Interface tension and chiral order parameter profile with dynamical quarks

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We investigate the free energy distribution across the interface of coexisting quark and hadron matter 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 a spatial volume $8^2\times 16$ we discuss the agreement between the differential and integral method in the pure gluonic case. With dynamical fermions it turns out that the interface tension is very small and we estimate an upper bound of $\alpha/T_c^3<0.1$. The chiral condensate indicates the same width of the domain wall as the Polyakov loop distribution and the other thermodynamical observables under consideration.

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I. INTRODUCTION

QCD thermodynamics on space-time lattices has demonstrated that matter can exist in two phases distinguishing between the confining hadron phase and the 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 opens up the possibility of the creation of an inhomogeneous universe which can now 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 and represents an input parameter for the probability of nucleation and the average distance between nucleation centers, and further effects the nucleosynthesis of light elements [3]. 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 which is 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 four-dimensional hypercubes of sizes $N_x\times N_y\times N_2\times 2$ have led to a definitely nonvanishing α for both methods [4,5] whereas on $N_x\times N_y\times N_z\times 4$ lattices the situation is more difficult [6]. In order to compare both methods we give a compilation of all existing data. We perform an independent analysis for $N_t=4$ relying on the differential method. The main objective of this paper is to study the situation in the presence of dynamical quark fields for which we choose the number of flavors $n_f=4$ and the mass $m=0.05$. This opens up the possibility to explore the domain wall in 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. II the formulas of the lattice version of the thermodynamical quantities are outlined. Section III presents our results with a discussion of the observables and a comparison with other recent work on this topic. In Sec. IV we summarize the physical interpretation of our results and give an outlook to future extensions on this subject.

II. 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,

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

by a path integral over the lattice action $S(U,\bar{\chi},\chi)=S_G(U)+S_F(U,\bar{\chi},\chi)$ [7,8]:

$$\begin{aligned} S_G&=\sum_x\left[\frac{1}{g_1^2}\frac{a_3}{a_0}(P_{01}+P_{02})+\frac{1}{g_2^2}\frac{a_0}{a_3}(P_{13}+P_{23})\right.\\ &\qquad\left.+\frac{1}{g_3^2}\frac{a_T^2}{a_0a_3}P_{03}+\frac{1}{g_4^2}\frac{a_0a_3}{a_T^2}P_{12}\right]\ ,\\ S_F&=a_0a_T^2a_3\frac{n_f}{4}\left[\sum_x m\bar{\chi}_x\chi_x\right.\\ &\qquad+\frac{1}{2}\sum_{x,\mu}\bar{\chi}_x\frac{\eta_\mu}{a_\mu}(U_{x\mu}\chi_{x+\mu}\\ &\qquad\left.-U^\dagger_{x-\mu,\mu}\chi_{x-\mu})\right]\ . \end{aligned} \tag{2.3}$$

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 [7]. 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 $\bar{\chi}_x, \chi_x$ at the sites of the lattice [8]. The fermionic action describes n_f flavors with mass m and the Dirac matrices reduce to phase factors $\eta_\mu=(-1)^{x_1+\cdots+x_{\mu-1}}$.

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

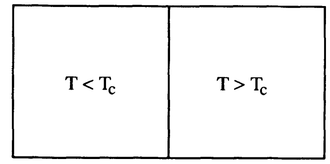

FIG. 1. Realization of a two-phase system with an interface at T_c. The phase transition occurs in the z direction at $n_z=8$ and $n_z=16$ due to periodic boundary conditions.

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

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 [4]:

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

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

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

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

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

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:

$$\epsilon_F \frac{V}{T} = \frac{n_f}{4} \langle \mathrm{tr}[D_0(D+m)^{-1}] \rangle - \tfrac{1}{16} N_c n_f + \tfrac{1}{4} m \langle\langle \bar{\chi}_x \chi_x \rangle\rangle_{T=0} ,$$

$$p_F \frac{V}{T} = -\frac{n_f}{4} \langle \mathrm{tr}[D_3(D+m)^{-1}] \rangle + \tfrac{1}{16} N_c n_f - \tfrac{1}{4} m \langle\langle \bar{\chi}_x \chi_x \rangle\rangle_{T=0} ,$$

$$\alpha_F \frac{A}{T} = \frac{n_f}{8} \langle \mathrm{tr}[(D_1+D_2-2D_3)(D+m)^{-1}] \rangle , \tag{2.10}$$

$$s_F V = (\epsilon_F + p_F) \frac{V}{T} - \alpha_F \frac{A}{T} .$$

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:

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

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.

