Surface tension in finite-temperature quantum chromodynamics

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In a first-order phase transition two phases can coexist at the critical point. The surface free energy α, associated with the interface separating the two phases, is an important parameter for the phenomenology of nucleation in supercooled matter and, more generally, for the whole dynamics of a system undergoing the phase transition. We report on a calculation of the surface tension in quenched QCD on lattices with volumes $6^2\times12\times2$, $8^2\times16\times2$, and $10^2\times20\times2$, as well as on $8^2\times16\times4$ and $12^2\times24\times4$. Our results have been obtained from a Monte Carlo simulation where one half of the lattice is adiabatically brought from one phase to the other by applying a temperature gradient, and where the variation of free energy is calculated at the same time through the average of the action. For $N_t=2$ lattices, we find $\alpha/T_c^3=0.23(3)$ and 0.28(9) on $8^2\times16$ and $10^2\times20$ spatial volumes, respectively. On the other hand, the results from lattices with $N_t=4$ are less well defined and are compatible with a vanishing surface tension. We discuss possible ways to improve the accuracy of the calculation with larger N_t. In particular we propose the use of the Wilson action supplemented with external Polyakov fields as a way to enhance the formation of the interface.

I. INTRODUCTION

The theoretical study of the quark-gluon plasma offers the exciting prospect of making predictions about a completely new state of matter, which may be reproducible in the laboratory through the collision of ultrarelativistic heavy ions.[1] The physics of the plasma also has important implications for cosmology, particularly for the formation of primordial H, He, D, and Li.[2-4] For these reasons a great deal of effort has been and is being invested in the exploration of quantum chromodynamics (QCD) at high temperature.[1] This is particularly true with regard to the numerical simulations of hot QCD on the lattice, which offer a systematic and nonperturbative way for deriving the properties of the quark-gluon plasma entirely from first principles.[5-7]

So far, lattice techniques have mostly been used to study equilibrium properties of hot hadronic matter. The calculated observables include the energy density, the pressure, the chiral condensate, baryonic susceptibilities, and screening lengths.[5-7] The temperature behavior of these and other observables has confirmed the long-suspected presence of a phase transition from a hot hadronic state to a quark-gluon plasma, that is, from a chirally broken, quark-confining phase to a chirally symmetric, deconfining phase. Most numerical simulations of the quenched approximation of QCD, including the recent studies on large spatial volumes,[7,8] support the notion of a first-order phase transition. Moreover, recent simulations of full QCD are also consistent with a first-order phase transition in the chiral limit, although the evidence is more tentative for lack of statistics and of runs on large volumes.[7,9] In such a case two different phases can coexist at the critical temperature and it becomes important to calculate the free energy per unit surface area associated with the interface, or surface tension α.

Surface tension is a fundamental parameter for the description of nucleation and therefore of the time evolution of hot hadronic matter as it proceeds through the transition. In homogeneous nucleation, for example,[10] a bubble of hadrons at temperature $T<T_c$ and pressure p' will be in hydrostatic equilibrium within a medium of supercooled plasma at temperature T and pressure p. Assuming spherical symmetry,

$$p-p'=\frac{2\alpha}{r_h}\ , \tag{1}$$

where r_h is the radius of the bubble. The probability for such a bubble to nucleate in the supercooled plasma will have the form

$$P(T)\propto\exp(-\Delta W/T)\ , \tag{2}$$

where ΔW is the free energy required to produce a bubble

of minimal radius $r \geq r_h$, i.e.,

$$\Delta W = -p'v' + pv' + \alpha A' , \tag{3}$$

and v' and A' are the volume and area of the bubble (see also Fig. 1). Using Eq. (1) and the fact that the bubble is spherical, one derives, for the probability,

$$P_r(T) \propto \exp\left[-\frac{16\pi}{3T_c} \frac{\alpha^3}{(p'-p)^2} \right] , \tag{4}$$

or, in terms of the latent heat H and $\eta \equiv (T_c - T)/T_c$ (using the Clapeyron-Clausius formula),

$$P_r(T) \propto \exp\left[-\frac{16\pi}{3} \frac{\alpha^3}{T_c H^2 \eta^2} \right] \tag{5}$$

(η is also called the "supercooling parameter"[3]).

The surface tension is also important for determining the average distance between nucleation centers.[3,11] In the process of nucleating, a bubble will release some of its latent heat into the surrounding plasma, thereby raising its temperature again and suppressing nucleation. In other words, a lesser surface tension means more nucleation, which in turn means more latent heat returned to the plasma and less nucleation elsewhere in the plasma. For example, Fuller, Mathews, and Alcock[3] obtain the following expression for the distance between nucleation sites:

$$d \approx (4 \times 10^4 \text{ m})(\sigma/\text{MeV}^3)^{3/2}(T_c/\text{MeV})^{-13/2} . \tag{6}$$

In a more general context, the value of the surface tension can be related to the tunneling rate between the degenerate vacua in the symmetry-broken phase due to the finite size of the lattice (tunneling would otherwise be absent at $V \to \infty$).[12-14] Here the tunneling is associated with domain walls of surface free energy αl^2 which separate the different vacua and it can be described as a transition between a symmetric and an antisymmetric combination:

$$|S\rangle = \frac{1}{\sqrt{2}}(|v_1\rangle + |v_2\rangle)$$

and

$$|A\rangle = \frac{1}{\sqrt{2}}(|v_1\rangle - |v_2\rangle) .$$

In a semiclassical approximation, the corresponding energy splitting is[12-14]

$$\Delta E \sim \sqrt{l}\, e^{-\alpha l^3} .$$

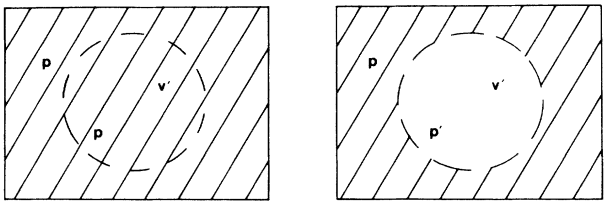

FIG. 1. Supercooled plasma at temperature T and pressure p, with and without a hadron bubble of volume v' and pressure p'.

