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CHIRAL INTERFACE FOR QCD WITH DYNAMICAL FERMIONS

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ABSTRACT

The free energy distribution across the interface of coexisting quark and hadron matter is studied in the framework of lattice QCD. We calculate the interface tension α with the "differential method" for pure SU(3) gauge theory and in the presence of dynamical quarks with four flavors. Using lattices with spatial volume 8^2x16 it turns out that α is very small and compatible with zero. The chiral condensate indicates the same width of the domain wall as the Polyakov loop distribution and the other thermodynamical observables.

Keywords: Lattice QCD; Dynamical quarks; Interface tension; Chiral condensate.

1. Introduction

It was the merit of QCD thermodynamics on space-time lattices to show that matter can exist in two phases, a confining hadron phase and a free quark-gluon plasma-phase. In pure gluonic QCD and in full QCD with four light dynamical fermions most numerical simulations support the fact that the phase transition is of first order[1,2] which implies that the two different phases can coexist at the critical temperature. This enables a mechanism to create an inhomogeneous universe and can be studied from the first principles of lattice QCD. The most important observable under consideration is the surface energy α between the quark-gluon plasma-state and the hadronic bubbles. The numerical value of α is a fundamental quantity for the inhomogeneity of the universe. It represents an input parameter for the probability of nucleation and the average distance between nucleation centers.[3] Further, it effects the nucleosynthesis of light elements. The thickness of the domain wall of a coexisting two-phase system can also be associated with the skin of the fireball of a quark-gluon plasma being currently under investigation in ultrarelativistic heavy-ion experiments.

To extract α one has to evaluate thermodynamical expressions demanding to differentiate the partition function with respect to the temperature, volume and interface area. This can be realized on the lattice by directly summing over plaquettes at fixed couplings (differential method) or by integrating the sum of plaquettes over the coupling (integral method). Lattice simulations of pure gluonic QCD on fourdimensional hypercubes of sizes $N_x \times N_y \times N_z \times 2$ have led to a non-vanishing $\alpha/T_c^3 \approx 0.24$ for both methods.[4,5] On $N_x \times N_y \times N_z \times 4$ lattices the situation is not clear and comprises a value of α/T_c^3 compatible with zero.[6,7] We perform an independent analysis for $N_t = 4$ relying on the differential method. A further aim of this paper is to study the situation in the presence of dynamical quarks for which we choose the number of flavors $n_f = 4$ and the mass $m = 0.05$. This allows to explore the domain wall between a two-phase system with spontaneously broken and restored chiral symmetry. In addition to the surface tension and other thermodynamical observables we calculate the distribution of the chiral condensate across the interface.

In Sec. 2 the formulae of the lattice version of the thermodynamical quantities are outlined. Sec. 3 presents our results with a discussion of the observables. In Sec. 4 we summarize the physical interpretation and give an outlook to future extensions on this subject.

2. Theory

Starting from the relation for the free energy F

$$F(T,V,A) = -T \ln Z(T,V,A), \tag{2.1}$$

we express the partition function Z

$$Z(T,V,A) = \int \prod dU_{x\mu} \prod d\overline{\chi}_x \prod d\chi_x \exp(-S(U,\overline{\chi},\chi)) \tag{2.2}$$

by a path integral over the lattice action $S(U,\overline{\chi},\chi)$ (Refs. 8, 9)

$$\begin{aligned} S(U,\overline{\chi},\chi) &= S_G(U) + S_F(U,\overline{\chi},\chi) \\ &= \sum_x \left[\frac{1}{g_1^2}\frac{a_3}{a_0}(P_{01}+P_{02}) + \frac{1}{g_2^2}\frac{a_0}{a_3}(P_{13}+P_{23}) + \frac{1}{g_3^2}\frac{a_T^2}{a_0 a_3}P_{03} + \frac{1}{g_4^2}\frac{a_0 a_3}{a_T^2}P_{12} \right] \\ &+ \frac{n_f}{4}\left[\sum_x m\overline{\chi}_x\chi_x + \frac{1}{2}\sum_{x,\mu}\overline{\chi}_x\frac{\eta_\mu}{a_\mu}\left(U_{x\mu}\chi_{x+\mu} - U^\dagger_{x-\mu,\mu}\chi_{x-\mu}\right)\right]. \end{aligned} \tag{2.3}$$

