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Quark number susceptibilities: Lattice QCD versus PNJL model ☆

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Abstract

Quark number susceptibilities at finite quark chemical potential are investigated in the framework of the Polyakov-loop-extended Nambu–Jona-Lasinio (PNJL) model. A detailed comparison is performed between the available lattice data, extrapolated using a Taylor expansion around vanishing chemical potential, and PNJL results consistently obtained from a Taylor series truncated at the same order. The validity of the Taylor expansion is then examined through a comparison between the full and truncated PNJL model calculations.
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Investigations of QCD thermodynamics using lattice simulations predict a transition from the hadronic to the quark–gluon phase around a critical temperature of 0.2 GeV, at vanishing quark chemical potential μ_q. This transition is signalled by a steep rise in energy density, pressure and entropy density as functions of the temperature, and known to be a crossover [1] when quarks are included.

Based on model calculations [2] as well as lattice QCD simulations [3], the existence of a critical point in the phase diagram is suggested. The precise location of this point is still under debate. It can possibly be identified by observables that are sensitive to singular parts of the free energy [4], such as quark number susceptibilities. Such susceptibilities have been studied both in lattice calculations [5,6], and using phenomenological models [7–10]. Both diagonal and off-diagonal susceptibilities can serve as useful diagnostics to elucidate the nature of strongly interacting matter [11].

The first lattice results for quark number susceptibilities at finite chemical potential have been obtained in [5] through the Taylor expansion method. An expansion of the pressure in powers of μ_q/T around $\mu_q = 0$ was performed up to fourth order in μ_q/T. Quark number susceptibilities were then obtained as second derivatives of the pressure with respect to the chemical potential. The presence of a peak in these observables at large chemical potentials has been interpreted as a signal of growing fluctuations in the baryon density, as the critical point is approached. Improvements were implemented in [6] by expanding the pressure up to sixth order in μ_q/T. In this case, the peak was shifted to a smaller temperature, and a dip was observed at $T \sim 1.05T_c$ which, together with the increased error bars in the extrapolated lattice data, made the presence of the peak less convincing.

In the present Letter we investigate quark number susceptibilities within the Polyakov-loop-extended Nambu–Jona-Lasinio (PNJL) model [12–15] which has recently been used successfully in comparisons with a variety of lattice QCD data [16–21]. In this model, quarks propagate in a temporal background gauge field representing Polyakov loop dynamics, while developing at the same time a dynamical mass through their coupling to the chiral condensate. Here we present results for the quark number susceptibilities at finite chemical potential. A comparison is first performed with truncated Taylor expansions in μ_q/T derived from lattice QCD. Then the convergence properties of the Taylor series are examined by comparison with the full, non-truncated PNJL result.

The Euclidean action of the two-flavor PNJL model is

$$
\begin{aligned}
&\mathcal{S}_E\big(\psi, \psi^\dagger, \phi\big) \\
&= \int_0^{\beta=1/T} \mathrm{d}\tau \int_V \mathrm{d}^3x \left[\psi^\dagger \partial_\tau \psi + \mathcal{H}\big(\psi, \psi^\dagger, \phi\big) \right] \\
&\quad - \frac{V}{T}\mathcal{U}(\phi, T).
\end{aligned} \tag{1}
$$

Here $\mathcal{H}$ is the fermionic Hamiltonian density given by:

$$
\mathcal{H} = -i\psi^\dagger(\vec{\alpha} \cdot \vec{\nabla} + \gamma_4 m_0 - \phi)\psi + \mathcal{V}(\psi, \psi^\dagger), \tag{2}
$$

where ψ is the $N_f = 2$ doublet quark field, $\vec{\alpha} = \gamma_0\vec{\gamma}$ and $\gamma_4 = i\gamma_0$ in terms of the standard Dirac γ matrices and $m_0 = \mathrm{diag}(m_u, m_d)$ is the quark mass matrix. $\mathcal{V}(\psi, \psi^\dagger)$ is an $SU(2) \times SU(2)$ invariant four-fermion interaction acting in the pseudoscalar–isovector/scalar–isoscalar quark–antiquark channel[1]

$$
\mathcal{V}(\psi, \psi^\dagger) = -\frac{G}{2}\big[(\bar\psi\psi)^2 + (\bar\psi i\gamma_5\vec{\tau}\psi)^2\big]. \tag{3}
$$

