Surface tension of nucleating hadrons using the free energy of an isolated quark

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We report on a new method of calculating the surface tension in quenched lattice QCD, in which an external field coupled to the Polyakov lines is applied to generate the interface between the confined and the deconfined phases. The free energy associated with the interface is then computed from an integral of the average Polyakov line with respect to the strength of the external field. We have tested this new approach on a $16\times16\times32$ spatial volume, using a temporal size of $N_t=4$ for which all previous attempts at computing the surface tension have failed. A clear signal has been seen, giving $\alpha/T_c^3=0.027(4)$, or $\alpha=5$ MeV/fm^2. This represents a very small cost in free energy for hadrons to nucleate from a hot plasma.

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I. INTRODUCTION

A major impediment to the identification of the quark-gluon plasma in heavy-ion collisions is the lack of theoretical knowledge concerning the time behavior of the plasma during cooling, especially near the critical temperature T_c where the transition into the hadronic phase takes place [1]. Although progress has been made by using relativistic hydrodynamics [2], important aspects of the transition remain unknown, in particular those relative to the hadronization of the plasma as it reaches T_c and below. The mounting numerical evidence in favor of a first-order transition both in quenched lattice QCD [3,5] and in full QCD with at least three flavors of light quarks [4,5] suggests that hadronization may take place through the nucleation of hadronic droplets in a supercooled plasma [6–9]. This possibility is all the more exciting since many features of nucleation processes can then be related to equilibrium quantities, for whose determination lattice techniques are especially well adapted. One example of the relation between equilibrium and nonequilibrium properties is found in the classical theory of nucleation, where the surface tension α plays a central role in determining the nucleation rates [8,9].

The past 2 years have seen the first results from the computation of the surface tension in quenched QCD, by numerical methods [10–14] as well as analytically, in the mean-field approximation [15]. When performed on $N_t=2$ lattices, the numerical studies have produced similar values: namely, $\alpha/T^3=0.12(2)$ [10] and 0.24(6) [13] on spatial volumes of $8^2\times16$ and larger. Huang, Potvin, Rebbi, and Sanielevici [10] have followed an approach where the free energy is obtained from the integration of the average action in the space of the coupling $\beta=6/g^2$ [16]. Kajantie, Kärkkäinen, and Rummukainen [13], on the other hand, have calculated the thermal average of a surface tension operator [12] obtained from a derivative of the partition function with respect to the area of the interface. This operator consists of differences of plaquettes parallel and perpendicular to the plane of the interface and bears some analogy to those operators that have been used for the calculation of the energy density and pressure [17]. The integral method is, in principle, exact, while the differential method is approximate. In the latter, one needs as input the derivatives of g^{-2} with respect to lattice dilatations [17], which are known only in the weak-coupling limit. As documented by several studies [18], the perturbative nature of the coefficients used in the differential approach severely limits its accuracy near the deconfinement transition, known to take place in the strong-coupling regime on $N_t=2$ and 4 lattices. Moreover, the integral method is more flexible, since, as shown below, any external field can be used to generate the interface provided that it induces the phase transition. This is a major advantage that has allowed us to overcome the difficulties previously encountered in the extension of the calculation to $N_t=4$. The differential method requires the simulation of QCD at fewer values of the coupling than in the integral method, where the range of integration, albeit restricted to a small interval

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around the transition, must nevertheless be filled by a sufficient number of integration points. Thus, the differential method appears *a priori* less costly in computer time, although such an advantage may be well offset by the need of working with substantially larger statistics and bigger volumes to reproduce the accuracy that the other method can provide with a judicious choice of the external field.

