Polyakov–Nambu–Jona-Lasinio model in finite volumes

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Abstract – We discuss the 2 + 1 flavor Polyakov loop enhanced Nambu–Jona-Lasinio model in a finite volume. The main objective is to check the volume scaling of thermodynamic observables for various temperatures and chemical potentials. We observe the possible violation of the scaling with system size in a considerable window along the whole transition region in the T-μq plane.

Introduction. – The hot and/or dense matter created in ultra-relativistic heavy-ion collisions is supposed to possess a rich phase structure. In the intermediate regime of temperature and baryon chemical potential in the range of few hundred MeV, the defining characters of the phases are the color confinement and chiral properties. While for low baryon densities the matter has a smooth crossover from color confined chiral symmetry broken phase to color deconfined chiral symmetry restored phase, at high enough baryon densities, this transition may be of first order. A critical end point seems to naturally occur in such a situation. Establishing this scenario forms an integral part of exploration in the international collaborative experiments at CERN and BNL and the upcoming experiments at GSI.

The matter formed in heavy-ion collision experiments has a finite volume, which depends on the size of the colliding nuclei as well as the center-of-mass energy (√s) and the centrality of collisions. The measurement of this system size is quite non-trivial. There are several estimates of the system size at freeze-out for different values of √s and different centralities from the measurement of HBT radii [1], which indicate that the freeze-out volume decreases as √s increases. The freeze-out volume was found to be in the range of 2000 fm³ to 3000 fm³. On the other hand, in the URQMD model [2] the volume of homogeneity has been calculated and compared with the experimentally available results in ref. [3]. The homogeneity volume [4,5] is given by the product of the HBT radii R_{out}, R_{side} and R_{long}, signifying the fraction of the fireball from which particles in a particular momentum window are emitted. The volume of homogeneity was obtained in the transverse momentum window of 300–400 MeV at different centralities and varying √s from 62.4 GeV to 2760 GeV. These UrQMD simulations show that the homogeneity volume has a power law scaling with multiplicity and varies in the range of 50–250 fm³. The ALICE Collaboration has also estimated the freeze-out volume to be in this range for different √s and different colliding nuclei [6]. Given that these are the freeze-out volumes, the initial volumes are expected to be much smaller [7,8].

Theoretical developments to understand the effects of finite volume on the strongly interacting matter are represented in refs. [9–31]. A general overview of the developments in this direction is reviewed in some of our recent work [32–34]. In case of high-energy heavy-ion collisions it was shown in ref. [35] that the finite-size effects give rise to important consequences in the later stage of evolution of the hadronic bubbles. In ref. [36], the authors have discussed the importance of finite-size scaling in order to properly locate the critical end point (CEP) on the phase diagram and emphasized on its use for the experimental data analysis program [37]. In ref. [32] some of us have studied the thermodynamic properties of strongly interacting matter in a finite volume using the Polyakov–Nambu–Jona-Lasinio (PNJL) model for 2 and 2+1 flavors. It was found that the crossover temperature at zero baryon density decreases with decrease in volume. Furthermore
the critical end point at finite temperature $T$ and chemical potential $\mu$ goes towards higher-$\mu$ and lower-$T$ domain as the system size is reduced. For a system confined to a lateral size $R = 2$ fm, it was found that the CEP vanishes and the whole phase boundary becomes a crossover line. We also discussed the possibility of chiral symmetry restoration in a color confined state for a system with finite size.

Fluctuations of conserved charges are sensitive indicators of the transition from hadronic matter to partonic state. Also the existence of the CEP may be signalled by the diverging behavior of fluctuations. From the chiral susceptibilities in the 2-flavor quark-meson model using a renormalisation group approach [38] the CEP was found to have lower temperature and higher chemical potentials with decreasing volume, similar to our results in the PNJL model [32]. Similar agreement was reported from baryon number susceptibility ratios via the Dyson-Schwinger approach using the 2-flavor model [31]. On the lattice, for a pure gluon theory, the Polyakov loop susceptibility has been calculated for a finite volume [39] showing that the transition temperature may increase with decreasing system size. In a lattice version of the 2-flavor PNJL model [40] the diagonal quark number susceptibility was found to decrease with increasing volume. Our recent studies in the mean-field approximation of the 2-flavor PNJL model [33] as well as in the hadron resonance gas model [34], give similar results. Additionally, we found that the volume scaling of susceptibility ratios is violated near the crossover region in the PNJL model and near the freeze-out surface in the hadronic model. It is therefore important to explore the situation in the 2+1 flavor PNJL model, which is reported in the present work.

