Meta-stable States in Quark-Gluon Plasma

Mridupawan Deka $^{a,b,*}$, Sanatan Digal $^{a,†}$ and Ananta P. Mishra $^{a‡}$

$^a$ Institute of Mathematical Sciences, Chennai- 600113, India
$^b$ Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

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Abstract

We study the meta-stable states in high temperature phase of QCD characterised 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 $\beta$ to observe these states. In particular, we find the value of the coupling ($\beta_m$) above which the meta-stable states appear. The resulting value of $\beta_m$ corresponds to temperature $T_m \gtrsim 750$ MeV for $N_f = 2$.

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* e-mail:Mridupawan.Deka@physik.uni-regensburg.de
† e-mail:digal@imsc.res.in
‡ e-mail:apmishra@imsc.res.in
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 ultra-relativistic 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 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 meta-stable states associated with it.

In the pure $SU(3)$ gauge theory, the deconfined phase exists in three degenerate states characterised 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 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 $\pm2\pi/3$) meta-stable.

We would like to emphasize that the $Z(3)$ meta-stable states are not the results of meta-stability near any first order transition. They are different from the meta-stable states that one observes near a first order phase transition. A closer analogy of the $Z(3)$ meta-stable states would be a state of magnetization anti-parallel to the external field.

The $Z(3)$ meta-stable states are expected to play 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 meta-stable bubble in the back-ground 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 thermalise to one of these meta-stable 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 meta-stable phases of super-horizon size may occur in the early Universe, and decay through bubble nucleation [3, 4].

There are several studies on $Z(3)$ meta-stable 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 meta-stable states for $T \geq T_c$ [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 meta-stable states. A lattice QCD study with fermions in the sextet representation has found meta-stable states, characterised by phase angle $(\pm2\pi/3, \pi)$, 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 meta-stable states. Contrary to the previous studies, we find that the meta-
stable states do not exist in the neighbourhood 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 LHC. The fact that $T_m > T_c$ may have important consequence(s) for the early Universe.

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

II. $Z(3)$ SYMMETRY IN THE PRESENCE OF DYNAMICAL QUARKS AND META-STABLE 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, $T = \beta^{-1}_T$. 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,

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

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

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

The expectation value of 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 $\beta_T = 1/T$ denotes the extent of Euclidean time. $A_\mu(\vec{x}, \tau) = A_\mu^a(\vec{x}, \tau) \lambda^a$ is the vector potential. The $\lambda^a$ 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 $\tau$. The gauge fields $A_\mu(\vec{x}, \tau)$ obey periodic boundary conditions in the Euclidean time direction, $A_\mu(\vec{x}, \beta_T) = A_\mu(\vec{x}, 0)$. These boundary conditions are maintained by a group of non-trivial gauge transformations [8] that are periodic up to a constant twist matrix, $z \in SU(N)$,

$$g(\vec{x}, \beta_T) = z g(\vec{x}, 0).$$

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 $\mathcal{G} \times Z(N)$, where $\mathcal{G}$ is the group of strictly periodic gauge transformations.

However, the Polyakov loop (which characterises the phases of pure gauge theory) transforms non-trivially 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

$$L(\vec{x}) \rightarrow z L(\vec{x}),$$

(4)

where,

$$z = \exp(2\pi i n/N) \mathbb{1} \in Z(N), \quad n \in \{0, 1, 2, \cdots, N-1\}.$$  

(5)

For temperatures above the critical temperature $T_c$, the high temperature phase or the deconfining phase is characterised 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,

$$\Psi \rightarrow g \Psi.$$  

(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) meta-stable 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 meta-stable states to exist in the neighbourhood of $T_c$.

### III. NUMERICAL PARAMETERS AND STUDIES

In principle meta-stable 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 “thermalising” to a meta-stable state is very small. Once the system thermalises to the absolute ground state the probability that it fluctuates to the meta-stable state decreases exponentially with the system size. So it is practical to choose initial configurations carefully so that they thermalise to the meta-stable states before decaying to the ground state. In order to have the system thermalized to a meta-stable state ($\text{Re} \, L < 0$ and $|\text{Im} \, L| > 0$), 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 MILC code) results in a stable state ($\text{Re} \, L > 0$), we need to select the initial configuration appropriately. As the meta-stable 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 meta-stable state. To generate the gauge field configurations, we have used the MILC code which uses the standard Hybrid R algorithm [15]. We have used the similar simulation parameters as 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 have selected one configuration each for the following cases:

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

The case (iii) has been taken into consideration additionally to study whether a meta-stable state could exist at $\theta = \pi$ [7], and the case (iv) to check whether we obtain the similar stable state if we start with a “fresh lattice”. Another method, we have employed, is by 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 iteration for updating a gauge configuration.

