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Metastable states in quark-gluon plasma

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We study the metastable states in the high temperature phase of QCD characterized by nonzero expectation values for the imaginary part of the Polyakov loop. We consider $N_f = 2$, 3 dynamical staggered quarks, and carry out simulations at various values of the coupling β to observe these states. In particular, we find the value of the coupling (β_m) above which the metastable states appear. The resulting value of β_m corresponds to temperature $T_m \gtrsim 750$ MeV for $N_f = 2$.

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I. INTRODUCTION

Experimental and theoretical studies of matter under extreme conditions is one of the active fields of research in recent times. Such a state of matter is created in ultrarelativistic heavy-ion collisions. The fireball created in these collisions leads to a state of deconfined quarks and gluons (quark-gluon plasma). With the increase in the collision energy, the fireball not only crosses the confinement-deconfinement transition temperature T_c but probes deeper into the deconfined phase. For example, in the heavy-ion collisions at the LHC the initial fireball temperature is expected to go up to $5T_c$ [1]. The increase in fireball temperature will result in the observation of new signals bearing the properties of the system at higher temperatures. Hence, it is important to study any possible prominent changes in the properties of the medium in the deconfinement phase away from T_c , which can be observed in experiments. In this context, we plan to study the explicit breaking of Z(3) symmetry, and the metastable states associated with it.

In the pure SU(3) gauge theory, the deconfined phase exists in three degenerate states characterized by three different values of the Polyakov loop. These three states are related to each other via the Z(3) rotations. So, in the deconfined phase, Z(3) symmetry is spontaneously broken. In the confinement phase, the Polyakov loop average vanishes restoring the Z(3) symmetry. For QCD with dynamical fermions, the Z(3) symmetry is explicitly broken, and the degeneracy between the three states is lifted [2]. Only the state for which the expectation value of the Polyakov loop is real becomes the ground state. It is not clear what happens to the other two states. For asymptotically large temperatures, one expects the gluons to dominate so that the effects of quarks can at most make the other two states (with Polyakov loop phase angle $\pm 2\pi/3$) metastable.

We would like to emphasize that the Z(3) metastable states are not the results of metastability near any first order transition. They are different from the metastable states that one observes near a first order phase transition. A closer analogy of the Z(3) metastable states would be a state of magnetization antiparallel to the external field.

The Z(3) metastable states are expected to play an important role both in the context of heavy-ion collision and in the early Universe. If these states indeed exist just above T_c , then they can have significant effects on the medium properties [1]. If a fluctuation in the form of a metastable bubble in the background of the stable phase costs free energy of the order of the temperature scale T, then such fluctuations will be present in the system. In the heavy-ion collision it is possible that the whole fireball may thermalize to one of these metastable states. This state will then decay through a first order phase transition even before the system cools down below T_c . It is also possible that the metastable phases of superhorizon size may occur in the early Universe and decay through bubble nucleation [3,4].

There are several studies on Z(3) metastable states at high temperatures in the presence of quarks. It has been shown that the contribution of massless quarks to the one loop effective potential leads to metastable states for $T \ge$ T_c [2,5]. These states have also been observed above the deconfinement transition in the Nambu-Jona-Lasinio model [6]. There are only a very few lattice QCD studies on these metastable states. A lattice QCD study with fermions in the sextet representation has found metastable states, characterized by phase angle ($\pm 2\pi/3, \pi$), close to T_c in the deconfinement phase [7]. However, in this work, we have considered $N_f = 2$, 3 staggered fermions in the fundamental representation to look for the metastable states. Contrary to the previous studies, we find that the metastable states do not exist in the neighborhood of T_c , but for temperatures $T_m \gtrsim 750$ MeV. Though this temperature may not be reached at the SPS and RHIC experiments, there is a possibility that these states are accessible at the LHC. The fact that $T_m > T_c$ may have important consequence(s) for the early Universe.

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The paper is organized as follows. In Sec. II, we review the Z(3) symmetry and metastable states in the presence of dynamical fermions. Our lattice simulation techniques are discussed in Sec. III. Results are presented in Sec. IV. We present our conclusions in Sec. V.

II. Z(3) SYMMETRY IN THE PRESENCE OF DYNAMICAL QUARKS AND METASTABLE STATES

In this section, we briefly discuss the pure SU(N) gauge theory at finite temperature and their symmetries. Later, we focus on the case with dynamical quarks and discuss their effects on the Z(N) symmetry [8,9].