The above phenomenon has also been studied numerically in the context of the four-dimensional Ising model by Jansen *et al.*[14]

In this paper we will report on the results of extensive simulations of quenched QCD on Euclidean finite lattices with time extent $N_t = 2$ and $N_t = 4$, aimed at calculating the surface tension. In Sec. II, we define the formalism and the algorithm we have used in our calculation. We also briefly review various alternative methods for calculating the surface tension which have been proposed over the years. We present and discuss our numerical results in Sec. III and also consider possible improvements on the calculation. Finally, Sec. IV will contain some concluding remarks.

II. THE SURFACE TENSION IN QCD

A. Definitions, algorithms

The concept of the surface tension α is very similar to that of the pressure p since it parametrizes the amount of work dW done on the system when the interface between the two phases is incremented by an area dA,

$$dW = \alpha\, dA , \tag{7}$$

in analogy with the work brought about by an increment of volume dv,

$$dW = -p\, dv . \tag{8}$$

In general, in a system described in terms of volume, temperature, and chemical potential, the variation of Helmholtz free energy at constant volume is related to α by

$$dF = -S\, dT - N\, d\mu + \alpha\, dA , \tag{9}$$

S being the entropy and N the number of particles. The change of internal energy E has a similar expression

$$dE = T\, dS + \mu\, dN + \alpha\, dA . \tag{10}$$

Connection with statistical mechanics is established through the formula

$$\beta F = -\ln Z . \tag{11}$$

The calculation of the surface tension by means of numerical simulations is in general more difficult than the calculation of quantities such as the internal energy, or the averages of Wilson or Polyakov loop factors, since it involves an evaluation of the free energy F, and therefore of the partition function Z itself.

Over the years, several methods for calculating the surface tension have been proposed and applied mostly in condensed-matter physics.[15] We review here those techniques which can be applied directly to QCD. One such group is based on a phenomenological theory of the interface profile proposed by Van der Waals[16] and refined by others.[17] The emphasis is on the matter density profile $\rho(x)$ describing the interface (Fig. 2), which is subsequently used in the calculation of the surface tension. This is done by assuming that a local Helmholtz free en-

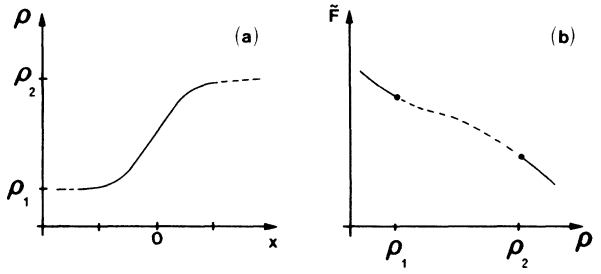

FIG. 2. The spatial dependence of (a) the particle density profile $\rho(x)$, and (b) the free energy $\tilde{F}$ defined in each phase and analytically continued at the transition point.

ergy can be expressed as

$$F(x)=\tilde{F}(\rho(x))+\tfrac{1}{2}A\left[\frac{d}{dx}\rho(x)\right]^2, \tag{12}$$

where $\tilde{F}$ is the free energy functional defined within each phase, analytically continued to the transition point (Fig. 2), and A is a temperature-dependent coefficient of the form $(T_c-T)^{\gamma-2\nu}$.[17] The function $\rho(x)$ can now be obtained by minimizing the surface tension

$$\alpha=-\int_{-\infty}^{\infty}x\frac{dF}{dx}dx\ ; \tag{13}$$

it can also be calculated directly by means of numerical simulations and subsequently used in Eqs. (12) and (13). This approach has many problems, related to limitations inherent to the assumptions implicit in Eq. (12): the use of the profile ρ as an unique parametrization, the use of the quadratic term and the continuity properties of $\tilde{F}$.[17] In particular, the use of ρ implies the risk of neglecting capillary waves on the interface and other important effects.

The advent of high-speed computers has made it possible to approach the problem from first principles. In the simulation of statistical systems, a direct calculation of the internal energy E as well as the integration of Eq. (10) can be implemented in a straightforward manner. The comparison of these results obtained on a lattice with and without the interface thus provides an estimate of the surface tension.[20] A possible problem, however, resides in having to integrate from $T=0$ or $T=\infty$, with the inherent loss of accuracy induced by the accumulation of errors over a large range of couplings.

There exist, on the other hand, methods aimed at computing differences of the free energy directly, without resorting to an integration all the way up to $T=\infty$ or down to $T=0$. In particular, there are those which can be characterized as "sampling" approaches.[19,21,22] In a method proposed by Bennett,[21] for example, the difference of free energies between two couplings β_1,β_2 can be written as

$$\Delta F_{12}=F|_{\beta_2}-F|_{\beta_1}=-\ln Z|_{\beta_2}+\ln Z|_{\beta_1}$$
$$=-\ln\left[\frac{\langle M(\beta_1 S-\beta_2 S)\rangle_{\beta_2}}{\langle M(\beta_2 S-\beta_1 S)\rangle_{\beta_1}}\right], \tag{14}$$

where M is defined as

$$M(x)=\min(1,e^{-x})\ . \tag{15}$$

The quantity ΔF_{12} is the result of two Monte Carlo simulations performed at β_1 and β_2, calculating the average of the function M. In the context of a surface-tension calculation, the two simulations would be for a system with and without the interface.[22]

Another method is that of Binder[19] based on the study of an order parameter that selects those configurations which possess a straight interface separating the lattice in two halves of equal volume and different phase:

$$\rho_{\text{int}}=\begin{cases}0 & \text{no interface,}\\ 1 & \text{with interface}\ .\end{cases} \tag{16}$$