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

IV. RESULTS AND DISCUSSIONS

A. How to observe the meta-stable states?

In this study the Polyakov loop expectation value $\langle L \rangle$ has been used to characterise different possible states of the system. In the absolute ground state $\langle L \rangle$ is real and positive. In the meta-stable states $\langle L \rangle$ is complex, with 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 auto-correlations 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 thermalised in a few hundred Monte-Carlo steps. During the thermalisation, all the measured observables change almost monotonically. Once the system is thermalised, all the physical observables fluctuate around their respective average values. We compute the histogram (probability distribution) of the Polyakov loop, $P(L)$. The meta-stable 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.
FIG. 1. Histograms of $\text{Im } L$ vs. no. of trajectories (a) Single peak at $\text{Im } L \neq 0$ indicating a meta-stable state only, (b) Double peak at $\text{Im } L \neq 0$ and $\text{Im } L = 0$ indicating a meta-stable state decaying into the ground state.

In Fig. 1(a), we show the histogram of $\text{Im } L$ (imaginary part of $L$) for two simulations with different random number sequences. The two $P(\text{Im } L)$ distributions are similar given the small length (a few thousands) of the Monte-Carlo histories. The peak positions are at a non-zero value of $\text{Im } L \sim -0.65$ which imply a meta-stable state. This being a meta-stable 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 run time. With another sequence of random numbers, the meta-stable decays to the ground state. This results in a second peak in $P(\text{Im } L)$ at $\text{Im } L \sim 0$ as seen in Fig. 1(b). Note that the peak position of the meta-stable state is at $\text{Im } L \sim -0.65$ which is same as that in Fig. 1(a). We find that $P(\text{Re } L, \text{Im } L)$ is independent of thermalisation apart from an overall normalisation factor. Random processes such as thermalisation can not give rise to such peaks.

Ideally the system should be allowed to explore all possible states in a single run. If there are meta-stable states, the distribution $P(\text{Re } L, \text{Im } L)$ will have three distinct peaks. The ratio of the peak heights of the meta-stable 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 meta-stable 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 meta-stable states. This is evident as we observe almost identical distributions $P(\text{Re } L, \text{Im } L)$ for different choices of initial configurations and random number sequences as they all thermalise to a particular meta-stable state.

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

In our simulations for $N_s = 32, N_T = 4$, with $\beta$ values up to $\beta_m \sim 5.80$, the system thermalises to the ground state irrespective of the initial configurations (listed in the previous section) (Fig. 2(a)). The system thermalises to the meta-stable states only for $\beta \geq \beta_m$ (Fig. 2(b)). One can argue that the meta-stable states are not observed below $\beta_m$ 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 slightly higher value in the meta-stable states than that of the ground state.

![Graphs showing Re L vs. number of trajectories for three different randomly chosen seeds at different beta values.](image)

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

Higher $\beta$ corresponds to higher temperature and larger quark mass [16, 18]. In the pure

![Graph showing Re L vs. number of trajectories at different beta values on a 32^3 x 4 lattice.](image)

**FIG. 3.** Re $L$ vs. number of trajectories at $\beta = 5.80$, and $\beta = 5.85$ on a $32^3 \times 4$ lattice.
$SU(3)$ 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 meta-stable state and the absolute ground state increases with $\beta$. As a result, the system in meta-stable state should spend on an average longer "Monte-Carlo time" in the meta-stable state. Considering different initial configurations and random number sequences (for a particular $\beta$ and $m_q$), we calculate the average Monte-Carlo time the system spends in the meta-stable states. We find that this time monotonically increases with $\beta$. For example, in Fig. 3 we have shown the case for $\theta = -2\pi/3$, and $\beta = 5.80$ and 5.85. For $\beta = 5.85$, the system stays longer in the meta-stable state than $\beta = 5.80$. For $\beta = 5.90$, the meta-stable state did not decay during the simulation we considered. In Figs. 4, we show Re$L$ vs. Im$L$ for different $\beta$ 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 meta-stable states. No other (meta)stable state was observed in our simulations, such as $\theta = \pi$ [7].

