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Quark cluster expansion model for interpreting finite-T lattice QCD thermodynamics

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Abstract: We present a unified approach to the thermodynamics of hadron-quark-gluon matter at finite temperatures on the basis of a quark cluster expansion in the form of a generalized Beth-Uhlenbeck approach with a generic ansatz for the hadronic phase shifts that fulfills the Levinson theorem. The change in the composition of the system from a hadron resonance gas to a quark-gluon plasma takes place in the narrow temperature interval of 150 – 185 MeV where the Mott dissociation of hadrons is triggered by the dropping quark mass as a result of the restoration of chiral symmetry. The deconfinement of quark and gluon degrees of freedom is regulated by the Polyakov loop variable that signals the breaking of the $Z(3)$ center symmetry of the color $SU(3)$ group of QCD. We suggest a Polyakov-loop quark-gluon plasma model with $\mathcal{O}(\alpha_s)$ virial correction and solve the stationarity condition of the thermodynamic potential (gap equation) for the Polyakov loop. The resulting pressure is in excellent agreement with lattice QCD simulations up to high temperatures.

Keywords: Polyakov quark-gluon plasma; hadron resonance gas; Beth-Uhlenbeck approach; lattice QCD thermodynamics

1. Introduction

Since continuum extrapolated lattice QCD (LQCD) thermodynamics results for physical quark masses became available [1–4] it has been a major goal to construct an effective low-energy QCD model that would reproduce them in the finite temperature and low chemical potential domain to high accuracy as a basis for extrapolations to the region of low temperatures and high baryochemical potentials where the sign problem still prevents LQCD obtaining benchmark solutions. To this end we construct here a cluster expansion model which reproduces the hadron resonance gas at low temperatures and the quark-gluon plasma (QGP) with $\mathcal{O}(\alpha_s)$ virial corrections at high temperatures.

We postulate a generic behaviour of the scattering phase shifts in these channels which are temperature dependent and embody the main consequence of chiral symmetry restoration in the quark sector: the lowering of the thresholds for the two- and three-quark scattering state continuous spectrum which triggers the transformation of hadronic bound states to resonances in the scattering continuum. The phase shift model is in accordance with the Levinson theorem which results in the vanishing of hadronic contributions to the thermodynamics at high temperatures.

We suggest a Polyakov-loop quark-gluon plasma model with $\mathcal{O}(\alpha_s)$ virial correction in order to obtain a satisfactory agreement with lattice QCD simulations up to high temperatures and solve the stationarity condition of the thermodynamic potential (gap equation) for the Polyakov loop.

2. Cluster virial expansion to quark-hadron matter

The main idea for unifying the description of the quark-gluon plasma (QGP) and the hadron resonance gas (HRG) phase of low-energy QCD matter is the fact that hadrons are strong,

nonperturbative correlations of quarks and gluons. In particular, mesons and baryons are bound states (clusters) of quarks and should therefore emerge in a cluster expansion of interacting quark matter as new, collective degrees of freedom.

For the total thermodynamic potential of the model, from which all other equations of state can be derived, we make the following ansatz

$$\Omega_{\text{total}}(T; \phi) = \Omega_{\text{QGP}}(T; \phi) + \Omega_{\text{MHRG}}(T), \quad (1)$$

where $\Omega_{\text{QGP}}(T; \phi) = \Omega_{\text{PNJL}}(T; \phi) + \Omega_{\text{pert}}(T; \phi)$ describes the thermodynamic potential of the quark and gluon degrees of freedom with a perturbative part $\Omega_{\text{pert}}(T; \phi)$ and a nonperturbative mean field part $\Omega_{\text{PNJL}}(T; \phi) = \Omega_{\text{Q}}(T; \phi) + \mathcal{U}(T; \phi)$ that can be decomposed into the quark quasiparticle contribution $\Omega_{\text{Q}}(\phi; T)$ and the gluon contribution that is approximated by a mean field potential $\mathcal{U}(T; \phi)$. Note that all these contributions to the QGP thermodynamic potential are intertwined by the traced Polyakov loop ϕ as the order parameter for confinement. The correlations beyond the mean field approximation which correspond to the hadronic bound states and their scattering state continuum are described by the Mott-HRG pressure $P_{\text{MHRG}}(T)$. This is a HRG pressure that takes into account the dissociation of hadrons by the Mott effect, when their masses would exceed the mass of the corresponding continuum of unbound quark states. A detailed description and numerical evaluation of these contributions will be given in the following.