In the gluonic part of the action, the plaquettes $P_{\mu\nu}$ are defined as

$$P_{\mu\nu} = P_{\mu\nu}(x) = \mathrm{tr}[2 - U_{x\mu}U_{x+\mu,\nu}U^\dagger_{x+\nu,\mu}U^\dagger_{x\nu} - \mathrm{h.c.}] \tag{2.4}$$

and $U_{x\mu}$ means the gauge field on a link of a hypercubic lattice. The factors $1/g_i^2$ denote the couplings for an anisotropic lattice with the so-called Karsch coefficients c_s, c_t, $\beta_0 = c_s + c_t$ entering the renormalization group equation.[8] The anisotropic couplings determine the corresponding lattice spacings a_i. In the fermionic part of the action, according to the Kogut-Susskind formulation the fermion fields are represented by single component Grassmann fields $\overline{\chi}_x, \chi_x$ at the sites of the lattice.[9]

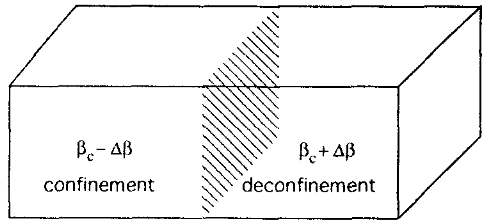

Fig. 1. Realization of a two-phase system with an interface at β_C. The phase transition occurs in the z direction at $n_z = 8$ and $n_z = 16$ due to periodic boundary conditions.

The fermionic action describes n_f flavors with mass m and the Dirac matrices reduce to phase factors $\eta_\mu = (-1)^{x_1+\ldots+x_{\mu-1}}$.

To perform QCD lattice-thermodynamics on a two-phase lattice of size $N_x \times N_y \times N_z \times N_t$ we place the interface in the (x,y) plane (see Fig. 1). To be able to take partial derivatives with respect to one variable while keeping two other variables constant we choose three different lattice constants a_0, $a_1 = a_2 = a_T$, a_3 which are all set equal after the derivation of the observables. The temperature, volume and interface size are given by

$$T = 1/N_t a_0, \qquad V = N_T^2 N_3 a_T^2 a_3, \qquad A = N_T^2 a_T^2. \tag{2.5}$$

Now we can proceed straightforward to derive the gluonic thermodynamical observables we are interested in, *i.e.* the energy ϵ_G, pressure p_G, surface energy α_G and entropy s_G (Ref. 4)

$$\begin{aligned}
\epsilon_G \frac{V}{T} &= \langle -T \frac{\partial S_G}{\partial T}\Big|_{A,V} \rangle \\
&= \langle \sum_x \Big[(\frac{1}{g^2} - c_s)(P_{12} + P_{13} + P_{23}) - (\frac{1}{g^2} + c_t)(P_{01} + P_{02} + P_{03}) \Big] \rangle, \\
p_G \frac{V}{T} &= \langle -V \frac{\partial S_G}{\partial V}\Big|_{A,T} \rangle \\
&= \langle \sum_x \Big[(\frac{1}{g^2} + c_t)(P_{03} + P_{13} + P_{23}) - (\frac{1}{g^2} - c_s)(P_{01} + P_{02} + P_{12}) \Big] \rangle, \\
\alpha_G \frac{A}{T} &= \langle A \frac{\partial S_G}{\partial A}\Big|_{T,V} \rangle \\
&= \langle \sum_x (\frac{1}{g^2} + \frac{1}{2}(c_t - c_s))(2P_{03} - P_{01} - P_{02} - 2P_{12} + P_{13} + P_{23}) \rangle, \\
s_G V &= (\epsilon_G + p_G)\frac{V}{T} - \alpha_G \frac{A}{T} \\
&= \langle \sum_x (\frac{1}{g^2} + \frac{1}{2}(c_t - c_s))(2P_{12} + P_{13} + P_{23} - P_{01} - P_{02} - 2P_{03}) \rangle.
\end{aligned} \tag{2.6}$$

To relate the energy and pressure to the $T = 0$ case we have to subtract the vacuum contribution given by the average plaquette $P_{av}(g^2)$ on a symmetric lattice, $\epsilon_{vac} = p_{vac} = -3\beta_0 P_{av}$. A further observable of interest is the Polyakov loop which on one hand represents the propagator in periodic time direction for a static quark

$$\langle L\rangle = \langle \frac{1}{3V}\sum_{\vec{x}} \mathrm{tr} \prod_{n_t=1}^{N_t} U_{x,\mu=0}\rangle \tag{2.7}$$

and on the other hand acts as an order parameter.