Both methods have been tried on $N_t=4$ lattices, with much less success than for $N_t=2$, however, as they failed to reveal any clear signal for a nonzero surface tension [10,13,14]. One reason may be the spatial size used, $8\times8\times16$ (or 40) and $12\times12\times24$, too small to generate a measurable discontinuity in the action, i.e., in the variable conjugate to the external field used to induce the transition [10]. Accordingly, we are proposing here to take fundamental advantage of the fact that arbitrary combinations of external fields can be used in the integral approach, provided they induce the transition, and to base the calculation of the surface tension on the expectation values of the Polyakov lines. It is a well-known fact that the Polyakov line exhibits a stronger discontinuity at the transition point than the action. This new technique should therefore be more sensitive to the phase transition in smaller systems. Our new approach is described in detail in the following section. The numerical results are described in Sec. III (a preliminary analysis was presented in [11]) and are followed, in Sec. IV, by a short discussion focusing on the comparison between the $N_t=4$ and 2 results.

II. EXTERNAL FIELD COUPLED TO POLYAKOV LINES

The computation of the surface tension is usually carried out by calculating the free energy F/kT associated with the presence of an interface separating two coexisting phases, in our case the low-temperature (hadronic) phase and the high-temperature (quark-gluon plasma) phase. In the integral approach, it is obtained from the integration with respect to some coupling constant driving the phase transition. In Ref. [10] the integration variable used was the bare coupling constant; here we will be using an external field coupled to the Polyakov lines.

Consider the lattice action

$$S=S_W+S_E \ , \tag{1}$$

where

$$S_E=-\tfrac{1}{2}\sum_{\mathbf{x}}[hL^*(\mathbf{x})+h^*L(\mathbf{x})] \ . \tag{2}$$

S_W is the standard Wilson action for SU(3) defined in terms of the compact gauge variables $U_\mu(x)=\exp[iA_\mu(x)]$. $L(\mathbf{x})$ is the Polyakov line [19]:

$$L(\mathbf{x})=\tfrac{1}{3}\mathrm{tr}\prod_{x_0=1}^{N_t}U_0(x_0,\mathbf{x}) \ . \tag{3}$$

The coupling h is a complex constant, taken to be independent of β. This new action describes quenched QCD in the presence of the external field h. The variation of free energy of the system can be obtained from the integral in h space of the thermal average of the Polyakov line, since

$$-V\langle \mathrm{Re}L\rangle=-\frac{d\ln Z}{d\,\mathrm{Re}h}=\frac{dF/kT}{d\,\mathrm{Re}h} \ , \tag{4}$$

$$-V\langle \mathrm{Im}L\rangle=-\frac{d\ln Z}{d\,\mathrm{Im}h}=\frac{dF/kT}{d\,\mathrm{Im}h} \ . \tag{5}$$

As in Ref. [10], the surface tension is obtained by first dividing the volume of the lattice into two halves, in which β and h can be set independently to β_1, β_2, h_1, h_2. An interface between an ordered phase, with a nonzero $\langle \mathrm{Re}L\rangle$, and a disordered phase, with a zero $\langle \mathrm{Re}L\rangle$, is then created and removed by a suitable path in the space of the variables β_1, β_2, h_1, h_2. As shown in Fig. 1, we start with a homogeneous system in the ordered phase with $\tilde{h}_1=\tilde{h}_2=\tilde{h}$ (where we have set $\mathrm{Im}h=0.0$ throughout and introduce the tilde to indicate real values for h) and $\beta_1=\beta_2=\tilde{\beta}$, where $\tilde{\beta}$ lies slightly below the critical value β_c. The interface is introduced by lowering $\tilde{h}_1$ adiabatically to zero. In practice, since $\tilde{\beta}$ is lower than β_c, this should be sufficient to bring one-half of the system to the disordered phase. In principle, the efficiency of the procedure in sampling the disordered phase can be increased by performing an excursion in β_i. A major advantage of our technique is the freedom of varying the parameters along a wide class of paths. Finally, the whole system is brought back to a homogeneous, now disordered phase, by lowering $\tilde{h}_2$ to zero as well, following the same path. As in [10], the surface tension of physical interest is obtained from the difference of the two paths, in the limits $V\to\infty$ followed by $\tilde{h}\to0$. In addition, $\tilde{\beta}$ should approach the infinite volume critical value β_c. In our calculation at finite volume we have taken $\tilde{\beta}$ sufficiently close to β_c so that we believe this is not a serious source of error.

