21 Color Molecular Dynamics for Dense Matter

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We propose a microscopic approach for quark many-body system based on molecular dynamics. Using color confinement and one-gluon exchange potentials together with meson exchange potentials between quarks, we construct nucleons and nuclear/quark matter. Dynamical transition between confinement and deconfinement phases are studied at high baryon density with this molecular dynamics simulation.

At high baryon density the nuclear matter is believed to undergo a phase transition to the quark matter because of the color Debye screening and the asymptotic freedom in quantum chromodynamics (QCD) [1]. Qualitative estimates using the Bag model [2] as well as the strong coupling lattice QCD [3] predict first order transition at baryon density ρ several times over the nuclear matter saturation density ($\rho_0 = 0.17\text{fm}^{-3}$). However, realistic studies of the high density matter based on the first principle lattice QCD simulations are not available yet due to technical difficulties [4]. In this situation any alternative attempts are welcome to unravel the nature of high density matter. In particular, how the nuclear matter composed of nucleons (which are by themselves composite three-quark objects) dissolve into quark matter at high baryon density is an interesting question to be studied. From the experimental and observational point of view, such transition may occur in the central core of neutron stars [5] and in high-energy heavy ion collisions [6].

In this paper, we propose a molecular dynamics (MD) simulation [7,8] of a system composed of many constituent quarks [9,10]. As a first attempt, we carry out MD simulation for quarks with SU(3) color degrees of freedom. Spin and flavor are fixed for simplicity, although there is no fundamental problem to include them. The time evolution of spatial and color coordinates of quarks are governed by the color confining potential, the perturbative gluon-exchange potential and the meson-exchange potential.

The confining potential favors the color neutral cluster (nucleon) at low density. However, as the baryon density increases, the system undergoes a transition to the deconfined quark matter, since the nucleons start to overlap with each other. Our color MD simulation (CMD) is a natural framework to treat such a percolation transition. The meson-exchange potential between quarks represents the nonperturbative gluon-exchange in the color singlet sector, the use of which is in line with the quark-meson coupling (QMC) model applied for studying the nuclear matter composed of quarks [11].

There exist several works on the quark many-body system in simulational approaches, such as Vlasovian plasma simulation with SU(2) Yang-Mils gauge field [12], Vlasov approach to the quarks with SU(3) colors [13], MD simulation with flip-flop potential [14,15], and MD simulation with chromodielectric model [16]. The quark-hadron phase transition and the dynamics of heavy-ion collisions have been studied in these models. Some of them use the two-body or many-body quark-quark potentials, while others solve the classical field equation for gluons. However, in all these simulations, color of each quark is fixed during the time-evolution, thus the non-Abelian nature of the color potential is frozen (Abelian approximation). On the other hand, our CMD solves the time-evolution of quark-colors as well as the spatial motion of quarks, and may give a new insight into the problem of quark-hadron transition.

We start with the total wave function of a system Ψ given as a direct product of single-particle quark wave-functions. The antisymmetrization is neglected at present.

$$\Psi = \prod_{i=1}^{3A} \phi_i(\mathbf{r})\chi_i, \tag{1}$$

$$\phi_i(\mathbf{r}) \equiv (\pi L^2)^{-3/4} \exp[-(\mathbf{r}-\mathbf{R}_i)^2/2L^2 - i\mathbf{P}_i\mathbf{r}], \tag{2}$$

$$\chi_i \equiv \begin{pmatrix} \cos\alpha_i \, e^{-i\beta_i} \, \cos\theta_i \\ \sin\alpha_i \, e^{+i\beta_i} \, \cos\theta_i \\ \sin\theta_i \, e^{i\varphi_i} \end{pmatrix}. \tag{3}$$

Here A is the total baryon number of a system, ϕ_i is the Gaussian wave packet with a fixed width L centered at position $\mathbf{R}_i$ and momentum $\mathbf{P}_i$. χ_i is a coherent state in the color SU(3) space parametrized by four angles, $\alpha_i, \beta_i, \theta_i$ and φ_i. Although general SU(3) vector has six real parameters, the normalization condition $|\chi_i| = 1$ and the unphysical global phase reduce the number of genuine parameters to four. Note that SU(2) spin coherent state parametrized by two angles has been used in the MD simulation of a many-nucleon system with spin degree of freedom [17].