The surface tension is then proportional to the probability of finding $\rho_{\text{int}}=1$: i.e.,

$$P(\rho_{\text{int}})=C\exp\left[-2S\frac{\alpha}{kT}\right]. \tag{17}$$

The goal is to compute this probability numerically, usually by sampling the different outcomes of the simulation. A limitation of this method, however, comes from the need to figure out the volume dependence of the constant C. Having to sample through the complete phase space could also be a problem when handling a large number of degrees of freedom as in QCD. This approach has been used recently in a study of the four-dimensional Ising model.[14]

A last class of algorithms is represented by those which calculate the surface tension directly without resorting to Eq. (11). In the theory of Lenard-Jones fluids for example, one can calculate the average of the so-called pressure stress tensor:[23]

$$\gamma=\int dz[p_{\text{normal}}(z)-p_{\text{tangent}}(z)]\ . \tag{18}$$

In the context of QCD and spin models, Kajantie and Kärkkäinen[24] and Kajantie, Kärkkäinen, and Rummukainen[25] have derived expressions which are similar in spirit. In quenched QCD, for example, the surface tension is calculated via the average of the following operator for an interface in the XY plane:

$$\frac{\alpha S}{kT}=\sum_n\left[\frac{1}{g^2}+\tfrac{1}{2}(c_t-c_s)\right](2P_{tz}-P_{tx}-P_{ty}$$
$$-2P_{xy}+P_{xz}+P_{yz})\ , \tag{19}$$

where $1-P_x^{\mu\nu}$ is the plaquette operator defined on an elementary square of lattice.[6] The accuracy of this approach is directly related to the possibility of obtaining accurate measurements of combinations of plaquettes with opposite signs. This may be problematic in cases where the plaquettes have roughly the same magnitude.

For the purpose of our own calculations, we have used a newly introduced, alternative method,[26] which attempts to maintain the most desirable features of the methods reviewed above, such as the derivation of the results from first principles, while avoiding, for instance, by restricting the integration to a small range of couplings, several of

the sources of error. The method is described in the following section.

B. Integrating with a mixed phase

Our procedure for deriving the surface tension is based on the direct calculation of the variation in free energy induced by the formation of an interface in a lattice, partitioned in two halves which are brought to different temperature.[26] The features which we believe are novel consist in the use of a temperature difference (other fields could also be varied) to induce the interface, accompanied by an integration of the internal energies of the two halves over a limited temperature range, for obtaining the variation of free energy. The advantages are found in the need to integrate only over a very small range of temperatures as well as in the control over the results coming from the fact that several paths, or even different fields, can be used to obtain in principle identical results (cf. Ref. 26). The difficulty one meets is that a limiting procedure, whereby the volume is sent to infinity while the temperature excursion across the critical point is sent to zero, must be followed for extracting the surface tension. This can be demanding in computer time, or, alternatively, can lead to some degree of ambiguity in the extrapolation to vanishing temperature difference if the volume is not large enough.

Equation (14) illustrates one way of obtaining the difference of the free energy between two points in coupling space by calculating the ratio of partition functions. That same difference can be calculated, on the other hand, via an integral of the average action S_g [SU(3) here], since according to Eq. (11):

$$\frac{\partial}{\partial\beta}(\beta F)=-\frac{\partial}{\partial\beta}\ln Z=\langle S_g\rangle_{S_g}\ , \tag{20}$$

where

$$\langle S_g\rangle_{S_g}=Z^{-1}\int[dU]S_g e^{-\beta S_g}\ . \tag{21}$$

More generally, a free-energy difference can be calculated from the average value of any operator O,

$$\frac{\partial}{\partial\lambda}(\beta F)=-\frac{\partial}{\partial\lambda}\ln Z=\langle\beta O\rangle_{S_{\rm new}}\ , \tag{22}$$

if coupled to the action as

$$S_{\rm new}=S_g+\lambda O\ . \tag{23}$$

Having defined the procedure we follow to calculate the variation of free energy, we must still specify how the interface is being set up on the lattice. The code for the numerical simulation of the system has been modified so that the whole lattice can be considered partitioned into two halves, where the couplings can be set independently: $\beta=\beta_1$ in the left half and $\beta=\beta_2$ in the right half [and $\beta=\frac{1}{2}(\beta_1+\beta_2)$ along the interface] (cf. Fig. 3). This is analogous to having the two halves maintained at two different temperatures. An interface between two different phases can, therefore, be generated by setting the couplings in the two halves below and above the critical point, namely $\beta_1=\beta_c-\delta$ and $\beta_2=\beta_c+\delta$.

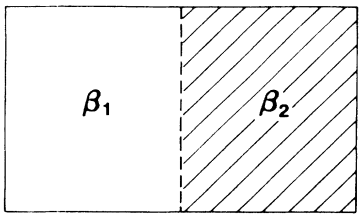

FIG. 3. Partition of the lattice during a Monte Carlo update.

At a finite value of the temperature difference δ, the free energy associated with the existence of the interface can be calculated via the integration of Eq. (20) along the path in coupling space illustrated in Fig. 4. More explicitly, it is obtained from the integral

$$\beta\Delta F_{V,\delta}=\frac{1}{2}\left[\int_{\beta^-}^{\beta^+}d\beta_1\langle S_1\rangle_{\beta_1,\beta^-}-\int_{\beta^-}^{\beta^+}d\beta_2\langle S_2\rangle_{\beta^+,\beta_2}\right]\ , \tag{24}$$

where $\beta^+\equiv\beta_c+\delta$ and $\beta^-\equiv\beta_c-\delta$. The surface tension is then obtained from the limit of infinite-volume and zero-temperature difference:

$$\beta\alpha=\beta\Delta F_s/2A\ , \tag{25}$$

$$\beta\Delta F_s=\lim_{\delta\to 0}\lim_{V\to\infty}\beta\Delta F_{V,\delta}\ . \tag{26}$$

In a numerical calculation the first of the integrals of Eq. (24) is obtained by performing a Monte Carlo simulation and measuring $\langle S\rangle$ in the right half, starting from a configuration at $\beta_1=\beta_2=\beta^-$, and slowly changing β_1 from β^- to β^+ while keeping β_2 fixed at β^-. The second integral is obtained similarly. The factor $\frac{1}{2}$ in Eq. (24) arises from the fact that, in the double difference, the free energy corresponding to the point $(\beta_1,\beta_2)=(\beta^+,\beta^-)$ is counted twice. Another factor $\frac{1}{2}$, appearing in Eq. (25), is included to account for the use of periodic boundary conditions which generate two interfaces of area A.

