# Surface tension in SU(3) at finite temperature

Nelson A. Alves
*Departamento de Física Matemática, Instituto de Física, Universidade de São Paulo, Caixa Postal 20516 01498 São Paulo, São Paulo, Brazil*
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In a first-order phase transition two phases can coexist in thermal equilibrium at the critical temperature with a stable interface inbetween. We explore the spectral density reweighting techniques to calculate the bulk free energy barrier $\Delta F$ and the surface tension $\alpha$ associated with this interface. We analyze data from a Monte Carlo simulation on $L_t L^3$ ($L_t=2,4$) lattices for the SU(3) deconfining phase transition. By combining different Monte Carlo simulations with finite-size scaling we establish a procedure to improve the evaluation of $\Delta F$.

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## I. INTRODUCTION

During recent years the lattice Monte Carlo (MC) calculations of QCD at finite temperature have led to a better understanding of its phase diagram [1]. Because of the first-order nature of the phase transition there exists a mixed phase at the critical temperature $T_c$, at which the hadronic phase and quark-gluon plasma phase can coexist. Corresponding to these coexisting bulk phases there is an interface tension. The free energy per unit surface area associated with this interface, or surface tension $\alpha$, is an important parameter to describe the dynamics of interfaces. It plays an important role in achieving a quantitative description of the nucleation process in the phase transition from quark-gluon phase to the hadronic phase in early Universe [2].

Recently, Monte Carlo methods have been proposed to calculate the surface tension in lattice QCD [3,4], and results have been reported to its pure SU(3) gauge sector. For $L_t=2$ the values are $\alpha/T_c^3=0.12(2)$, using the path method in the $\beta$ coupling space [3,5], and $\alpha/T_c^3=0.08(2)$ for the operator method [4].

For $L_t=4$ the values are less conclusive and the results have been compatible with zero due to large statistical error [4]. The recent generalization of the path method gave the first estimate for the surface tension [5] $\alpha/T_c^3=0.024(4)$. This confirms the trend of a weaker first-order transition as one increases $N_t$ from 2 to 4 in SU(3) deconfining phase transitions [6].

Here we also address the same problem: the calculation of the free energy and the surface tension in SU(3) at finite temperature.

For this purpose we apply an alternative method [7,8] which exploits the finite-size scaling (FSS) of the barrier between the coexisting phases at the critical point by means of the energy probability distribution. This method is extended to the continuous energy distribution obtained in previous investigations of SU(3) deconfining phase transitions on $L_t L^3$ ($L_t=2,4$) lattices [9]. The simulations were done by using the MC updating of Ref. [10] and to obtain the energy distribution at the critical point we apply the reweighting technique [11].

We show that an improvement can be reached when we combine MC simulations at different couplings in such a way that the error of the calculated quantity is minimized [9]. This improvement is more relevant for $L_t=4$, where the signal for the transition is pronounced only for large lattice sizes. However, the suppression of tunnelings increases with the lattice size and in that case we would need a sufficiently long MC run to include many tunneling events. To overcome this difficulty the multicanonical MC algorithm was recently proposed [12] to enhance configurations dominated by the interface. Nevertheless for $L_t=4$ a good estimate of the probability distribution was achieved when one combines MC simulations obtained in a small neighborhood of the critical $\beta$, which enabled us to evaluate $\Delta F$ and $\alpha$.

In Sec. II we review the spectral density reweighting technique and our procedure of patching different MC simulations to obtain the energy distribution at the critical $\beta$. In Sec. III we present our estimates of the bulk free energy and the surface tension for $L_t=2$ and 4, while Sec. IV contains a summary and conclusions.

## II. SPECTRAL DENSITY MC CALCULATIONS AND SURFACE TENSION

We simulated the SU(3) Wilson action

$$S=\sum_p S_p \quad \text{with } S_p=\tfrac{1}{3}\mathrm{Tr}(U_p)\ , \tag{2.1}$$

where $U_p$ is the ordered product of link matrices around the plaquette $p$ on a $L_t L^3$ lattice, with periodic boundary conditions. $\beta$ is related to the coupling constant, $\beta=6/g^2$, and the temperature is given by $T=1/aL_t$, for a lattice with spacing $a$.

We measured the action $S$ and introduced a convenient normalization, the action per plaquette $s=S/V_p$, where $V_p=6L_t L^3$ is the total number of plaquettes.

Because of the continuous nature of SU(3) action density we collected all measurements after every sweep through the lattice to a disk. Thus we avoided the initial introduction of a histogramming as a storage method. This storage procedure provided us with the full empiri-

 

cal time series of configurations for each MC simulation.