The time evolution of a system is given by solving equations of motion for $\{\mathbf{R}_i, \mathbf{P}_i, \alpha_i, \beta_i, \theta_i, \varphi_i\}$ derived from the time-dependent variational principle

$$\frac{\partial \mathcal{L}}{\partial q} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}, \tag{4}$$

with the classical Lagrangian

$$\mathcal{L} = \langle\Psi|i\hbar\frac{d}{dt} - \hat{H}|\Psi\rangle \qquad (5)$$

$$= \sum_i[-\dot{\mathbf{P}}_i\mathbf{R}_i + \hbar\dot{\beta}_i\cos 2\alpha_i\ \cos^2\theta_i - \hbar\dot{\varphi}_i\sin^2\theta_i] - H, \qquad (6)$$

where $H = \langle\Psi \mid \hat{H} \mid \Psi\rangle$. The explicit form of equations of motion reads :

$$\dot{\mathbf{R}}_i = \frac{\partial H}{\partial \mathbf{P}_i}, \quad \dot{\mathbf{P}}_i = -\frac{\partial H}{\partial \mathbf{R}_i}, \qquad (7)$$

$$\dot{\beta}_i = -\frac{1}{2\hbar\sin 2\alpha_i\ \cos^2\theta_i}\frac{\partial H}{\partial \alpha_i}, \qquad (8)$$

$$\dot{\theta}_i = \frac{1}{2\hbar\sin\theta_i\ \cos\theta_i}\frac{\partial H}{\partial \varphi_i}, \qquad (9)$$

$$\dot{\alpha}_i = \frac{1}{2\hbar\sin 2\alpha_i\ \cos^2\theta_i}\frac{\partial H}{\partial \beta_i} - \frac{\cos 2\alpha_i}{2\hbar\sin 2\alpha_i\ \cos^2\theta_i}\frac{\partial H}{\partial \varphi_i}, \qquad (10)$$

$$\dot{\varphi}_i = -\frac{1}{2\hbar\sin\theta_i\ \cos\theta_i}\frac{\partial H}{\partial \theta_i} + \frac{\cos 2\alpha_i}{2\hbar\sin 2\alpha_i\ \cos^2\theta_i}\frac{\partial H}{\partial \alpha_i}. \qquad (11)$$

As for the color-dependent quark-quark interaction, we employ the one-gluon exchange and the linear confining potentials. In the usage of linear or quadratic confining potential, a long range color Van der Waals force is known to arise. The string-flip model or flip-flop model are the possible candidates for avoiding this unphysical interaction (see e.g. [18]). It is not clear, however, at the moment how to combine these models with CMD in a practical manner.

To take into account the nonperturbative gluon exchange in the color singlet channel and simultaneously to reproduce the essential part of the nuclear force between color-singlet baryons (namely, the state-independent short range repulsion and the medium range attraction), we include the σ+ω meson-exchange potential acting between quarks according to ref. [11].