The quarks move in a background color gauge field $\phi \equiv A_4 = iA_0$, where $A_0 = \delta_{\mu 0}g\mathcal{A}_a^\mu t^a$ with the $SU(3)_c$ gauge fields $\mathcal{A}_a^\mu$ and the generators $t^a = \lambda^a/2$. The matrix valued, constant field ϕ relates to the (traced) Polyakov loop as follows:

$$
\Phi = \frac{1}{N_c}\mathrm{Tr}\left[\mathcal{P}\exp\left(i\int_0^\beta \mathrm{d}\tau\, A_4\right)\right] = \frac{1}{3}\mathrm{Tr}\,e^{i\phi/T}. \tag{4}
$$

In a convenient gauge (the so-called Polyakov gauge), one can choose a diagonal representation for the matrix ϕ,

$$
\phi = \phi_3\lambda_3 + \phi_8\lambda_8, \tag{5}
$$

which leaves only two independent variables, ϕ_3 and ϕ_8.

The term $-(V/T)\mathcal{U}$ of the action (1) involves the effective potential $\mathcal{U}(\Phi, \Phi^*, T)$ which controls the thermodynamics of the Polyakov loop. An improved form for this effective potential was introduced in our previous work [20]. It involves the logarithm of $J(\Phi)$, the Jacobi determinant which results from integrating out six non-diagonal $SU(3)$ generators while keeping the two diagonal ones, $\phi_{3,8}$, to represent Φ:

$$
\begin{aligned}
&\frac{\mathcal{U}(\Phi, \Phi^*, T)}{T^4} \\
&= -\frac{1}{2}a(T)\Phi^*\Phi + b(T)\ln\big[1 - 6\Phi^*\Phi \\
&\quad + 4(\Phi^{*3} + \Phi^3) - 3(\Phi^*\Phi)^2\big]
\end{aligned} \tag{6}
$$

with

$$
a(T) = a_0 + a_1\left(\frac{T_0}{T}\right) + a_2\left(\frac{T_0}{T}\right)^2, \\
b(T) = b_3\left(\frac{T_0}{T}\right)^3. \tag{7}
$$

The logarithmic divergence of $\mathcal{U}(\Phi, \Phi^*, T)$ as $\Phi, \Phi^* \to 1$ automatically limits the Polyakov loop Φ to be always smaller than 1, reaching this value asymptotically only as $T \to \infty$. The parameters a_i and b_3 are taken from Ref. [20], where they were determined to reproduce lattice data for the thermodynamics of pure gauge lattice QCD up to about twice the critical temperature.[2] The resulting parameters are

$$
a_0 = 3.51, \qquad a_1 = -2.47, \qquad a_2 = 15.22,
$$
$$
b_3 = -1.75.
$$

The critical temperature T_0 for deconfinement in the pure gauge sector is fixed at 270 MeV in agreement with lattice results.

The NJL part of the model involves three parameters: the bare quark mass which we take equal for u- and d-quarks, the coupling strength G and a three-momentum cutoff Λ. We take those from Ref. [14]:

$$
m_{u,d} = 5.5 \text{ MeV}, \qquad G = 10.1 \text{ GeV}^{-2},
$$
$$
\Lambda = 0.65 \text{ GeV},
$$

fixed to reproduce the pion mass and decay constant in vacuum and the chiral condensate as $m_\pi = 139.3$ MeV, $f_\pi = 92.3$ MeV and $\langle\bar\psi_u\psi_u\rangle = -(251 \text{ MeV})^3$.