We start with the pure SU(N) gauge theory at finite temperature, $T = \beta_{\tau}^{-1}$. In this case, one uses static fundamental charges (infinitely heavy test quarks) to probe into the dynamics of the pure glue system. The static fundamental charges are described by the Polyakov loop [10,11] which is defined as the trace of the thermal Wilson line,

$$L(\vec{x}) = \frac{1}{N} \operatorname{Tr} \mathbf{W}(\vec{\mathbf{x}}), \tag{1}$$

with the thermal Wilson line operator, $L(\vec{x})$, defined as

$$\mathbf{W}(\vec{\mathbf{x}}) = P \exp\left[ig \int_0^{\beta_\tau} A_0(\vec{x}, \tau) d\tau\right]. \tag{2}$$

The expectation value of the Polyakov loop $\langle L(\vec{x}) \rangle$ is an order parameter for confinement-deconfinement transition in the pure glue theory. Here, P denotes path ordering of the exponential, g is the gauge coupling, and $\beta_{\tau}=1/T$ denotes the extent of Euclidean time. $A_{\mu}(\vec{x},\tau)=A_{\mu}^{a}(\vec{x},\tau)\lambda^{a}$ is the vector potential. The λ^{a} are the $N^{2}-1$ Hermitian generators of the SU(N) algebra in the fundamental representation. $A_{0}(\vec{x},\tau)$ is the time component of the vector potential at spatial position \vec{x} and Euclidean time τ . The gauge fields $A_{\mu}(\vec{x},\tau)$ obey periodic boundary conditions in the Euclidean time direction, $A_{\mu}(\vec{x},\beta_{\tau})=A_{\mu}(\vec{x},0)$. These boundary conditions are maintained by a group of nontrivial gauge transformations [8] that are periodic up to a constant twist matrix, $z \in SU(N)$,

$$g(\vec{x}, \beta_{\tau}) = zg(\vec{x}, 0). \tag{3}$$

These matrices z form the center Z(N) of the gauge group SU(N), where Z(N) is a cyclic group of order N. Thus the pure SU(N) gauge theory at finite temperature has the complete symmetry $G \times Z(N)$, where G is the group of strictly periodic gauge transformations.

However, the Polyakov loop (which characterizes the phases of pure gauge theory) transforms nontrivially under the Z(N) transformations, though the Euclidean action is invariant under the transformations. Under the global Z(N) symmetry transformations, $L(\vec{x})$ transforms as

$$L(\vec{x}) \to zL(\vec{x}),$$
 (4)

where

$$z = \exp(2\pi i n/N) 1 \in Z(N),$$

$$n \in \{0, 1, 2, \dots, N-1\}.$$
(5)

For temperatures above the critical temperature T_c , the high temperature phase or the deconfining phase is characterized by $\langle L(\vec{x}) \rangle \neq 0$, corresponding to the finite free energy of an isolated heavy test quark, and thus breaks the Z(N) symmetry spontaneously. At temperatures below T_c (in the confining phase), $\langle L(\vec{x}) \rangle = 0$, thereby restoring the Z(N) symmetry [9].

We now come to the effect of matter fields in fundamental representation on Z(N) symmetry. In the fundamental representation of SU(N), the quark fields transform as

$$\Psi \to g\Psi$$
. (6)

As a result, the fermion part of the action is not invariant under the twisted transformations pertaining to the Z(N) symmetry. Thus in full QCD, the fermion part of the action breaks the Z(N) symmetry while the pure gauge part respects it.

The effect of quarks on the Z(N) symmetry has been discussed in detail in [5,12]. It has been advocated that one can take the effect of quarks in terms of explicit breaking of Z(3) symmetry [12–14]. This leads to a unique ground state and two (possible) metastable states in the deconfinement phase [2]. It has also been argued that the effects of quarks in terms of explicit symmetry breaking may be small, and the pure glue theory may be a good approximation [14]. However, we will see later that the explicit symmetry breaking due to quarks is too large for the metastable states to exist in the neighborhood of T_c .