We first give a brief description of the PNJL model followed by the results for the fluctuations and correlations.

Model. — The NJL model [41–46] gives a satisfactory description of strongly interacting matter at zero temperature and chemical potentials. However this is a model with global color conservation and therefore no confinement of color charges appear at non-zero temperatures and densities. A suitable modification is done by introducing a background field that mimics the behavior of the Polyakov loop to bring in the effects of confinement [47–55]. Considerable progress has been made to have an understanding of strongly interacting matter using the PNJL model (see, e.g., [32,33,56–73]). Here we have considered 2 + 1 flavor PNJL model including up to six-quark interactions [32,74]. To include the effect of finite volumes, a non-zero lower momentum cutoff $p_{\text{min}} = \pi / R = \lambda$ is introduced. Here $R$ is the lateral size of a cubic volume $V = R^3$. This is a simple approach as compared to more sophisticated approaches needed to compute the proper density of states as discussed for various systems in refs. [9–15]. In principle there should be an infinite sum over discrete momentum values. However, for simplification, we consider integration over continuous values of momentum. Alternatively, surface and curvature effects should have been included in the continuous momentum variables which are beyond the scope of the present work. The essential physical effects are expected to remain similar. Most likely we are going to make an underestimation of finite-size effects in the quantities we evaluate. We have also not considered any modification of the model parameters with the expectation that much of those effects would show up in the mean values of the quantum fields. This is exactly in the line of neglecting the temperature and chemical potential dependence of model parameters in most of the related literature. Within this approximation, the thermodynamic potential is now given by [32,74],

$$\Omega = U' (\Phi, \bar{\Phi}, T) + 2g_S \sum_{f=u,d,s} \sigma_f^2 - \frac{g_D}{2} \sigma_u \sigma_d \sigma_s$$

$$+ \sum_{f=u,d,s} \left[ \int_\Lambda d^3 p \left( \frac{p^2}{2\pi^2} V_f - 2T \int_\Lambda d^3 p \left( \frac{p^2}{2\pi^2} \right)^3 \right) \right] \times \left\{ \ln \left[ 1 + 3 \left( \Phi + \Phi e^{-(3\Delta f - 3\mu_f)/T} \right) e^{-(3\Delta f - 3\mu_f)/T} + e^{-(3\Delta f - 3\mu_f)/T} \right] \right\} \right]$$

(1)

Here $\Phi$ and $\bar{\Phi}$ are the Polyakov loop field and its conjugate, respectively. The condensate fields of different flavors ($f = u, d, s$) are given by $\sigma_f = \langle \bar{\psi}_f \psi_f \rangle = -\frac{3M_f}{4\Lambda} \int_\Lambda \frac{d^3 p}{E_f} dp$, where $E_f = \sqrt{p^2 + M_f^2}$ is the corresponding quasiparticle energy with quasiparticle mass $M_f = m_f - g_S\sigma_f + g_D\sigma_u\sigma_d\sigma_s$. The NJL parameters are the 4-quark coupling $g_S$, the 6-quark coupling $g_D$ and the ultraviolet cutoff $\Lambda$. The Polyakov loop potential is given by

$$\frac{U' (\Phi, \bar{\Phi}, T)}{T^4} = \frac{-b_2(T)}{2} \Phi \bar{\Phi} - \frac{b_3}{6} (\Phi^3 + \bar{\Phi}^3) - \frac{b_4}{4} (\Phi \bar{\Phi})^2 - \kappa \ln[1 - 6\Phi \bar{\Phi} + 4(\Phi^3 + \bar{\Phi}^3) - 3(\Phi \bar{\Phi})^2]$$

(2)

where, $b_2(T) = a_0 + a_1 (\frac{T}{T_0}) + a_2 (\frac{T}{T_0})^2 + a_3 (\frac{T}{T_0})^3$. Here $a_0, a_1, a_2, T_0$, $b_3$ and $b_4$ are constants which may be obtained by fitting the temperature dependence of the Polyakov loop and pressure in pure gauge theory in the lattice framework [49]. The thermodynamic potential $\Omega$ is first extremized with respect to the $\sigma$ and $\Phi$ fields to estimate the mean-field values at desired temperature and chemical potential. The values of the mean fields are plugged back into $\Omega(T, \mu)$ to obtain the mean thermodynamic potential.