III. RESULTS

For the pure gluonic system we approximated the path integral by 25 000 Monte Carlo iterations around $\beta_c = 6/g_c^2$ for several values of $\Delta\beta = 0.05$, 0.10, 0.15, 0.20 (0.25) on a hypercubic lattice [9]. In Figs. 2–4 we compare the results on lattices with spatial volume $8\times8\times16$ and two different time elongations $N_t=2$ and $N_t=4$, respectively. The Polyakov loop (see Fig. 2) as an order parameter of the gauge spin system changes smoothly from zero to a finite value. Since we plot the absolute value $|\langle L \rangle|$ without the factor $\frac{1}{3}$ we find a positive number in the confinement compartment which is not only due to the spreading of the hot phase. In Fig. 3 our results for the thermodynamical quantities are presented. All observables are influenced by the interface induced between $8 \le n_z < 9$. 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. Energy and pressure are plotted with vacuum corrections from an 8^4 lattice [4] and approach the Stefan-Boltzmann limit for an ideal gas at high temperatures. The difference between the cold and the hot phase is less clearly seen with increasing time elongation due to the smaller magnetization of the plaquette operator (2.4). In the $N_t=4$ case discretization artifacts become increasingly important and especially energy and pressure are difficult to be resolved. The entropy in Fig. 3 also increases towards the hot phase. Finally, the distribution of the surface energy $\alpha(z)$ which has no direct physical meaning is plotted.

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. 4 the surface energy normalized to physical units is compared with some other recent data obtained by the integral method [5] and the differential method [4,10]. There is a remarkable agreement between the data points 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 spacelike and timelike plaquettes decreases with increasing elongation in time the interface tension becomes more difficult to be extracted. All computations for time extension $N_t=4$ yield 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 $16\times16\times32\times4$ lattice to $\alpha/T_c^3 = 0.024 \pm 0.004$ [6]. Our data points agree within error bars with those of Refs. [4,10] but are systematically lower for both time extensions and especially for $\Delta\beta = 0.05$. Performing a linear extrapolation to $\Delta\beta = 0$ we find $\alpha/T_c^3 = -0.14 \pm 0.12$ for $N_t=2$ and $\alpha/T_c^3 = -0.68 \pm 0.40$ for $N_t=4$. Since both analyses rely on the differential method the deviation is a consequence

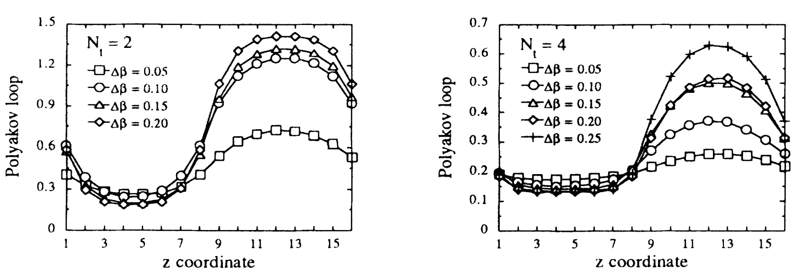

FIG. 2. Distribution of the Polyakov loop for pure gluonic QCD across the interface for two time elongations $N_t=2$ and $N_t=4$, respectively, and for two-phase systems with various coupling (temperature) gradients $2\Delta\beta$.