The total Hamiltonian is thus written as

$$\hat{H} = \sum_i \sqrt{m^2 + \hat{\mathbf{p}}_i{}^2} + \frac{1}{2}\sum_{i,j\neq i}\hat{V}_{ij}, \qquad (12)$$

$$\hat{V}_{ij} = -\sum_{a=1}^{8} t_i^a t_j^a V_{\mathrm{C}}(\hat{r}_{ij}) + V_{\mathrm{M}}(\hat{r}_{ij}), \qquad (13)$$

$$V_{\mathrm{C}}(r) \equiv Kr - \frac{\alpha_{\mathrm{s}}}{r}, \qquad (14)$$

$$V_{\mathrm{M}}(r) \equiv -\frac{g_{\sigma q}^2}{4\pi}\frac{e^{-\mu_\sigma r}}{r} + \frac{g_{\omega q}^2}{4\pi}\frac{e^{-\mu_\omega r}}{r}, \qquad (15)$$

where $t^a = \lambda^a/2$ with λ^a being the Gell-Mann matrices, V_{C} is the confinement and one-gluon exchange terms, and V_{M} is the meson exchange term [19]. We introduce a smooth infrared cutoff to the confining potential in $V_{\mathrm{C}}(r)$ to prevent the long-range interaction beyond the size of a box in which we carry out MD simulations. We choose the cutoff scale $r_{\mathrm{cut}} = 3.0$ fm, which is approximately half of the length of the box. Typical values of the parameters in the quark model for baryons read [19], $m = 320$ MeV (the constituent-quark mass), $\alpha_{\mathrm{s}} = 1.25$ (the QCD fine structure constant), and $K = 0.75$ GeV/fm (the string tension). The meson-quark coupling constants $g_{\sigma(\omega)q}$ are estimated from the meson-nucleon couplings $g_{\sigma(\omega)N}$ using the additive quark picture: $g_{\sigma q} = g_{\sigma N}/3 = 3.53$ and $g_{\omega q} = g_{\omega N}/3 = 5.85$. The meson masses are taken to be $\mu_\omega = 782$ MeV and $\mu_\sigma = 550$ MeV.

Some comments are in order here on the evaluation of the matrix elements $H = \langle\Psi \mid \hat{H} \mid \Psi\rangle$.

(i) Because of the lack of the anti-symmetrization of quark wave function, the interaction between quarks in a color-singlet baryon is underestimated by factor 4 when one takes the matrix element of $t_i^a t_j^a$. To correct this, we use effective couplings $K^{\mathrm{eff}} = 4K$ and $\alpha_s^{\mathrm{eff}} = 4\alpha_s$ throughout the CMD simulation.

(ii) The size of the quark wave-packet L is chosen to be 0.35 fm corresponding to the r.m.s. radius of the constituent quark 0.43 fm. This is consistent with the typical value expected from the dynamical breaking of chiral symmetry [20]. This value is used in the matrix element of the gluonic interaction V_{C}. At the same time, the meson-quark coupling is intrinsically nonlocal, since σ and ω have their own quark structure. Besides, the meson-exchange interaction between nucleons with the nucleon form-factor should be properly reproduced by the superposition of the meson-exchange interaction between quarks. To take into account these facts, we use $L^{\mathrm{eff}} = 0.7$ fm (corresponding to the r.m.s. radius of 0.86 fm) in the matrix element of V_{M}.

(iii) $H = \langle\Psi \mid \hat{H} \mid \Psi\rangle$ generally contains a kinetic energy originating from momentum variances of wave packets. However, when the width of the wave packet is fixed as a time-independent parameter, this kinetic energy is spurious and neglected in the present calculation.

Let us now describe how to simulate the simplest three-quark system, i.e. the nucleon, in CMD. We first search for a three-quark state obeying the color neutrality condition

$$\sum_{i=1}^{3}\langle\chi_i|\lambda^a|\chi_i\rangle = 0 \qquad (a = 1,\cdots,8). \qquad (16)$$

This is satisfied by solving a cooling equation of motion in the color space with a potential proportional to $\sum_{i,j\neq i}\sum_{a=1}^{8}\langle\chi_i|\lambda^a|\chi_i\rangle\langle\chi_j|\lambda^a|\chi_j\rangle$ with random initial values of χ_i. During this cooling procedure, spatial coordinates of quarks are fixed, e.g. at the three corners of a triangle.