The model parameters used here are [32], $a_0 = 6.75$, $a_1 = -1.95$, $a_2 = 2.625$, $a_3 = -7.44$, $b_3 = 0.75$, $b_4 = 7.5$, $T_0 = 190$ MeV, $\kappa = 0.13$, $m_u = m_d = 5.5$ MeV, $m_s = 134.76$ MeV, $\Lambda = 631$ MeV, $g_S\Lambda^2 = 3.67$ and $g_D\Lambda^2 = 9.33$. The crossover temperatures for the different system sizes studied here is given in table 1.
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Fig. 1: (Color online) Variation of second- and fourth-order susceptibilities as a function of $T/T_c$, for quark (left column), electric charge (middle column) and strangeness (right column). The volume dependence of $c_4^2$ has been plotted in the inset.

Table 1: Crossover temperatures corresponding to various system sizes as extracted in a 2+1 flavor PNJL model at vanishing chemical potential.

| $R$ (fm) | 2    | 3    | 4    | $\infty$ |
|---------|------|------|------|----------|
| $T_c$ (MeV) | 160  | 174  | 178  | 181      |

Results. – The globally conserved charges in the 2+1 flavor matter are the quark number $q$, the electric charge $Q$ and the strangeness $S$. The fluctuations of these charges are related to the respective susceptibilities via the fluctuation-dissipation theorem, and are obtained as the moments of different orders from the corresponding chemical potential dependence of the free energy. Close to zero chemical potential these are given by

$$ c_n^X(T) = \frac{1}{n!} \left. \frac{\partial^n(\Omega(T,\mu_X)/T^4)}{\partial(\mu_X)^n} \right|_{\mu_X=0}, \quad (3) $$

where, $X$ stands for either of $q$, $Q$ or $S$. These susceptibilities have been computed in first principle QCD calculations on the lattice [75–82] as well as in calculations with hard thermal loops [83–91] for large system sizes. Suitable estimates of these fluctuations are also given by various QCD inspired models (see, e.g., [51–53,61,69,92–99]). In the context of finite volumes a study of fluctuations was done by some of us in ref. [33]. Here we present the corresponding results in a 2 + 1 flavor PNJL model.

To evaluate the fluctuations in the PNJL model, we first compute the thermodynamic potential $\Omega$ at any particular temperature and with chemical potentials in a range of $-300 \text{ MeV} \leq \mu_X \leq 300 \text{ MeV}$ with an interval of 0.1 MeV. The scaled thermodynamic potential $\Omega_{SB}$, is then expanded in a Taylor series around $\mu_X/T = 0$. The fluctuations of various orders may be extracted directly from the coefficients of the series expansion. We have in fact fitted the scaled thermodynamic potential with a truncated Taylor series using the GNUPLOT software [51]. To obtain the best fit parameters up to the 4th order, we have checked the least squares by varying the order of polynomials from 6 to 10 as well as varying the range of $\mu_X/T$ around zero. The final least squares for the lowest system size were less than $10^{-9}$ and much smaller ($\sim 10^{-11}$) for $R = 3$ fm, 4 fm and $\infty$. The whole procedure was repeated for the different temperatures in the range of $0.5 < T/T_c < 2.5$.

