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Thermodynamics of the PNJL model

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Abstract. QCD thermodynamics is investigated by means of the Polyakov-loop-extended Nambu–Jona–Lasinio (PNJL) model, in which quarks couple simultaneously to the chiral condensate and to a background temporal gauge field representing Polyakov loop dynamics. The behaviour of the Polyakov loop as a function of temperature is obtained by minimising the thermodynamic potential of the system. A Taylor series expansion of the pressure is performed. Pressure difference and quark number density are then evaluated up to sixth order in the quark chemical potential and compared to the corresponding lattice data. The validity of the Taylor expansion is discussed within our model through a comparison between the full results and the truncated ones.

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1 Introduction

QCD thermodynamics has been the subject of intense investigations in recent years. Thanks to lattice simulations, the equation of state of strongly interacting matter is now at hand as a function of temperature T and in a limited range of quark chemical potential μ. Improved multi-parameter re-weighting techniques [1, 2], Taylor series expansion methods [3–5] and analytic continuation from imaginary chemical potential [6–9] provide lattice data for the pressure, entropy density, quark density and selected susceptibilities. In response to these lattice simulations, many phenomenological models have been proposed [10–24], both to give an interpretation of the available lattice data in terms of effective degrees of freedom and to explore those regions of the phase diagram that cannot be reached on the lattice yet.

In this context, encouraged by the successful description of $N_c = 2$ QCD obtained in the Nambu–Jona–Lasinio model [25], we have investigated recently full QCD thermodynamics at zero and finite quark chemical potential in the framework of a Polyakov-loop-extended Nambu–Jona–Lasinio (PNJL) model [26–32] in which quarks develop quasiparticle masses by propagating in the chiral condensate, while they couple at the same time to a homogeneous background (temporal) gauge field representing Polyakov loop dynamics.

The "classic" NJL model incorporates the chiral symmetry of two-flavour QCD and its spontaneous breakdown at $T < T_c$. Gluonic degrees of freedom are "integrated out" and replaced by a local four-point interaction of quark colour currents. Subsequent Fierz transformations project this interaction into various quark–antiquark and diquark channels. The colour singlet $q\bar{q}$ modes of lowest mass are identified with the lightest mesons. Pions properly emerge as Goldstone bosons at $T < T_c$. However, the local $SU(N_c)$ gauge invariance of QCD is now replaced by a global $SU(N_c)$ symmetry in the NJL model, so that the confinement property is lost. Consequently, standard NJL-type models are bound to fail in attempts to describe $N_c = 3$ thermodynamics around T_c (and beyond) for non-zero quark chemical potential μ.

The deconfinement phase transition is well defined in the heavy-quark limit where the Polyakov loop serves as an order parameter. In the presence of dynamical quarks the $Z(3)$ center symmetry of the $SU(3)$ gauge group is explicitly broken. No rigorous order parameter is established for the deconfinement transition in this case [33], but the Polyakov loop still serves as an indicator of a rapid crossover towards deconfinement.

In the present paper we explore the capability of an updated PNJL model to describe the essentials of QCD thermodynamics around and above T_c. We use a modified version of our previous PNJL model [31, 32], with an improved effective potential for the Polyakov loop field. One of our main tasks here is to check the validity of the Taylor expansion approach at finite chemical potential μ. The presently available lattice simulations that we want to compare our results with provide the equation of state of two-flavour QCD at finite quark chemical potential by means of a Taylor expansion around $\mu = 0$ up to sixth order in μ. Our PNJL model enables us to produce both the full

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result at finite μ and the Taylor expansion around $\mu = 0$. In this way we can draw conclusions about the range of applicability of the Taylor expansion and its convergence properties.