With the available time series, the reweighting technique allows us to calculate an estimator $\bar{f}(\beta)$ for the physical observable $f$, in a small neighborhood $\Delta\beta$ of the simulated point $\beta_0$:

$$\bar{f}(\beta)=\frac{F}{Z} \quad \text{with } F=\sum_{n=1}^{N} f_n \exp(\Delta\beta S_n) ,$$
$$Z=\sum_{n=1}^{N} \exp(\Delta\beta S_n) \quad \text{and } \Delta\beta=\beta-\beta_0, \tag{2.2}$$

where $N$ is the total number of measurements. This range will depend on whether our statistics obtained at $\beta_0$ can still give meaningful results at the distance $\Delta\beta$. We defined this appropriated range depending on which percentage of our statistics we expect to be representative of an importance sampling at the new coupling $\beta$. This translates into a relevant interval $\Delta\beta=\beta_{\max}-\beta_{\min}$ where one can apply the reweighting technique. This interval was obtained from our empirical action density values by using the concept of $q$ tiles $s_q$ [9,13], with $q=0.025$.

When one has runs at different $\beta_0^i$ values ($\beta_0^{i+1}>\beta_0^i$, $i=1,\ldots,P$) we can presumably combine them to improve our estimate for $\bar{f}(\beta)$. Various methods have been proposed for patching [14–17]. However, for our purposes of combining different histograms we patch only the ones whose validity $\beta$ ranges overlap and this leads to a very straightforward approach [9].

Any valid estimator for $f$ can be obtained as a linear combination:

$$\bar{f}(\beta)=\frac{\sum_{i=1}^{P} a_i F_i}{\sum_{i=1}^{P} a_i Z_i} , \tag{2.3}$$

where the non-negative weight factors $a_i=a_i(\beta)$ are chosen in a way of minimizing the error of the final calculated physical observable $f$.

We impose the normalization

$$\sum_{i=1}^{P} w_i=1 \quad \text{with } w_i=a_i Z_i , \tag{2.4}$$

and Eq. (2.3) becomes

$$\bar{f}=\sum_{i=1}^{P} w_i \bar{f}_i \quad \text{with } \bar{f}_i=\frac{F_i}{Z_i} . \tag{2.5}$$

The optimal choice for the normalized weight factors $w_i$ is simply the inverse variance of $\bar{f}_i$, which can be estimated as the empirical error bars,

$$w_i \sim \frac{1}{(\Delta\bar{f}_i)^2} , \tag{2.6}$$

from each MC simulation at $\beta_0^i$. The overall constant is fixed by the normalization condition (2.4).

In the following, we shall make the corresponding histogram for the observable $f$ probability distribution.

In order to obtain the histogram we divide the allowed ranges for $f$ and $s$ into intervals of equal width, the histogram bins. We label these intervals by the values $s_j$ and $f_k$. It is a natural description for spin systems where the number of bins is the number of states.

The relative number of times a set of measurements falls into a given bin is proportional to the probability of observing the system in the state labeled by $s_j$ and $f_k$:

$$n_{jk}=\frac{N(s_j,f_k)}{\sum_{j,k} N(s_j,f_k)} , \tag{2.7}$$

where $N(s_j,f_k)$ is the number of configurations in the histogram bin and $n_{jk}$ is the empirical frequency distribution. In MC simulations $n_{jk}$ is an approximation to the probability distribution and represents a measuring for the probability $P(s_j,f_k;\beta_0)$ to observe the system in the state with energy $s_j$ and observable value $f_k$ with coupling $\beta_0$.

In terms of the canonical distribution, the above equation can be reweighted to give the probability at $\beta$:

$$P(s_j,f_k;\beta)=\frac{n_{jk} e^{-(\beta_0-\beta)s_j V_p}}{\sum_{jk} n_{jk} e^{-(\beta_0-\beta)s_j V_p}} , \tag{2.8}$$

where the denominator accounts for the normalization factor.

Now we restrict ourselves to the action per plaquette probability distribution. This distribution, for first-order transition, has a double maximum corresponding to two coexisting phases at $s=\epsilon_1$ and $s=\epsilon_2$, and separated by a minimum at $s=\epsilon_m$. For a fixed lattice size $L$ it is described by $P_L(s;\beta)$.

