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Quantum Color Dynamic Simulations of the Strongly Coupled Quark-Gluon Plasma

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A strongly coupled plasma of quark and gluon quasiparticles is studied by combination of Path integral Monte Carlo and quantum Wigner dynamics simulations. This method extends previous classical nonrelativistic simulations based on a color Coulomb interaction to the quantum regime. First results for the momentum-momentum autocorrelation function and diffusion constant are presented.

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1 Introduction

Determining the properties of the quark-gluon plasma (QGP) is one of the main challenges of strong-interaction physics, both theoretical [1] and experimental [2]. 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 [3], is that the deconfined quark-gluon matter behaves as almost perfect fluid rather than as a perfect gas, as it could be expected from the asymptotic freedom.

From the theory side, the most fundamental way to compute properties of strongly interacting matter is provided by lattice QCD, see Refs. [4, 5]. Interpretation of these very difficult and long computations requires application of various QCD motivated, albeit schematic, models simulating various aspects of the full theory and allowing for a deeper physical understanding. In a previous paper [6] we presented first applications of the Path integral Monte Carlo (PIMC) method to simulations of a nonideal quark-gluon plasma (QGP) which showed good agreement of the PIMC equation of state with lattice data for the 2+1 flavor case. In this contribution we extend the analysis to dynamic properties by performing first exploratory quantum molecular dynamics (QMD) simulations of the QGP. This MD method extends previous classical nonrelativistic simulations [7] based on a color Coulomb interaction to the quantum regime.

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2 Theoretical model

Our model is based on precisely the same assumptions as those in Ref. [7] which are summarized as follows:

- I:** All particles (quarks and gluons) are heavy, i.e., $m > T$, where m is the mass of a particle and T , the temperature, and therefore they move non-relativistically. This assumption is based on the analysis of lattice data [8,9].
- II:** Since the order of magnitude of quark and gluon masses, deduced from the lattice data [8,9] is the same, we do not distinguish these masses and put them equal. Moreover, because of the latter we do not distinguish between quark flavors.
- III:** The interparticle interaction is dominated by a color-electric Coulomb interaction, see Eq. (2). Magnetic effects are neglected as sub-leading ones in the nonrelativistic limit.
- IV:** The color operators t^a are substituted by their average values, i.e. by classical color $3D$ unit vectors, relying on the fact that the color representations are large. Time evolution of these color vectors is described by Wong's dynamics [10].

The quality of these approximations and their limitations were discussed in Ref. [7]. Aiming at a first test of this model in QMD simulations, we consider the QGP only at zero baryon density. Thus, this model requires the following quantities as an input:

1. the temperature dependence of the quasiparticle mass, $m(T)$,
2. the density of particles, $n(T)$, at a given temperature [Following [7], we assume that the numbers of quarks, antiquarks and gluons are approximately equal as the number of effective degrees of freedom in thermodynamical quantities is such that roughly all three species are equally represented.],
3. the coupling constant, $g^2(T)$, at a given temperature, see Eq. (2) [Note that, because of the running coupling in the QCD, g^2 generally depends on T].

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

3 Color Wigner dynamics

The basis of our consideration is the Wigner representation of the von Neumann equation – the Wigner-Liouville equation (WLE). To derive the WLE for the full density matrix of the N -particle system $\rho(x_N|y_N)$ we introduce center of mass and relative coordinates in standard manner, $\vec{q} \equiv \vec{q}_N \equiv (\vec{x}_N + \vec{y}_N)/2$ and $\vec{r} \equiv \vec{r}_N \equiv \vec{x}_N - \vec{y}_N$. Note that all these quantities are $3N$ -dimensional vectors. The Wigner distribution function (WF) is defined by $f(\vec{p}, \vec{q}, t) = \frac{1}{(2\pi\hbar)^{6N}} \int \rho(\vec{q} - \frac{\vec{r}}{2}, \vec{q} + \frac{\vec{r}}{2}) e^{i\vec{p}\vec{r}/\hbar} d\vec{r}$, so the WLE can be written in the form [11]:

