Quantum simulations of strongly coupled quark-gluon plasma

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A strongly coupled quark-gluon plasma (QGP) of heavy constituent quasiparticles is studied by a path-integral Monte-Carlo method. This approach is a quantum generalization of the classical molecular dynamics by Gelman, Shuryak, and Zahed. It is shown that this method is able to reproduce the QCD lattice equation of state. The results indicate that the QGP reveals liquid-like rather than gas-like properties. Quantum effects turned out to be of prime importance in these simulations.

1. INTRODUCTION

Investigation of properties of the QGP is one of the main challenges of strong-interaction physics, both theoretically and experimentally. Many features of this matter were experimentally discovered at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven. The most striking result, obtained from analysis of these experimental data [1], is that the deconfined quark-gluon matter behaves as an almost perfect fluid rather than a perfect gas, as it could be expected from the asymptotic freedom.

There are various approaches to studying QGP. Each approach has its advantages and disadvantages. The most fundamental way to compute properties of the strongly interacting matter is provided by the lattice QCD [2–4]. Interpretation of these very complicated computations requires application of various QCD motivated, albeit schematic, models simulating various aspects of the full theory. Moreover, such models are needed in cases when

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the lattice QCD fails, e.g. at large baryon chemical potentials and out of equilibrium. While some progress has been achieved in the recent years, we are still far away from having a satisfactory understanding of the QGP dynamics.

A semi-classical approximation, based on a point like quasi-particle picture has been introduced in [5]. It is expected that the main features of non-Abelian plasmas can be understood in simple semi-classical terms without the difficulties inherent to a full quantum field theoretical analysis. Independently the same ideas were implemented in terms of molecular dynamics (MD) [6]. Recently this MD approach was further developed in a series of works [7, 8]. The MD allowed one to treat soft processes in the QGP which are not accessible by perturbative means.

A strongly correlated behavior of the QGP is expected to show up in long-ranged spatial correlations of quarks and gluons which, in fact, may give rise to liquid-like and, possibly, solid-like structures. This expectation is based on a very similar behavior observed in electrodynamic plasmas [7, 9]. This similarity was exploited to formulate a classical non-relativistic model of a color Coulomb interacting QGP [7] which was numerically analyzed by classical MD simulations. Quantum effects were either neglected or included phenomenologically via a short-range repulsive correction to the pair potential. Such a rough model may become a critical issue at high densities, where quantum effects strongly affects properties of the QGP. Similar models have been used in electrodynamic plasmas and showed poor behavior in the region of strong wave function overlap, in particular at the Mott density. For temperatures and densities of the QGP considered in Ref. [7] these effects are very important as the quasiparticle thermal wave length is of order the average interparticle distance.

In this paper we extend previous classical nonrelativistic simulations [7] based on a color Coulomb interaction to the quantum regime. We develop an approach based on path integral Monte Carlo (PIMC) simulations of the strongly coupled QGP which self-consistently takes into account the Fermi (Bose) statistics of quarks (gluons). Following an idea of Kelbg [11], quantum corrections to the pair potential are rigorously derived [12]. To extend the method of quantum potentials to a stronger coupling, an "improved Kelbg potential" was derived, which contains a single free parameter, being fitted to the exact solution of the quantum-mechanical two-body problem. Thus, the method of the improved Kelbg potential is able to describe thermodynamic properties up to moderate couplings [13]. However, this approach may fail, if bound states of more than two particles are formed in the system. This re-

sults in a break-down of the pair approximation for the density matrix, as demonstrated in Ref. [13]. A superior approach, which does not have this limitation, consists in use the original Kelbg potential in the PIMC simulations which effectively map the problem onto a high-temperature weakly coupled and weakly degenerate one. This allows one to rigorously extend the analysis to strong couplings and is, therefore, a relevant choice for the present purpose.

This method has been successfully applied to strongly coupled electrodynamic plasmas [14, 15]. Examples are partially-ionized dense hydrogen plasmas, where liquid-like and crystalline behavior was observed [16, 17]. Moreover, also partial ionization effects and pressure ionization could be studied from first principles [18]. The same methods have been also applied to electron-hole plasmas in semiconductors [19, 20], including excitonic bound states, which have many similarities to the QGP due to smaller mass differences as compared to electron-ion plasmas.

The main goal of this article is to test the developed approach for ability to reproduce known lattice data [2, 3] and to predict other properties of the QGP, which are still unavailable for the lattice calculations. To this end we use a simple model [7] of the QGP consisting of quarks, antiquarks and gluons interacting via a color Coulomb potential. First results of applications of the PIMC method to study of thermodynamic properties of the nonideal QGP have already been briefly reported in [21, 22]. In this paper we present a comprehensive report on the thermodynamic properties.