If we start with three quarks in triangular position obtained above and kick each quark by the same amount of energy keeping the total momentum zero, the quarks start to have a breathing motion in 2-dimensional plane. Due to the total color conservation the color-neutrality is maintained during this time evolution.

By an initial kick to give the time-averaged kinetic energy of 76 MeV, the total energy of the nucleon become 1206 MeV. Accordingly, the r.m.s. radius of the nucleon reads 0.46 fm using L (which corresponds to the size of the quark-core of the nucleon) or 0.87 fm using L^{eff} (which corresponds to the physical nucleon size for meson-exchange interaction). The "nucleon" here is certainly a semiclassical object which should be regarded as a mixture of the ground and excited states of three quarks. We use a collection of these nucleons as an initial condition for the CMD simulation of many quarks. Since the interaction among quarks in matter will eventually randomize the internal motion of quarks in the initial nucleon, the final result is not sensitive to the way how we kick the quarks.

Now, let us study the phase change from the confined hadronic system to the deconfined quark matter. We simulate the infinite matter under the periodic boundary condition and see how the system responds to the change of the baryon density as well as to the energy deposition from outside.

To start with, nucleons constructed above are randomly distributed in a box with the periodic boundary condition. At this stage, the total system is in its excited state. The minimum-energy state of matter is obtained by the frictional cooling procedure, namely we solve a cooling equation of motion with frictional terms. During the cooling, spatial and color motion of quarks in the nucleon are artificially frozen, and the following equations are solved:

$$\dot{\mathbf{R}}_i = \frac{1}{3}\sum_{j\in\{i\}}\left[\frac{\partial H}{\partial \mathbf{P}_j} + \mu_R \frac{\partial H}{\partial \mathbf{R}_j}\right], \tag{17}$$

$$\dot{\mathbf{P}}_i = \frac{1}{3}\sum_{j\in\{i\}}\left[-\frac{\partial H}{\partial \mathbf{R}_j} + \mu_P \frac{\partial H}{\partial \mathbf{P}_j}\right], \tag{18}$$

$$\dot{\alpha}_i = \dot{\beta}_i = \dot{\theta}_i = \dot{\varphi}_i = 0, \tag{19}$$

where damping coefficients μ_R and μ_P are negative and $\{i\}$ means a set of three quarks in a nucleon to which i belongs. Under this cooling procedure, the system approaches to a stable configuration with minimum energy. The system does not collapse due to the repulsive part of the meson exchange potential V_{M}.

After the system reached its energy-minimum by the cooling, internal color and spatial motion of quarks are turned on and the normal equation of motion is solved for several tens of fm/c so that the system gets equilibrated. Since our treatment of particle motion is classical, we cannot simulate the exact ground state with Fermi motion. Our prescription should be recognized as a classical description of approximate ground state. When we study the excited state of the system, additional random motion are assigned to nucleons in this "ground state" so that the system has a given excitation energy E^*.

We use the following criterion of confinement as

$$\begin{cases} |\mathbf{R}_i - \mathbf{R}_j| < d_{\mathrm{cluster}} \quad (i,j = 1,2,3), \\ \displaystyle\sum_{a=1}^{8}\left[\sum_{i=1}^{3}\langle\chi_i|\lambda^a|\chi_i\rangle\right]^2 < \varepsilon. \end{cases} \tag{20}$$

If three quarks within a certain distance d_{cluster} are white with an accuracy ε, they are considered to be confined. All quarks are checked by this criterion without duplications. The actual numerical values we use are $d_{\mathrm{cluster}} = 1$ fm and $\varepsilon = 0.05$.

Snapshots of matter in equilibrium for different baryon densities are displayed in Fig. 1. Quarks in the confined states are shown with white and those in the deconfined state with gray. As ρ increases, fraction of deconfined quarks increase. This is not a trivial consequence and is a unique feature of the CMD simulation. In fact, one may naively expect that, as the density increases, confinement criterion becomes easier to be fulfilled since more quarks are around. However, the use of the color coherent state allows the color excitation even in a three-quark cluster and does not necessarily favor the formation of color singlet clusters at high densities.