Similarly, we treat the fermionic part of the thermodynamical observables. After integration over the fermionic fields one obtains the fermion determinant

$$\exp(-S_F^{eff}) = \frac{n_f}{4}\det[D(U)+m], \tag{2.8}$$

with the covariant derivative

$$D_{\mu,xy}(U) = \frac{\eta_\mu}{2a_\mu}[U_{x\mu}\delta_{x+\mu,y} - U^\dagger_{x-\mu,\mu}\delta_{x-\mu,y}]. \tag{2.9}$$

Performing the thermodynamical differentiations we get the fermionic parts of the thermodynamical observables, *i.e.* the energy ϵ_F, pressure p_F, surface energy α_F and entropy s_F. The derivation was given for the first time for Wilson fermions in Ref. 4 and is formulated here for Kogut-Susskind fermions

$$\begin{aligned}
\epsilon_F\frac{V}{T} &= \frac{n_f}{4}\langle \mathrm{tr}[D_0(D+m)^{-1}]\rangle - \frac{1}{16}N_c n_f + \frac{1}{4}m\langle\langle\overline{\chi}_x\chi_x\rangle\rangle_{T=0},\\
p_F\frac{V}{T} &= -\frac{n_f}{4}\langle \mathrm{tr}[D_3(D+m)^{-1}]\rangle + \frac{1}{16}N_c n_f - \frac{1}{4}m\langle\langle\overline{\chi}_x\chi_x\rangle\rangle_{T=0},\\
\alpha_F\frac{A}{T} &= \frac{n_f}{8}\langle \mathrm{tr}[(D_1+D_2-2D_3)(D+m)^{-1}]\rangle,\\
s_F V &= (\epsilon_F + p_F)\frac{V}{T} - \alpha_F\frac{A}{T}.
\end{aligned} \tag{2.10}$$

The fermionic vacuum contribution for the energy and pressure is considered explicitly for gauge group $SU(N_c)$. In the fermionic system the chiral order parameter appears which is related to spontaneous chiral symmetry breaking and is a measure for the virtual quark density

$$\langle\langle\overline{\chi}_x\chi_x\rangle\rangle = \frac{n_f}{4V}\langle \mathrm{tr}(D+m)^{-1}_{xx}\rangle. \tag{2.11}$$

Single brackets mean path integration over the gauge field after fermionic integration whereas double brackets denote additional fermionic integration. The total expectation value of a thermodynamical observable O consists of the gluonic and fermionic parts

$$O = O_G + O_F. \tag{2.12}$$

The simulations are realized on a system with one half in the hadron phase at an inverse gluon coupling $\beta = \beta_c - \Delta\beta$ and the other half in the quark phase at $\beta = \beta_c + \Delta\beta$ (see Fig. 1). The partition wall is set to the critical coupling β_c. Thus, the interface is forced by construction and is not created dynamically. To obtain the physical expectation value for a coexisting two-phase system, one has to extrapolate the observables to the critical point.

3. Results

For the pure gluonic system we approximated the path integral by 25000 Monte Carlo iterations around β_c with several values of $\Delta\beta = 0.05, 0.10, 0.15, 0.20, 0.25$ on a hypercubic lattice.[10] For QCD with dynamical quarks we performed 5000 iterations using the pseudofermionic algorithm[11] with 50 fermionic steps and scanned over $\Delta\beta = 0.05, 0.10, 0.15, 0.20, 0.25, 0.30$. The dynamical quark field has flavor number $n_f = 4$ and mass $m = 0.05$. In the fermionic simulation we used the corrected Karsch coefficients.[12]

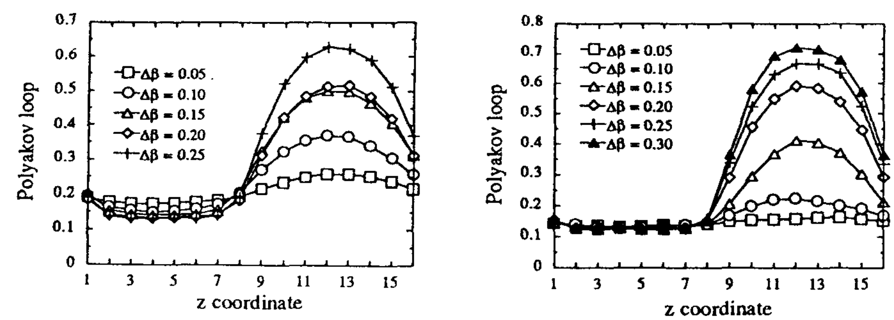

Fig. 2. Distribution of the Polyakov loop for pure gluonic QCD (left plot) and for full QCD (right plot) with four flavors across the interface. The two-phase systems have time elongation $N_t = 4$ and various coupling (temperature) gradients.