III. NUMERICAL PARAMETERS AND STUDIES

In principle metastable states should occur in any simulation run. Given enough time the system will explore all of the configuration space. But the probability that an arbitrary initial configuration temporarily "thermalizing" to a metastable state is very small. Once the system thermalizes to the absolute ground state the probability that it fluctuates to the metastable state decreases exponentially with the system size. So it is practical to choose the initial configurations carefully so that they thermalize to the metastable states before decaying to the ground state. In order to have the system thermalized to a metastable state (ReL < 0 and |ImL| > 0), the trial configuration should not be far away from this state. Otherwise, it will thermalize to the absolute ground state. Since a random configuration (termed as "fresh" in the MILC code) results in a stable state (ReL > 0), we need to select the initial configuration appropriately. As the metastable states arise from the Z(3) symmetry so they are expected to be close to the Z(3) rotation of the absolute ground state. This fact can be used to find an initial configuration which may thermalize to the metastable state. To generate the gauge field configurations, we have used the MILC code which uses the standard HYBRID R ALGORITHM [15]. We have used simulation parameters similar to those in [7,16].

As a first step, we have performed a pure gauge calculation on a lattice of size $16^3 \times 4$ near critical temperature ($\beta = \beta_c = 5.6925$ [17]) starting with a "fresh lattice." We then selected one configuration each for the following cases:

- (i) Re $L \ll 0$ and Im $L \gg 0$, i.e. $\theta \simeq 2\pi/3$.
- (ii) Re $L \ll 0$ and Im $L \ll 0$, i.e. $\theta \simeq -2\pi/3$.
- (iii) Re $L \ll 0$ and Im $L \sim 0$, i.e. $\theta \simeq \pi$.
- (iv) Re $L \gg 0$ and Im $L \sim 0$, i.e. $\theta = 0$.

Case (iii) has been taken into consideration additionally to study whether a metastable state could exist at $\theta=\pi$ [7], and case (iv) to check whether we obtain a similar stable state if we start with a "fresh lattice." Another method, we have employed, is using an initial configuration with all the temporal links on a fixed time slice set to $e^{\pm 2\pi i/3}\mathbf{I}$. The pure gauge calculations have been performed using the MILC code. We have considered 4 over-relaxation steps for each of the heat-bath iterations for updating a gauge configuration.

We have used each of the gauge configurations (one for each θ) so obtained as an initial configuration to thermalize and calculate the Polyakov loop in the presence of 2 and 3-flavor quarks for a series of β values, $5.2 \le \beta \le 6.0$. For this purpose, we have again used the MILC code with dynamical staggered fermion action. The numerical calculations have been performed with quark mass $am_{u,d} = 0.01$, so that $m_{u,d}/T = 0.04$. Our microcanonical time step size has been $\Delta \tau \sim 0.01$, and the trajectory length (microcanonical time step \times steps per trajectory) has been $\tau \sim 0.8$. Each gauge configuration has been analyzed after 10 heat-bath iterations. For each β , we have collected 2500 gauge configurations.

0.25 0.2 0.15 0.05 0.05 0.05 0.05 0.05 0.05 0.05 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0.08 0.09 0

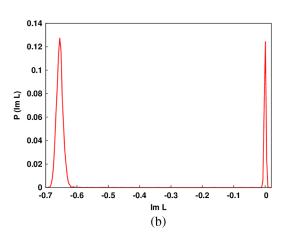


FIG. 1 (color online). Histograms of ImL vs number of trajectories (a) Single peak at ImL \neq 0 indicating a metastable state only, (b) Double peak at ImL \neq 0 and ImL = 0 indicating a metastable state decaying into the ground state.

IV. RESULTS AND DISCUSSIONS

A. Method to observe the metastable states

In this study the Polyakov loop expectation value $\langle L \rangle$ has been used to characterize different possible states of the system. In the absolute ground state $\langle L \rangle$ is real and positive. In the metastable states $\langle L \rangle$ is complex, with the phase of $\langle L \rangle$ close to $\pm \frac{2\pi}{3}$.

In a typical Monte Carlo simulation, a sequence of statistically significant configurations is generated. This sequence constitutes the Monte Carlo history. In order to reduce the autocorrelations between the consecutive configurations, measurements are performed on every 10th configuration in the Monte Carlo history. In all the different simulations, the initial configuration is thermalized in a few hundred Monte Carlo steps. During the thermalization, all the measured observables change almost monotonically. Once the system is thermalized, all the physical observables fluctuate around their respective average values. We compute the histogram (probability distribution) of the Polyakov loop, P(L). The metastable states are local minima in the free energy which are stable against small fluctuations. As a result, they appear as well-defined peaks in P(L). Distinct multiple peaks in P(L) correspond to different possible states of the system.