We notice that the calculation of the difference $\Delta F_{V,\delta}$ will always produce a nonzero result, irrespective of the existence of a surface tension. This is because the finite-

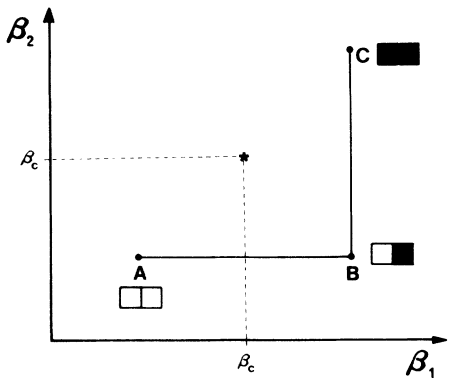

FIG. 4. Path in coupling space for the calculation of the surface tension.

temperature discontinuity will force an interface onto the system in any circumstance. A zero surface tension (at T_c) will simply imply a smooth limit to zero as $\delta \to 0$. On the other hand, a nonzero surface tension will manifest itself in a discontinuous jump in the action. More specifically, the left half of the lattice will undergo a rather sudden transition from the hadronic to plasma phase at a value of β slightly larger than β_c, at $\beta^> \equiv \beta_c + \Delta^>$, when the right half is maintained in the hadron phase at β^- [see the first integral in Eq. (24)]. Similarly, in the presence of a nonvanishing surface tension, the right half will also undergo an abrupt transition from the hadronic to the plasma phase when the left half is kept in the plasma phase, but this will occur at β smaller than β_c, i.e., $\beta^< = \beta_c - \Delta^<$ [see the second integral in Eq. (24)]. This effect is illustrated in Fig. 5. The relationship between the surface tension and the magnitude of the shift in β will be made more explicit below. Let us point out that these jumps will occur for a temperature difference large enough to prevent the system from being overwhelmed by the metastability of the two phases, which normally occur at β_c on a finite volume. There will be some minimum value for δ, which we denote by γ, below which metastability effects take over and make the interface unstable; this will be marked by the point where the slope in $\Delta F_{\delta,V}$ versus δ exhibits a crossover (Fig. 6). One expects γ to be proportional to the inverse power of the ratio $L = V/A$. As shown in Fig. 6, the crossover for δ smaller than $\gamma(L)$ demands that the $\delta \to 0$ limit in Eq. (26) be taken from the range $\delta > \gamma$; a linear extrapolation can then be taken as $\delta \ll 1$. Moreover, as also suggested by Eq. (26), it is important to repeat the calculation on larger volumes, where $\gamma(L'' > L') < \gamma(L')$. The facts that the crossover does indeed approach the $\delta = 0$ axis as $V \to \infty$ and that data from increasingly larger volumes do overlap provide the best legitimization for the extrapolation $\delta \to 0$. This has been shown explicitly in the context of the Potts model[26] and more recently in the Ising model[27] (see also Ref. 28).

It must be remarked that in QCD using two different

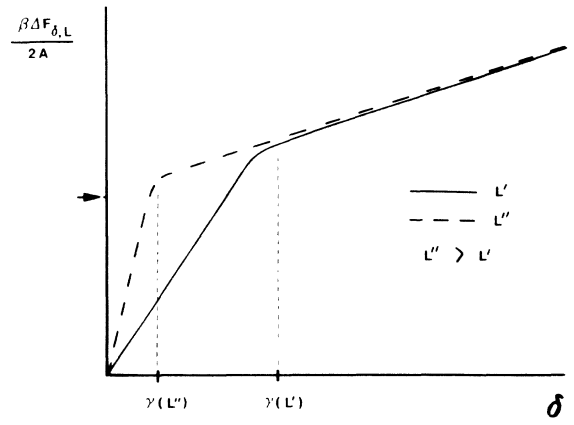

FIG. 6. Anticipated δ dependence of the free energy difference $\Delta F_{V,\delta}$, and definition of the parameter $\gamma(L)$. The extrapolation $\delta \to 0$ from the range $\gamma < \delta \ll 1$ yields the surface free energy at the current volume.

values of the coupling at different locations on the lattice not only changes the physical value of the length of the temporal axis but that of the spatial volume as well. Integrating along a path in coupling space such as the one illustrated in Fig. 4 implies a distortion of the lattice and the introduction of extra volume effects. Ultimately, however, these effects will vanish as the two limits in Eq. (26) are implemented. This corresponds to the fact, already mentioned above, that different paths in parameter space can be equivalently used to derive the surface tension (here the spatial volumes of the two halves are also seen to vary along the paths, because of the distortion of the lattice), an obvious advantage of the method. On a large volume, γ should be small, allowing an extrapolation with $\delta \ll 1$.

It is important to stress that the success of this method rests on the accurate determination of (1) the discontinuity in the action at β_c and (2) the shift of critical coupling ($\Delta^>$ and $\Delta^<$) when one-half of the lattice is changing

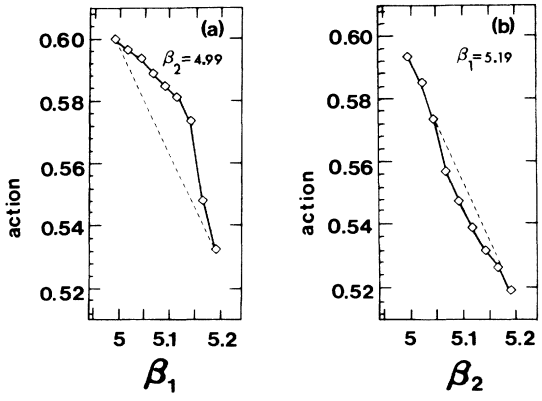

FIG. 5. Variation of the averaged action with respect to β, as two halves evolve along the path of Fig. 4 and Eq. (24). The data were produced on an $8 \times 8 \times 16 \times 2$ lattice, where $\beta_c = 5.095$; here $\delta = 0.10$.