After performing a bosonization of the PNJL action and introducing scalar and pseudoscalar auxiliary fields, σ and $\vec{\pi}$, the PNJL thermodynamic potential becomes:

$$
\begin{aligned}
&\Omega\big(T, \mu_q, \sigma, \Phi, \Phi^*\big) \\
&= \mathcal{U}\big(\Phi, \Phi^*, T\big) + \frac{\sigma^2}{2G} \\
&\quad - 2N_f \int \frac{\mathrm{d}^3 p}{(2\pi)^3}\Big\{T\ln\big[1 + 3\Phi e^{-(E_p-\mu_q)/T} \\
&\quad + 3\Phi^* e^{-2(E_p-\mu_q)/T} + e^{-3(E_p-\mu_q)/T}\big] \\
&\quad + T\ln\big[1 + 3\Phi^* e^{-(E_p+\mu_q)/T} + 3\Phi e^{-2(E_p+\mu_q)/T} \\
&\quad + e^{-3(E_p+\mu_q)/T}\big] + 3\Delta E_p\theta\big(\Lambda^2 - \vec{p}^2\big)\Big\},
\end{aligned} \tag{8}
$$

where the quark quasiparticle energy is $E_p = \sqrt{\vec{p}^2 + m^2}$ and the dynamical (constituent) quark mass is the same as in the standard NJL model: $m = m_0 - \sigma = m_0 - G\langle\bar\psi\psi\rangle$. The last term in the previous equation involves the difference ΔE_p between the quasiparticle energy E_p and the energy of free fermions (quarks). It is understood that for three-momenta $|\vec{p}|$ above the cutoff Λ where NJL interactions are "turned off", σ is set to zero.

In general, the Euclidean action $\mathcal{S}_E$ is formally complex in the presence of the temporal gauge field ϕ [22,23]. It is real only at vanishing chemical potential, $\mu_q = 0$. At nonvanishing chemical potential one has in addition $\langle\Phi\rangle \neq \langle\Phi^*\rangle$ [24]. Fluctuations beyond mean field are at the origin of $\langle\Phi\rangle \neq \langle\Phi^*\rangle$ for $\mu_q \neq 0$ (see the more detailed discussion in [20]). This Letter deals with self-consistent solutions and predictions of the

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[1] The scalar diquark interaction that has been considered in [20] is not relevant in the present discussion since the range of chemical potentials explored here is lower than the critical μ_q for diquark condensation.

[2] At much higher temperatures, where transverse gluons begin to dominate, the PNJL model is not supposed to be applicable.
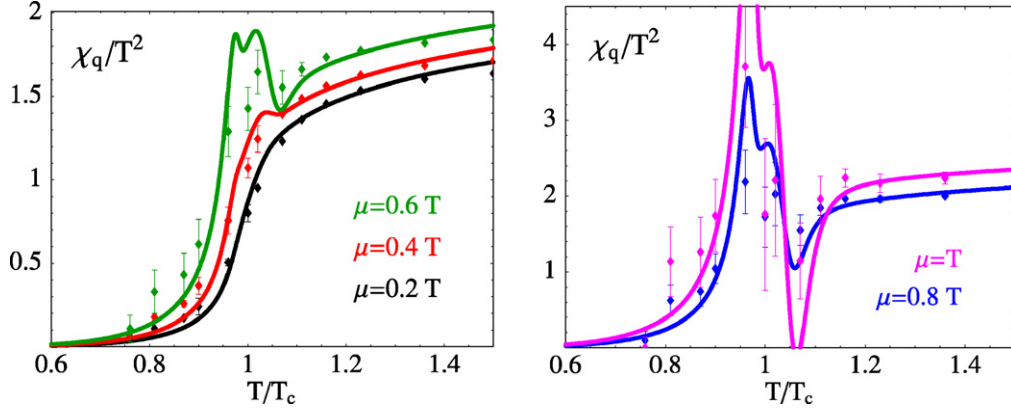
Fig. 1. Scaled quark number susceptibility χ_q as function of T/T_c for different values of μ_q/T. The curves are PNJL model results obtained from the Taylor series expansion in μ_q/T around $\mu_q = 0$ (see Eq. (12)). Corresponding lattice data are taken from Ref. [6].