2.1. Beth-Uhlenbeck model for HRG with Mott dissociation

For the MHRG part of the pressure of the model, we have $P_{\text{MHRG}}(T) = -\Omega_{\text{MHRG}}(T)$

$$P_{\text{MHRG}}(T) = \sum_{i=M,B} P_i(T), \quad (2)$$

where the sum extends over all mesonic (M) and baryonic (B) states from the particle data group (PDG), comprising an ideal mixture of hadronic bound and scattering states in the channel i that are described by a Beth-Uhlenbeck formula. Then the partial pressure of the hadron species i reads

$$P_i(T) = \mp d_i \int_0^\infty \frac{dp}{2\pi^2} p^2 \int_0^\infty \frac{dM}{\pi} T \ln \left(1 \mp e^{-\sqrt{p^2 + M^2}/T} \right) \frac{d\delta_i(M; T)}{dM}, \quad (3)$$

where d_i is the degeneracy factor. For the phase shift of the bound states of N_i quarks in the hadron i we adopt the simple model that is in accordance with the Levinson theorem

$$\delta_i(M; T) = \pi [\Theta(M - M_i) - \Theta(M - M_{\text{thr},i}(T))] \Theta(M_{\text{thr},i}(T) - M_i). \quad (4)$$

Inserting (4) into (3) results in

$$P_i(T) = \mp d_i \int_0^\infty \frac{dp}{2\pi^2} p^2 T \left[\ln \left(1 \mp e^{-\sqrt{p^2 + M_i^2}/T} \right) - \ln \left(1 \mp e^{-\sqrt{p^2 + M_{\text{thr},i}(T)^2}/T} \right) \right] \Theta(M_{\text{thr},i}(T) - M_i). \quad (5)$$

The temperature dependent threshold mass of the 2- (3-) quark continuum for mesonic (baryonic) bound state channels i is

$$M_{\text{thr},i}(T) = \sqrt{2} [(N_i - N_s)m(T) + N_s m_s(T)], \quad (6)$$

where $N_s = 0, 1, \dots$, N_i is the number of strange quarks in hadron i . The factor $\sqrt{2}$ originates from quark confinement in the following way. In the confining vacuum, the quarks are not simple plane waves with arbitrarily long wavelength, but due to the presence of bag-like boundary conditions their wavelength shall not exceed a certain length scale. Therefore, a minimal quark momentum applies

to the quark dispersion relations $E_{q,\min}(T) = \sqrt{m_q^2(T) + p_{q,\min}^2}$, which for the choice $p_{q,\min} = m_q(T)$ results in $E_{q,\min}(T) = \sqrt{2}m_q(T)$. For details, see [5]. The chiral condensate is defined as

$$\langle \bar{\psi}\psi \rangle_{q,T} = -\frac{\partial \Omega(T)}{\partial m_q}, \quad q = u, d, s, \quad (7)$$

where m_l (m_s) is the current-quark mass in the light (strange) quark sector, $l = u, d$. It is an order parameter for the dynamical breaking of the chiral symmetry that is reflected in the corresponding temperature dependence of the dynamical quark masses $m_q(T)$.

In our present model, we do not treat the dynamical quark mass as an order parameter that should follow from the solution of an equation of motion (gap equation) that minimizes the thermodynamic potential like in the case of the Polyakov-loop variable ϕ , but we will use the quantity $\Delta_{l,s}(T)$ from simulations of 2+1 flavor lattice QCD as an input. This quantity has been introduced in [6] with the definition

$$\Delta_{l,s}(T) = \frac{\langle \bar{\psi}\psi \rangle_{l,T} - (m_l/m_s) \langle \bar{\psi}\psi \rangle_{s,T}}{\langle \bar{\psi}\psi \rangle_{l,0} - (m_l/m_s) \langle \bar{\psi}\psi \rangle_{s,0}}, \quad (8)$$