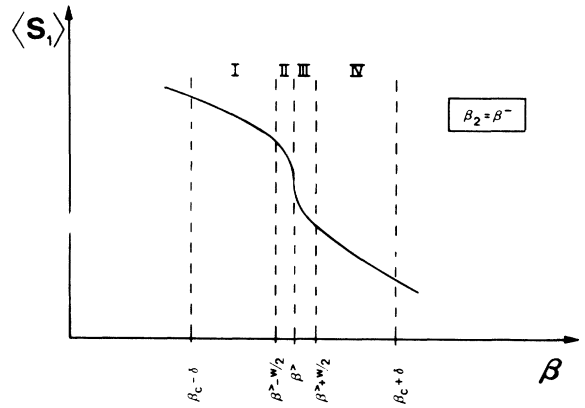

FIG. 7. Four distinct regimes for the slope of the action in lattice half No. 1 (a similar subdivision can be defined for $\langle S_2 \rangle$).

phases. As shown by the data later on, this will depend largely on the aspect ratio N_s/N_t. The dependence of the surface tension on the action discontinuity and on the coupling shifts can be uncovered by trying to evaluate directly the integrals of Eq. (24), using a small number of assumptions. In a first step, each integral is divided into four distinct regions, depending on the magnitude of the slope of the average action (see Fig. 7): regions I and IV, where $(1/VN_t)\partial\langle S_i\rangle/\partial\beta_i$ is always finite and (space-time) volume independent, and regions II and III, where $(1/VN_t)\partial\langle S_i\rangle/\partial\beta_i$ go to infinity as $VN_t\to\infty$. Implicit here is the assumption that the width of regions II and III combined is equal to w. Moreover, it is assumed that V is large enough so that $\gamma,\delta\ll 1$ and also that $\delta > w$. Finally, because of periodic boundary conditions,

$$\int_{\beta^-}^{\beta^+} d\beta_2 \langle S_2\rangle_{\beta^+,\beta_2} = \int_{\beta^-}^{\beta^+} d\beta_1 \langle S_1\rangle_{\beta_1,\beta^+} . \tag{27}$$

In the case where $\delta > \gamma$, using Eq. (27) and partitioning the integrals of Eq. (24) according to the regions defined above, we get

$$\frac{\beta\Delta F_{V,\delta}}{2A} = \frac{1}{4A}\left[\left[\int_{\beta^-}^{\beta^>-\gamma} d\beta_1\langle S_1\rangle_{\beta_1,\beta^-} + \int_{\beta^>-\gamma}^{\beta^>+\gamma} d\beta_1\langle S_1\rangle_{\beta_1,\beta^-} + \int_{\beta^>+\gamma}^{\beta^+} d\beta_1\langle S_1\rangle_{\beta_1,\beta^-}\right] - \left[\int_{\beta^-}^{\beta^<-\gamma} d\beta_1\langle S_1\rangle_{\beta_1,\beta^+} + \int_{\beta^<-\gamma}^{\beta^<+\gamma} d\beta_1\langle S_1\rangle_{\beta_1,\beta^+} + \int_{\beta^<+\gamma}^{\beta^+} d\beta_1\langle S_1\rangle_{\beta_1,\beta^+}\right]\right] . \tag{28}$$

Taylor expansions of the averages $\langle S_1\rangle$ around the points β^-, $\beta^>$, $\beta^<$, and β^+ are then carried out, and keeping the zeroth- and first-order terms allows an explicit integration. In the limit $V\to\infty$, where γ and $\delta\to 0$, the products of the form

$$(\gamma,\beta^>\pm\gamma, \text{ or } \beta^<\pm\gamma)^2\frac{\partial\langle S_i\rangle}{\partial\beta_i}$$

will vanish in regions I and IV. Moreover, if the values of $\langle S_1\rangle$ and of its derivatives on both sides of the singularity dividing regions II and III are assumed to be the same at $\beta^>$ (and $\beta^<$), we obtain

$$\begin{aligned}\frac{\beta\Delta F_{V,\delta}}{2A} = \frac{1}{4A}(\{&\langle S_1\rangle_{\beta^-,\beta^-}(\beta^>-\beta_c+\delta-\gamma)\\ &-\langle S_1\rangle_{\beta^+,\beta^+}(\beta_c-\beta^<+\delta-\gamma)\\ &-\langle S_1\rangle_{\beta^-,\beta^+}[(\beta^>-\beta_c)-(\beta_c-\beta^<)]\\ &+2\gamma(\langle S_1\rangle_{\beta^>,\beta^-}-\langle S_1\rangle_{\beta^<,\beta^+})\}) .\end{aligned} \tag{29}$$

Extrapolating to $\delta\to 0$ is still not easy at this stage since factors such as $\langle S_1\rangle_{\beta^-,\beta^-}$ have a nontrivial δ dependence. On the other hand, one can take advantage of the fact that since $V\to\infty$, Eq. (29) should be a good approximation to the surface tension for $\delta=\gamma$. In terms of the action density s_1,

$$\begin{aligned}\beta\alpha = \frac{N_t}{4}\Bigg[&\left[\frac{V_1}{A}(\beta^>-\beta_c)\langle s_1\rangle_{\beta^-,\beta^-} - \frac{V_1}{A}(\beta_c-\beta^<)\langle s_1\rangle_{\beta^+,\beta^+}\right]\\ &-\frac{V_1}{A}\langle s_1\rangle_{\beta^-,\beta^+}[(\beta^>-\beta_c)-(\beta_c-\beta^<)]\\ &+2\gamma\frac{V_1}{A}(\langle s_1\rangle_{\beta^>,\beta^-}-\langle s_1\rangle_{\beta^<,\beta^+})\Bigg] .\end{aligned} \tag{30}$$

At this point the surface tension should be a constant in the $V\to\infty$ limit. That implies that the critical coupling shifts $\beta^>-\beta_c$, $\beta_c-\beta^<$ have to vary like A/V_1. It also implies that $\gamma\sim A/V_1$.[29] According to Eq. (30), an accurate evaluation of the surface tension requires a clear discontinuity in the action and also a measurable shift in the critical coupling.