mean-field equations

$$\frac{\partial \operatorname{Re} \Omega}{\partial \varphi} = 0 \qquad (9)$$

with $\varphi = \sigma, \phi_3, \phi_8$. At this mean field level, the additional constraint of ϕ_i being real implies that the action is minimized by $\phi_8 = 0$. It follows that $\Phi \sim \operatorname{Tr} \exp(i\lambda_3\phi_3/T)$ is real (i.e. $\Phi = \Phi^*$ at the mean field level). The temperature dependence of the Polyakov loop and chiral condensate, obtained from Eq. (9) can be found in Ref. [20]. In a forthcoming paper [25] we demonstrate the stability of results to fluctuations beyond mean field (which imply $\langle\Phi\rangle \neq \langle\Phi^*\rangle$). We anticipate at this point that the effects of such fluctuations do not produce qualitative changes in our conclusions, in particular those concerning the susceptibilities discussed in the following.

A Taylor expansion of the pressure in μ_q/T has been performed in Ref. [20] in order to compare with corresponding lattice data [6]. The pressure is written as a series

$$\frac{p(T, \mu_q)}{T^4} = \sum_{n=0}^{\infty} c_n(T) \left(\frac{\mu_q}{T}\right)^n,$$

$$c_n(T) = \frac{1}{n!} \left.\frac{\partial^n (p(T, \mu_q)/T^4)}{\partial(\mu_q/T)^n}\right|_{\mu_q=0}. \qquad (10)$$

The Taylor expansion coefficients c_2, c_4 and c_6, calculated in the PNJL model, turn out to agree very well with the corresponding lattice data.

The PNJL model calculations can provide useful insights concerning the convergence of the expansion (10). The sign problem at non-zero chemical potential restricts lattice QCD thermodynamics to extrapolations including only the first few terms of Eq. (10), whereas the model is not restricted to such truncations. In Ref. [18] we have shown that, for the pressure, very good agreement is reached between the full result and the truncated one, already at fourth order in μ_q/T and up to $\mu_q/T \sim 1$. In the case of the quark number density, the agreement is still very good at small chemical potentials, but discrepancies are observed at large μ_q/T in the vicinity of the phase transition.

In the present Letter we investigate the quark number susceptibilities defined as

$$\frac{\chi_q(T, \mu_q)}{T^2} = \frac{\partial^2 (p/T^4)}{\partial(\mu_q/T)^2}. \qquad (11)$$

The isospin-symmetric case is considered, with equal chemical potential for up and down quarks. The full result for χ_q is compared with the truncated one given by the Taylor expansion

$$\frac{\chi_q(T, \mu_q)}{T^2} = 2c_2 + 12c_4 \left(\frac{\mu_q}{T}\right)^2 + 30c_6 \left(\frac{\mu_q}{T}\right)^4. \qquad (12)$$

In Fig. 1 we show a comparison between truncated PNJL result obtained from Eq. (12), and the corresponding lattice data, consistently expanded to the same order in μ_q/T. One finds remarkably good agreement between the lattice data and the PNJL predictions. At large chemical potential $\mu_q/T \sim 1$ we observe, consistently with the lattice data, a pronounced peak slightly below T_c, followed by a dip around $T \sim 1.05 T_c$. This feature was also discussed in [6].

Fig. 2 presents a study of the convergence of the Taylor expansion in $\tilde{\mu} = \mu_q/T$. A comparison is made between full PNJL results and those truncated at fourth and sixth order in $\tilde{\mu}$, for a sequence of chemical potentials $0.4 \leqslant \mu_q/T \leqslant 1$. For low chemical potentials, the agreement between the full result and the truncated one is rather good. Only in the case of $\mu_q/T = 0.6$ and in the region of T around the phase transition, the first discrepancies start to appear.