It should be pointed out that this procedure can be used with any external fields in S, provided that they generate the correct phase transition near the zero-field limit. In other words, because we are ultimately interested in

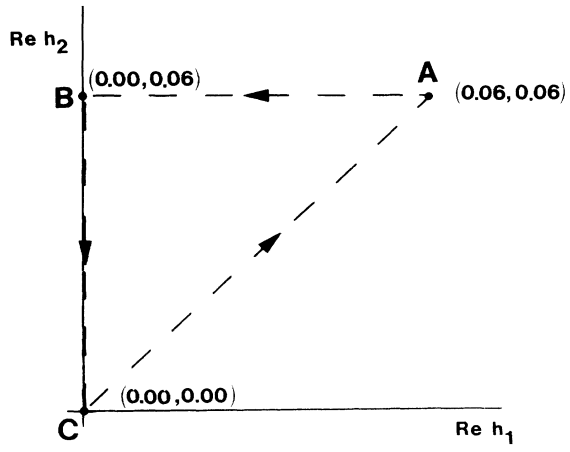

FIG. 1. Integration path for the computation of the surface tension.

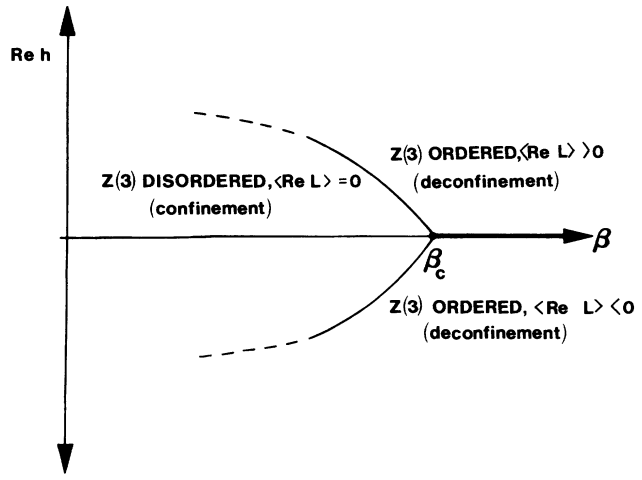

FIG. 2. Conjectured phase diagram of quenched QCD with an external Polyakov field. A first-order phase transition is represented by a solid line; phase transition of unknown character corresponds to dashed lines.

the surface tension between the Z_3-ordered and -disordered phases at β_c, and because the external field S_E is used to generate and stabilize the interface, it is essential that the correct phase transition be recovered in the limit of a zero external field. This condition is satisfied with the use of the Polyakov line (2). The phase diagram of such an extended QCD can be understood as follows: the first-order phase transition is well established in the absence of the external fields ($h=0$) [3]. It is natural to expect that this first-order transition point will continue itself into the domain of finite h, at least for small enough h. This line of first-order transition is illustrated in Fig. 2 and defines the values of the coupling h_c (or $\mathrm{Re}h_c$). On the other hand, the line in the range $\beta > \beta_c$ separates two different types of ordered states: $\langle \mathrm{Re}L \rangle > 0$ and $\langle \mathrm{Re}L \rangle < 0$. The whole situation is analogous to the three-dimensional three-state Potts model [20].

There are two main sources of systematic errors to worry about: namely, large integration steps and low statistics. Both give rise to hysteresis effects which will bias the computation of the Polyakov line averages. These effects are particularly important near the critical coupling h_c. Hysteresis can be easily revealed in the calculation of the net free energy around any closed loop, such as the loop ABC in Fig. 1; because on finite size systems the free-energy is a nonsingular thermodynamic potential, it must have a zero variation around any closed loop. In order to reduce potential hysteresis effects, it is best to use an integration measure $d(\mathrm{Re}h)$ ten times smaller near the transition line as the measure away from it. Likewise, the statistics in the line averages should also be increased near h_c.