In fig. 1 we present the 2nd- and 4th-order susceptibilities for all the conserved charges as a function of $T/T_c$. From the inset we observe the saturation of $c_4^2$ with increasing system size around $T_c$. As in the case of the 2-flavor system [33], the qualitative behavior of the susceptibilities for a small system size is similar to that for infinite volumes, though quantitatively there are significant finite-size effects. These effects are clearly visible for the 2nd-order susceptibilities in the range of $0.8T_c < T < 2T_c$, and for the 4th-order susceptibilities in the range of $0.8T_c < T < 1.2T_c$. Therefore if the experimentally produced fireballs thermalize and cool down to a temperature close to $T_c$, one should consider freeze-out volume as a fitting parameter along with the temperature and various chemical potentials to fit the freeze-out multiplicity ratios (see, e.g., [100] and references therein). Within the ambit of the present model, we find that the finite-volume effects would be important if the system freezes out with a size less than $R \sim 5$ fm.

To find the relevant length scales in the different temperature regimes we have also checked the scaling of the susceptibilities with the corresponding mass scales in the model. For $T < T_c$ the relevant length scale is the temperature-dependent pion mass ($m_\pi R$) and for $T > T_c$, the electric charge (middle column) and strangeness (right column). The volume dependence of $c_4^2$ has been plotted in the inset.
the corresponding scale is the temperature-dependent constituent quark mass \( M_q \), where \( M_q \) is the average constituent mass for the three flavors). For demonstration we have shown these scaling behavior in fig. 2. The relevant masses were reported by some of us in [32]. We find that for very low temperatures as well as very high temperatures the mass scaling is satisfied. But in a significant temperature range close to \( T_c \) the scaling is violated.

It should be noted here that for comparing theoretical computations like in the thermal model [100], lattice QCD [101], etc. with experimental data, one usually considers ratios of thermodynamic observables. This helps in situations where the volume is not directly measured and the free energy is assumed to be simply proportional to the volume of the system and therefore scales out in the ratios. In fact it has been argued [101] that in such a situation the susceptibility ratios are expected to be not only spectrum independent but dependent only on the ratio of \( \mu_q/T \). Therefore lattice QCD results corroborates hadron resonance gas results very well for temperatures below \( T_c \).

With this expectation, attempts to match experimentally obtained fluctuation ratios with theoretical predictions are also undertaken [102]. On the other hand, some of us have reported that a finite-size system of hadron gas may show some departure from volume scaling essentially in the electric charge sector [34]. Therefore it is important to check the extent of volume scaling in the PNJL model. In this regard what we find is that the susceptibilities themselves being derivatives of the free energy density are still volume dependent. Therefore the free energy is not necessarily proportional to the volume of the system. So a correlated measurement of the particle multiplicities and the various susceptibilities may provide suitable estimates of the finite sizes of the produced strongly interacting matter with \( R < 5 \text{ fm} \). Recently, with the assumption of volume scaling, an estimate of system size has been extracted from the fluctuation and correlations measured by the ALICE Collaboration at \( \sqrt{s} = 2.76 \text{ TeV} \) confronting with the corresponding computations in lattice QCD [103].

On the other hand, if the multiplicity ratios and ratios of fluctuations are to be employed to make contact between theory and experiment then it is important to find out if the volume scaling violation occurs for such ratios. Otherwise no unique value of the system volume may be found. In fig. 3 we have plotted the ratios of fourth- to second-order fluctuations for different conserved charges as a function of temperature. It may be observed that the scaling of the ratios with the system volume holds as a function of temperature. For all the conserved charges there is a significant violation of the volume scaling essentially in the electric charge sector the magnitude of violation is high compared to the strangeness sector, which however shows the scaling violation for the largest temperature range.
the derivative ∂\(\Omega\) at any given temperature within the range

\[\mu_q \leq 50 \text{ MeV}\]

in an interval of 0.1 MeV. For obtaining the derivative we obtain the observables. The correlations are obtained as

\[C_{X,Y}^{i,j} = \frac{1}{i! j!} \frac{\partial^{i+j} (-\Omega/T^4)}{\partial (\mu'_X)^i \partial (\mu'_Y)^j},\]

(4)

where, X and Y stands for q, Q and S with X ≠ Y. We compute the correlation coefficients using numerical differentiation. We obtain the thermodynamic potential \(\Omega\) at any given temperature within the range \(-50 \text{ MeV} \leq \mu_X, \mu_Y \leq 50 \text{ MeV}\) in an interval of 0.1 MeV. For obtaining the derivative \(\partial^{i+j} (\Omega/T^4)\), we compute it for various values of \(\Delta(\mu_X/T) = \Delta(\mu_Y/T)\) and consider the value when the derivative reaches a saturation. We repeat the whole procedure for the entire temperature range so as to obtain first-order correlations of conserved charges as functions of temperature around zero chemical potentials.