and was used later on, e.g., in [1,2]. Further, we assume for the temperature-dependent light quark mass

$$m(T) = m(0)\Delta_{l,s}(T) + m_l, \quad (9)$$

with $m_l = 5.5$ MeV being the current-quark mass, and for the strange quark mass we adopt

$$m_s(T) = m(T) + m_s - m_l = m(0)\Delta_{l,s}(T) + m_s, \quad (10)$$

with $m_s = 100$ MeV. The LQCD result for the temperature dependence of the chiral condensate [1,2] can be fitted by

$$\Delta_{l,s}(T) = \frac{1}{2} \left[1 - \tanh \left(\frac{T - T_c}{\delta_T} \right) \right], \quad (11)$$

where $T_c = 154$ MeV is the common pseudocritical temperature of the chiral restoration transition of both LQCD Collaborations and $\delta_T = 26$ MeV is its width for the data from Ref. [1], while $\delta_T = 22.7$ MeV for those from Ref. [2], see Fig. 1. For our present applications in modelling the QCD thermodynamics, we will use the fit of the chiral condensate (11), but with the modern value of $T_c = 156.5 \pm 1.5$ MeV [7]. We have checked that the results for the total pressure of our model are practically inert against changing the value of δ_T within the above range of variation. Inserting (9) and (10) into (6) we get

$$\begin{aligned} M_{\text{thr},i}(T) &= \sqrt{2} [N_i m(T) + N_s (m_s(T) - m(T))] \\ &= \sqrt{2} [m_s N_s + m_l (N_i - N_s) + m(0) N_i \Delta_{l,s}(T)], \end{aligned} \quad (12)$$

and using (9) results in

$$M_{\text{thr},i}(T) = \sqrt{2} \left\{ m_s N_s + m_l (N_i - N_s) + m(0) N_i \left[\frac{1}{2} - \frac{1}{2} \tanh \left(\frac{T - T_c}{\delta_T} \right) \right] \right\}. \quad (13)$$

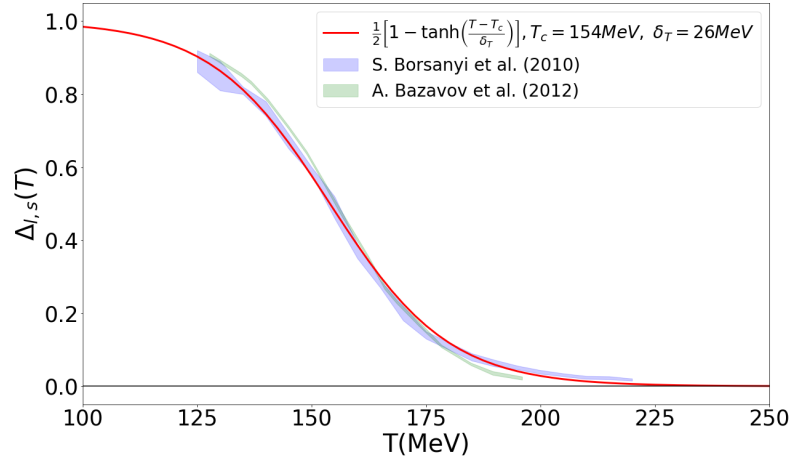


Figure 1. Comparison of the fit (11) for the temperature dependence of the chiral condensate $\Delta_{I,S}(T)$ and the Lattice QCD data for it from the Wuppertal-Budapest Collaboration [1] and the hotQCD Collaboration [2]. .