III. RESULTS

The computations were carried out on the Boston University Connection Machine 2, using a $\frac{1}{4}$ configuration or 16 384 processors. In such a configuration, a Metropolis code written in C updates a 16^4 lattice in quenched QCD at a sustained rate of 300 Mflops. For the purpose of calculating the surface tension, a lattice of size $16\times16\times32\times4$ was considered. On such a space-time volume, the transition point has been located at $\beta_c=5.690$ [3,21]. As shown in Fig. 1, the values of the Polyakov couplings were taken in the range $0<\mathrm{Re}h<0.06$ and the value of the gauge coupling set to $\beta=5.685$. $\mathrm{Im}h$ was set to zero throughout the calculation. The integration steps were of magnitude $d(\mathrm{Re}h)=0.01$–0.02 away from h_c, and $d(\mathrm{Re}h)=0.001$–0.002 in its vicinity. 8000–15 000 iterations away from h_c, and 50 000–80 000 iterations near h_c were accumulated for each value of the pairs $(\mathrm{Re}h_1, \mathrm{Re}h_2)$, measuring $\mathrm{Re}L$ every 10 sweeps. At $\beta=5.685$, h_c is located at $\mathrm{Re}h\sim0.004$.

The update of the lattice configurations were performed with the overrelaxed Metropolis algorithm [22]. The standard checkerboard algorithm cannot be used in the presence of Polyakov fields in the action because, unlike S_W which has only nearest-neighbor interactions, S_E spans the full lattice in the temporal direction. The update procedure was therefore performed using the checkerboard pattern on the space-time plaquettes on time slices 1,2 and 3,4 separately.

The computation of the surface tension hinges on the subtraction of the net free energy associated with the legs AB and BC in Fig. 1, requiring two numbers computed with high accuracy. At $\tilde{h}=0.06$, for example, they have values $\delta F=0.686$ and 0.616, respectively (in units of α/T^3), leading to a surface tension $\alpha/T^3=0.070$. An accuracy of 1 part in 10^3 is therefore needed in such a computation. The calculation of the free energy along the closed path ABC will require a similar accuracy; in our example ($\tilde{h}=0.06$), one obtains $\delta F=0.002(8)$ along the largest closed path available, a value consistent with zero as expected.

The values of the surface tension for $\tilde{h}<0.06$ and its extrapolation to zero Polyakov coupling are displayed in Fig. 3 and Table I. The statistical errors were computed

TABLE I. The surface tension vs $\mathrm{Re}h$. The error is the combined systematic and statistical errors. The asterisk and dagger refer to extrapolated values to $\mathrm{Re}h=0$ by using the data of $\mathrm{Re}h>0.006$ and $\mathrm{Re}h>0.008$, respectively.

$\mathrm{Re}h$	α/T_c^3	Error
0.002	0.004	0.007
0.004	0.015	0.007
0.006	0.028	0.007
0.008	0.032	0.007
0.010	0.036	0.007
0.020	0.044	0.006
0.030	0.050	0.005
0.040	0.055	0.005
0.050	0.062	0.005
0.060	0.070	0.004
0	0.027*	0.004
0	0.029†	0.005

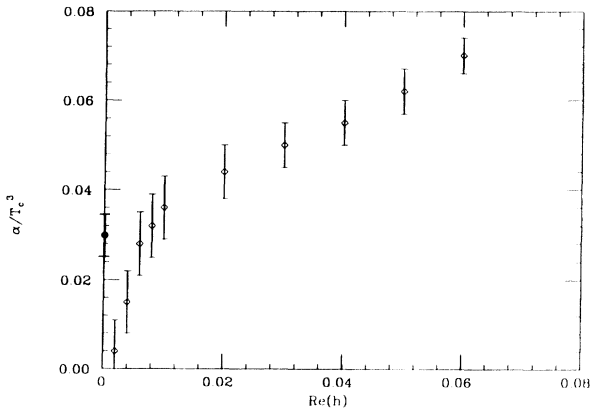

FIG. 3. α/T_c^3 vs $\tilde{h}$. The solid line is the result of its extrapolation to $\tilde{h}\to 0$ from $\tilde{h}>0.01$.