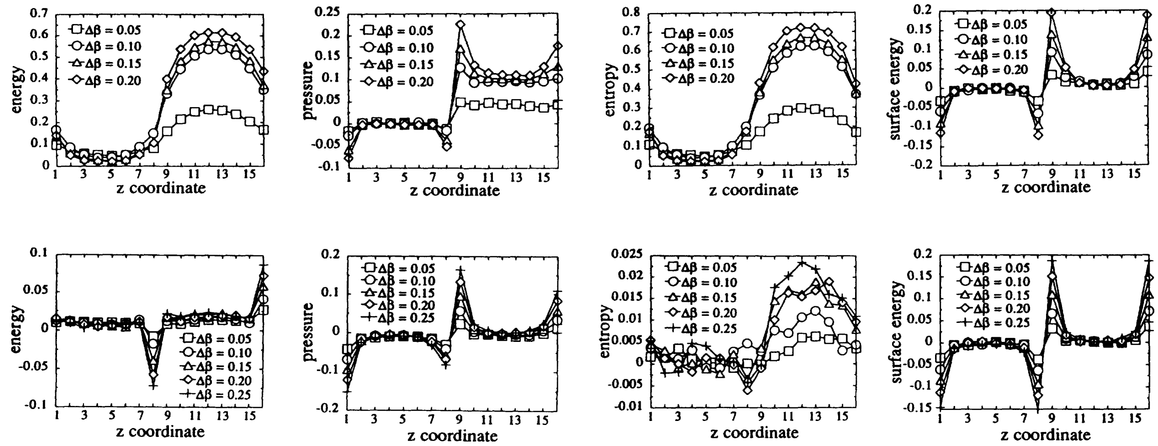

FIG. 3. Theromodynamical observables for pure gluonic QCD as a function of the z coordinate for $N_t = 2$ (first row) and $N_t = 4$ (second row) with different temperature gradients.

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. Omitting the data points for $\Delta\beta = 0.05$ we get $\alpha/T_c^3 = -0.14 \pm 0.12$ for $N_t = 2$ and $\alpha/T_c^3 = -0.37 \pm 0.40$ for $N_t = 4$. The choice of the smallest reliable $\Delta\beta$ and the numerical extrapolation $\Delta\beta \rightarrow 0$ represent a serious problem [11].

For QCD with dynamical quarks we approximated the path integral by 5000 Monte Carlo iterations using the pseudofermionic algorithm [12] with 50 fermionic steps and scanned several values of $\Delta\beta = 0.05$, 0.10, 0.15, 0.20, 0.25, 0.30. The dynamical quark field has flavor number $n_f = 4$ and mass $m = 0.05$ [9]. For the fermionic simulation we used the corrected Karsch coefficients [13]. In Fig. 5 we present the Polyakov loop and the chiral order parameter. A clear change is seen at the transition point from confinement to deconfinement. The Polyakov loop has a nonvanishing expectation value due to the broken Z_3 symmetry from the fermions in the confining phase. The 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 we approach the coexisting phases at $\Delta\beta \rightarrow 0$. 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 Polyakov loop distribution. The order parameter with dynamical quarks has not reached a plateau as in pure gluonic studies on larger lattices indicating a width of the domain wall of 2.5 fm [4,10]. The lattice results can be compared with a study of the σ model which predicts a width of about 4.5 fm [14].

Next we discuss the gluonic and fermionic contributions to the total thermodynamical observables in Fig. 6. We start with the distribution of the energy. Its gluonic part exhibits discretization effects at the transition point from the vacuum contribution. The fermionic part has a smooth behavior and clearly shows both phases, confinement and deconfinement. The vacuum corrections have been determined from a consistent fermionic simulation of an 8^4 lattice with the same parameters. The total energy as a sum of the gluonic and fermionic part has discretization effects. In the deconfining phase the energy is in accordance with the Stefan-Boltzmann limit of an ideal gas with a tendency of overshooting [15].

We turn to the z component of the pressure in Fig. 6. Discretization effects are clearly visible and show a similar behavior as the pressure in a single-phase SU(3) system at the transition point which is due to the perturbative β function entering the definition [15]. At high temperatures the ideal gas relation $\epsilon = 3p$ holds. The next plot presents the profile of the entropy. The discretization effects are partially compensated because pressure and surface energy enter into the entropy with different signs. For all thermodynamical observables it is found that the gluonic and fermionic contributions are of the same size.