2. THERMODYNAMICS OF QGP

2.1. Basics of the model

Our model is based on a resummation technique and lattice simulations for dressed quarks, antiquarks and gluons interacting via the color Coulomb potential. The assumptions of the model are similar to those of Ref. [7]:

I. All color quasi-particles are heavy, i.e. their mass (m) is higher than the mean kinetic energy per particle. For instance, at zero net-baryon density it amounts to $m > T$, where T is a temperature. Therefore these particles move non-relativistically. This assumption is based on the analysis of lattice data [23, 24].

II. Since the particles are non-relativistic, interparticle interaction is dominated by a color-electric Coulomb potential. Magnetic effects are neglected as sub-leading ones.

III. Relying on the fact that the color representations are large, the color operators are substituted by their average values, i.e. by classical color vectors, the time evolution of which is described by Wong's dynamics [25].

The quality of these approximations and their limitations were discussed in Ref. [7]. Thus, this model requires the following quantities as an input:

1. the quasiparticle mass, m, and

2. the coupling constant g^2.

All the input quantities should be deduced from the lattice data or from an appropriate model simulating these data.

3. SIMULATIONS OF QGP

To test the developed approach we consider the QGP only at zero baryon density and further simplify the model by additional approximations, similarly to Ref. [7]:

IV We replace the grand canonical ensemble by a canonical one. The thermodynamic properties in the canonical ensemble with given temperature T and fixed volume V are fully described by the density operator $\hat{\rho} = e^{-\beta \hat{H}}$ with the partition function defined as follows

$$Z(N_q, N_{\bar{q}}, N_g, V; \beta) = \frac{1}{N_q! N_{\bar{q}}! N_g!} \sum_{\sigma} \int_V dr dQ \, \rho(r, Q, \sigma; \beta), \tag{1}$$

with $N_q = N_{\bar{q}}$ and hence $N_B = 0$. The density matrix ρ in this expression is calculated using the path integral Monte Carlo approach [21, 22, 27, 28]. In order to preserve the thermodynamical consistency of this formulation, thermodynamic quantities should be calculated through respective derivatives of the logarithm of the partition function (1) in which N_a are indepenent variables.

V Since the masses of quarks of different flavors extracted from lattice data are very similar, we do not distinguish between quark flavors. Moreover, we take the quark and

gluon quasi-particle masses being equal because their values deduced from the lattice data [23, 24] are very close.

VI Because of the equality of masses and approximate equality of number of degrees of freedom of quarks, antiquarks and gluons, we assume that these species are equally represented in the system: $N_q = N_{\bar{q}} = N_g$.

VII For the sake of technical simplicity, the $SU(3)$ color group is replaced by $SU(2)$.

Thus, this simplified model requires an additional quantity as an input:

3. the density of quasi-particles $(N_q + N_{\bar{q}} + N_g)/V = n(T)$ as a function of the temperature.

Although this density is unknown from the QCD lattice calculations and we use it as a fit parameter, it is very important to partially overcome constrains of the above simplifications. First, it concerns the use of the $SU(2)$ color group, which first of all reduces the degeneracy factors of the quark and gluon states, as compared to the $SU(3)$ case, and thereby reduces pressure and all other thermodynamic quantities. A proper fit of the density allows us to remedy this deficiency of the normalization. Second, in fact we consider the system of single quark flavor, i.e. all quarks are identical, which also reduces the normalization of all thermodynamic quantities. The density fit cures the deficiency of this normalization, though the excessive anticorrelation of quarks remains.

Ideally the parameters of the model should be deduced from the QCD lattice data. However, presently this task is still quite ambiguous. Therefore, in the present simulations we take a possible (maybe, not the most reliable) set of parameters. Following Refs. [7, 24], the parametrization of the quasi-particle mass is taken in the form

$$m(T)/T_c = 0.9/(T/T_c - 1) + 3.45 + 0.4T/T_c \tag{2}$$

where $T_c = 175$ MeV is the critical temperature. This parametrization fits the quark mass at two values of temperature obtained in the lattice calculations [23]. According to [23] the masses are quite large: $m_q/T \simeq 4$ and $m_g/T \simeq 3.5$. These are essentially larger than masses required for quasi-particle fits [29, 30] of the lattice thermodynamic properties of the QGP: $m_q/T \simeq 1$–2 and $m_g/T \simeq 1.5$–3. Moreover, the pole quark mass $m_q/T \simeq 0.8$ was reported in recent work [31], as deduced from lattice calculations. Nevertheless, in spite of the fact that it obviously produces too high masses, we use parametrization (2) in order to be compatible

with the input of classical MD of Ref. [7]. The T-dependence of this mass is illustrated in Fig. 1*a*.