2 The model

The Lagrangian of the Polyakov-loop-extended Nambu–Jona–Lasinio (PNJL) model is written in the following way:

$$\mathcal{L} = \bar{\psi}\left(\mathrm{i}\gamma_\mu D^\mu - \hat{m}_0\right)\psi + \frac{G}{2}\left[\left(\bar{\psi}\psi\right)^2 + \left(\bar{\psi}\mathrm{i}\gamma_5\tau\psi\right)^2\right] - \mathcal{U}\left(\Phi, \Phi^*, T\right), \tag{1}$$

where $\psi = (\psi_u, \psi_d)^{\mathrm{T}}$ is the quark field, $\hat{m}_0 = \mathrm{diag}(m_0, m_0)$ is the isospin-symmetric bare quark mass matrix, and we define

$$D^\mu = \partial^\mu - \mathrm{i}A^\mu \quad \text{with} \quad A^\mu = \delta^\mu_0 A^0, \quad A^0 = g\mathcal{A}^0_a\frac{\lambda_a}{2}, \tag{2}$$

with $A_0 = -\mathrm{i}A_4$; λ_a are the eight Gell-Mann matrices. A local, chirally symmetric scalar–pseudoscalar four-point interaction of the quark fields is introduced with an effective coupling strength G. The potential $\mathcal{U}\left(\Phi, \Phi^*, T\right)$ in the Lagrangian (1) governs the dynamics of the Polyakov loop $\Phi = \mathrm{Tr_c}(L)/3$ and its conjugate $\Phi^* = \mathrm{Tr_c}(L^\dagger)/3$. The matrix L is written in terms of the temporal gauge fields:

$$L = \left[\mathcal{P}\exp\left(\mathrm{i}\int_0^\beta A_4\,\mathrm{d}\tau\right)\right] = \exp\left[\frac{\mathrm{i}A_4}{T}\right]. \tag{3}$$

In a convenient gauge (the so-called Polyakov-gauge) the Polyakov loop matrix can be given a diagonal representation [28]. Note that in the chiral limit ($\hat{m}_0 \to 0$), this Lagrangian is invariant under the chiral flavour group, $SU(2)_{\mathrm{L}} \times SU(2)_{\mathrm{R}}$, just like the original QCD Lagrangian.

The effective potential $\mathcal{U}\left(\Phi, \Phi^*, T\right)$ must obey the following general features: it must satisfy the $Z(3)$ center symmetry, like the pure gauge QCD Lagrangian; besides, in accordance with lattice predictions for the behaviour of the Polyakov loop, $\mathcal{U}$ must have an absolute minimum at Φ=0 at small temperatures, while above the critical temperature ($T_0 \simeq 270\,\mathrm{MeV}$ in pure gauge QCD), the minimum is shifted to a finite value of Φ. In the limit $T \to \infty$ we have $\Phi \to 1$. In our previous works [31,32] we have chosen the simplest possible form for $\mathcal{U}$, namely a polynomial in Φ, Φ^*. An improved effective potential, following [28], replaces the fourth order term by $\log[J(\Phi)]$, where $J(\Phi)$ is the Jacobi determinant which results from integrating out six non-diagonal group elements while keeping the two diagonal ones to represent L. We therefore use the following ansatz for $\mathcal{U}$:

$$\frac{\mathcal{U}\left(\Phi, \Phi^*, T\right)}{T^4} = -\frac{1}{2}b_2\left(T\right)\Phi^*\Phi + b_4\left(T\right)\log\left[1 - 6\Phi^*\Phi + 4\left(\Phi^{*3} + \Phi^3\right) - 3\left(\Phi^*\Phi\right)^2\right], \tag{4}$$

with

$$b_2\left(T\right) = a_0 + a_1\left(\frac{T_0}{T}\right) + a_2\left(\frac{T_0}{T}\right)^2, \quad b_4\left(T\right) = b_4\left(\frac{T_0}{T}\right)^3. \tag{5}$$

Through its logarithmic divergence as $\Phi, \Phi^* \to 1$, this ansatz guarantees that the Polyakov loop will be automatically constrained to be always smaller than 1, reaching this asymptotic value as $T \to \infty$.

Following the procedure of [31], a precision fit of the parameters a_i, b_i is performed to reproduce the lattice data for pure gauge QCD thermodynamics and the behaviour of the Polyakov loop as a function of temperature. The results of this combined fit are shown in Figs. 1 and 2 (dotted line). The corresponding parameters are listed in Table 1. The critical temperature T_0 for deconfinement in the pure gauge sector is fixed at 270 MeV, in agreement with the lattice results. The NJL part of the model involves some free parameters, which we take from [31], where they were fixed to reproduce some physical quantities in the hadronic sector. These parameters, and the corresponding physical quantities, are listed in Table 2.