The right panel of Fig. 2 shows a comparison between the full PNJL result (continuous line), the one truncated at fourth order (dashed line) and the one truncated at sixth order (dotted line) for $\mu_q/T = 1$. Evidently, the Taylor series converges badly in the region around the phase transition. The full result shows a peak, not a divergence, around $T/T_c \sim 0.9$, indicating that the critical temperature for the phase transition decreases with increasing chemical potential. The coefficient c_6 is sizeable around the phase transition, so that the sixth-order contribution differs significantly from that of fourth order. The dip above T_c occurring at sixth order is entirely an effect of the truncation of the series. It is absent in the full result. It reflects the corresponding dip exhibited by c_6: in the fourth-order result (dashed line) it is in fact absent as well. The height of the
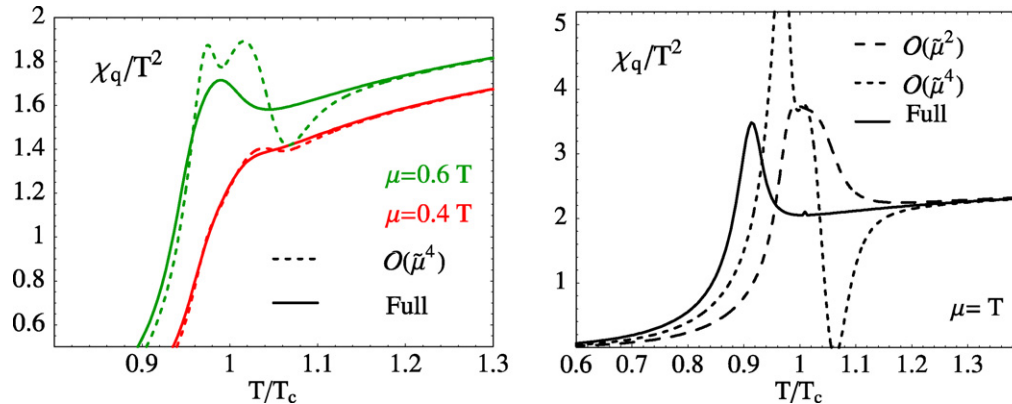
Fig. 2. Left: comparison between the full and truncated PNJL results for two different (small) chemical potentials. Right: comparison between full and truncated results, at different orders, for $\mu_q/T = 1$ (see Eq. (12)).

peak in the full result is much reduced as compared to the corresponding one found at sixth order. No divergence is observed in the full result. In fact, our model predicts that the phase transition is a crossover, for this value of μ_q. The position of the calculated critical point [20] in the (T, μ) plane is at (0.13, 0.31) GeV. As shown in [20], the location of this point depends sensitively on the quark mass and on the effects induced by the Polyakov loop. The present analysis indicates that the truncated χ_q can be misleading in the sense that it incorrectly suggests the possibility of a first-order transition which is not realized in the full susceptibility.

From the present work we can draw the following conclusions. The available lattice results for quark number susceptibilities at finite chemical potential, obtained from a Taylor expansion in μ_q/T around $\mu_q = 0$, can be successfully reproduced in the framework of the PNJL model through an analogous Taylor expansion truncated at the same order in μ_q/T. The comparison between the full PNJL result at finite chemical potential and the truncated one shows good convergence of the Taylor series up to $\mu_q/T \leqslant 0.4$–0.6. For larger values of μ_q/T, significant discrepancies are observed between full and truncated results in the region around the phase transition. The singular behaviour of the susceptibilities observed in the sixth-order result is not present in the full calculation. The transition predicted by our model for $\mu_q/T = 1$ is still a crossover, reflected by the finite height of the peak in the corresponding quark number susceptibilities.

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