$$\frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \frac{\partial f}{\partial \vec{q}} - \frac{\partial U(q)}{\partial \vec{q}} \frac{\partial f}{\partial \vec{p}} = \int_{-\infty}^{\infty} ds f(\vec{p} - \vec{s}, \vec{q}, t) \omega(\vec{s}, \vec{q}), \quad (1)$$

where $\omega(\vec{s}, q) = \vec{F}(q) \frac{d\delta(\vec{s})}{d\vec{s}} + \frac{4}{(2\pi\hbar)^{6N}} \int d\vec{q} U(q - \vec{q}) \sin\left(\frac{2\vec{s}\vec{q}}{\hbar}\right)$, and $\vec{F}(\vec{q}) = -\partial U(q)/\partial \vec{q}$ is the classical force. Obviously, the force term in ω exactly cancels the last term on the lhs of Eq. (1). Retaining these terms allows us to write the WLE as the classical Liouville equation [lhs of Eq. (1)] plus a quantum correction [all terms on the rhs of Eq. (1)] which vanish for $\hbar \rightarrow 0$. This form allows us to identically transform Eq. (1) into an integral equation [11], $f(\vec{p}, \vec{q}, t) = f_0(p_0, q_0) + \int_0^t d\tau \int_{-\infty}^{\infty} d\vec{s} f(p_\tau - \vec{s}, q_\tau, \tau) \omega(\vec{s}, q_\tau)$. The first contribution describes quantum dynamics and is given by the initial WF $f_0(p, q) \equiv f(p, q, 0)$, but taken at arguments $p_0 \equiv \vec{p}(0)$ and $q_0 \equiv \vec{q}(0)$, being classical trajectories $p_\tau \equiv \vec{p}(\tau)$ and $q_\tau \equiv \vec{q}(\tau)$ (solutions of the Hamilton equations associated to the WLE and connecting points (\vec{p}, \vec{q}) at time t and points (p_0, q_0) at time 0):

$$\frac{d\vec{p}_\tau}{d\tau} = F[\vec{q}_\tau(\tau)]; \quad \frac{d\vec{q}_\tau}{d\tau} = \frac{\vec{p}_\tau(\tau)}{2m}, \quad \text{with } \vec{p}_\tau(\tau = t; p, q, t) = p; \vec{q}_\tau(\tau = t; p, q, t) = q.$$

Notice that even the first term describes the evolution of a *quantum* many-body state if the initial WF $f_0(p, q)$ is chosen appropriately and contains all powers of Planck's constant. The integral term describes the perturbation of the classical trajectories due to effects of quantum ($[p, q]$) uncertainty.

As a next step let us consider the classical dynamics of particles having color dynamic variables Q beside the normal spatial and momentum coordinates. As a simple example, let us consider Wong's color dynamics of the variables Q , which are 3D unit vectors as we mentioned before. For the considered in this paper quark-gluon plasma media the interaction between particles is described by a color Coulomb potential with the Hamiltonian written as $\hat{H} = \hat{K} + \hat{U}^c$, where we introduced the kinetic and color Coulomb interaction energy operators:

$$\hat{K} = \sum_{t=1}^N \frac{p_t^2}{2m_t}, \quad \hat{U}^c = \frac{1}{2} \sum_{p=1}^N \sum_{t=1}^N \frac{C_{pt} g^2 \langle Q_p | Q_t \rangle}{4\pi |r_p - r_t|}. \quad (2)$$

Here the constants $C_{pt} = C_{tp}$ are products of eigenvalues of the Casimir operator [7], g^2 is the coupling constant g^2 , and $\langle Q_p | Q_t \rangle$ is scalar product of two vectors Q_p and Q_t .

