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SURFACE TENSION IN HOT LATTICE QCD

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ABSTRACT

We review the results of recent calculations of the surface tension in lattice QCD for flat and spherical interfaces separating coexisting phases of hadronic matter and quark-gluon plasma. We compare these results with the the Bag model calculation of Mardor and Svetitsky and discuss their implications for the 'Swiss Cheese' instability. Presented by J. Potvin.

1. Introduction

Recent lattice simulations of quenched and full QCD suggest that the phase transition between hadronic matter and quark-gluon plasma may be weakly 1st order (and possibly 2nd order in 2 flavor QCD).[1] First order phase transitions are particularly interesting since they feature metastable states which decay by nucleating droplets of stable matter. In strongly first order phase transitions the lifetime of such a decay is calculated from classical nucleation theory[2,3] and depends on the value of the surface tension on a flat interface separating macroscopic domains of hadronic matter and quark-gluon plasma. As reviewed in the following section, several lattice calculations of the surface tension in quenched QCD have given a value of order $\alpha = 50 MeV/fm^2$ or less.[4–11] Compared to the scale of the strong interactions such a value is very small, confirming further the weak character of the phase transition.

Weak first order phase transitions are outside the range of validity of classical nucleation theory. Studying droplet decay will therefore require a more detailed knowledge of the droplets' free energy at various droplet sizes.[3] One standard parametrization of the radius-dependence of the free energy is the following:

$$\Delta F(R) = -\Delta f\ V + \alpha_{oo} A - 8\pi C R + \ldots.. \tag{1}$$

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were V, A and R are the droplet's volume, surface and radius respectively; f is the bulk free energy difference between the metastable and the stable states and the factor $8\pi C$ is the so-called curvature coefficient. Computing the value of the curvature coefficient on gluonic and hadronic droplets has motivated some of the most recent lattice work in finite temperature QCD.[12,13] These will be discussed in Section 3 below.

The droplet surface free energy being size-dependent may imply a phase kinetics (i.e. droplet time-evolution) very different from the kinetics characteristic of classical nucleation. An example is the 'Swiss cheese' instability suggested by Mardor and Svetitsky[14], in which droplets of sizes smaller than the size of the 'saddle-point' configuration in the classical theory may exist as metastable states (these sub-critical droplets are unstable in the classical theory). Because scenarios like the Swiss Cheese instability depend on the precise size-dependence of the free energy, lattice calculations are particularly useful in determining the likely forms of droplet evolution as we will see in Section 4.

2. Surface Tension of Flat Interfaces

Most of the studies done so far have focused on studying the surface free energy in quenched QCD.[4–6,8–11] Work in QCD with 4 flavors of dynamical (heavy) fermions was done by Hackel et al.[7]

The surface tension of a flat interface separating hadronic and quark-gluon phases is calculated from the free energy needed to create a macroscopic interface of surface area $A = 2\ L^2$ on a $L * L * 2L$ spatial lattice with periodic boundary conditions (see figure 1). It is sufficient to compare F_{12}, the free energy associated with a mixed phase system containing equal volumes of phase 1 (hadronic matter) and phase 2 (gluonic plasma), with the free energy (F_1, F_2) associated with each bulk phase separately. By parametrizing $(F_{12} - F_1)$ and $(F_{12} - F_2)$ as a superposition of a volume term and a surface term, the contributions from the bulk free energy can be subtracted out, giving:

$$\Delta F_s = \frac{[V_1(F_{12} - F_1) - V_2(F_2 - F_{12})]}{V_1 + V_2}. \tag{2}$$

V_1 and V_2 correspond to the volume occupied by phase 1 and 2 respectively. A similar formula can be used in the case of droplets of phase 1 immersed in bulk matter of phase 2 (or vice versa), using instead V_{in} and V_{out}, the volumes inside and outside the droplet respectively. Eq. (2) is equivalent to an experiment in which the system is initially in phase 1 and is allowed to 'grow' the other phase in one half of the lattice, leading to a mixed phase. The interface is then allowed to "melt" when the rest of the system is transformed to the second phase.