In Fig. 1(a), we show the histogram of ImL (imaginary part of L) for two simulations with different random number sequences. The two P(ImL) distributions are similar given the small length (a few thousands) of the Monte Carlo histories. The peak positions are at a nonzero value of $ImL \sim -0.65$ which imply a metastable state. This being a metastable state, it will decay to the ground state if the simulations were continued further. In Fig. 1(a), we see only one peak because the state did not decay during our runtime. With another sequence of random numbers, the metastable state decays to the ground state. This results in a second peak in P(ImL) at $ImL \sim 0$ as seen in Fig. 1(b). Note that the peak position of the metastable

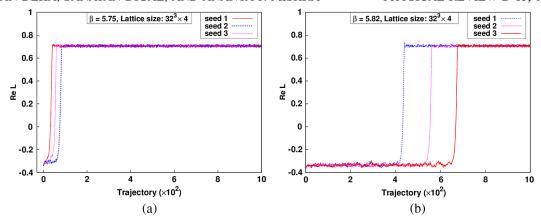


FIG. 2 (color online). ReL vs number of trajectories for three different randomly chosen seeds at (a) $\beta = 5.75$, and (b) $\beta = 5.82$ for the 2-flavor case.

state is at $\text{Im}L \sim -0.65$ which is same as that in Fig. 1(a). We find that P(ReL, ImL) is independent of thermalization apart from an overall normalization factor. Random processes such as thermalization cannot give rise to such peaks.

Ideally the system should be allowed to explore all possible states in a single run. If there are metastable states, the distribution P(ReL, ImL) will have three distinct peaks. The ratio of the peak heights of the metastable state to the ground state will be given approximately by the exponential of the difference in free energies of these two states. Thereby, this ratio will be vanishingly small for large volumes. This translates to the vanishing probability of observing these metastable states starting from any arbitrary initial configuration. These states can only be observed by starting from suitable initial configurations. We believe such a method of study has no bearing on the properties of the metastable states. This is evident as we observe almost identical distributions P(ReL, ImL) for different choices of initial configurations and random number sequences as they all thermalize to a particular metastable state.

We have already mention that the physics we study here is different from the metastability observed near the critical point of a first order transition. For a first order transition, the metastable (stable) state becomes stable (metastable) as the system passes through the critical point. The metastable states are observed close to the transition point. On the other hand, the Z(3) metastable states exist away from the phase transition point as we discuss below.

B. Studies with a given volume

In our simulations for $N_s = 32$, $N_\tau = 4$, with β values up to $\beta_m \sim 5.80$, the system thermalizes to the ground state irrespective of the initial configurations (listed in the previous section) [Fig. 2(a)]. The system thermalizes to the metastable states only for $\beta \geq \beta_m$ [Fig. 2(b)]. One can argue that the metastable states are not observed below β_m

because the thermal fluctuations are large compared to the barrier height between these states and the stable state. In effect this situation can be described by an effective potential without any local minima. We mention here that the chiral condensate takes a slightly higher value in the metastable states than that of the ground state.

Higher β corresponds to higher temperature and larger quark mass [16,18]. In the pure SU(3) gauge theory, the barrier height between the Z(3) states increases with temperature. This should also be true in full QCD, since gluons dominate at higher temperatures. So it is expected that the barrier height between the metastable state and the absolute ground state increases with β . As a result, the system in the metastable state should spend on average a longer "Monte Carlo time" in the metastable state. Considering different initial configurations and random number sequences (for a particular β and m_q), we calculate the average Monte Carlo time the system spends in the metastable states. We find that this time monotonically increases with β . For example, in Fig. 3 we have shown the case

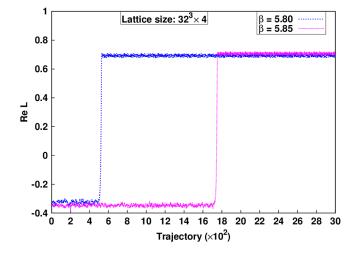


FIG. 3 (color online). ReL vs number of trajectories at $\beta = 5.80$, and $\beta = 5.85$ on a $32^3 \times 4$ lattice.