The bulk free energy barrier associated with these coexisting phases can then be calculated as [8]

$$\Delta F(L)=\ln\frac{P_L(\epsilon_1;\beta_h)}{P_L(\epsilon_m;\beta_h)} , \tag{2.9}$$

where the finite lattice critical point $\beta=\beta_h(L)$ is defined by

$$P_L(\epsilon_1;\beta_h)=P_L(\epsilon_2;\beta_h) . \tag{2.10}$$

To estimate the surface tension $\alpha$ we further need to know the $L$ dependence of $\Delta F$. For sufficiently large $L$, the two phases are separated for domain walls [7], whose energy is proportional to the total area $2A$. We then have $\Delta F(L)/2A=\alpha L_t$. To take into account possible linear corrections to the bulk free energy we fit our data to

$$\frac{\Delta F(L)}{2AL_t}=\alpha+\frac{\alpha_1}{L} . \tag{2.11}$$

The condition (2.10) defines a critical coupling for finite lattices. However, this definition should also lead to the infinite lattice critical point as obtained by other methods. Thus we also investigate the $\beta$ dependence on $L$ through the FSS fit:

$$\beta_h(L)=\beta_c+\frac{a}{L^3} . \tag{2.12}$$

The comparison with results obtained by other methods is a good test for this procedure in defining the critical coupling at which we have equal heights in the empirical distributions.

## III. NUMERICAL RESULTS

To avoid the initial introduction of a step size to define the histogram bin and consequently to reweight (2.8) with $s_j$ as the average value on that interval, it is preferable to reweight size zero bins. This means we are reweighting every entry $s_j^{(i)}$ with the proper Boltzmann factor to a new coupling $\beta$, which belongs to the validity range, $\beta \in [\beta_{\min}, \beta_{\max}]$. This is done by identifying $s_j^{(i)}$ with its Boltzmann factor. At this stage we can get a pictorial representation for the energy histogram by distributing the reweighted entries on ordered energy intervals.

Our statistical analysis were carried out using the jackknife method. This method was applied to the probability distributions and the reported errors were calculated with 20 jackknife bins.

Table I presents our data $L_t=2$. These results rely on 120 000 measurements for each data point. Although this case has been recently studied [18], we also apply patching here. We have simulated two different points for $L=12$, $\beta_0=5.092$ and 5.095. These two measurement series were patched and gave the result

$$\Delta F(12)=3.49(29) \tag{3.1a}$$

at

$$\beta_h(12)=5.0934(7)\ . \tag{3.1b}$$

At this coupling, each time series contributed with weights 0.37 and 0.63, respectively, in order of increasing $\beta_0$. To fit (2.11) we have used our data from Table I, but the result for $L=12$ was substituted by the patched value in (3.1a), which represents our best estimate for $\Delta F(12)$. This fit gives, in units of $T_c$,

$$\frac{\alpha}{T_c^3}=0.078(8) \tag{3.2a}$$

and

$$\frac{\alpha_1}{T_c^3}=-0.38(6) \tag{3.2b}$$

for the linear correction. The goodness of fit [19] is $Q=0.24$. Although we have good agreement with previous calculations for $\alpha$, the correction term (3.2b) seems to be important. This may be due to the fact that we are working with rather small lattice sizes and in this situation we might have deviations introduced by interface shapes other than planar ones [7].

To estimate the infinite volume critical $\beta$ for $L_t=2$, we use the FSS fit (2.12). We obtain $\beta_c=5.0938(7)$, with $Q=0.50$. This value is in very good agreement with the more recent FSS results obtained by other methods [9].

TABLE I. $L_t=2$ data and their reweighting $\beta$ range. $\beta_h$ and the bulk free energy $\Delta F$ were obtained, respectively, from Eqs. (2.10) and (2.9).

| $L$ | $\beta_0$ | $[\beta_{\min},\beta_{\max}]$ | $\beta_h(L)$ | $\Delta F(L)$ |
|---|---|---|---|---|
| 6 | 5.094 | [5.026, 5.155] | 5.0910(14) | 0.32(06) |
| 8 | 5.090 | [5.042, 5.122] | 5.0914(11) | 0.89(09) |
| 10 | 5.090 | [5.050, 5.108] | 5.0938(11) | 2.24(24) |
| 12 | 5.092 | [5.064, 5.107] | 5.0935(07) | 3.42(31) |
| 12 | 5.095 | [5.078, 5.114] | 5.0934(07) | 3.63(40) |

Now we address our attention to $L_t=4$. A complete overview of our data can be found in Ref. [9].

We had to restrict our analysis to larger available lattice sizes, i.e., $L=20$ and 24. This is because for smaller lattices it was hardly possible to distinguish a double peak structure in the energy distributions and our tentative to calculate $\Delta F$ gave results compatible with zero due to their large error bars. This fact had already been investigated [20] and for lattice sizes up to 16 the conclusion of a second-order behavior could be drawn [6].