Before passing to the actual calculations, we summarise basic assumptions behind (1) and comment on limitations to be kept in mind. In fact the PNJL model (1) is quite schematic in several respects. It reduces gluon dynamics to

(a) chiral point couplings between quarks, and

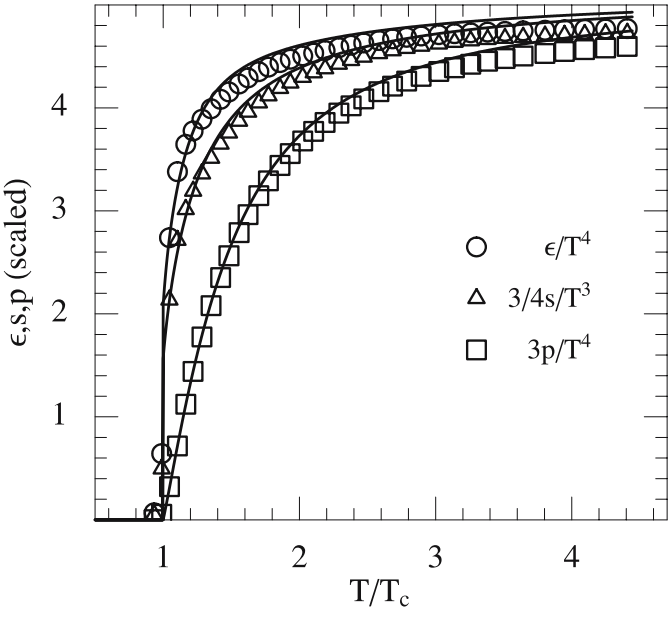

Fig. 1. Scaled pressure, entropy density and energy density as functions of the temperature in the pure gauge sector, compared to the corresponding lattice data taken from [34]

Table 1. Parameter set used in this work for the Polyakov loop potential (4) and (5)

a_0	a_1	a_2	b_4
3.51	−2.47	15.22	−1.75

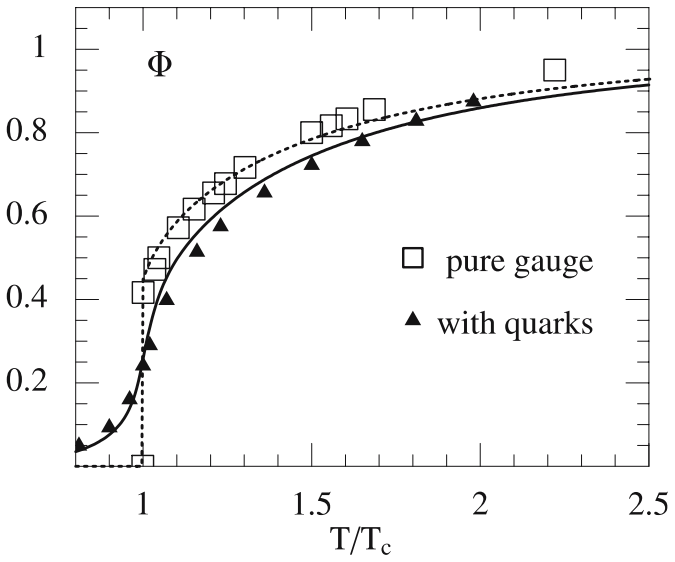

Fig. 2. *Dotted line*: PNJL fit of Polyakov loop as a function of temperature in the pure gauge sector, compared to the corresponding lattice results (*empty symbols*) taken from [35]. *Continuous line*: PNJL model prediction of the Polyakov loop behaviour as a function of the temperature, in the presence of dynamical quarks. The corresponding lattice data (*full symbols*) are taken from [36]

Table 2. Parameter set used in this work for the NJL model part of the effective Lagrangian (1) and the resulting physical quantities. For these values of the parameters we obtain a constituent quark mass $m = 325$ MeV

Λ [GeV]	G [GeV^{-2}]	m_0 [MeV]
0.651	10.08	5.5
$\lvert\langle\bar{\psi}_u\psi_u\rangle\rvert^{1/3}$ [MeV]	f_π [MeV]	m_π [MeV]
251	92.3	139.3

(b) a simple static background field representing the Polyakov loop.