As shown before in Ref. [13,14], the solution of the integral equation for $f(p, q, t)$ can be transformed into an iteration series. Now the first term of the iteration series has additional color variables Q and takes the form $f_0[p, q, Q] \equiv f_0[p(0), q(0), Q(0)]$. Here the arguments $p_0 \equiv \vec{p}(0)$, $q_0 \equiv \vec{q}(0)$ and $Q_0 \equiv \vec{Q}(0)$ are the classical trajectories connecting points $(\vec{p}, \vec{q}, \vec{Q})$ at time t with points (p_0, q_0, Q_0) at time 0

$$\frac{d\bar{p}_\tau}{d\tau} = F(\tau); \quad \frac{d\bar{q}_\tau}{d\tau} = \frac{\bar{p}_\tau(\tau)}{2m}; \quad \frac{d\bar{Q}_k^a(\tau)}{d\tau} = G_k^a(\tau), \quad (3)$$

with $\bar{p}_\tau(\tau = t) = p$; $\bar{q}_\tau(\tau = t) = q$; $\bar{Q}_\tau(\tau = t) = Q$. Here $G_k^a(\tau) = \sum_{t=1}^N \sum_b \sum_c f^{abc} \frac{C_{kt} g^2 Q_k^b Q_t^c}{4\pi |r_k - r_t|}$, where f^{abc} are structure constants of the color group related to Wong's dynamics.

4 Wigner representation of time correlation functions

According to the Kubo formula the dynamic conductivity or diffusion constant are defined by the real part of Fourier transform of the current-current correlation function. Our starting point is the general operator expression for the canonical ensemble-averaged time correlation function [12]: $C_{FA}(t) = Z^{-1} \text{Tr} \left\{ \hat{F} e^{i\hat{H}t_c/\hbar} \hat{A} e^{-i\hat{H}t_c/\hbar} \right\}$, where \hat{H} is the Hamiltonian of the system expressed as a sum of the kinetic energy operator, \hat{K} , and the potential energy operator, \hat{U}^c . Time is taken to be a complex quantity, $t_c = t - i\hbar\beta/2$, where $\beta = 1/k_B T$ is the inverse temperature with k_B denoting the Boltzmann constant. The operators \hat{F} and \hat{A} are quantum operators of the dynamic quantities under consideration and $Z = \text{Tr} \left\{ e^{-\beta\hat{H}} \right\}$ is the partition function. The Wigner representation of the time correlation function in a v -dimensional space can be written as $C_{FA}(t) = (2\pi\hbar)^{-2v} \int \int d\mu_1 d\mu_2 F(\mu_1) A(\mu_2) W(\mu_1; \mu_2; t; i\hbar\beta)$, where we introduce the short-hand notation for the phase space point, $\mu_i = (p_i, q_i)$, ($i = 1, 2$), and p and q comprise the momenta and coordinates, respectively, of all particles in the system. $W(\mu_1; \mu_2; t; i\hbar\beta)$ is the spectral density expressed as $W(\mu_1; \mu_2; t; i\hbar\beta) = Z^{-1} \int \int d\xi_1 d\xi_2 e^{i\frac{p_1\xi_1}{\hbar}} e^{i\frac{p_2\xi_2}{\hbar}} \times \left\langle q_1 + \frac{\xi_1}{2} \left| e^{i\hat{H}t_c/\hbar} \right| q_2 - \frac{\xi_2}{2} \right\rangle \left\langle q_2 + \frac{\xi_2}{2} \left| e^{-i\hat{H}t_c/\hbar} \right| q_1 - \frac{\xi_1}{2} \right\rangle$, and $A(\mu)$ denotes Weyl's symbol [11] of operator \hat{A} : $A(\mu) = \int d\xi e^{-i\frac{p\xi}{\hbar}} \left\langle q - \frac{\xi}{2} \left| \hat{A} \right| q + \frac{\xi}{2} \right\rangle$, and similarly for the operator \hat{F} . Hence the problem of the numerical calculation of the canonically averaged time correlation function is reduced to the computation of the spectral density.