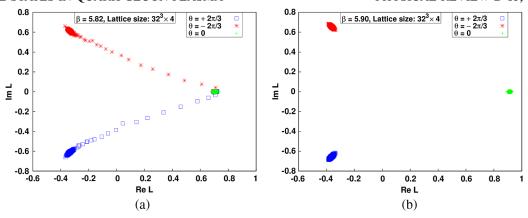


FIG. 4 (color online). Imaginary vs real part of the Polyakov loop for two different values of β .

for $\theta = -2\pi/3$, and $\beta = 5.80$ and 5.85. For $\beta = 5.85$, the system stays in the metastable state longer than $\beta = 5.80$. For $\beta = 5.90$, the metastable state did not decay during the simulation we considered. In Fig. 4, we show ReL vs ImL for different β values. We see that for $\beta = 5.90$ [Fig. 4(b)], there are no fluctuations between different minima. With various different trial configurations and different seeds, we found only two metastable states. No other (meta)stable state was observed in our simulations, such as $\theta = \pi$ [7].

C. Volume and N_{τ} studies

We extend our studies to different spatial volumes, V's, and temporal extent, N_{τ} 's, in order to investigate whether the finite volume effects play any significant role in the observation of the metastable states. We consider $V=16^3$, 24^3 , 32^3 and $N_{\tau}=4$, 6. For a particular choice of $(V,N_{\tau},n_f$ and $m_q)$, we always find a β_m above which there are metastable states. For a fixed N_{τ} , the value of β_m remains almost the same as volume changed. The average value of |L| in the metastable (stable) state remains the same as we increase V from 16^3-32^3 , as seen in Fig. 5. For the different volumes we considered, the Polyakov loop susceptibility does not have any dependence on the size of the system. This is expected since at $\beta=\beta_m$, the system is away from

the transition region. The corresponding correlation length is expected to be very small compared to the system size. So we hardly see any finite size effects. In Fig. 5, it can be seen that the average value of |L| and its fluctuations decrease when N_{τ} changes from 4 to 6. This behavior is observed in both the metastable and the ground states. In our estimate for β_m , we find the value increases with N_{τ} . For example, for $V=32^3$ we find that $\beta_m\sim5.80(5.89)$ for $N_{\tau}=4(6)$. The β function [18] results show that a fixed temperature scale corresponds to a higher β for larger N_{τ} in the β range of our study. Interestingly, we find that the two β_m 's obtained for $N_{\tau}=4$, 6 correspond to the temperature scales close to each other. However, a quantitative comparison between different N_{τ} results will require higher statistics than the present simulations.

In all the volumes under our study, we find a similar pattern in the behavior of the Polyakov loop in the metastable and stable states. As expected, β_m increases with N_τ . But we would like to mention that our study of the thermodynamic and continuum limit is far from complete. With the increase in the size of the system, the metastable states should take longer *average* Monte Carlo time to decay to the stable state. In our simulations with a small number of seeds, we do see that the metastable states take

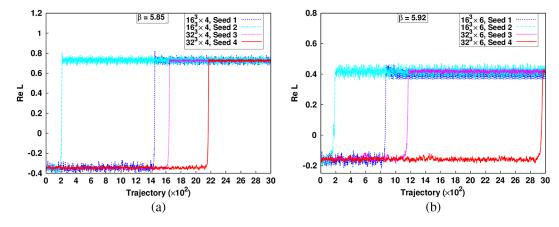


FIG. 5 (color online). ReL vs number of trajectories for $V = 16^3$, 32^3 at (a) $\beta = 5.85$, $N_{\tau} = 4$ and (b) $\beta = 5.92$, $N_{\tau} = 6$.

longer average MC time to decay with the increase in volume. However, a quantitative estimate of the volume dependence of the average decay time will need simulations with a large number of different seeds. We mention here that the same β corresponds to lower physical temperature for higher N_{τ} . This can lead to smaller decay time for the metastable states for higher N_{τ} (see Fig. 5).

D. n_f and m_q dependence

We have repeated our simulations for the 3-flavors of degenerate quarks. In this case, the metastable states appear at higher values of β_m compared to that of the 2flavor. Apart from higher β_m , all other findings are similar to those of the 2-flavor case. So, we have not shown any results for the 3-flavor here. We have also considered higher values of (m/T) in our simulations. For infinitely heavy quark masses, there is no explicit symmetry breaking of Z(3). So, we expect that higher the quark mass smaller is the explicit symmetry breaking. For a larger mass $am_{u,d} = 0.1$, the Monte Carlo histories for $\beta =$ 5.80 has been shown in Fig. 6 together with $am_{u,d} =$ 0.01 for the same β and seed. We see that the metastable state with $am_{u,d} = 0.1$ decays later than that of $am_{u,d} =$ 0.01. This suggests that β_m is smaller for higher (m/T) and approaches the pure gauge transition point for $m_q \to \infty$.