In practice, the free energy is obtained from a suitable derivative of the partition function Z, since $F = -\ln Z$. (Here, F/k_BT has been rescaled to F). Some investigators have used a derivative with respect to a change of the interface's surface.[6] Others have used a derivative with respect to the gauge coupling β ($\beta = 6/g^2$) [4] or to

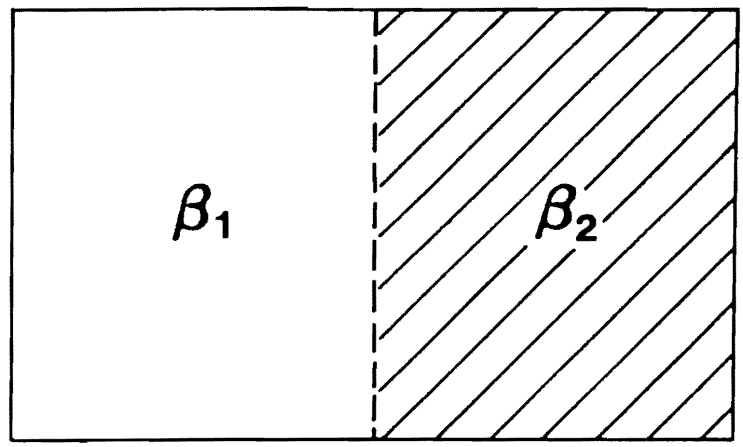

Fig. 1. A mixed phase configuration on a lattice, created by a small gauge coupling (temperature) difference across the interface (ref. [4]).

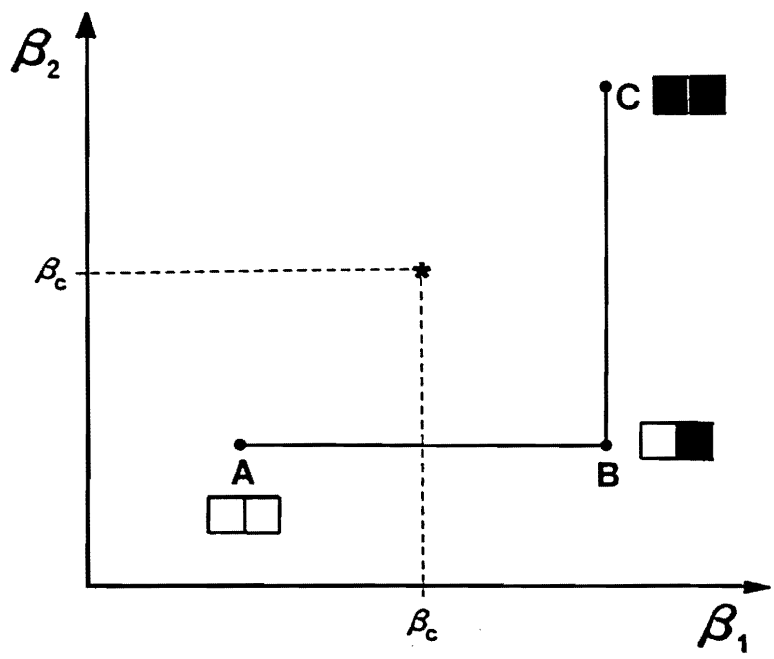

Fig. 2. Path in coupling space for the calculation of the surface tension.

external Polyakov line couplings[5] in order to simulate an actual creation/destruction of phases through small changes of temperature or external fields. Others have explicitely calculated the probability to generate a two-phase system.[8-10]

Derivatives of the partition function are usually obtained from Monte Carlo simula An example is the average action $\langle S \rangle$ calculated from the derivative of $\ln Z$ with respect to β. The free energy is then simply obtained from the following integral:

$$F(\beta'') - F(\beta') = \int_{\beta'}^{\beta''} d\beta \, \langle S \rangle_\beta \tag{3}$$

The calculation of the hadronic and quark-gluon droplets free energy is obtained from the integral of $\langle S \rangle$ along paths shown in figure 2. Each path is defined by tuning the gauge coupling β inside V_1 (β_1) and inside V_2 (β_2) in succession (changing the coupling is equivalent to increasing and/or decreasing the temperature). In order to have a stable interface the integration starts at temperatures slightly smaller than T_c, that is $\beta = \beta_c - \delta\beta$ and ends at temperature slighlty higher, or $\beta = \beta_c + \delta\beta$.[4] To obtain the physical value of the surface free energy, the calculation is repeated for smaller values of the temperature difference $\delta\beta$, and an extrapolation to zero-$\delta\beta$ is performed in the end.