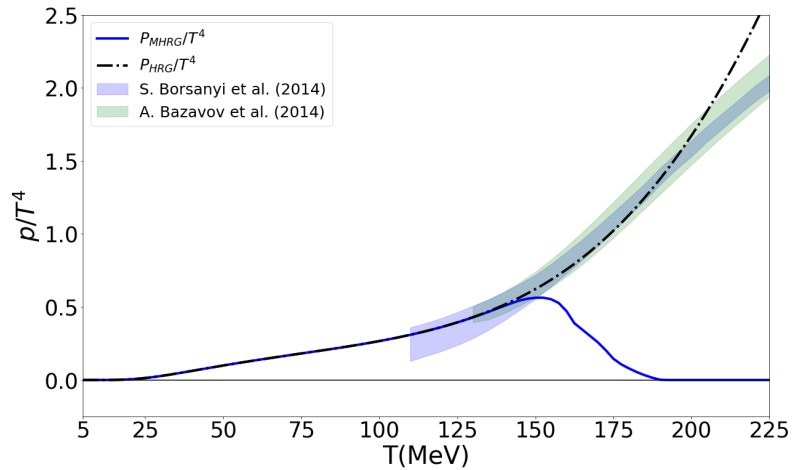


Figure 2. Pressure as a function of the temperature for the hadron resonance gas (HRG) model with stable hadrons (red line) and for the HRG with Mott dissociation of hadrons (MHRG) according to the simple phase shift model (4) employed in the present work. These results are compared to the lattice QCD data from the [HotQCD Collaboration] [4] (green band) and the [Wuppertal-Budapest Collaboration] [3] (blue band).

2.2. Polyakov-loop improved Nambu–Jona-Lasinio model

The underlying quark and gluon thermodynamics is divided into a perturbative contribution $\Omega_{\text{pert}}(T)$ which is treated as virial correction in two-loop order following Ref. [8] and a nonperturbative part described within a PNJL model in the form

$$P_{\text{PNJL}}(T; \phi) = P_Q(T; \phi) + \mathcal{U}(T; \phi), \quad (14)$$

where the quark quasiparticle contribution is given by

$$P_Q(T; \phi) = 4N_c \sum_{q=u,d,s} \int \frac{dp}{2\pi^2} \frac{p^2}{3} T \ln \left[1 + 3\phi(1 + Y_q)Y_q + Y_q^3 \right], \quad Y_q = e^{-\sqrt{p^2 + m_q^2(T)}/T}, \quad (15)$$

and the Polyakov-loop potential $\mathcal{U}(T; \phi)$ takes into account the nonperturbative gluon background in a meanfield approximation using the polynomial fit of Ref. [9]

$$\mathcal{U}(T; \phi) = \frac{b_2(T)}{2} \phi^2 + \frac{b_3}{3} \phi^3 - \frac{b_4}{4} \phi^4, \quad (16)$$

where the temperature-dependent coefficient $b_2(T)$ is given by

$$b_2(T) = a_0 + a_1 \left(\frac{T_0}{T} \right) + a_2 \left(\frac{T_0}{T} \right)^2 + a_3 \left(\frac{T_0}{T} \right)^3, \quad (17)$$

and the coefficients are given in Table 1.

Table 1. Set of values for the Polyakov-loop potential $\mathcal{U}(T; \phi)$ [9].

a_0	a_1	a_2	a_3	b_3	b_4
6.75	-1.95	2.625	-7.44	0.75	7.5

2.3. Perturbative contribution

It is well known that the lattice QCD thermodynamics at high temperatures $T \sim 1$ GeV does follow a Stefan-Boltzmann like behaviour $\propto T^4$, but with a 15 – 20% reduction of the effective number of degrees of freedom. It has been observed, e.g., in Ref. [8], that this deviation can be described by the virial correction to the pressure due to the quark-gluon scattering at $\mathcal{O}(\alpha_s)$ shown in Fig. 3. Here we modify the standard expression [10] of the form

$$\Omega_{\text{pert}}(T; \phi) = -\frac{8}{\pi} \alpha_s T^4 \left[I(T; \phi) + \frac{3}{\pi^2} (I(T; \phi))^2 \right] \quad (18)$$

by introducing the modified integral

$$I(T; \phi) = \int_{\Lambda/T}^{\infty} dx \, x f_{\phi}(x), \quad (19)$$

where the generalized Fermi distribution function of the PNJL model for the case of vanishing quark chemical potential considered here is defined as

$$f_{\phi}(x) = [\phi(1 + 2Y)Y + Y^3] / [1 + 3\phi(1 + Y)Y + Y^3], \quad Y = \exp(-x) \quad (20)$$

and $\Lambda = m_l(T)$ is the momentum range below which nonperturbative physics dominates and is accounted for by the dynamically generated quark mass. We use here a temperature dependent, regularized running coupling [11–13]

$$\alpha_s = \frac{g^2}{4\pi} = \frac{12\pi}{11N_c - 2N_f} \left(\frac{1}{\ln(r^2/c^2)} - \frac{c^2}{r^2 - c^2} \right), \quad (21)$$

where $r = 3.2T$, $c = 350$ MeV and $N_c = N_f = 3$.