For $L=20$, we simulated three points: $\beta_0=5.690$, 5.691, and 5.692. Only for $\beta_0=5.691$ did we obtain a nonzero compatible value, $\Delta F(20)=0.11(09)$ at $\beta_h(20)=5.6914(6)$, although its error is quite large. In this case patching does not improve this calculation presumably because we still have a weak signal for the transition. In Fig. 1 we present the distributions for $L_t=24$. We carried out 180 000 measurements for each simulated point: $\beta_0=5.691$ and 5.693. As we can observe, these runs do not show a clear double peak structure because they do not contain enough configurations of both phases. This fact is related to the critical slowing down due to the presence of the interface between the bulk phases, leading to a fast suppression of tunnelings with increasing lattice size.

At the right side of Fig. 1 we present the reweighted histograms. The calculation of $\Delta F$ also gives a value compatible with zero. In Fig. 2 we show the two patched distributions, which now we believe contain enough information for both phases. Each run contributed respectively with weights 0.38 and 0.62, in order of increasing $\beta_0$. Equation (2.10) then defines the critical coupling at

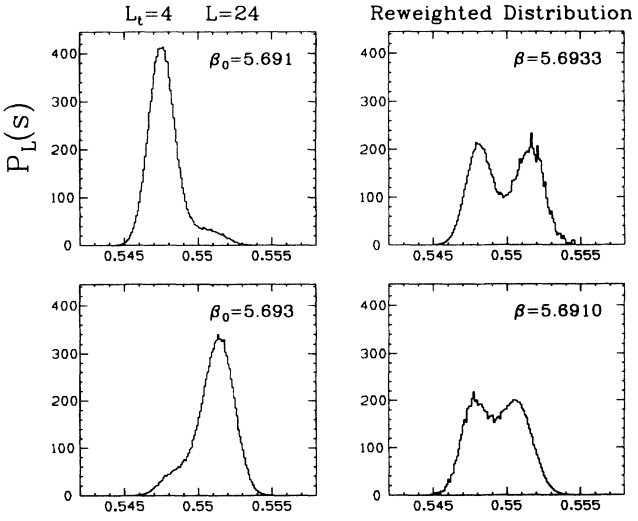


FIG. 1. Histograms for the action per plaquette distribution probabilities. The left side shows the distributions obtained with MC data for $L_t=4$ and $L=24$, with couplings $\beta_0=5.691$ and 5.693. The right side shows the same distributions reweighted to critical couplings, defined according to Eq. (2.10).

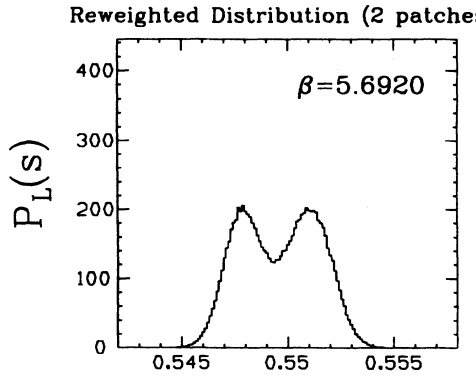


FIG. 2. Histogram for the reweighted distribution obtained when we combine the action per plaquette distribution probabilities of Fig. 1 (left side).

$$\beta_h(24)=5.6920(3)\ . \tag{3.3}$$

At this coupling we obtained

$$\Delta F(24)=0.47(12)\ , \tag{3.4a}$$

corresponding to

$$\frac{\alpha}{T_c^3}=0.007(2)\ . \tag{3.4b}$$

This lattice size gives a lower value than the first calculation [5]. However, to obtain a FSS estimate we would need larger lattice sizes and in this case patching can give an important contribution to the $\Delta F$ evaluation.

## IV. SUMMARY AND CONCLUSIONS

We investigated the distribution probability method to calculate the bulk free energy associated with coexistent phases when one introduces patching. The distributions were obtained from a time series of a continuous variable and single entries were reweighted to the critical point. For a strong first-order transition, as seems to be the case for $L_t=2$, we were able to estimate the surface tension using the FSS fit (2.11). However, for $L_t=4$, the double peak structure becomes pronounced only for lattices larger than 16. This turns out to be a more difficult case. By combining different MC simulations on both sides of the critical coupling, it was possible to obtain a more representative distribution for the transition which enabled us to estimate $\Delta F$ and $\alpha$.

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