To obtain the integral equation for W let us introduce a pair of dynamic p, q -trajectories $\{\bar{q}_\tau(\tau; p_1, q_1, t), \bar{p}_\tau(\tau; p_1, q_1, t)\}$ and $\{\tilde{q}_\tau(\tau; p_2, q_2, t), \tilde{p}_\tau(\tau; p_2, q_2, t)\}$ starting at $\tau = t$ from the initial condition $\{q_1, p_1\}$ and $\{q_2, p_2\}$ propagating in 'negative' and 'positive' time direction, respectively:

$$\frac{d\bar{p}_\tau}{d\tau} = \frac{1}{2} F[\bar{q}_\tau(\tau)]; \quad \frac{d\bar{q}_\tau}{d\tau} = \frac{\bar{p}_\tau(\tau)}{2m}, \quad \text{with } \bar{p}_\tau(\tau = t) = p_1; \quad \bar{q}_\tau(\tau = t) = q_1,$$

$$\frac{d\tilde{p}_\tau}{d\tau} = -\frac{1}{2} F[\tilde{q}_\tau(\tau)]; \quad \frac{d\tilde{q}_\tau}{d\tau} = -\frac{\tilde{p}_\tau(\tau)}{2m}, \quad \text{with } \tilde{p}_\tau(\tau = t) = p_2; \quad \tilde{q}_\tau(\tau = t) = q_2,$$

where $F(q) \equiv -\nabla\tilde{U}$ with \tilde{U} being the total potential, i.e. the sum of all pair interactions U_{ab} . Then, as has been proven in [13], W obeys the following integral equation: $W(\mu_1; \mu_2; t; i\hbar\beta) = \bar{W}(\bar{p}_0, \bar{q}_0; \tilde{p}_0, \tilde{q}_0; i\hbar\beta) + \frac{1}{2} \int_0^t d\tau \int ds W(\bar{p}_\tau - s, \bar{q}_\tau; \tilde{p}_\tau, \tilde{q}_\tau; \tau; i\hbar\beta) \varpi(s, \bar{q}_\tau) - \frac{1}{2} \int_0^t d\tau \int ds W(\bar{p}_\tau, \bar{q}_\tau; \tilde{p}_\tau - s, \tilde{q}_\tau; \tau; i\hbar\beta) \varpi(s, \tilde{q}_\tau)$,

where $\varpi(s, q) = \frac{4}{(2\pi\hbar)^v \hbar} \int dq' \tilde{U}(q - q') \sin\left(\frac{2sq'}{\hbar}\right) + F(q)\nabla\delta(s)$, and $\delta(s)$ is the Dirac delta function. This equation has been supplemented by an initial condition for the spectral density at $t = 0$: $W(\mu_1; \mu_2; 0; i\hbar\beta) = \bar{W}(\mu_1; \mu_2; i\hbar\beta)|_{t=0} \equiv \bar{W}$. The τ -integrals connect the points $\bar{p}_\tau, \bar{q}_\tau; \tilde{p}_\tau, \tilde{q}_\tau$ at time τ of the mentioned above dynamic p,q-trajectories with the points $p_1, q_1; p_2, q_2$ at time t whereas in \bar{W} the trajectories are to be taken at $\tau = 0$ (denoted by the subscript "0"). The function \bar{W} can be expressed in the form of a finite difference approximation of the path integral [13–15]:

$$\bar{W}(\mu_1; \mu_2; i\hbar\beta) \approx \int \int d\tilde{q}_1 \dots d\tilde{q}_n \int \int dq'_1 \dots dq'_n \Psi(\mu_1; \mu_2; \tilde{q}_1, \dots, \tilde{q}_n; q'_1, \dots, q'_n; i\hbar\beta),$$

$$\text{with } \Psi(\mu_1; \mu_2; \tilde{q}_1, \dots, \tilde{q}_n; q'_1, \dots, q'_n; i\hbar\beta) \equiv \frac{1}{Z} \left\langle q_1 \left| e^{-\epsilon\hat{K}} \right| \tilde{q}_1 \right\rangle e^{-\epsilon U(\tilde{q}_1)} \left\langle \tilde{q}_1 \left| e^{-\epsilon\hat{K}} \right| \tilde{q}_2 \right\rangle e^{-\epsilon U(\tilde{q}_2)} \dots \dots$$

