Model A Dynamics and the Deconfining Phase Transition for Pure Lattice Gauge Theory

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We consider model A dynamics for a heating quench from the disordered (confined) into the ordered (deconfined) phase of SU(3) lattice gauge theory. For $4 N_s^3$ lattices the exponential growth factors of low-lying structure function modes are calculated. The linear theory of spinodal decompositions is compared with the data from an effective model and the Debye screening mass is estimated from the critical mode. Further, the quench leads to competing vacuum domains, which make the equilibration of the QCD vacuum after the heating non-trivial. We investigate the influence of such domains on the gluonic energy density.

1. Introduction

In Ref. [1,2] it is argued that a heating quench of QCD from its confined phase of disordered Polyakov loops into its deconfined phase of ordered Polyakov loops leads to vacuum domains of distinct $Z_3$ triality, and one ought to be concerned about non-equilibrium effects due to heating of the system. This comes because the heating is a rapid quench and the QCD high temperature vacuum carries structures which are similar to the low temperature phase of analogue spin models.

Here we report a similar investigation for SU(3) lattice gauge theory and preliminary results about the influence of such domains on the gluonic energy density and pressure of pure SU(3) lattice gauge theory. The Markov chain Monte Carlo (MC) process provides model A (Glauber) dynamics in the classification of Ref. [3]. As time step a sweep of systematic updating with the Cabibbo-Marinari [4] heat-bath algorithm and its improvements of Ref. [5,6] is used (no over-relaxation, to stay in the universality class of Glauber dynamics). Although this is certainly not the physical dynamics of QCD, in the present state of affairs it appears important to collect qualitative ideas about eventual dynamical effects. For this purpose the investigation of any dynamics, which actually allows for its study ought to be useful.

2. Preliminaries

We report numerical results for the structure factors (or functions) defined by

$$\hat{S}(\vec{k}, t) = \left\langle \hat{u}(\vec{k}, t) \hat{u}(\vec{k}'', t) \right\rangle =$$

$$\int \left\langle u(\vec{r}, t) u(\vec{r}', t) \right\rangle \exp \left( i\vec{k} \cdot (\vec{r} - \vec{r}') \right) d\vec{r} d\vec{r}'. \quad (1)$$

Here $u(\vec{r}, t)$ is the relevant fluctuation about some average. For gauge systems we deal with fluctuations of the Polyakov loop (for analogue spin systems with fluctuations of the magnetization). The time $t$ corresponds to the dynamical process, i.e., in our case the Markov chain MC time. Within the linear theory the differential equation

$$\frac{\partial \hat{u}(\vec{k}', t)}{\partial t} - \omega(\vec{k}') \hat{u}(\vec{k}', t) = g(\vec{k}') \quad (2)$$

with $g(k) = -\Gamma f_0' \sum_{\vec{r}} \exp(i\vec{k} \cdot \vec{r})$

can be derived, where $\Gamma$ is the response coefficient and $f_0'$ the derivative of the coarse-grained

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free energy density with respect to the fluctuation variable. The general solution of Eq. (2) is
\[
\dot{u}(\vec{k}, t) = C \exp \left( \frac{\omega(\vec{k}) t}{\omega(\vec{k})} \right) - \frac{g(\vec{k})}{\omega(\vec{k})} 
\]
(3)
with \( \omega(\vec{k}) = -\Gamma \left( K \vec{k}^2 + f_0'' \right) \).

Where \( K \) is the lowest order expansion coefficient of the free energy density about its minimum \( f_0 \), i.e. \( K > 0 \). If \( f_0'' > 0 \) holds, Eq. (4) implies that the amplitude of any fluctuation approaches a constant exponentially fast with time. But if the second derivative is negative, then one sees an exponential growth of the fluctuations for momentum modes smaller than the critical value
\[
|\vec{k}| < \kappa_c = |\vec{k}_c| = \left[ -\frac{f_0''}{K} \right]^{1/2}. 
\]

The equation of motion for the structure factor is derived by taking the time derivative of \( S(\vec{k}, t) \) and using Eq. (2)
\[
\frac{\partial \hat{S}(\vec{k}, t)}{\partial t} = \left\{ 2 \dot{u}(\vec{k}, t) \hat{u}^*(\vec{k}, t) \omega(k) \right\} + \left\{ (\hat{u}^*(\vec{k}, t) + \hat{u}(\vec{k}, t)) g(k) \right\}. 
\]

The average of fluctuations about the mean of the fluctuation variable has to be zero \( \left\{ \dot{u}(\vec{k}, t) \right\} = 0 \). Thus (6) becomes
\[
\frac{\partial \hat{S}(\vec{k}, t)}{\partial t} = 2 \omega(\vec{k}) \hat{S}(\vec{k}, t), 
\]
with the solution
\[
\hat{S}(\vec{k}, t) = \hat{S}(\vec{k}, t = 0) \exp \left( 2\omega(\vec{k}) t \right). 
\]

Again, for \( f_0'' < 0 \) low momentum modes grow exponentially. The value of the critical momentum is the same as for the fluctuations. Originally the linear theory was developed for model B. Details for model A can be found in Ref. [2].