On the other hand, if $\delta<\gamma$, the free energy difference $\Delta F_{V,\delta}$ has a different expression. Here, Eq. (24) becomes

$$\frac{\beta\Delta F_{V,\delta}}{2A} = \frac{1}{4A}\left[\int_{\beta^>-\delta}^{\beta^>+\delta} d\beta_1\langle S_1\rangle_{\beta_1,\beta^-} - \int_{\beta^<-\delta}^{\beta^<+\delta} d\beta_1\langle S_1\rangle_{\beta_1,\beta^+}\right] . \tag{31}$$

As with the case $\delta>\gamma$, Taylor expansions are once again used for the integrals Eq. (31). Keeping the lowest order in δ, and using the action density s_1,

$$\frac{\beta\Delta F_{V,\delta}}{2A} = \frac{1}{2A}N_tV_1\delta(\langle s_1\rangle_{\beta^>,\beta^-}-\langle s_1\rangle_{\beta^<,\beta^+}) . \tag{32}$$

Since $\delta<\gamma$, finite-volume metastability mixes the two phases and the difference of the two action densities in the right-hand side of Eq. (32) is very small. There, the surface tension vanishes as $\delta\to 0$ on finite-size lattices. Note the volume dependence of the slope in Eq. (32), which has been confirmed in numerical simulations of the Potts model.[26]

III. NUMERICAL RESULTS

A. An estimate

Unlike hadronic spectroscopy, there is no empirical data, nor any model calculations of the surface tension which could be used in the comparison with the numerical results reported below. But an order-of-magnitude estimate can be attempted using bag-model and current lattice results. The starting point is Eq. (1), which relates α

to the pressure difference inside and outside a hadronic bubble of radius r immersed in supercooled plasma. The meaning of Eq. (1) is that for a finite value of the surface tension, the minimum radius increases to infinity as $\Delta p \to 0$ or as $T \to T_c$. Assuming a radius of 1 fm in the range $T < T_c$, one obtains

$$\alpha/T_c^3 \sim 0.5 \times (1 \text{ fm}) \times \Delta p/T_c^3 . \quad (33)$$

The right-hand side of Eq. (33) vanishes as $\Delta p \to 0$ or $T \to T_c$. This estimate may, however, be meaningful if the temperature dependence of Δp changes by at most an order of magnitude in the range of temperature $T < T_c$. In the following, the equation of state of the bag and the Kallman models[6,30] for both hadronic and plasma phases at $T < T_c$ are used to get such a temperature dependence. For the pressure difference, one gets

$$\text{bag: } \Delta p/T_c^3 = 1.42 \times T_c[1-(T/T_c)^4] ,$$

$$\text{Kallman: } \Delta p/T_c^3 = 1.42 \times T[1-(T/T_c)^3] .$$

On the other hand, one can also use the Clapeyron-Clausius equation[10]

$$\Delta p/H = 1 - T/T_c$$

and write

$$\Delta p/T_c^3 = (H/T_c^4)T_c(1-T/T_c) .$$

Using lattice data for the latent heat H (Ref. 8),

$$\Delta p/T_c^3 = 2.1 T_c(1-T/T_c) .$$

Inserting these three relationships back into Eq. (33) produces the estimates shown in Table I, assuming 1 fm $\times T_c \sim 1$, a value commonly found in lattice SU(3).[6] One first weakness of these estimates may come from the use of 1 fm as a typical radius over a large range of temperature. The assumed value for T_c may also be at fault. Finally, one has all the weaknesses associated with the phenomenological models used here. However, the calculation suggests that it is not unreasonable to expect values of the surface tension in the vicinity of 0.1–0.5.

These values may be compared with the result of a mean-field lattice calculation by Frei and Patkós:[31]

$$\alpha\xi^3 \simeq 0.8$$

(ξ is the correlation length). On the other hand, a recent lattice calculation by Kajantie *et al.*[32] on a $8^2 \times 40 \times 2$ volume has given

$$\alpha/T_c^3 = 0.24(6) .$$

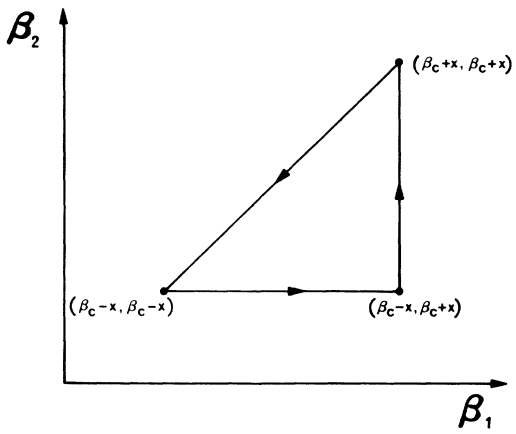

FIG. 8. Closed path for the study of the systematic errors in the integration of Eq. (24).

B. Monte Carlo simulations and error analysis

We have applied the integral approach to the calculation of the surface tension in quenched QCD on several volumes, namely, $6^2 \times 12 \times 2$, $8^2 \times 16 \times 2$, $10^2 \times 20 \times 2$, $8^2 \times 16 \times 4$, and $12^2 \times 24 \times 4$. The Monte Carlo updating was based on the Metropolis algorithm described in Ref. 33. The integrals of Eq. (24) were implemented by using steps $\Delta\beta$ in the range 0.005 to 0.02, depending on β_1 and β_2, the smaller step size being used when closer to the discontinuity at β_c. For each volume, 20 to 40 values of the pair (β_1,β_2) were simulated with 10 000 to 30 000 iterations each. The average action was calculated every 10 iterations.