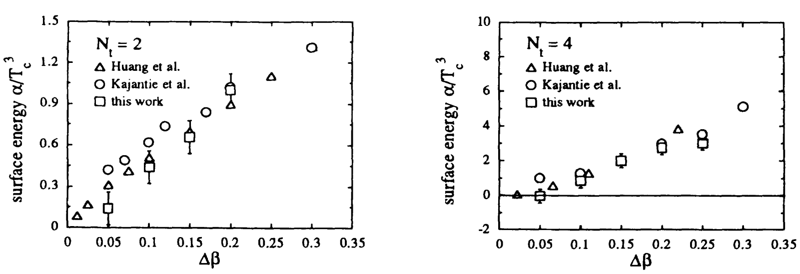

FIG. 4. Compilation of all available results for the surface energy α/T_c^3 in pure QCD on an $8 \times 8 \times N_z$ lattice with $N_t = 2$ and $N_t = 4$ [4–6,10]. Error bars are inserted for our results and denote mean standard deviation.

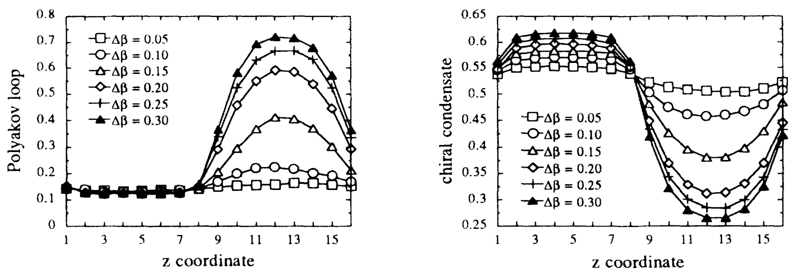

FIG. 5. Profiles of the Polyakov loop and the chiral condensate for full QCD with four flavors and for various two-phase systems.

Now we look at the profile of the surface energy in Fig. 6. In the region of the phase transition the surface energy has a nonvanishing value. In comparison to the gluonic part having a positive and a negative peak, only a single positive peak is detected for the fermionic contribution. Thus, the total surface energy is stabilized by the fermionic contribution.

The physical expectation value of the surface energy is the sum of its profile in the z direction. The left plot in Fig. 7 shows the surface energy 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 a linear fit yields $\alpha/T_c^3=\alpha_G/T_c^3+\alpha_F/T_c^3 = -2.98-0.88=-3.86\pm0.38$. There might be several reasons for this negative value. (i) The physical reason is that the phase transition for $n_f=4$ with mass $m=0.05$ is only weakly first order. (ii) For technical reasons we have to perform our simulations for $N_t=4$ implying $\beta_c=5.01$ far away from the continuum limit. As a consequence the lattice constant is rather large and part of the interaction falls through the mesh points lowering the interface tension. (iii) From the algorithmical point of view the application of the pseudofermionic method is known to bring more disorder to the gauge field configurations [16]. Thus, effectively a higher quark mass is simulated weakening the order of the phase transition. (iv) A methodological shortcoming of the differential method is the use of the Karsch-Trinchero coefficients being computed at weak coupling. But a recent analysis of the influence of these coefficients for pure gauge theory with $N_t=2$ has shown that they lead to an *increase* of α by a factor of 3 [17]. In the right plot we compare our $N_t=4$ computations with and without dynamical fermions. Altogether, we find that the surface energy has a small numerical value decreasing with increasing time elongation and is lower than in the pure gluonic case, $\alpha/T_c^3<0.1$.