In Fig. 2 we compare our results on lattices with space-time volume $8 \times 8 \times 16 \times 4$ with (right plot) and without (left plot) dynamical fermions. The Polyakov loop is an order parameter for the pure gauge spin-system and changes smoothly from zero to a finite value. Since we plot the absolute value $|\langle L \rangle|$ without the factor $1/3$ we find a positve number in the confinement compartment which is not only due to the spreading of the hot phase. Also in the presence of dynamical quarks a clear change is seen at the transition point from confinement to deconfinement. Here the Polyakov loop has a non-vanishing expectation value due to the broken Z_3 symmetry from the fermions in the confining phase.

The chiral order parameter is presented Fig. 3. Chiral symmetry is broken in the confinement and restored in the deconfinement. For the chiral order parameter profile crossing the interface at $n_z = 8$ we find an increase of the wall thickness when

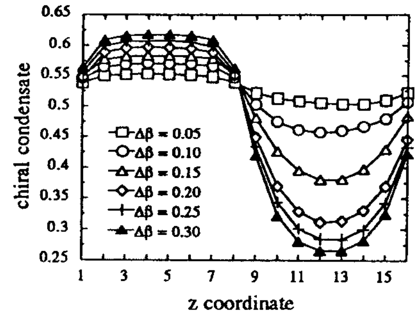

Fig. 3. Profiles of the chiral condensate for full QCD with four flavors and for various two-phase systems.

we approach the coexisting phases at $\Delta\beta \to 0$. For $\Delta\beta = 0.3$ the width is about 5 lattice spacings a which corresponds to roughly 1 fm. It turns out that the chiral condensate has the same width as the corresponding Polyakov loop distribution. The order parameter with dynamical quarks has not reached a plateau like in pure gluonic studies on larger lattices indicating a width of the domain wall of 2.5 fm.[4,6] The lattice results can be compared with a study of the σ model which predicts a width of about 4.5 fm.[13]

In Fig. 4 our results for the thermodynamical quantities are presented with the pure gluonic case placed to the left and full QCD to the right. All observables are influenced by the interface induced between $8 \leq n_z < 9$. The kinks are due to the discretization effects depending on the local construction of the operators[4] and are decreasing with $\Delta\beta \to 0$. Error bars corresponding to the mean standard deviation have been computed and it was seen that they exceed the symbols in general only around the interface. For all thermodynamical observables in full QCD vacuum it is found that the gluonic and fermionic contributions are of the same size.

We start with the distribution of the energy. The vacuum corrections have been determined from a consistent simulation of an 8^4 lattice with the same parameters. The difference between the cold and the hot phase is less pronounced with increasing time elongation due to the smaller magnetization of the plaquette operator (2.4) (Refs. 4, 5). In the $N_t = 4$ case discretization artefacts become increasingly important and especially energy and pressure are difficult to be resolved. In the deconfining phase the energy is in accordance with the Stefan-Boltzmann limit of an ideal gas with a tendency of overshooting.[14] We turn to the z component of the pressure in Fig. 4. Discretization effects at the phase transition are clearly visible. At high temperatures the ideal gas relation $\epsilon = 3p$ holds. The next plots present the profile of the entropy which also increases towards the hot phase. The discretization effects are partially compensated because pressure and surface energy enter into the entropy with different signs. Finally, the distribution of the surface energy $\alpha(z)$ which has no direct physical meaning is plotted in Fig 4. In the region