(m/T) is fixed in our simulations. But for realistic simulations, one should fix the quark masses. This amounts to considering a smaller (m/T) at higher β . Smaller (m/T) will decrease the barrier height between the metastable and ground state. On the other hand, the pure gauge effects will make the barrier height grow at higher β . We expect that the pure gauge effects will take over the explicit symmetry breaking term for $\beta > \beta_m$. The value of β_m we get, should be the lower bound for all the quark masses for which $am_{u,d}(\beta_m) \leq 0.01$.

The quark masses we have considered are larger compared to that of the physical u, d quarks. So, if we ignore the strange quark, the β_m for QCD with u, d quarks will be

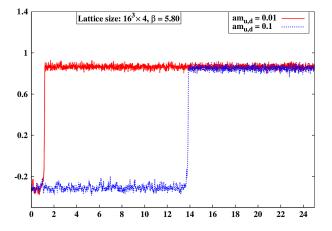


FIG. 6 (color online). ReL vs number of trajectories at $\beta = 5.80$ with masses at $am_{u,d} = 0.01$ and $am_{u,d} = 0.1$.

higher than the value we got from our 2-flavor simulations. Inclusion of strange quark will only increase the β_m . From this, we can conclude that β_m for a realistic case of light u, d quarks, and a heavy strange quark will be larger than the value for our 2-flavor calculations. Note that β_m is larger than the β_c for the quark-hadron transition. As a result, the metastable states do not appear near the quark-hadron transition but at larger temperatures.

E. Estimate of temperature scale T_m for the metastable states

Now we make an estimate of the temperature T_m corresponding to β_m and am_q . This requires the β function which relates these bare parameters to the lattice cutoff, a. The β function for $N_f = 2$ which is appropriate for the action we have used has been studied in detail in [18] in the range $5.2 \le \beta \le 5.6$. However, the values of β_m that are of interest to us lie outside this range. But we naively used the same β function as in [18] to make an estimate of T_m . This gives us $T_m = T$ ($\beta_m = 5.80$, $am_a = 0.01$) \simeq 750 MeV. This temperature should be compared with the phase transition temperature which is about 200 MeV. For a better estimate, we should have lattice results for the $\beta(a)$ close to β_m . However, we believe that this will not drastically reduce T_m . As we have argued before, β_m will be larger for realistic quark masses with $N_f = 2 + 1$, 3. So, it is likely that the actual value of T_m will be larger than our estimate.

Previous studies have suggested that the explicit symmetry breaking due to quarks is small [14]. But as we can see here that the explicit symmetry breaking is strong enough to make the Z(3) states with nonzero phase angle unstable below T_m . The value of $T_m > 750$ MeV suggests that these states will not be excited at the RHIC. There is a possibility, however, that they will be observed at the LHC. During thermalization a local region or the whole of the fireball may be trapped in one of the metastable states. The regions in the metastable phase can then decay through bubble nucleation or via spinodal decomposition, depending on dynamical evolution of the system [2,3]. It would be interesting to explore the possible consequence of the decay of the metastable phases. For temperature above T_m the system is dominated by gluons and Z(3) is effectively restored. This allows for various types of domain walls, static or otherwise [19]. These solutions become unstable below T_m .

V. CONCLUSION

We have done full QCD simulations with the $N_f = 2$, 3-flavor of degenerate quarks to study metastable states in the neighborhood of T_c . It has been found that the β value above which the metastable states appear is close to critical value of β for the pure gauge confinement-deconfinement transition. We estimate the temperature scale to be

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 $T_m > 750$ MeV (for $N_f = 2$) above which metastable states can appear. So, we expect that these metastable states may be observed at the LHC. There is a nontrivial change in the shape of the effective potential for the Polyakov loop as the system cools through T_m . Below T_m , there are no local minima in the effective potential. So, the metastable states, Z_3 domain walls become unstable. This may have important consequences for systems such as the fireball in heavy-ion collisions or the early Universe.

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