C. Volume and $N_\tau$ studies

We extend our studies to different spatial volumes, $V$’s, and temporal extent, $N_\tau$’s, in order to investigate whether the finite volume effects play any significant role in the observation of the meta-stable 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 $\beta_m$ above which there are meta-stable states. For a fixed $N_\tau$, the value of $\beta_m$ remains almost the same as volume changed. The average value of $|L|$ in the meta-stable(stable) state remains the same as we increase $V$ from $16^3 - 32^3$ as seen in Figs. 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 it’s fluctuations decrease when $N_\tau$ changes from 4 to 6. This behavior is observed in both the meta-stable and the ground states. In our estimate for $\beta_m$, we find the value increases with $N_\tau$. For example, for $V = 32^3$ we find that $\beta_m \sim 5.80(5.89)$ for $N_\tau = 4(6)$. The $\beta$–function [18] results show that a fixed temperature
scale corresponds to a higher $\beta$ for larger $N_\tau$ in the $\beta$ range of our study. Interestingly, we find that the two $\beta_m$’s obtained for $N_\tau = 4, 6$ correspond to the temperature scales close to each other. However, a quantitative comparison between different $N_\tau$ results will require higher statistics than the present simulations.

In all the volumes we study, we find a similar pattern in the behavior of the Polyakov loop in the meta-stable and stable states. As expected, $\beta_m$ increases with $N_\tau$. But we would like to mention that our study of thermodynamic and continuum limit is far from complete. With the increase in the size of the system, the meta-stable 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 meta-stable states take 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 a large number of simulations with different seeds. We mention here that same $\beta$ corresponds to lower physical temperature for higher $N_\tau$. This can lead to smaller decay time for the meta-stable states for higher $N_\tau$ (see Fig. 5).

D. $n_f$ and $m_q$ dependence

We have repeated our simulations for 3–flavors of degenerate quarks. In this case, the meta-stable states appear at higher values of $\beta_m$ compared to that of 2–flavor. Apart from higher $\beta_m$, all other findings are similar to those of 2-flavor case. So, we have not shown any results for 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 $\beta$ and seed. We see that the meta-stable state with $am_{u,d} = 0.1$ decays later than that of $am_{u,d} = 0.01$. This suggests that $\beta_m$ 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 \(\beta\). Smaller \((m/T)\) will decrease the barrier height between the meta-stable and ground state. On the other hand, the pure gauge effects will make the barrier height grow at higher \(\beta\). We expect that the pure gauge effects will take over the explicit symmetry breaking term for \(\beta > \beta_m\). The value of \(\beta_m\) 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 \(\beta_m\) for QCD with \(u,d\) quarks will be higher than the value we got from our 2-flavor simulations. Inclusion of strange quark will only increase the \(\beta_m\). From this, we can conclude that \(\beta_m\) for 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 \(\beta_m\) is larger than the \(\beta_c\) for the Quark-Hadron transition. As a result the meta-stable states do not appear near the Quark-Hadron transition but at larger temperatures.

**E. Estimate of temperature scale \(T_m\) for the meta-stable states**

Now we make an estimate of the temperature \(T_m\) corresponding to \(\beta_m\) and \(am_q\). This requires the \(\beta\)--function which relates these bare parameters to the lattice cutoff, \(a\). The \(\beta\)--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 \(\leq \beta \leq 5.6\). However, the values of \(\beta_m\) which is of interest to us lie outside this range. But we naively used the same \(\beta\)--function as in [18] to make an estimate of \(T_m\). This gives us \(T_m = T(\beta_m = 5.80, am_q = 0.01) \simeq 750\) MeV. This temperature should be compared with the phase transition temperature which is about 700 MeV. For a
better estimate, we should have lattice results for the $\beta(a)$ close to $\beta_m$. However, we believe that this will not drastically reduce $T_m$. As we have argued before, $\beta_m$ 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 non-zero phase angle unstable below $T_m$. The value of $T_m > 750$ MeV suggests that this states will not be excited in RHIC. There is a possibility, however, that they will be observed at LHC. During thermalization a local region or the whole of the fireball may be trapped in one of the meta-stable states. The regions in meta-stable 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 meta-stable 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 $N_f = 2, 3$—flavor of degenerate quarks to study meta-stable states in the neighborhood of $T_c$. It has been found that the $\beta$ value above which the meta-stable states appear is close to critical value of $\beta$ for the pure gauge confinement-deconfinement transition. We estimate the temperature scale to be $T_m > 750$ MeV (for $N_f = 2$) above which meta-stable states can appear. So, we expect that these meta-stable states may be observed at LHC. There is a non-trivial 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 meta-stable 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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