During our simulations the structure functions are averaged over rotationally equivalent momenta and the notation \( S_{n_i} \) is used to label structure functions of momentum
\[
\vec{k} = \frac{2\pi}{L} \vec{n} \quad \text{where} \quad |\vec{n}| = n_i. 
\]

We recorded the modes (including the permutations) \( n_1: (1, 0, 0) \), \( n_2: (1, 1, 0) \), \( n_3: (1, 1, 1) \), \( n_4: (2, 0, 0) \), \( n_5: (2, 1, 0) \), \( n_6: (2, 1, 1) \), \( n_7: (2, 2, 0) \), \( n_8: (2, 2, 1) \) and \( (3, 0, 0) \), \( n_9: (3, 1, 0) \), \( n_{10}: (3, 1, 1) \), \( n_{11}: (2, 2, 2) \), \( n_{12}: (3, 2, 0) \), \( n_{13}: (3, 2, 1) \), \( n_{14}: (3, 2, 2) \), \( n_{15}: (3, 3, 0) \), \( n_{16}: (3, 3, 1) \), \( n_{17}: (3, 3, 2) \), \( n_{18}: (3, 3, 3) \). Note that there is an accidental degeneracy in length for \( n_8 \).

3. Numerical Results

In Fig. 1 the time evolution of the first structure function mode after a heating quench from \( \beta = 5.5 \rightarrow 5.92 \) in pure SU(3) lattice gauge theory is depicted. For the \( 4 \times 16^3 \) lattice the pseudo-transition value is \( \beta_c = 5.6908 \) and for the larger lattices the value is expected to be close-by. Our results are averages over 10,000 repetitions of the quench for the \( 4 \times 16^3 \) lattice and 4,000 repetitions for the \( 4 \times 32^3 \) lattice. The \( 4 \times 64^3 \) lattices are still running: Presently there are only 60 repetitions and only some structure function maxima are presently reached. Notable in Fig. 1 is the strong increase of the maxima \( S_{n_{max}} \) with lattice size. In our normalization non-critical behavior corresponds to a fall-off \( \sim 1/N_s^3 \) and a second order phase transition to a slower fall-off \( \sim 1/N_s^x \) with \( 0 < x < 3 \). As the \( N_s \rightarrow \infty \) limit is bounded by a constant, our figure shows that with our lattice sizes the asymptotic behavior has not yet been reached.

To determine the critical mode \( \kappa_c \) we fit the
initial increase of the structure functions. The results are combined in Fig. 2 and indicate $a k_c = 2\pi n_c/N_c \approx 0.34$ (from the figure $n^2_c/N^2_c \approx 0.003$). Using results of Miller and Ogilvie [10], we have $m_D = \sqrt{3} k_c$, where $m_D$ is the Debye screening mass at the temperature in question. The relation $k_c/T_f = N_c a k_c$, where $T_f$ is the final temperature after the quench, allows us to convert to physical units. For our quench we have $T_f/T_c = 1.57$ and get

$$m_D = \sqrt{3} N_c a k_c T_f = 3.7 T_c.$$  

(10)

For pure SU(3) lattice gauge theory $T_c = 265 (1)$ MeV holds, assuming $\sigma = 420$ MeV for the string tension, while for QCD the cross-over temperature appears to be around $T_c \approx 165$ MeV, see [13] for a recent review.

In Fig. 1 we observe that not only the height of the peaks increases with lattice size, but also the time $t_{\text{max}}$, $S_{n_1}^{\text{max}} = S_{n_1} (t_{\text{max}})$, which it takes to reach them. Whereas $S_{n_1}^{\text{max}}$ has finally to approach a constant value, $t_{\text{max}}$ is expected to diverge with lattice size due to the competition of vacuum domain of distinct $Z_3$ triality.

Using Fortuin-Kasteleyn (FK) clusters, the competition of such distinct vacuum domains can be made visible for the analogue Potts models [2]. The states of the three-dimensional, three-state Potts model substitute then for the $Z_3$ trialities of SU(3) lattice gauge theory. In Fig. 3 we compare the evolution of geometrical and FK clusters for a quench of this model from its disordered into its ordered phase. We plot the evolution of the largest clusters for the three Potts magnetizations in zero external magnetic field $h$. While the system grows competing FK clusters of each magnetization before one becomes dominant, geometrical clusters do not compete. This picture is unfavorable for the use of geometrical clusters of Polyakov loops in gauge theories, for which the FK definition does not exist.

The process of competitions between the largest FK clusters of different magnetization leads for the proper transition ($h = 0$) to a divergence of the equilibration time in the limit of infinite systems, an effect known in condensed matter physics [3]. Potts studies [2] with an external magnetic field show that a major slowing down effect survives for $h \neq 0$. As the influence of an external magnetic field on the Potts model is similar to that of quarks on SU(3) gauge theory this indicates that the effect may be of relevance for QCD studies of the crossover region.