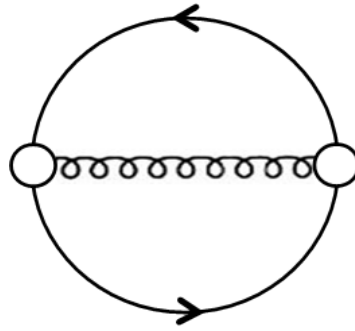


Figure 3. Two-loop diagram for the contribution of the one-gluon exchange interaction to the thermodynamic potential of quark matter.

3. Stationarity condition for the Polyakov loop

The pressure follows from the thermodynamic potential under the condition of stationarity w.r.t. variations of the order parameters. Since the chiral condensate is fixed by the fit (11) to the numerical result from lattice QCD, the Polyakov loop ϕ is the only free order parameter in the system to be varied this condition means

$$P_{\text{QGP}}(T) = - \min_{\phi} \{ \Omega_{\text{QGP}}(T; \phi) \} . \quad (22)$$

It is realized by demanding

$$\frac{d\Omega_{\text{QGP}}(T; \phi)}{d\phi} = \frac{dU(T; \phi)}{d\phi} + \frac{d\Omega_Q(T; \phi)}{d\phi} + \frac{d\Omega_{\text{pert}}(T; \phi)}{d\phi} = 0 , \quad (23)$$

where the separate contributions come from the variations of the Polyakov loop potential

$$\frac{dU(T; \phi)}{d\phi} = b_2(T)\phi + b_3\phi^2 - b_4\phi^3 , \quad (24)$$

the quark quasiparticle pressure

$$\frac{d\Omega_Q(T; \phi)}{d\phi} = 4N_c \sum_{q=u,d,s} \int \frac{dp}{2\pi^2} p^2 \frac{(1 + Y_q)Y_q}{1 + 3\phi(1 + Y_q)Y_q + Y_q^3} , \quad (25)$$

with $Y_q = \exp[-\sqrt{p^2 + m_q^2(T)}/T]$, and the $\mathcal{O}(\alpha_s)$ quark loop contribution

$$\frac{d\Omega_{\text{pert}}(T; \phi)}{d\phi} = -\frac{8}{\pi} \alpha_s T^4 \left[\frac{dI(\phi, T)}{d\phi} + \frac{6}{\pi^2} I(\phi, T) \frac{dI(\phi, T)}{d\phi} \right] , \quad (26)$$

where

$$\frac{dI(T; \phi)}{d\phi} = \int_{\Lambda/T}^{\infty} dx \, x \frac{df_{\phi}(x)}{d\phi} , \quad (27)$$

and

$$\frac{df_{\phi}(x)}{d\phi} = \frac{Y + 2Y^2 - 2Y^4 - Y^5}{(1 + 3\phi(1 + Y)Y + Y^3)^2} = \frac{(1 + 2Y)Y - (2 + Y)Y^4}{(1 + 3\phi(1 + Y)Y + Y^3)^2} , \quad Y = \exp(-x) . \quad (28)$$

The equation resulting from the stationarity condition (23) can be dubbed "gap equation" for ϕ since it has a similar structure as the quark mass gap equation, known from Nambu–Jona-Lasinio models. The solution of this gap equation gives the temperature dependence of the traced Polyakov loop ϕ that is shown in Fig. 4 in comparison to the lattice QCD data for the renormalized Polyakov loop from the TUMQCD Collaboration [14] and the Wuppertal-Budapest Collaboration [1].