by first using the jackknife method [23] on the data sample of $\langle \mathrm{Re}L \rangle$. Jackknife block sizes of $\tilde{N}=10$–50 measurements (away from h_c) and 750 measurements (near h_c) were ultimately chosen. The statistical error on the value of the surface tension was then obtained by adding in quadrature the errors on $\langle \mathrm{Re}L \rangle$ along the same integration path.

Table I and Fig. 3 quote the combined statistical and systematic error on the value of the surface tension. The systematic error is due to the integration step and has been estimated to be of order 0.001 (in units of T_c^3) by computing the contribution of the next-higher-order term in Simpson's rule. The effect of such a systematic error is a upward or downward shift in the data of Fig. 3.

The presence of a break in the slope of the surface tension in Fig. 3 is a finite-size effect, arising from the inability of the system to support a stable interface on a $16\times16\times32$ spatial volume when the applied field $\tilde{h}$ on the Polyakov loop is too small. This minimum field [16] $\tilde{h}=\gamma$ is approximately $\gamma=0.01$ for our lattice. The extrapolation to $\tilde{h}\to 0$ is therefore carried out by fitting a straight line in the range $\tilde{h}>0.01$, for which one obtains $\alpha(\tilde{h}=0)/T_c^3=0.027(4)$, the value of the surface tension in quenched QCD with $N_t=4$. Measured in lattice units, this result is about 40 times smaller than that of the $N_t=2$ case, thus explaining the difficulties encountered in the previous studies [10,12–14] which have used the action to compute the free energy.

Knowing the value of the surface tension allows us to estimate the value of γ for arbitrary lattice sizes, provided that γ is small and α near the infinite volume limit. Indeed, the point at which the bulk volume free energy is approximately equal to $\mathrm{Re}h\times\langle \mathrm{Re}L \rangle$ and also equal to the cost in free energy due to the formation of the interface gives $\gamma d\langle \mathrm{Re}L \rangle=(2S/2V)\alpha/T$. Applying this criterion to the results of the present simulation gives a check on the internal consistency of our calculation, and indeed gives $\gamma=0.01$.

Other effects of the finite lattice size within the region of interface stability can be studied by considering the profile of the Polyakov line averages with respect to coordinate z, as shown in Fig. 4. Whereas the line develops a clear and wide plateau in the region of nonzero Polyakov coupling, such is not the case in the region of zero $\tilde{h}$, where no plateau is seen but a broad minimum located at the midpoint of the half-lattice. Longer lattices are clearly needed to simulate properly a disordered half in the presence of a polarized one [13]. However, this finite-size effect has less severe consequences in the integration approach since only the average of the Polyakov line in the half-lattice with nonzero strength $\tilde{h}$ (the right half) is con-