Systematic errors may be induced if there are hysteresis effects. However, it is easy to check whether these errors are acceptably low for the chosen thermalization rate and integration step size by evaluating the net free energy change along any closed contour in coupling space, which we know should be identically zero (Fig. 8). On a lattice of volume $12^2 \times 24 \times 4$ we have obtained $\beta\Delta F_{V,\delta}/2AT_c^3 = 0.01 \pm 0.30$ for the largest triangular path ($x = 0.12$).

The statistical errors on the surface tension have been estimated by adding in quadrature the statistical error at each point of the integration. We have verified that the separation of 10 iterations between measurements guarantees sufficiently decorrelated results. The main source of error, of course, is due to the finiteness of the integration step. We have estimated it by using first- and second-order summations for the integral. In general, the

TABLE I. Estimate of α/T_c^3 (here 1 fm $\times T_c \sim 1.0$).

Model	$T/T_c = 1.00$	$T/T_c = 0.95$	$T/T_c = 0.80$	$T/T_c = 0.50$	$T/T_c = 0.0$
Bag	0.00	0.13	0.42	0.67	0.71
Kallman	0.00	0.10	0.28	0.32	0.00
C-C/Lattice	0.00	0.05	0.21	0.53	1.05

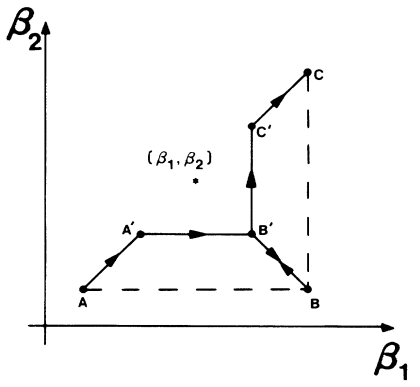

FIG. 9. Computer-time-saving paths in coupling space. Once the free energy corresponding to the path $A'B'C'$ has been evaluated, that of path ABC can be computed more cheaply by using $AA'B'C'C$.

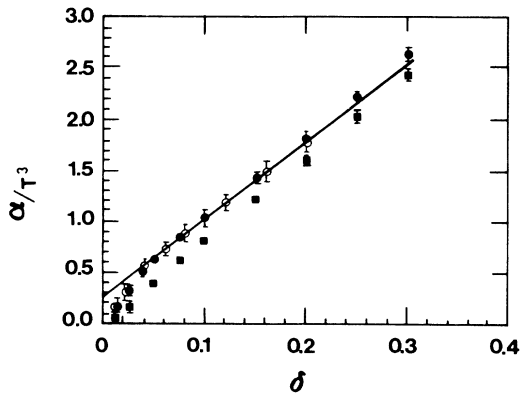

FIG. 10. The surface tension vs δ for $N_t=2$, with spatial volume $6\times6\times12$ (■), $8\times8\times16$ (●), and $10\times10\times20$ (○). The straight line is to guide the eye.

results from the two formulations agreed well within a few percent of error.

The difference of the free energy is, as suggested in Eq. (20), like a potential difference, depending only on the end points of any paths in coupling space. For that reason it is possible to use paths which are less costly in computer time than the basic wedgelike path pictured in Fig. 4. Typically, we have used paths such as the one illustrated in Fig. 9, which include the results of the simulations already done for another value of δ.

Let us now present our results, in terms of the number of time sites N_t.

$N_t=2$. Figure 10 and Table II show the resulting surface tension, rescaled by T^3, as a function of δ. The two largest volumes provide consistent values for the extrapolation to $\delta\to0$ performed in the range $\delta>0.025$:

$$\frac{\alpha}{T_c^3}=\begin{cases}0.229(29) & \text{on } 8^2\times16,\\ 0.277(88) & \text{on } 10^2\times20\ .\end{cases} \tag{34}$$

In contrast, the $6\times6\times12\times2$ data seem to extrapolate to a value consistent with zero. The difference between the $N_s=6$ and the $N_s=8,10$ results is due to the fact that there is too much tunneling in the smallest volume to keep a stable interface. The above result is consistent with the estimates shown in Table I. It also agrees well with that of Kajantie *et al.*;[32] however, the slope in the (nonphysical) regime $\delta\neq0$ is different in both studies. Let us recall that in Ref. 32 the surface tension is calculated directly from the derivative of $\ln Z$ with respect to an element of area in the plane of interface [see Eq. (19)]. It is possible that the vacuum contributions are handled differently, as evidenced by the comparison between the results of the two methods in QCD and in the Potts model.[28]

$N_t=4$. The data for the simulations performed on $8\times8\times16\times4$ and $12\times12\times24\times4$ volumes are shown in Fig. 11 and Table III. There is no indication of a finite surface tension for the extrapolation to $\delta\to0$. We notice

TABLE II. The surface tension for $N_t=2$.

δ	α/T_c^3, $(6\times6\times12)$	α/T_c^3, $(8\times8\times16)$	α/T_c^3, $(10\times10\times20)$
0.010			0.168(84)
0.012	0.067(66)	0.171(60)	
0.020			0.312(84)
0.025	0.175(54)	0.336(51)	
0.050	0.406(36)	0.624(36)	0.648(75)
0.075	0.621(24)	0.827(30)	
0.080			0.888(75)
0.100	0.819(12)	1.023(18)	1.032(90)
0.120			1.176(93)
0.150	1.208(24)	1.403(27)	
0.160			1.488(99)
0.200	1.613(36)	1.795(39)	1.776(105)
0.250	2.016(51)	2.208(51)	
0.300	2.433(63)	2.630(63)	
0.000[a]	0.017(25)	0.229(26)	0.277(88)

[a]Extrapolated values.