This picture cannot be expected to work beyond a limited range of temperatures. At large T, transverse gluons are known to be thermodynamically active degrees of freedom, but they are ignored in the PNJL model. To what extent this model can reproduce lattice QCD thermodynamics is nonetheless a relevant question. We can assume that its range of applicability is, roughly, $T \leq (2-3)T_c$, based on the conclusion drawn in [37] that transverse gluons start to contribute significantly for $T > 2.5\,T_c$.

3 Results

3.1 PNJL model at mean-field level

After performing a bosonization of the PNJL Lagrangian and introducing the auxiliary fields σ and π, the thermodynamic potential as a result is found to be as follows:

$$\begin{aligned}
&\Omega\left(T,\mu,\sigma,\Phi,\Phi^*\right)\\
&=\mathcal{U}\left(\Phi,\Phi^*,T\right)+\frac{\sigma^2}{2G}-2N_f\int\frac{\mathrm{d}^3p}{(2\pi)^3}\left\{3E_p\theta\left(\Lambda^2-\mathbf{p}^2\right)\right.\\
&+T\ln\left[1+3\Phi e^{-\left(E_p-\mu\right)/T}+3\Phi^* e^{-2\left(E_p-\mu\right)/T}+e^{-3\left(E_p-\mu\right)/T}\right]\\
&+T\ln\left[1+3\Phi^* e^{-\left(E_p+\mu\right)/T}+3\Phi e^{-2\left(E_p+\mu\right)/T}\right.\\
&\left.\left.+e^{-3\left(E_p+\mu\right)/T}\right]\right\}, \qquad (6)
\end{aligned}$$

where the quark quasiparticle energy is $E_p=\sqrt{\mathbf{p}^2+m^2}$ and the dynamical (constituent) quark mass is the same as in the standard NJL model: $m = m_0 - \langle\sigma\rangle = m_0 - G\langle\bar{\psi}\psi\rangle$.

In general, the fields Φ and Φ^* (and their thermal expectation values) are different at non-zero quark chemical potential [38]. We demonstrate in a forthcoming paper [39] that $\Phi \neq \bar{\Phi}^*$ at $\mu \neq 0$ is primarily a consequence of quantum fluctuations of the fields around their mean-field values. In the present work we stay at the mean-field limit which consistently implies $\Phi = \Phi^*$.

Minimising $\Omega(T,\mu,\sigma,\Phi)$ determines the chiral condensate σ and the Polyakov loop Φ as functions of the temperature and the quark chemical potential. Figure 2 shows the temperature dependence of the Polyakov loop at $\mu = 0$ for two situations: first for the pure gauge case (dotted line), and secondly for the case including quarks (full line). While the pure gauge lattice results have been used to fix the effective potential for the Polyakov loop field as explained previously, the case with inclusion of quarks is a prediction of the model without any additional tuning of parameters. The resulting agreement with the corresponding lattice data incorporating dynamical quarks [36] is striking.

Notice that, while the Polyakov loop shows a discontinuity at the critical temperature in the pure gauge system indicating a first order deconfinement phase transition, this turns into a smooth crossover when quarks are introduced. At the same time the critical temperature is reduced from $T_0 = 270$ MeV in the pure gauge case to around $T_c = 215$ MeV in the presence of quarks (not evident from Fig. 2 since the horizontal axis is scaled by T_c).

3.2 Comparison with lattice results

In our previous work [31] we have compared predictions of the PNJL model concerning QCD thermodynamics, at zero and finite μ, with the corresponding lattice data. At non-zero chemical potential the lattice "data" are deduced from a Taylor expansion of the thermodynamic quantities in powers of μ/T around $\mu = 0$. For this reason, following also [40], we perform the same expansion in the PNJL model, and compare the lattice expansion coefficients to those calculated in our model. We have

$$\begin{aligned}
\frac{p\left(T,\mu\right)}{T^4}&=\sum_{n=0}^{\infty}c_n\left(T\right)\left(\frac{\mu}{T}\right)^n;\\
c_n\left(T\right)&=\frac{1}{n!}\frac{\partial^n\left(p\left(T,\mu\right)/T^4\right)}{\partial\left(\mu/T\right)^n}\bigg|_{\mu=0}. \qquad (7)
\end{aligned}$$