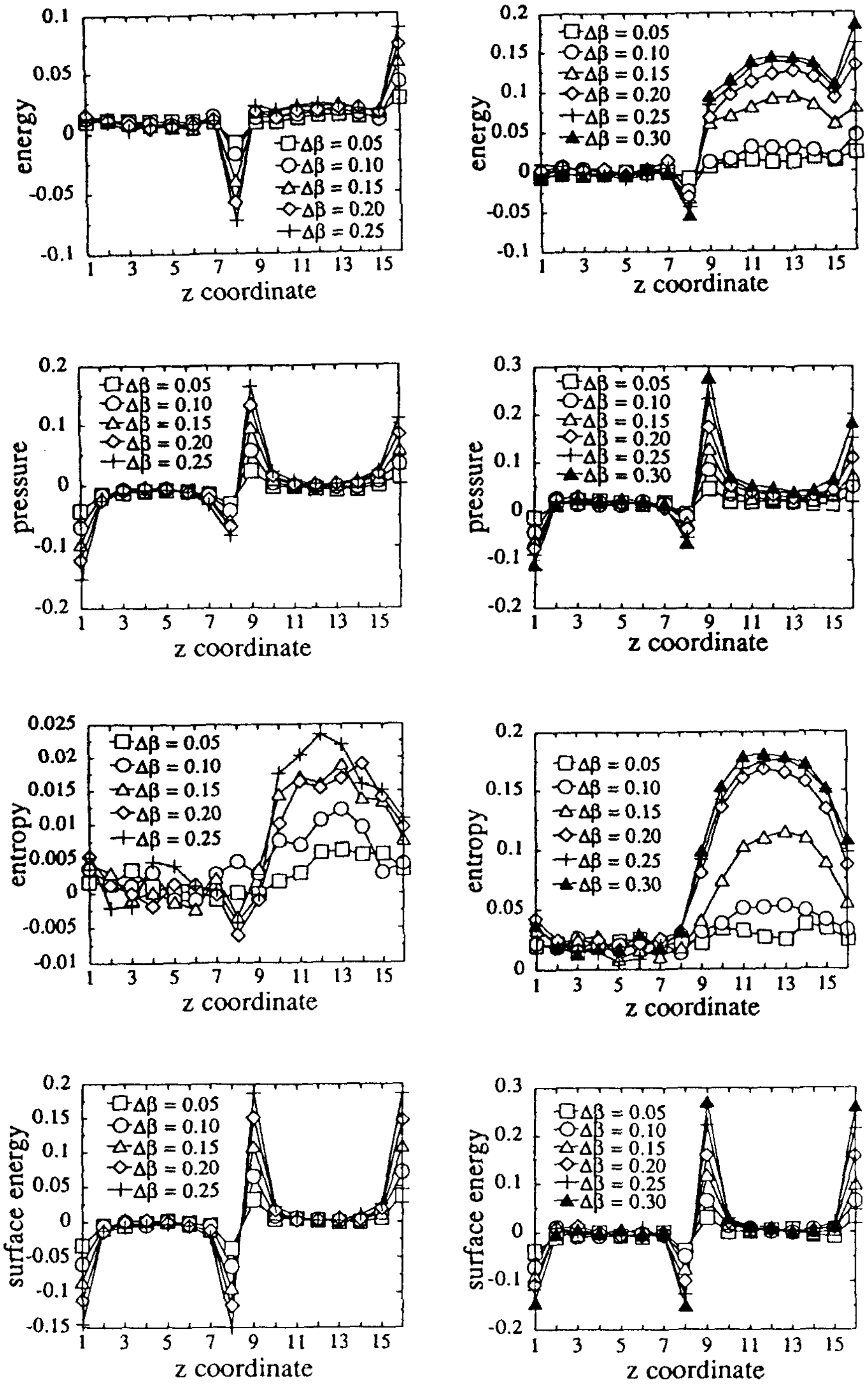

Fig. 4. Thermodynamical observables for pure gluonic QCD as a function of the z coordinate (left plots) and for QCD with four dynamical quarks (right plots) at different temperature gradients.

of the phase transition the surface energy has a non-vanishing value. In full QCD the total surface energy is stabilized by the fermionic contribution.

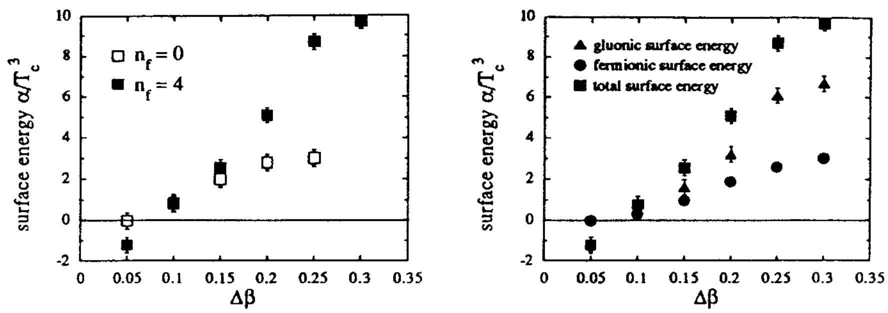

Fig. 5. Surface energy for full QCD with $n_f = 4$ in comparison to the pure gluonic case (left plot). Gluonic and fermionic contributions to the total surface energy in the presence of dynamical quarks (right plot). Error bars denote mean standard deviation.