Figure 2 shows "confined ratio of quarks",

$$R \equiv \frac{\text{(number of confined quarks)}}{\text{(total quark number)}}, \tag{21}$$

in the approximate ground state. With increase of the baryon density ρ, matter shows a transition from hadronic phase to the quark phase which is well characterized by R in Fig.2. The order of the phase transition, which should be examined in terms of the pressure of the system, is a future problem to be studied.

So far we have discussed only the cold matter close to the ground state at finite baryon density, which is relevant for the physics of e.g. neutron stars. On the other hand, to study the excited state of matter such as that created in the high-energy heavy ion collisions, not only the thermal motion of quarks, but also $q\bar{q}$ creation/annihilation processes and the dynamical gluons should be included. Here, as a first step toward this goal, we study the "thermal" property of the system with only the quark degrees of freedom.

Figure 3 shows the same quantity as Fig. 2 but with a variation of excitation energy E^*. The hadronic matter and the quark matter are characterized by R. Although no sudden transition of R between two phases is observed, R becomes less than 20% for all densities for $E^* > 200$ MeV/q.

We fit the kinetic energy distribution of quarks in the excited matter by the classical Boltzmann distribution with a normalization factor $\mathcal{N}$

$$\frac{dN}{dE_{\mathrm{kin}}} = \mathcal{N}\frac{p^2 dp}{dE_{\mathrm{kin}}} e^{-E_{\mathrm{kin}}/T^*}, \tag{22}$$

$$E_{\mathrm{kin}} = \sqrt{p^2 + m^2} - m. \tag{23}$$

Then, we can define an effective temperature T^* for given E^*. Note that T^* is not really a physical temperature of the system, but is a measure of the averaged kinetic energy per quark. In Fig. 4, T^* is plotted as a function of E^*. For $E^* > 300$ MeV/q, T^* depends almost linearly on E^* irrespective of baryon density, while, for $E^* = 100 \sim 200$ MeV/q, T^* for low-density matter increases rather slowly as a function of E^*. In fact, this corresponds exactly to the region where the confined ratio of low-density matter changes in Fig. 3. This implies that, during the deconfinement process, the energy deposit from outside is consumed to melt confined clusters (i.e., nucleons), which suppresses the effective temperature T^*.

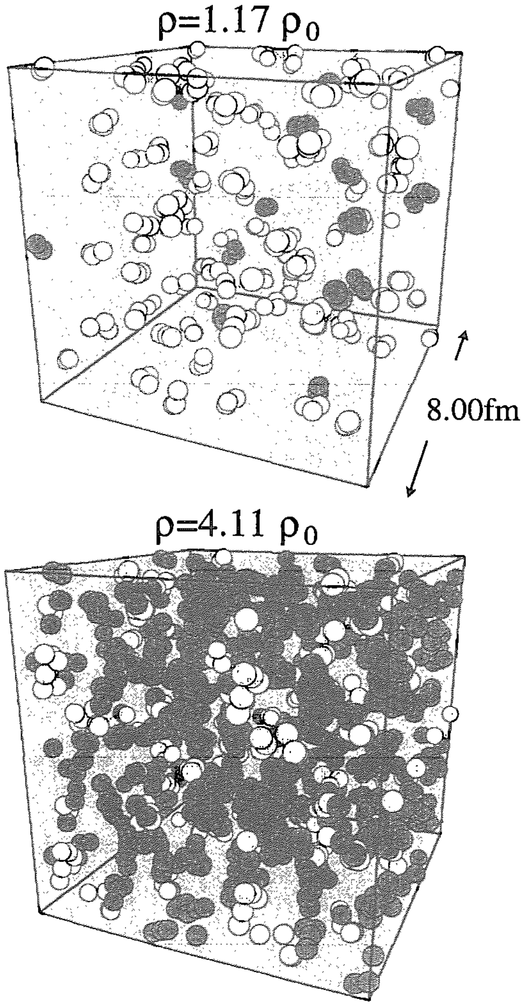

FIG. 1. Perspectives of matter with baryon density at $1.17\rho_0$ and $4.11\rho_0$. White/gray particles indicate quarks in the confined/deconfined state. Some white clusters near the boundary contain only one or two quarks. This is due to the periodic boundary condition, and they are actually a part of 3-quark clusters.