The coupling constant, i.e. $\alpha_s = g^2/(4\pi)$, used in the simulations is displayed in Fig. 1*a* as well. As seen, α_s well complies with phenomenologic QCD estimations [32] of its values. Notice that in previous publications [21, 22] the factor $(N_c^2 - 1)$, where N_c is the number of colors in the $SU(N_c)$ color group, was accidentally included in g^2, when displaying it corresponding figures. In fact, this factor is a part of Casimirs defining the normalization of the color vectors in the color group.

The density of quasi-particles, which is additionally required within the canonical-ensemble approach, was chosen on the condition of the best agreement of the calculated pressure with the corresponding lattice result, see Fig. 1*b*. It was taken to be $n(T) = 0.24T^3$. From the first glance, it is a very low density. For example, in the classical simulations of Ref. [7] it was taken as $n(T)/T^3 = 6.3$, which corresponds to the density of an ideal gas of *massless* quarks, antiquarks and gluons. Since the quasi-particles are very heavy in the present model (as well as in that of Ref. [7]), the latter density looks unrealistically high. Even in quasi-particle models [29, 30], where the masses are lower, the density turns out to be $n(T)/T^3 \approx 1.4$. Since Eq. (2) gives even larger masses than those in Refs. [29, 30] and in view of the adopted large coupling, the chosen value of $n(T)$ does not look too unrealistic.

Thus, although the chosen set of parameters is still debatable, it is somehow self-consistent. In the future we are going to get rid of the $n(T)$ parameter, by applying the grand-canonical approach, and by using more moderate (and maybe realistic) sets of parameters.

Calculation of the equation of state (Fig. 1*b*) was used to optimize the parameters of the model in order to proceed to predictions of other properties concerning the internal structure and in the future also non-equilibrium dynamics of the QGP. The plasma coupling parameter is defined as

$$\Gamma = \frac{\overline{q_2} g^2}{4\pi r_s T}\,, \tag{3}$$

where r_s is the the Wigner-Seitz radius, defined such that $4\pi r_s^3/3 = n$, and $\overline{q_2}$ the quadratic Casimir value averaged over quarks, antiquarks and gluons, $\overline{q_2} = N_c^2 - 1$ is a good estimate for this quantity. The plasma parameter is a measure of ratio of the average potential to the average kinetic energy. It is also presented in Fig. 1*a*. It turns out to be of the order of

unity which indicates that the QGP is a strongly coupled Coulomb liquid rather than a gas. In the studied temperature range, $1 < T/T_c < 3$, the QGP is, in fact, quantum degenerate, since the degeneracy parameter $\chi_a = n_a \lambda_a^3$ (where the thermal wave length, λ, is defined in the previous section) varies from 0.1 to 1.7, see Fig. 1*a*.

Fig. 2 additionally presents the entropy (S) and trace anomaly ($\varepsilon - 3P$) of the QGP computed in the PIMC method. In order to avoid the numeric noise, the derivative of a smooth interpolation between the PIMC points (see Fig. 1*b*) was taken. These results are compared to lattice data of Refs. [2, 4]. It is not surprising that agreement with the lattice data is also good, since it is a direct consequence of the good reproduction of the pressure.

Details of our path integral Monte-Carlo simulations have been discussed elsewhere in a variety of papers and review articles, see, e.g. [33] and references therein. The main idea of the simulations consists in constructing a Markov process of configurations which differ by the particle coordinates. Additionally to the case of electrodynamic plasmas, here we randomly sample, according to the group measure, the color variables Q of all particles until convergence is achieved. We use a cubic simulation box with periodic boundary conditions. The number of particles was taken as $N = N_q + N_{\bar{q}} + N_g = 40 + 40 + 40 = 120$, and the number of beads, $n = 20$. Calculation of the equation of state (Fig. 1*b*) was used to optimize the parameters of the model in order to proceed to predictions of other properties concerning the internal structure and in the future also non-equilibrium dynamics of the QGP.