To get the surface energy α we have to integrate its distribution along the z axis. The phase transition occurs twice due to periodic boundary conditions. Thus, we have to divide the sum by two in order to obtain the surface energy for one confinement-deconfinement transition. In Fig. 5 the surface energy α/T_c^3 is normalized to physical units. In the left plot we compare our $N_t = 4$ computations with and without dynamical fermions. We find that the surface energy has a small numerical value in both cases, $\alpha/T_c^3 < 0.1$. We discuss our gluonic results and compare them with some other recent data obtained by the integral method[5] and the differential method.[4] There is a remarkable agreement if one keeps in mind that the two methods are completely different. For $N_t = 2$ the differential method[4] yields a value of $\alpha/T_c^3 = 0.24 \pm 0.06$ and the integral method[5] gives $\alpha/T_c^3 = 0.12 \pm 0.02$. Because the difference between the space like and time like plaquettes decreases with increasing elongation in time the interface tension becomes more difficult to be extracted. All computations for time extension $N_t = 4$ have given a value of α compatible with zero; an exception is the extension of the integral method employing Polyakov lines to stabilize the interface which leads on a $16 \times 16 \times 32 \times 4$ lattice to $\alpha/T_c^3 = 0.024 \pm 0.004$.[7] Our data points agree within error bars with those of Refs. 4, 6 but are systematically lower especially for $\Delta\beta = 0.05$. Since both analyses rely on the differential method the deviation is a consequence of the shorter z elongation of our system, $N_z = 16$ compared to $N_z = 40$. For small coupling gradients $\Delta\beta$ the two phases begin to intermix and the resolution of the surface energy becomes unstable. The choice of a smallest reliable $\Delta\beta$ and the numerical extrapolation $\Delta\beta \to 0$ represent a serious problem.[15] The right plot in Fig. 5 shows the gluonic and fermionic contributions to the total surface energy $\alpha = \alpha_G + \alpha_F$ normalized to T_c^3 in the presence of dynamical quarks as a function of the coupling gradient $\Delta\beta$. One finds that the fermionic part is smaller than the gluonic one. The extrapolated surface energy for a coexisting two-phase system is hard to extract and compatible with zero.

4. Summary

This paper contains a first trial to extract the interface tension in the presence of dynamical quarks. We derived the corresponding expressions for Kogut-Susskind fermions in the framework of the differential method and made an exploratory computation of α. Our simulations were performed on a lattice of moderate spatial volume $8^2 \times 16$. We started with the pure SU(3) case and time extension $N_t = 4$. Switching on dynamical fermions with four flavors we found that the gluonic and fermionic contributions to the interface tension are of comparable size. The extrapolation to the coexisting two-phase system represents a great difficulty, especially with increasing time elongation and on our moderate lattice size with limited statistics. Important for astrophysics, we can predict $\alpha/T_c^3 \sim 0.1$ as an upper bound for the interface tension. Further, we studied the fermionic behavior of different thermodynamical observables together with the order parameters of confinement and chiral symmetry. We made a crude estimate of the thickness of the domain wall, which is for $\Delta\beta = 0.3$ about 5 lattice spacings corresponding roughly to 1 fm. The wall thickness increases towards the coexisting two-phase system which might give some first principle information for heavy-ion experiments.

For future investigations beside larger lattices and higher statistics more sophisticated methods should be considered. We propose in analogy to the method which uses an external Polyakov loop field hL for stabilizing the interface, to employ the internal chiral condensate $m\bar{\psi}\psi$ of the fermionic action.[7] In this way, by differentiating the partition function with respect to m, the surface energy could be extracted in case of full QCD from the chiral condensate relying on the integral method. Another possibility might be to use the multicanonical algorithm and the tunneling probability between metastable states to calculate the tension of a dynamically created interface.[16]

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