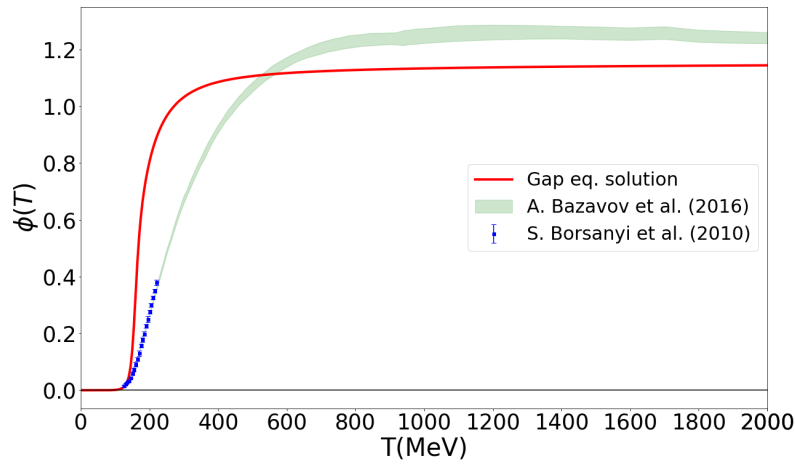


Figure 4. The traced Polyakov loop ϕ from the solution of the stationarity condition (23) on the thermodynamical potential as a function of temperature (magenta solid line) compared with the lattice results for the renormalized Polyakov loop the TUMQCD Collaboration [14] (green band) and the Wuppertal-Budapest Collaboration [1] (blue symbols).

4. Results

4.1. Pressure

The main result of this work is a unified approach to the pressure of hadron-quark-gluon matter at finite temperatures that is in excellent agreement with lattice QCD thermodynamics, see Fig. 5. The nontrivial achievement of the presented approach is that the Mott dissociation of the hadrons described by the MHRG model pressure conspires with the quark-gluon pressure described by the Polyakov-loop quark-gluon model with $\mathcal{O}(\alpha_s)$ corrections in such a way that the resulting pressure as a function of temperature yields a smooth crossover behaviour. By virtue of the Polyakov-loop improved perturbative correction, the agreement with the lattice QCD thermodynamics extends to the high temperatures of $T = 1960$ MeV reported in Ref. [15], see Fig. 6.

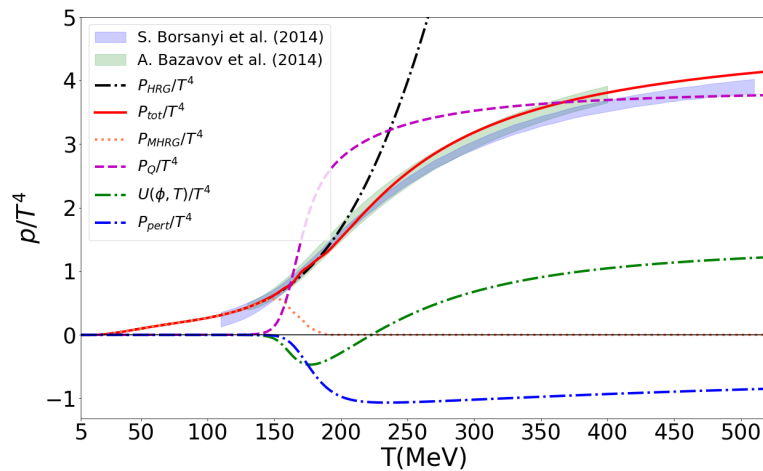


Figure 5. The temperature dependence of the total scaled pressure (red solid line) and its constituents: MHRG (coral dotted line), quark (dashed magenta line), Polyakov-loop potential $\mathcal{U}(T; \phi)$ (dash-dotted green line), perturbative QCD contribution (dash-dotted blue line) compared to the lattice QCD data: [HotQCD Collaboration] [4] (green band) and [Wuppertal-Budapest Collaboration] [3] (blue band).