$$e^{-\epsilon U(\tilde{q}_n)} \left\langle \tilde{q}_n \left| e^{-\epsilon\hat{K}} \right| q_2 \right\rangle \varphi(p_2; \tilde{q}_n, q'_1) \times \left\langle q_2 \left| e^{-\epsilon\hat{K}} \right| q'_1 \right\rangle e^{-\epsilon U(q'_1)} \left\langle q'_1 \left| e^{-\epsilon\hat{K}} \right| q'_2 \right\rangle e^{-\epsilon U(q'_2)} \dots \dots$$

$$e^{-\epsilon U(q'_n)} \left\langle q'_n \left| e^{-\epsilon\hat{K}} \right| q_1 \right\rangle \varphi(p_1; q'_n, \tilde{q}_1),$$

where $\varphi(p; q', q'') \equiv (2\lambda^2)^{v/2} \exp\left[-\frac{1}{2\pi} \left\langle \frac{p\lambda}{\hbar} + i\pi \frac{q' - q''}{\lambda} \left| \frac{p\lambda}{\hbar} + i\pi \frac{q' - q''}{\lambda} \right\rangle\right]$, and $\langle x|y \rangle$ denotes the scalar product of two vectors \vec{x}, \vec{y} .

The function Ψ has to be generalized to properly account for spin statics effects. This gives rise to an additional spin part of the density matrix and antisymmetrization of one off-diagonal matrix element.

Inclusion of the color variable in the approximation allowing for the first term of iteration series gives expressions: $W(\mu_1, Q_1; \mu_2, Q_2; t; i\hbar\beta) = \bar{W}(\bar{p}_0, \bar{q}_0, \bar{Q}_1(0); \tilde{p}_0, \tilde{q}_0, \tilde{Q}_2(0); i\hbar\beta)$ with equation of motion $\frac{d\bar{p}_\tau}{d\tau} = \frac{1}{2}F(\tau); \frac{d\bar{q}_\tau}{d\tau} = \frac{\bar{p}_\tau(\tau)}{2m}; \frac{d\bar{Q}_k^a(\tau)}{d\tau} = \frac{1}{2}G_k^a(\tau)$ with $\bar{p}_\tau(\tau = t) = p_1; \bar{q}_\tau(\tau = t) = q_1, \bar{Q}_\tau(\tau = t) = Q_1$, $\frac{d\tilde{p}_\tau}{d\tau} = -\frac{1}{2}F(\tau); \frac{d\tilde{q}_\tau}{d\tau} = -\frac{\tilde{p}_\tau(\tau)}{2m}, \frac{d\tilde{Q}_k^a(\tau)}{d\tau} = -\frac{1}{2}G_k^a(\tau)$ with $\tilde{p}_\tau(\tau = t) = p_2; \tilde{q}_\tau(\tau = t) = q_2, \tilde{Q}_\tau(\tau = t) = Q_2$, where $F(q) \equiv -\nabla\tilde{U}$ with \tilde{U} being the sum of all pair interactions with the diagonal quantum effective color Kelbg potential

$$\Phi^{pt}(\mathbf{r}_p, \mathbf{r}_p, \mathbf{r}_t, \mathbf{r}_t, Q_p, Q_t, \Delta\beta) = \Phi^{pt}(|\mathbf{r}_{pt}|, Q_p, Q_t, \Delta\beta)$$

$$= \frac{C_{pt} g^2 \langle Q_p | Q_t \rangle}{4\pi\lambda_{pt} x_{pt}} \left[1 - e^{-x_{pt}^2} + \sqrt{\pi} x_{pt} (1 - \text{erf}(x_{pt})) \right], \quad (4)$$

where $x_{pt} = |\mathbf{r}_p - \mathbf{r}_t|/\bar{\lambda}_{pt}$. Note that the color Kelbg potential approaches the color Coulomb potential at distances larger than the De Broglie wavelength. Most importantly, it is finite at zero distance, removing in a natural way the classical divergences which makes any artificial cut-offs obsolete. Here $G_k^a(\tau) = \sum_{t=1}^N \sum_b \sum_c f^{abc} \frac{C_{kt} g^2 Q_k^b Q_t^c}{4\pi\lambda_{kt} x_{kt}} \left[1 - e^{-x_{kt}^2} + \sqrt{\pi} x_{kt} (1 - \text{erf}(x_{kt})) \right]$, where f^{abc} are structure constants of color group.