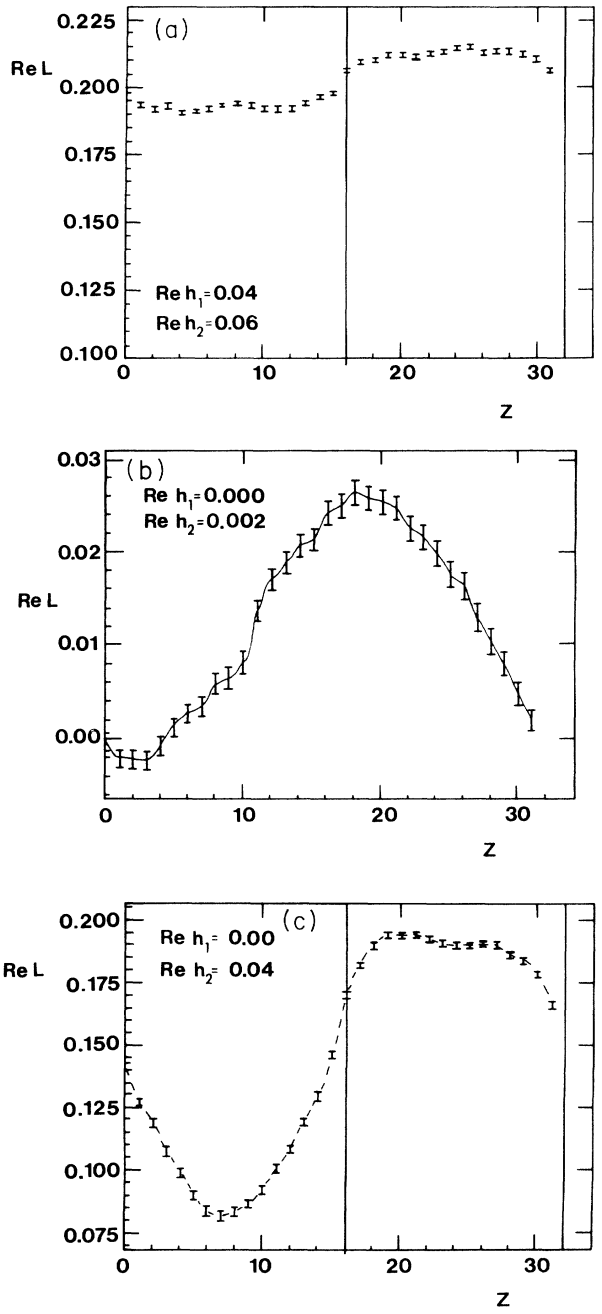

FIG. 4. Profiles of the Polakov line (real part) along the coordinate normal to the interface.

sidered in the integration path BC. In fact, since most of the calculation has a nonzero Polyakov strength, these finite-size effects will be minimized because the external field imposes a well-defined length scale of about $N_z/2$. Of course, this scale is destroyed by metastability at small $\tilde{h} < \gamma$, as shown in Fig. 4.

IV. CONCLUSIONS

Previous simulations on small spatial volumes using plaquettes as derivatives of the free energy were unable to get a meaningful value for the surface tension [10,12–14] on $N_t=4$ lattices. Those results indicate that a much larger spatial volume, perhaps as large as $24^2\times 48$, would have to be considered in order to see clearly the discontinuity in the plaquette at the transition point. A new method was presented here as an alternative for medium sized lattices, where the interface and the free energy are defined in terms of Polyakov line averages. In addition to relying on a more sensitive variable at the phase transition, this method is, in principle, exact and less sensitive to finite volume effects. By simulating quenched QCD on a $16\times 16\times 32\times 4$ lattice, a value of $\alpha/T^3=0.027(4)$ was obtained. This result can be compared with the result from $N_t=2$ lattices (using the integral approach), $\alpha/T^3=0.12(2)$ [10]. No scaling due to asymptotic freedom is seen as yet. This situation is similar to the lack of scaling observed with $T_c/\Lambda_{\rm QCD}$, which change by as much as 60% by going from $N_t=2$ to 8 [19,21]. This should not be surprising given the relatively strong value of the gauge coupling β at which the phase transition is located for $N_t=2$ and 4 lattices. Longer temporal extensions are clearly needed to see asymptotic scaling.

It is interesting to note how small the value of the surface tension is when expressed in physical units. In quenched $N_t=4$ lattice QCD, $T_c=200$ MeV [4], so that $\alpha=5$ MeV/fm^2. Although the computations reported here are still far from the continuum limit and did not include the effects of the internal quark loops, the result indicates that only a very small amount of free energy is required for hadrons to nucleate from the quark-gluon plasma, thus diminishing the importance of supercooling and other nucleation effects in plasma dynamics.

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