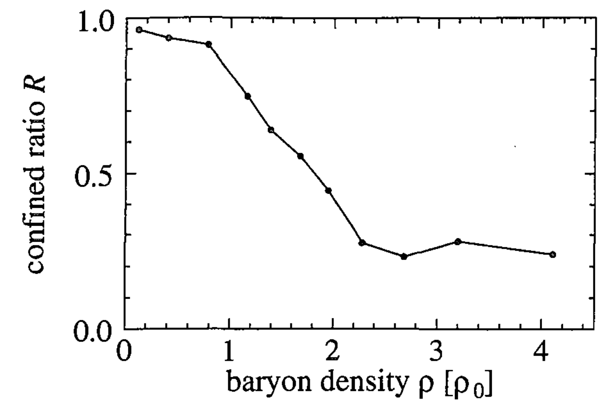

FIG. 2. Confined ratio of quarks as a function of baryon density ρ.

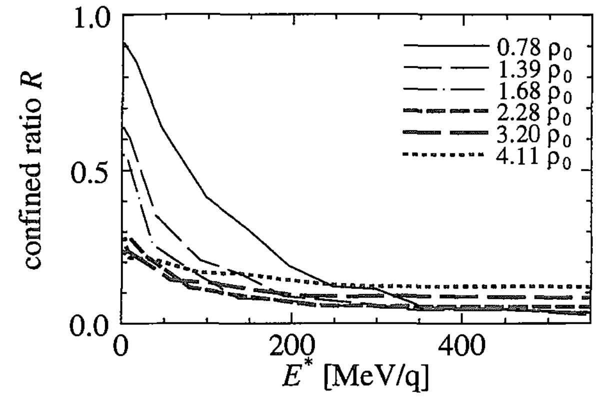

FIG. 3. Confined ratio of quarks as a function of E^* for several different baryon densities.

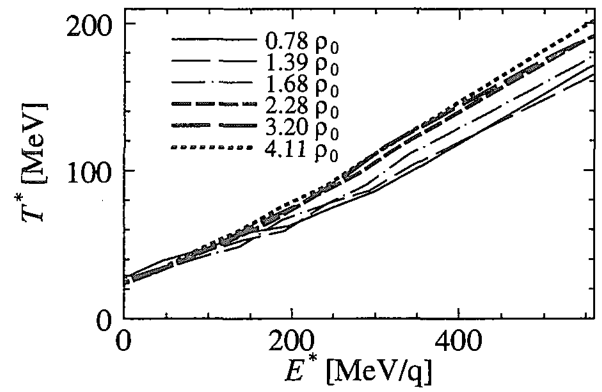

FIG. 4. Baryon density and excitation energy dependence of the effective temperature extracted from the Boltzmann fit of the kinetic energy distribution.

Here we show the preliminary calculation on finite system. To make the "nucleus", we first prepare a given number of white baryons and distribute them in a sphere. Then we cool the system in the same way as explained for the infinite matter. Figure 5 shows the density profile of

$A = 66$ nucleus. Its binding energy is written in the figure. Since we have not yet included the Fermi motion of nucleons, the binding energy is too large. The time evolution of confined ratio during the collision of two $A = 66$ nuclei is displayed in Fig. 6. Instead of the bombarding energy, the CM velocity β of two nuclei is used to distinguish the violence of the collision. One can see in the figure that more quarks are deconfined for more violent collisions. The life time of the deconfined state is rather long compared to that generally believed. We consider this feature is due to the lack of $q\bar{q}$ creation/annihilation process in our simulation.