Lattices of several volumes have been used for surface tension studies, namely lattices with 2 and 4 times slices (or $N_t = 2, 4$) with spatial volumes ranging from $6*6*12$ up to $16*16*32$,[4,5] from $8*8*16$ to $8*8*40$,[6,7] and finally from $12*12*6$ up to $12*12*12$ (on a $N_t = 2$ lattice),[8] and $12*12*12$ on $N_t = 2$ as well as $20*20*20$, $24*24*24$ on $N_t = 4$.[10]

The computation of the surface tension has a recent history. The world data can be listed as follows:

First, on $N_t = 2$ lattices, $\alpha/T^3 = 0.12(2)$ [ref.4] , 0.08(1) [ref. 6 (approximate error)] , 0.071(8) [ref. 8], 0.140(6) [ref. 9] and, 0.078(8) [ref. 10].

On $N_t = 4$ lattices, on the other hand: $\alpha/T^3 = 0.024(4)$ [ref. 5] and 0.007(2) [ref. 10].

We see that all studies are consistent with the statement that the surface tension is indeed small in QCD. There are some discrepencies between the different methods of computation however. Because the results within each group of methodologies do not agree, it is hard at this time to identify clearly each source of systematic error. Here it seems that errors due to small lattice volume, Monte Carlo sampling, ignorance of the so-called Karsch coefficients at intermediate coupling, etc. may be affecting the results in an uneven manner. More work is clearly needed here to determine how large a lattice or how long a Monte Carlo run need to be in order to see agreeement between these different methods.

It is important to point out that all the recent computations of the surface tension in the 3-dimensional Ising model agree nicely over a wide range of temperatures. [15] On the other hand, a major disagreement do exist in the 2-dimensional 7-state Potts model between the 'integral' method[16] and the probability distribution method.[8] The source of the discrepency is not understood at the moment.

It seems clear that the surface tension on lattices with 2 and 4 time slices differ substancially, indicating lack of scaling. This is consistent with the scaling properties of other physical parameters . In the case of the transition temperature T_c for example, studies have shown that scaling appears only on lattices with more than 10 time slices ($N_t = 10$).[17]

A computation of the surface tension in 4-flavor QCD has been performed by Hackel et al.[7] These authors have used the derivative with respect to a change of the interface area to compute the free energy.[6] They have obtained a very small (negative) value, also consistent with zero within errors. It is worth mentioning that Hackel et al. have found that the value of the surface tension results from a delicate balance between the (positive) contribution of the gluonic degrees of freedom and the (negative) contribution of the fermionic degrees of freedom. Much remains to be done, however, regarding the estinate of the systematic errors present in this calculation, since approximate algorithms were used for both the computation of the surface tension and the Monte Carlo update of the gauge configurations.

3. Surface Tension of Spherical Interfaces

Unlike the surface tension of a flat interface (or wall), the definition of the surface tension on a droplet is more ambiguous. The reason rests with the fact that at $T = T_c$, walls are macroscopic objects which are stable in the infinite volume limit. Droplets, on the other hand, are unstable objects which either shrink or grow during the phase transition. Of course, stable droplets do exist in macroscopic sizes in the real world, when a pressure difference between the droplet's interior and exterior balances out the surface tension. In principle, such an environment could be created in supercooled and superheated matter.