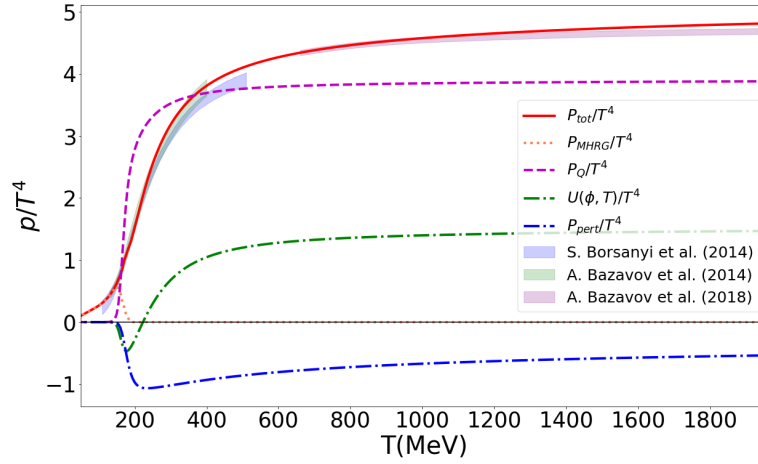


Figure 6. The temperature dependence of the total scaled pressure (red solid line) and it's constituents: MHRG (coral dotted line), quark (dashed magenta line), Polyakov-loop potential $U(\phi, T)$ (dash-dotted green line), perturbative QCD contribution (dash-dotted blue line) compared to the lattice QCD data: [HotQCD Collaboration] [4] (green band) and [Wuppertal-Budapest Collaboration] [3] (blue band), and the high-temperature result [15] (magenta band).

4.2. Quark number susceptibilities

In the present work we did not yet consider the generalization of the approach to finite chemical potentials which would then allow to evaluate the (generalized) susceptibilities as derivatives of the pressure with respect to the corresponding chemical potential in appropriate orders. On that basis ratios of susceptibilities can be formed as they indicate different aspects of the QCD transition between the limiting cases of a HRG and a QGP. Here we would like to discuss as an outlook to these extensions of the approach one of the simplest susceptibility ratios, namely the dimensionless ratio of quark number density to quark number susceptibility

$$R_{12}(T) = \left. \frac{n_q(T)}{\mu_q \chi_q(T)} \right|_{\mu_q=0}, \quad (29)$$

where $n_q(T) = \partial P(T, \mu_q) / \partial \mu_q|_{\mu_q=0}$ and $\chi_q(T) = \partial^2 P(T, \mu_q) / \partial \mu_q^2|_{\mu_q=0}$. This ratio (29) has two well-known limits. At low temperatures, in the hadron resonance gas phase it is given by

$$R_{12}^{HRG}(T) = \frac{T}{3\mu_q} \tanh\left(\frac{3\mu_q}{T}\right), \quad (30)$$

while in the QGP phase for massless quarks it approaches

$$R_{12}^{QGP}(T) = \frac{1 + (1/\pi^2)(\mu_q/T)^2}{1 + (3/\pi^2)(\mu_q/T)^2}. \quad (31)$$

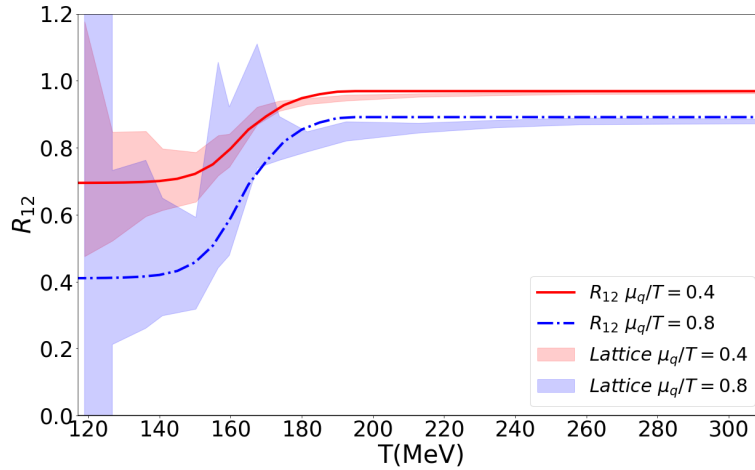


Figure 7. The dimensionless ratio of quark number density to quark number susceptibility $R_{12}(T) = n_q(T)/(\mu_q \chi_q(T))|_{\mu_q=0}$ as a function of temperature for $\mu_q/T = 0.4$ (red solid line) and $\mu_q/T = 0.8$ (blue dash-dotted line) compared to the lattice QCD data [16] $\mu_q/T = 0.4$ (red band), $\mu_q/T = 0.8$ (blue band). For details, see text.