The time correlation functions are linear functionals of the spectral density, for them the same series representation holds, $C_{FA}(t) = (2\pi\hbar)^{-2v} \int \int d\mu_1 dQ_1 d\mu_2 dQ_2 \phi(\mu_1; \mu_2) W(\mu_1, Q_1; \mu_2, Q_2; t; i\hbar\beta)$, where $\phi(\mu_1; \mu_2) \equiv F(\mu_1)A(\mu_2)$.

Using this approach we can compute averages of arbitrary operators in standard way and obtain any dynamic macroscopic property of the correlated quantum particles without approximations related to the existence of different small physical parameters. Naturally, the true particle number N is replaced by a greatly reduced number N_{sim} which is of the order 50 – 100 in the MC cell with periodic boundary conditions. The solution scheme is a combination of Quantum Monte Carlo and classical Molecular Dynamics methods: Quantum MC is used to generate the correlated initial state, MD generates the p-q-Q trajectories. In this work, we take into account only the first term of the iteration series, which is related to the propagation of the initial quantum distribution according to the Hamiltonian equation of motion and classical color dynamics. This term, however, does not describe pure classical dynamics but accounts for quantum effects as noted above. The remaining terms of the iteration series, due to the convolution structure, describe momentum jumps which account for higher-order corrections to the classical dynamics of the quantum distribution, which are expected to be relevant in the limit of high density. This approach allows us to generate, in a controlled way, various kinds of quantum dynamics and initial conditions of the many-body system.

5 Numerical results

Very important aspect of the strongly coupled quark – gluon plasma is the dramatic change in transport properties in comparison to weakly coupled plasmas. As a first test of the developed method we have calculated the QGP momentum autocorrelation function and its Fourier transform, presented by Figs. 1 and 2 respectively. The diffusion constant is proportional to the integral of this function or the Fourier transform at zero frequency. We used the same parameters as those in ref. [6]: the temperature dependence of the quasiparticle mass was chosen according to $m(T)/T_c = 0.9/(T/T_c - 1) + 3.45 + 0.4T/T_c$ [7,9], where $T_c = 175$ MeV is the critical temperature of the phase transition to the QGP, whereas the coupling constant $g^2(T) \approx 6$ was taken T -independent. The calculations were performed at temperature $T = 3T_c$ with the mean interparticle distance $r_s = \langle r \rangle / \sigma = 0.28$. Here time is shown in units $t_0 = \hbar/k_B T_c$, while the mass unit and the length scale are defined as $m_0 = k_B T_c / c^2$ and $\sigma = \hbar c / T_c = 1.16$ fm. For the preliminary results presented below we used a cubic simulation box with periodic boundary conditions. The number of particles was equal to $N = N_q + N_{\bar{q}} + N_g = 40 + 40 + 40 = 120$, and the number of high-temperature factors (beads [19,20]), $n = 20$.

