investigate the influence of shape variations, choosing a cubic system.
(35) In a system with size $L$ and temperature $T$, the region where the scaling becomes important is characterized by $L \sim \xi_\infty(T) = (\text{length scale})t^{-\nu}$.
(36) The reduced temperature $t$ is a dimensionless measure of the distance to the critical point when no other external parameter is considered. In the presence of other external parameters, such as $\mu$, one should redefine this distance accordingly: $t \mapsto \sqrt{t^2 + (\mu - \mu_c)^2}/\mu_c$.
(37) The authors of Ref. [22] found, surprisingly, two critical points for QCD under this approximation, in a region of parameter space already investigated by HIC experiments. However, in this specific application, the scaling relation [4] is oversimplified into a necessary but not sufficient condition for FSS and the maximum collapse observed is well beyond the propagated errorbars. Inspired by the precision observed in extensive FSS analyses in statistical physics, we expect the genuine scaling phenomenon to manifest inside the experimental errorbars. Furthermore, a robust statement of scaling observation should be based on data with larger statistics, including different carefully chosen observables simultaneously and further studies within statistical models to guarantee minimum interference of the thermal background and the existence of the full scaling hypothesis.
(38) In this case the proper normalization will include not only the dimension scaling associated with the exponent $\gamma_x$ (which constrains in principle a small anomalous contribution), but also the factors, such as mesonic couplings, involved in the connection of the pion fluctuations to the correlation functions of the order parameter of the chiral transition.
(39) It is interesting to note that when performing a scaling analysis, the scaling variable needs to be defined only up to $L$- and $t$-independent multiplicative factors. Therefore, the knowledge of the actual size of the system during the phase conversion process is not needed, as long as we have an observable that scales with it (like the square root of the number of participants in the case of HIC, with an approximately 2d initial geometry).