An evaluation of (29) for the present model for the QCD pressure would require its extension to finite μ_q which we will perform in a subsequent work. In the present model we will use our knowledge of the composition as a function of temperature to define a proxy for (29) by interpolating between the two known limits (29) and (29) with the partial pressure of the HRG, $x_{HRG}(T) = P_{MHRG}(T)/P_{tot}(T)$, as

$$R_{12}(T) = x_{HRG}(T)R_{12}^{HRG}(T) + [1 - x_{HRG}(T)]R_{12}^{QGP}(T). \quad (32)$$

The result is shown in Fig. 7 for two values of μ_q/T for which lattice QCD results in the two-flavor case [16] are shown for a comparison.

5. Discussion and Conclusions

The main result of the present work is a unified approach to the thermodynamic potential of hadron-quark-gluon matter at finite temperatures that is in excellent agreement with lattice QCD thermodynamics on the temperature axis of the QCD phase diagram. The key ingredient to this approach is the quark cluster decomposition of the thermodynamic potential within the Beth-Uhlenbeck approach [17] which allowed to implement the effect of Mott dissociation to the hadron resonance gas phase of low-temperature/low-density QCD. Such a MHRG model description includes, in principle, the information about the spectral properties of all hadronic channels with their discrete and continuous part of the spectrum, encoded in the hadronic phase shifts. Instead of solving the equations of motion, a coupled hierarchy of Schwinger-Dyson equations in the one-, two-, and many-quark channels selfconsistently (a formidable task of finite-temperature quantum field theory!), we applied here a very schematic model for the in-medium phase shifts that is in accordance with the Levinson theorem and sufficiently general to be applicable for all multi-quark cluster channels. This phase shift model requires just the knowledge of the vacuum mass spectrum which can come from the particle data group tables, or from relativistic quark models, and the medium dependence of the multi-quark continuum threshold.

The latter requires the knowledge of the quark mass (i.e. the chiral condensate) with its medium dependence as an order parameter of the chiral symmetry breaking and restoration. Since a quark mean field model of the (P)NJL type is not sufficient as it lacks the backreaction from the hadron resonance gas on the quark propagator properties, we employ here the chiral condensate measured in continuum-extrapolated, full lattice QCD with physical current quark masses as an input. This procedure restricts the applicability of the present model to small chemical potentials only, where

lattice QCD data for the chiral condensate are available. In a further development of the model, a beyond-mean-field derivation of the quark selfenergy shall be given. Furthermore, at the same level of approximation the corresponding sunset-type diagrams for the Φ functional of the 2PI approach should be derived and evaluated. This allows to calculate the generalized polarization-loop integrals which determine the analytic properties of the multi-quark states. These can be equivalently encoded in the corresponding medium-dependent phase shifts of the generalized Beth-Uhlenbeck approach, as has been demonstrated in particular examples for pions, diquarks [18,19] and nucleons [20] within the Polyakov-loop generalized NJL model.

Another important aspect of the present approach is that it leads to a relativistic density functional theory for QCD matter in the QCD phase diagram, with the known limits of the HRG and pQCD manifestly implemented. Such an approach allows to predict the existence and location of critical endpoints in the QCD phase diagram, as it had been demonstrated, e.g., in Ref. [21], where in dependence on a free parameter could have besides the critical endpoint of the liquid-gas transition in the nuclear matter phase another endpoint for the deconfinement transition or none. This "crossover all over" case of the QCD phase diagram is impossible to address with two-phase approaches that use a Maxwell construction for the phase transition. Other models that are in use for analyses of the critical behaviour of QCD (see, e.g., [22,23]) do impose it by assuming a so-called "switch function" between HRG and QGP phases. They are valuable tools but do not have a predictive power.

With these perspectives for the further development of the approach developed here, we conclude this work.

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