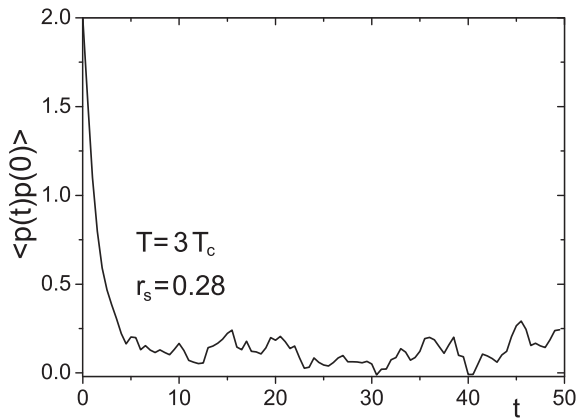


Fig. 1 Momentum-momentum autocorrelation functions

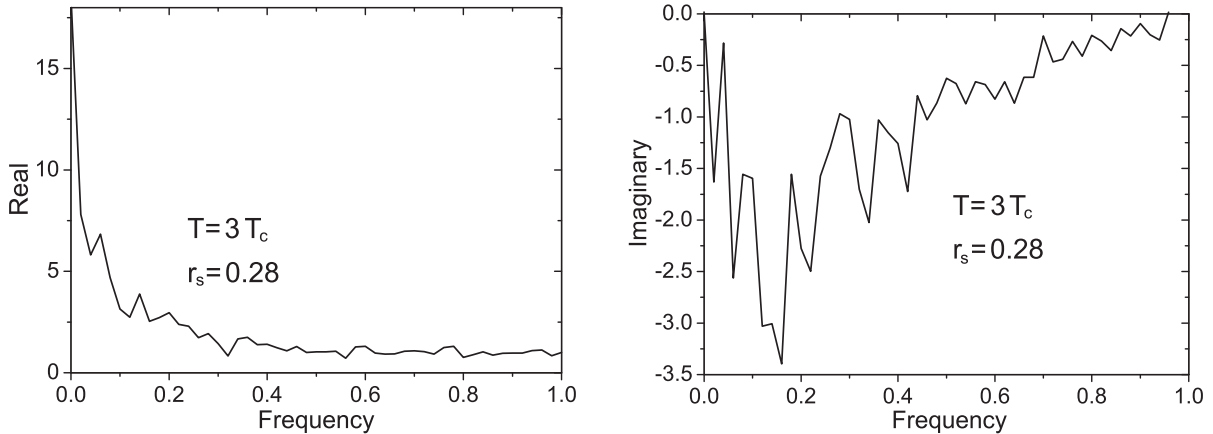


Fig. 2 Real and imaginary parts of the Fourier transform of the momentum-momentum autocorrelation function of Fig. 1.

At zero frequency the Fourier transform of autocorrelation function is proportional to the value of the diffusion constant. Figs. 1 and 2 show also decaying oscillations of quasiparticles in maniparticle complexes existing at this conditions. Figs. 2 present spectrum of dynamic oscillation of qusiparticles in many-particle clusters existing at these conditions and allow to estimate the typical decaying time and typical frequencies.

6 Discussion

Experimental data on the quark-gluon plasma and the hadronization transition give rise to numerous challenges to the theory, see, e.g. [3, 16] and references therein. Of particular interest is the question why the quark-gluon matter behaves as an almost perfect fluid rather than as a perfect gas, as it could be expected from the asymptotic freedom. Quantum Monte Carlo simulations [6] and quantum molecular dynamics based on the quasiparticle picture with color Coulomb interactions help us to answer this question. Our simulation results indicate that the ratio of the potential to kinetic energy is of the order of $1 \dots 3$, depending on the temperature. This certainly corresponds to a liquid-like rather than a gas-like behavior.

In Ref. [6] we have shown that the PIMC method captures main trends of the equation of state (even near the critical temperature) and may also yield valuable insight into the internal structure of the QGP, in particular into the pair correlation functions. However, the PIMC method is not able to yield dynamical and transport properties of the QGP. One way to achieve this is to develop semiclassical molecular dynamics simulations. In contrast to previous MD simulations where quantum effects were included phenomenologically via a short range potential [7] a more systematic approach has been developed for electron-ion plasmas [17–19] where an effective quantum pair potential has been derived from quantum Monte Carlo data which should also be possible in application to the QGP. Here, instead we have developed another more rigorous approach to study the dynamical and transport properties of strongly coupled quark gluon systems which is based on the Wigner formulation of quantum dynamics and presented first results for the momentum-momentum autocorrelation functions.

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