Our results for the coefficients c_2 and c_4 are shown in Fig. 3. Once a limited set of input parameters is fitted to lattice QCD in the pure gauge sector and to pion properties in the hadronic sector, the PNJL model evidently provides a very good description of the lattice data for the expansion coefficients of the Taylor series. The results for c_6 (not shown here) are also in very good agreement with the lattice data and will be found in a forthcoming paper [41].

From these coefficients the Taylor-expanded pressure (7) is reconstructed and the quark number density follows:

$$\frac{n_q}{T^3} = 2c_2\left(\frac{\mu}{T}\right) + 4c_4\left(\frac{\mu}{T}\right)^3 + 6c_6\left(\frac{\mu}{T}\right)^5 + \dots \qquad (8)$$

Figure 4 displays results for the pressure difference, $\Delta p = p(T,\mu) - p(T,\mu=0)$, and for the quark number density, both expanded around $\mu = 0$ up to sixth order in the quark chemical potential, consistently with the corresponding lattice data. The full computation of the pressure and quark number density at finite chemical potential cannot be performed on the lattice, but this is of course possible in our model. We can thus investigate the convergence properties of the Taylor series and study discrepancies between the full and truncated results. This study is shown in Fig. 5. The continuous lines (full results) are compared to second order (dashed) and fourth order (dotted) expansions in μ/T. Evidently the series converges rapidly for small chemical potentials: the second order differs by less

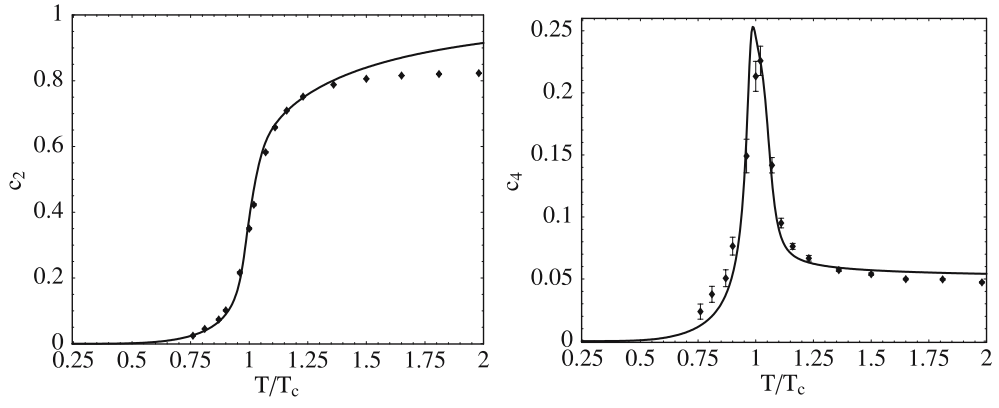

Fig. 3. Expansion coefficients c_2 and c_4: the PNJL model results are compared with the corresponding lattice results taken from [5]