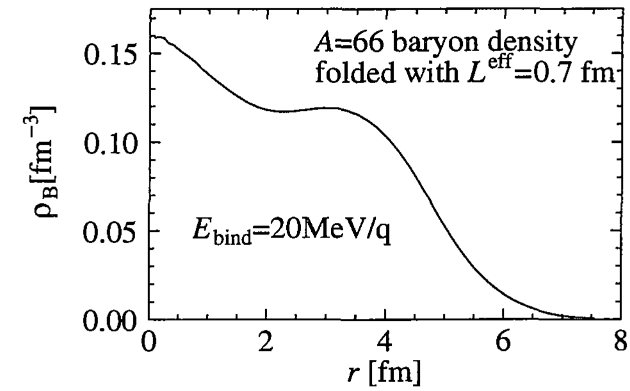

FIG. 5. Density profile of $A = 66$ nucleus.

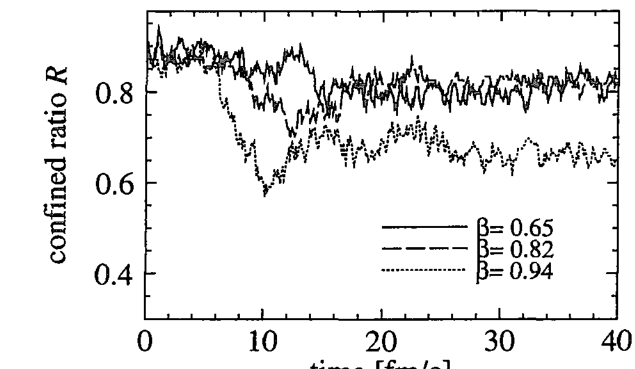

FIG. 6. Time evolution of confined ratio during the collision of two $A = 66$ nuclei.

In summary, we have proposed a color molecular dynamics (CMD) simulation of a system with many constituent quarks. The system is approximated by the product of wave packets with SU(3) color coherent state. Adopting the effective interaction between quarks we study the transition from nuclear matter to quark matter under the periodic boundary condition. At low baryon density ρ, the system is in the confined phase where most of the quarks are hidden inside the color singlet nucleons. However, as we increase ρ, the partial deconfinement takes place due to the disintegration of color-singlet clusters both in the coordinate space and in the color space. This can be seen explicitly in Fig. 1 and in the confined ratio Fig. 2. The similar conclusions also hold for finite excitation energies E^* (Fig. 3 and Fig. 4), although the $q\bar{q}$ process and dynamical gluons are not included yet.

The results of this paper are still in the qualitative level and are limited to the cold matter. The refinement of interaction parameters and inclusion of flavor and spin degrees of freedom are necessary for quantitative discussions. The use of the antisymmetrized quark wave function [21] and the medium modification of the constituent-quark mass associated with the partial restoration of chiral symmetry are also important future problems. For the discussion of hot matter, inclusion of $q\bar{q}$ creation/annihilation and the dynamical gluons are essential. In spite of all these reservations, the method proposed in this paper gives a starting point to study the statistical feature of the hadron-quark transition as well as to examine finite nuclei and the dynamics of heavy-ion collisions.

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22 Quark Dynamics on Phase-Space

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Abstract

We discuss the dynamics of quarks within a Vlasov approach. We use an interquark (qq) potential consistent with the indications of Lattice QCD calculations and containing a Coulomb term, a confining part and a spin dependent term. Hadrons masses are shown to arise from the interplay of these three terms plus the Fermi motion and the finite masses of the quarks. The approach gives a lower and an upper bound for hadrons. The theoretical predictions are shown to be in fairly good agreement with the experimental data.

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