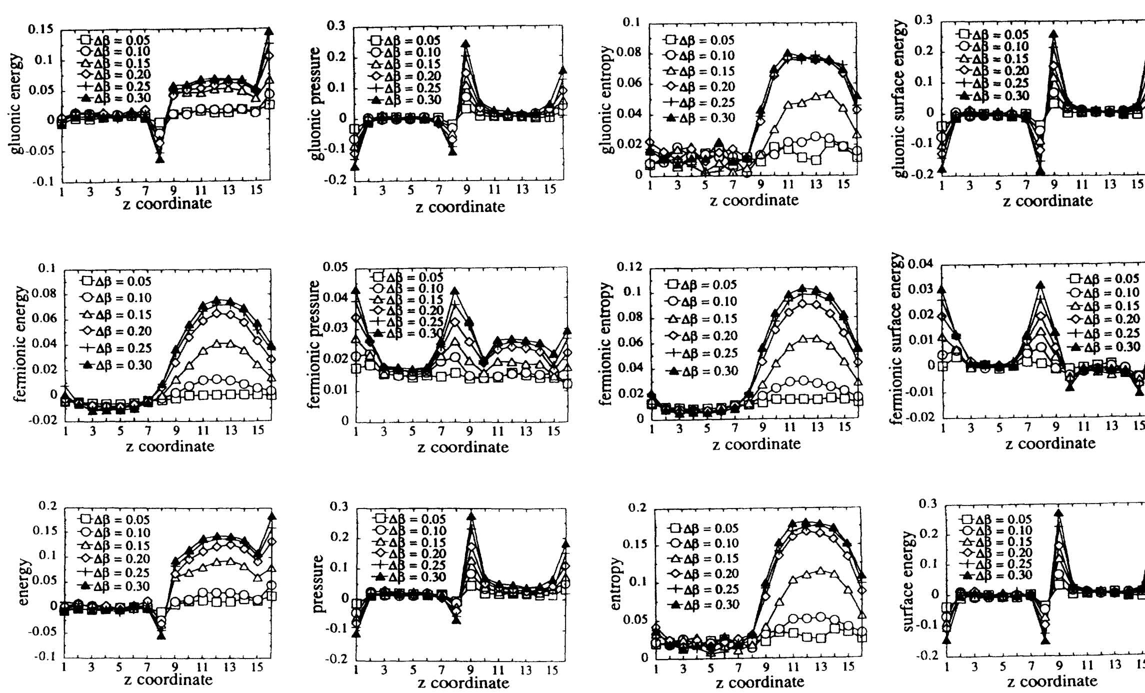

FIG. 6. Thermodynamical observables for QCD with four dynamical quarks as a function of the z coordinate for different temperature gradients. The first row of the plots displays the gluonic contribution and the second row the fermionic part while the third row gives the sum (see text).

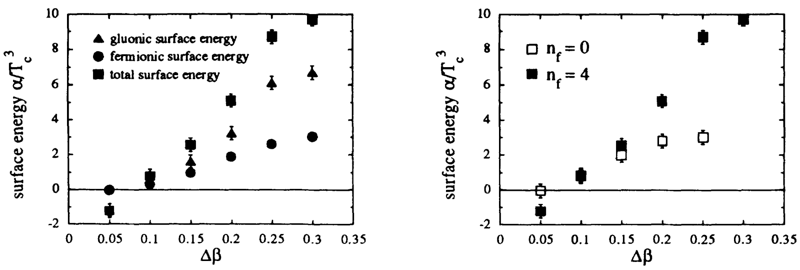

FIG. 7. Total interface tension α/T_c^3 in the presence of dynamical quarks with $n_f=4$ and its gluonic and fermionic contribution (left plot). Comparison of the interface in full QCD with the pure gluonic case (right plot). Error bars denote mean standard deviation.

IV. SUMMARY

This study contains the 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 extensions $N_t=2$ and $N_t=4$, respectively, and presented a compilation of existing data obtained both with the differential and integral method. There is a remarkable agreement between all computations although the extrapolation to the coexisting two-phase system represents a great difficulty, especially with increasing time elongation. Switching on dynamical fermions with four flavors and $N_t=4$ we found that the gluonic and fermionic contributions to the interface tension are of comparable size but again difficult to extrapolate to $T\rightarrow T_c$, at least on our moderate lattice size with limited statistics. Important for astrophysics, we can predict $\alpha/T_c^3\approx 0.1$ 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-principles information for heavy-ion experiments.

For future investigations other than 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 [6]. 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 [18]. A further extension of this subject is to study the curvature term in the free energy of spherical hadronic or quark bubbles in the presence of dynamical quarks [19].

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