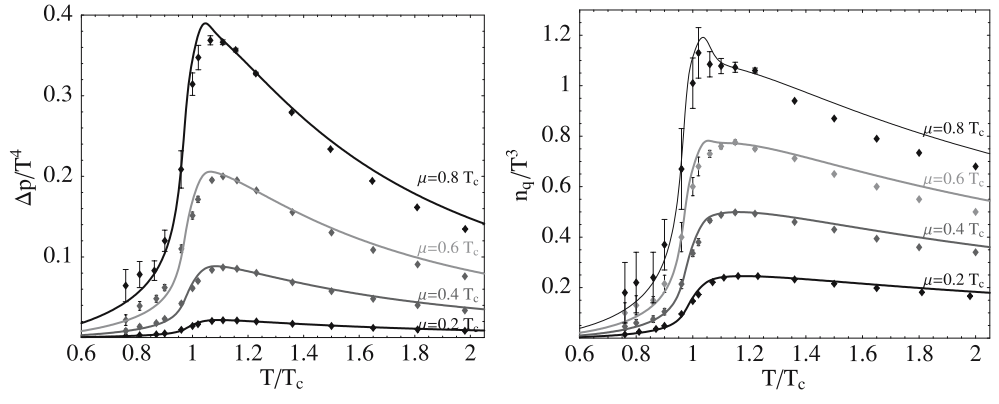

Fig. 4. Scaled pressure difference (*left*) and quark number density (*right*) as functions of T/T_c for different values of μ/T_c. In both cases the lattice data, obtained from a Taylor expansion to sixth order in the quark chemical potential [5], are compared to the PNJL model results, also obtained from a Taylor expansion up to sixth order in the quark chemical potential

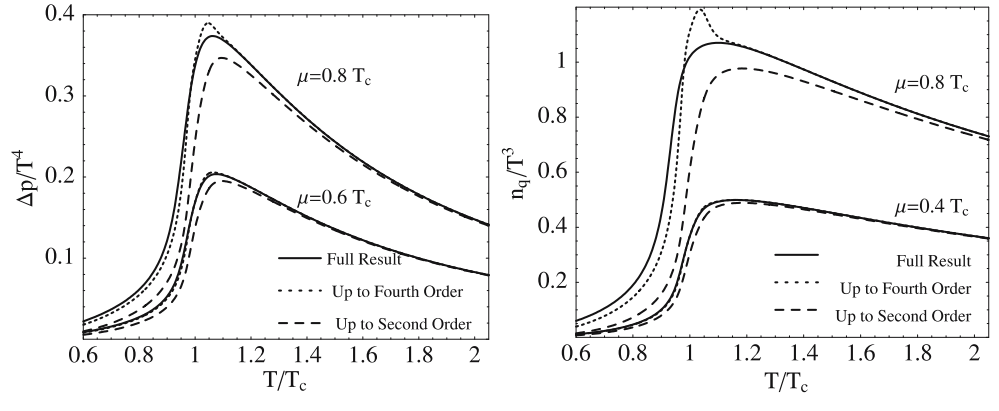

Fig. 5. Pressure difference (*left*) and quark number density (*right*) as functions of T/T_c for two different values of the quark chemical potential. The full result (continuous line) is compared to the Taylor expansion up to second (*dashed line*) and fourth order (*dotted line*) in the quark chemical potential

than 5% from the full result, and the fourth order basically coincides with the solid curve. It is nevertheless also evident that when μ/T_c becomes larger, of order 1, the Taylor expansion develops problems around T_c. In this region, in fact, the expansion coefficient c_4 is rather large, and for this reason the fourth order contribution overshoots the full one around T_c. When T becomes larger, the coefficient c_4 drops, and for this reason the agreement between the full result and the truncated one is again very good.

4 Conclusions

The PNJL model represents a minimal synthesis of the two basic principles that govern QCD at low temperatures: spontaneous chiral symmetry breaking and confinement. The respective order parameters (the chiral quark condensate and the Polyakov loop) are given the meaning of collective degrees of freedom. Quarks couple to these collective fields according to the symmetry rules dictated by QCD itself. Once a limited set of input parameters is fitted to lattice QCD in the pure gauge sector and to pion properties in the hadron sector, the quark–gluon thermodynamics above T_c up to about twice the critical temperature is well reproduced. In particular, the coefficients of the Taylor expansion in μ/T are in remarkably good agreement with the ones coming from lattice simulations. The PNJL model correctly describes the step from the first order deconfinement transition observed in pure gauge lattice QCD to the crossover transition when $N_f = 2$ light-quark flavours are added. The predicted behaviour of the Polyakov loop as a function of temperature in the presence of two quark flavours is in surprisingly good agreement with the corresponding lattice data: a highly non-trivial result.

The Taylor-expanded pressure difference and quark number density of the system has been calculated up to sixth order in the quark chemical potential. The agreement with corresponding lattice data is again very good. Finally, a comparison between the full result for these two quantities and the truncated one has been performed. We observe fast convergence of the expansion in powers of μ/T at small chemical potential. At larger chemical potentials, comparable to T_c, limitations in the applicability of the Taylor expansion become apparent.

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