4. CONCLUSION

Quantum Monte Carlo simulations based on the quasiparticle picture of the QGP are able to reproduce the lattice equation of state (even near the critical temperature) and also yield valuable insight into the internal structure of the QGP. Our results indicate that the QGP reveals liquid-like (rather than gas-like) properties even at the highest considered temperature of $3T_c$. At temperatures just above T_c we have found that bound quark-antiquark states still survive. Quantum effects turned out to be of prime importance in these simulations.

Our analysis is still too simplified and incomplete. It is still confined only to the case of zero baryon chemical potential. The input of the model also requires refinement. Work on these problems is in progress. We have also performed first simulations of dynamic properties of the QGP based on quantum Wigner dynamics. In particular, these allow us to deduce the

viscosity of the QGP. However, the brief format of the present contribution does not allow us to report on the respective results.

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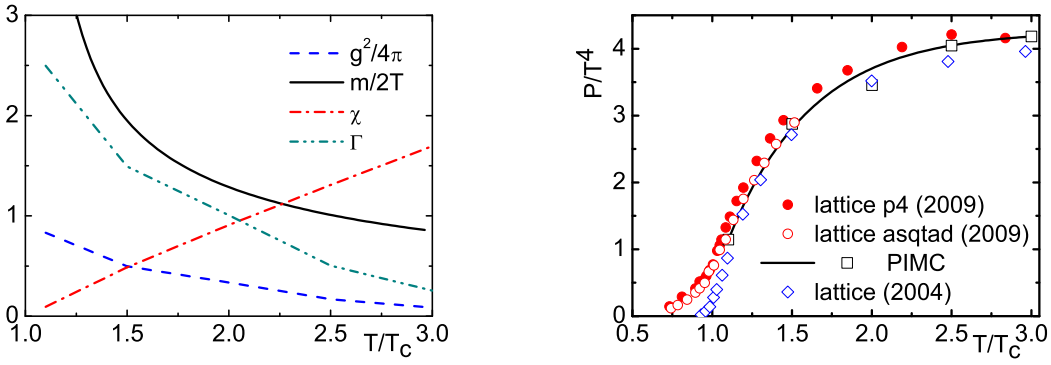

Figure 1. (a) Temperature dependence of the model input quantities, coupling constant g^2 and mass-to-temperature ratio (scaled by $1/2$), the plasma coupling parameter Γ [see Eq. (3)] and the degeneracy parameter χ. The χ parameters for different species are equal, since their masses and densities are assumed to be equal. (b) Equation of state (pressure versus temperature) of the QGP from PIMC simulations (open squares) compared to lattice data of Refs. [2, 4]. The solid line is a smooth interpolation between the PIMC points. Results of the HotQCD Collaboration [2] are presented by filled circles, while results of the Budapest group [4], open circles. Different kinds of circles (filled and open) correspond to different dicretization schemes of the QCD action (p4 and asqtad, see [2] for detailes).

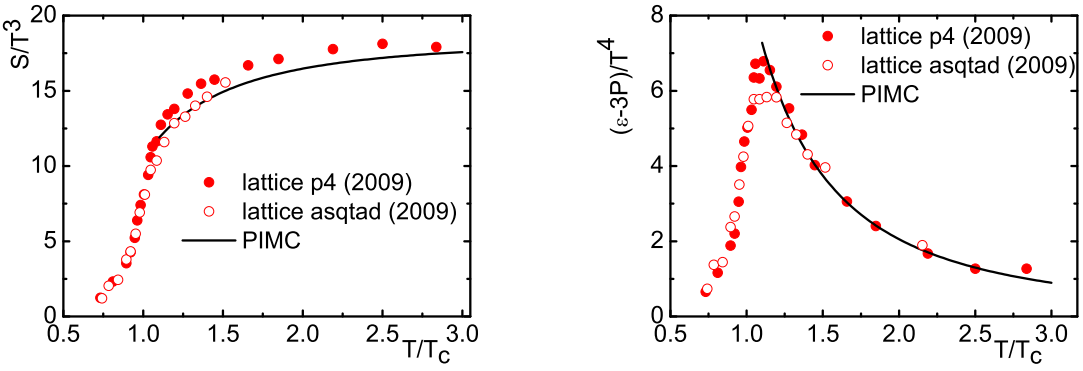

Figure 2. Entropy (a) and trace anomaly (b) of the QGP from PIMC simulations (solid line) compared to lattice data of Refs. [2, 4]. Notation is the same as in the right panel of Fig. 1.

FIGURE CAPTIONS

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Fig. 2: Entropy (a) and trace anomaly (b) of the QGP from PIMC simulations (solid line) compared to lattice data of Refs. [2, 4]. Notation is the same as in the right panel of Fig. 1.