For gauge theories a satisfactory cluster definition is presently not available. Nevertheless the underlying mechanism is expected to be the same as in the spin models. To study its influence on the gluonic energy $\epsilon$ and pressure $p$ densities, we like to calculate these quantities at times $t \leq t_{\text{max}}$.

Let us first summarize the equilibrium procedure of Ref. [9,11] (in earlier work [12,14] the pressure exhibited a non-physical behavior after the deconfining transition and the energy density approached the ideal gas limit too quickly due to the fact that anisotropy coefficients were calculated perturbatively). We denote expectation
values of spacelike plaquettes by $P_\sigma$ and those involving one time link by $P_\tau$. The energy density and pressure can then be cast into the form

$$(\varepsilon + p)/T^4 = 8N_c N_f g^{-2} \left[ 1 - \frac{g^2}{2}[c_\sigma(a) - c_\tau(a)] \right] (P_\sigma - P_\tau) \tag{11}$$

and

$$(\varepsilon - 3p)/T^4 = 12N_c N_f^4 [c_\sigma(a) - c_\tau(a)] [2P_0 - (P_\sigma + P_\tau)], \tag{12}$$

where $P_0$ is the plaquette expectation value on a symmetric ($T = 0$) lattice and anisotropy coefficients $c_{\sigma,\tau}(a)$ are defined as follows:

$$c_{\sigma,\tau}(a) \equiv \left( \frac{\partial g_{\sigma,\tau}^{-2}}{\partial g} \right)_{\xi=1}. \tag{13}$$

They are related to the QCD $\beta$-function in a simple way

$$a \frac{dg^{-2}}{da} = -2(c_\sigma(a) + c_\tau(a)). \tag{14}$$

One needs to calculate the $\beta$-function and anisotropy coefficients non-perturbatively to obtain meaningful results. In the range above the phase transition this is carried out in [9]. Using integral methods and Padé fits from [11] one finds the spatial anisotropy coefficient

$$c_\sigma(a) = c_\sigma(0) \frac{1 + d_1 g^2 + d_2 g^4}{1 + a_0 g^2}, \tag{15}$$

with $d_0 = -0.64907$, $d_1 = -0.61630$ and $d_2 = 0.16965$, where from perturbative calculations $c_\sigma(0) = 0.150702 N_c - 0.146711 / N_c$. Thus, taking data for the $\beta$-function from Table 3 of [9] and evaluating $c_\sigma(a)$ and $c_\tau(a)$ from Eqs. (13) and (14) we can calculate the energy density $\varepsilon$ and pressure $p$ using Eqs. (11) and (12) for arbitrary values of the coupling $\beta$ above $\beta_c$.

To normalize to zero temperature, plaquette values from the symmetric $N_\tau = N_\sigma$ lattice are needed in Eq. (12). For the quench this leaves us with the question whether we should perform the quench also on the symmetric lattice and use $P_0$ from the corresponding time evolution, or whether we should take the equilibrium value at $\beta = 5.92$ for $P_0$. Fortunately, the empirical answer is that it does not matter. When one is far

![Figure 4. SU(3) gluonic energy density: (a) with $P_0$ calculated from the time series after the quench and (b) using the equilibrium value of $P_0$.](image1)

![Figure 5. SU(3) gluonic energy density $P(\epsilon)$ histograms: (a) with competing vacuum domains present and (b) after reaching equilibrium.](image2)

Finally, we compare in Fig. [5] for the $N_\sigma = 16$ lattice the gluonic energy distribution in equilibrium at $\beta = 5.92$ with the one obtained after 148 time steps. We find a shift towards lower gluonic energies and the width of the probability density is slightly broader for the time evolution after the quench than in equilibrium. One also has to take into account that the geometry of relativistic heavy ion experiments experiments is reasonably approximated by $N_\tau/N_\sigma = \text{const}$, $N_\sigma \to \infty$, rather than by $N_\tau = \text{const}$, $N_\sigma \to \infty$. 
4. Summary and Conclusions

Structure functions allow to identify the transition scenario. For our quench from the disordered into the ordered phase of SU(3) lattice gauge theory we find spinodal decomposition. Relying on the linear theory of spinodal decomposition, we have calculated the critical mode $k_c$. From it the Debye screening mass $m_D$ at temperature $T$ is determined using phenomenological arguments of Miller and Ogilvie [10].

With increasing lattice size $N_{\sigma}$ the time to reach the structure function maxima diverges. Relying on a study of Fortuin-Kasteleyn clusters in Potts models [2], we assume that the reason is that vacuum domains of distinct $Z_3$ trialities compete. These could be the relevant configurations after the heating quench in relativistic heavy ion experiments. We have initiated a study of the gluonic energy and pressure densities on such configurations.

All our results rely on using a dissipative, non-relativistic time evolution, believed to be in the Glauber universality class. The hope is that the thus created non-equilibrium configurations may exhibit some features, which are in any dynamics typical for the state of the system after the quench. This hope could get more credible by studying a Minkowskian time evolution of Polyakov loops and finding similar features. Such a study appears to be possible [15] within a relativistic Polyakov loop model which was introduced by Pisarski [10].

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