In fig. 4 we have plotted the ratios of correlations to fluctuations for different conserved charges. The volume scaling violation in this case is quite small for all the sectors except for the smallest system size. We note that here the correlations and fluctuations are derivatives of the same order of the free energy.

The fluctuations of the conserved charges can also be extracted for non-zero chemical potentials. Here we have considered net quark density \(c^q_1\) and quark number fluctuations \(c^q_2\) for simplicity. These quantities are also the simplest to analyze from the experimental data at least in terms of net proton number and its fluctuations [102]. We compute the thermodynamic potential as a function of \(\mu_q\) in a range of \(0 < \mu_q < 400 \text{ MeV}\) with an interval of 0.1 MeV for a set of temperatures. Then using the method of numerical derivative we obtain the observables.

The quark number density itself was found to have a volume dependence. The ratio \(c^q_1/c^q_2\) is displayed in fig. 5 for a few representative values of temperature. Since the quark number is very small for low values of \(\mu_q\) we present our results in the range \(100 \text{ MeV} < \mu_q < 400 \text{ MeV}\). For high temperatures the ratio is monotonically increasing. On the other hand for \(T < 200 \text{ MeV}\) we observe a dip in a certain window of \(\mu_q\). Incidentally these windows of \(\mu_q\) correspond to those close to the phase boundary [32]. The dips occur due to the shooting up of the quark number fluctuations in these regions. For \(T < 100 \text{ MeV}\) there is even a discontinuity indicating the existence of the first-order line in the phase diagram for the corresponding system size. We observe that for high temperatures the volume scaling is maintained even for large chemical potentials. However as we go down below \(T \sim 200 \text{ MeV}\) the volume scaling is violated in the transition region of the corresponding temperature. Thus we may infer that the violation of volume scaling, if any, always occurs close to the transition region, where large correlation lengths come into play and lead to the separate finite-size behavior of the derivatives of the free energy.

**Conclusion.** To conclude, we have studied the volume dependence of the free energy density of \(2+1\) flavor strongly interacting matter in terms of various second- and fourth-order fluctuations of the conserved charges, as well as the quark number density at finite temperature and chemical potentials. We observed volume scaling violations at two levels. Firstly, the free energy density is itself volume dependent for \(R < 5 \text{ fm}\) within a certain range of \(T\) and \(\mu_q\), as given by the behavior of the susceptibilities. Secondly, the ratio of these derivatives themselves show violation of volume scaling in a small window of \(T\) and \(\mu_q\) all along the transition region in the \(T, \mu_q\) phase diagram. The addition of one more flavor in our treatment did not change any qualitative features of the quark number fluctuations compared to the the 2-flavor system [33],

![Fig. 5: (Color online) Ratios of net quark number density to the quark number fluctuations as functions of the quark chemical potential at different temperatures.](Image 39x775 to 549x775)

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though the quantitative results are significantly different. The 2nd-order strangeness susceptibility has a substantial contribution to the quark number fluctuation. On the other hand, the 4th-order strangeness susceptibility has a sub-dominant contribution to the corresponding quark number susceptibility. As a result the volume scaling violation in the ratio of 4th-order to 2nd-order quark number fluctuations is somewhat smaller in the 2+1 flavor system compared to the 2-flavor system. However a clearer signal of volume scaling violation is now observed in the ratios of strangeness susceptibilities themselves, which is sustained in a much wider range of temperatures. We have also been able to extract various charge correlations. The ratios of these correlations with the 2nd-order fluctuations violate volume scaling only for very small system sizes. We have further extended our studies to non-zero chemical potentials. An interesting feature observed is that the first-order phase transition nature is itself manifestly dependent on the system size, as can be seen from the quark number to quark susceptibility ratios. For very small systems the first-order phase boundary is completely washed out. Further investigations in these directions are required with the computation of higher-order moments that we wish to carry out in the future.

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