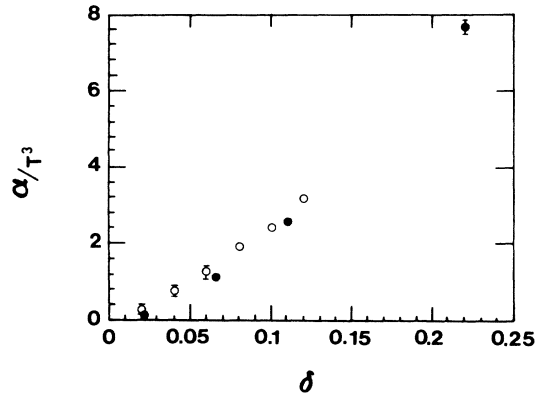

FIG. 11. The surface tension vs δ for $N_t=4$, with spatial volume $8\times8\times16$ (●) and $12\times12\times24$ (○).

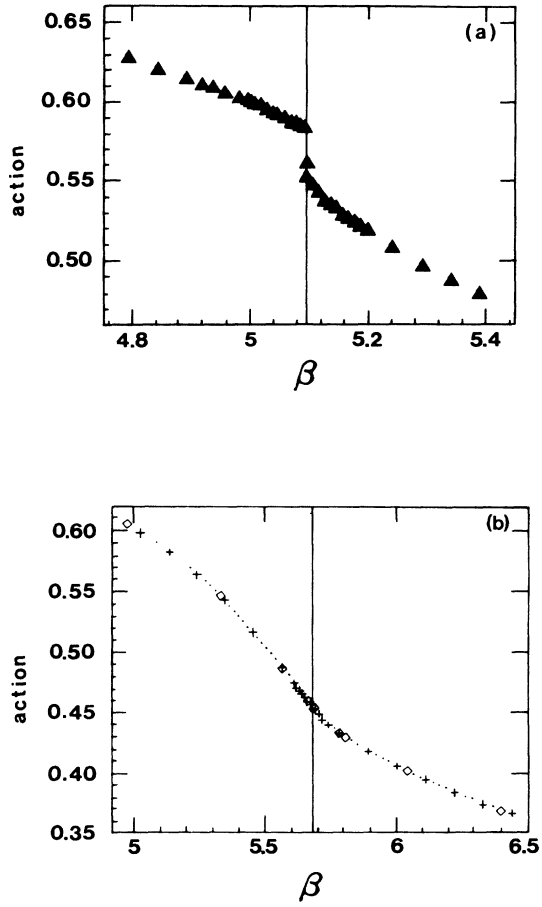

FIG. 12. Action density as a function of the coupling constant β: (a) $N_t=2$ (triangles), (b) $N_t=4$ (diamonds and crosses).

that, with $N_t=4$, our lattice gives no sign of an appreciable discontinuity of the action at the critical point (assuming, of course, a first-order phase transition[7]). This lack of discontinuity is illustrated in Fig. 12, which should be contrasted with the corresponding graph for $N_t=2$. Our difficulty in extracting a finite surface tension may depend on the weakness of the discontinuity in the observable, namely, the action, that we have used as integrand in the evaluation of the free energy. Let us mention that the lack of evidence for a measurable value of the surface tension is also consistent with the latest calculation of Kajantie *et al.* on an $8^2\times40\times4$ lattice.[34]

Assuming that there is a finite surface tension and that the negative result for $N_t=4$ is due to limitations in the present calculation, the situation should be improved by going to larger lattices. Better results could also be obtained without going to extremely large lattices, by computing the free energy from Polyakov lines instead. Indeed, using the action

$$S=S_g+\sum_{\mathbf{x}}(h^*L_{\mathbf{x}}+hL_{\mathbf{x}}^*)\ , \tag{35}$$

where S_g is the standard Wilson pure gauge action, $L_{\mathbf{x}}$ the Polyakov line,[6] and $h=h^R+ih^I$ the corresponding coupling constant, the free energy can be obtained from Eq. (22). The surface tension is obtained from a procedure analogous to the temperature-partitioned lattice method outlined in the previous section. Given the well-known fact that the Polyakov line exhibits a discontinuity sharper than that of the plaquettes on volumes greater than $8^3\times4$, this alternative approach promises interesting results on the $N_t=4$ lattices studied here.[35]

TABLE III. The surface tension for $N_t=4$.

δ	α/T_c^3, $(8\times8\times16)$	α/T_c^3, $(12\times12\times24)$
0.020		0.280(143)
0.022	0.084(164)	
0.040		0.760(122)
0.060		1.241(96)
0.066	1.111(83)	
0.080		1.920(77)
0.100		2.431(55)
0.110	2.580(46)	
0.120		3.185(77)
0.220	7.660(184)	

IV. CONCLUSIONS

We have reported the results of a calculation of the surface tension in quenched QCD, on $N_t=2$ and $N_t=4$ lattices. The algorithm used in this work was based on free energy differences calculated by means of an integration of the action in coupling space; the interface was generated by setting the two halves of the lattice at two different temperatures. In the case of $N_t=2$ we were able to obtain a nonzero value for α/T_c^3, which agreed with the recent calculation of Kajantie *et al.*[32] For $N_t=4$ lattices, however, no evidence of a finite surface tension was obtained. We briefly discussed possible reasons for this

negative result (spatial volume too small, given the weakness of the discontinuity of the action) and the use of the Polyakov lines as a way out of this problem.

Much remains to be done in the study of phase interfaces in QCD, in addition to the above calculation on larger volumes. One interesting issue in the context of lattice SU(3) theory is the calculation of the surface tension between domains of gluon plasma in different Z_3 vacua, denoted by α^{gg}, and its relationship with the surface tension between hadronic and gluon-plasma phases calculated in this work ($\alpha=\alpha^{gh}$). Recently, Frei and Patkós[36] have studied the possibility of having perfect wetting, i.e.,

$$\alpha^{gg}\approx 2\alpha^{gh} , \tag{36}$$

at least within the mean-field approximation. The techniques described in this paper can be applied directly to the study of such phenomena, particularly by using external Polyakov fields [see Eqs. (22) and (35)] in order to establish an interface between two deconfined Z_3 vacua.[35]

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