Another ambiguity in the definition of a droplet's free energy has to do with the location of the droplet's surface when the interface has a finite thickness w. This problem can also be solved for macroscopic droplets supporting a pressure difference across their interface by using Laplace's equation $\Delta p = 2\alpha/R$ as a constraint.[3,18,19]

The radius dependence of a stable droplet surface tension was first computed by Gibbs.[3,18,19] Following general thermodynamics and using Laplace's equation, one can derive this radius dependence in terms of the wall surface tension α_{oo} and of the surface thickness w (assumed to be thin), thus obtaining the Tolman-Gibbs equation:

$$\alpha = \frac{\alpha_{oo}}{1 + 2w/R} \quad . \tag{4}$$

As discussed in reference [19], it can be argued that the Tolman-Gibbs formula holds for slowly growing non-equilibrium macroscopic droplets as well.

Practically speaking, it is very difficult to adequately simulate metastable states or slowly growing droplets in lattice QCD simulations because of limitations on the system's volume and on the actual identification of metastable states (not to mention the definition of real time in Eucledian field theories). One alternative is to artificially create a droplet of a given size at $T = T_c$ using some external fields or

by applying a (small) temperature difference across the interface. The problem is of course whether this is at all meaningful, particularly in the case of small (microscopic) droplets. However this procedure may be justified for large droplets which feature flat walls on a microscopic scale. These artificially created droplets would correspond to droplets which in the real world are in equilibrium or grow at a very slow rate. These assumptions can be checked indirectly by comparing the surface free energies obtained from the use of different types of external fields and/or by comparing with the large R-limit of the Tolman-Gibbs equation (Eq. (4)) as will be done below.

Two series of calculations in quenched $N_t = 2$ lattice QCD have been performed recently,[12,13] in wich droplets were created by tuning the gauge coupling (and hence the temperature) inside the droplet to artificially stabilize its surface. Huang et al.[12] have measured the derivative of the partition function with respect to the gauge coupling β and integrated with respect to β in order to obtain the free energy. Kajantie et al.[13] have computed the derivative with respect to the droplet's radius R and integrated with respect to R to compute F. Both studies have used Eq. (1) to extract the value of the curvature coefficient; in both cases also, an extrapolation to a zero value of the stabilizing temperature difference had to be performed.

The values of the surface tension obtained in reference [12] are shown in figure 3: $\alpha/{T_c}^3 = -0.060(7), -0.042(5), +0.055(14)$ for hadronic droplets with radii $R = 4, 5, 8$ respectively, and $\alpha/{T_c}^3 = 0.000, -0.076(5), +0.061(14)$ for gluonic droplets with radii $R = 4, 5, 8$. These values were obtained directly from the integration of the action, without using equation (1). The results are compared with the Tolman-Gibbs formula (Eq. 4), using a value for the interface width of $w = 4$,[6] and a wall surface tension of $\alpha_{oo}/{T_c}^3 = 0.12(2)$.[4] The agreement with the Tolman-Gibbs formula for $R > 5$ is rather surprising given the fact that no free parameters were available. Perhaps the size of $R = 8$ droplets could be considered as macroscopic; given the droplet width $w = 4$,[6] droplets with radii smaller than 5 are clearly microscopic.

It is important to notice that having $w = 4$ implies that the definition of a droplet's radius is ambiguous at T_c (Laplace's equation cannot be used at T_c).[19] However, one can estimate the error due to this ambiguity by using calculus of variations with respect to the transformation $R \to R + \delta$ on the surface term of the droplet's total free energy. One finds an error of $\frac{R}{(R+w/2)} - 1$, or, of about 20 percent for $R = 8$ droplets and up to 60 percent for $R = 4, 5$. Qualitatively, the ambiguity due to interface thickness does not change the picture shown in figure 3.

Kajantie, Karkkainen and Rummukainen[13] have expressed their computed free energy using equation (1) as an ansatz. The values of the curvature coefficients thus obtained were $C = -0.076(25)$ and $C = +0.076(120)$ (in units of T^3) for hadronic and gluonic droplets respectively. Their data on hadronic droplets have smaller errors than the data on gluonic droplets. These numbers can be compared with the Bag model calculation of Mardor and Svetitsky[14] (see also Section 4. below) which predicts $C = -0.0707$ (hadronic) and $C = +0.0707$ (gluonic), thus showing a nice agreement particularly in the case of the hadronic droplets.

A consistency check can be made by comparing the coefficient of the surface-dependent term which should be identical to the flat wall surface tension: Kajantie

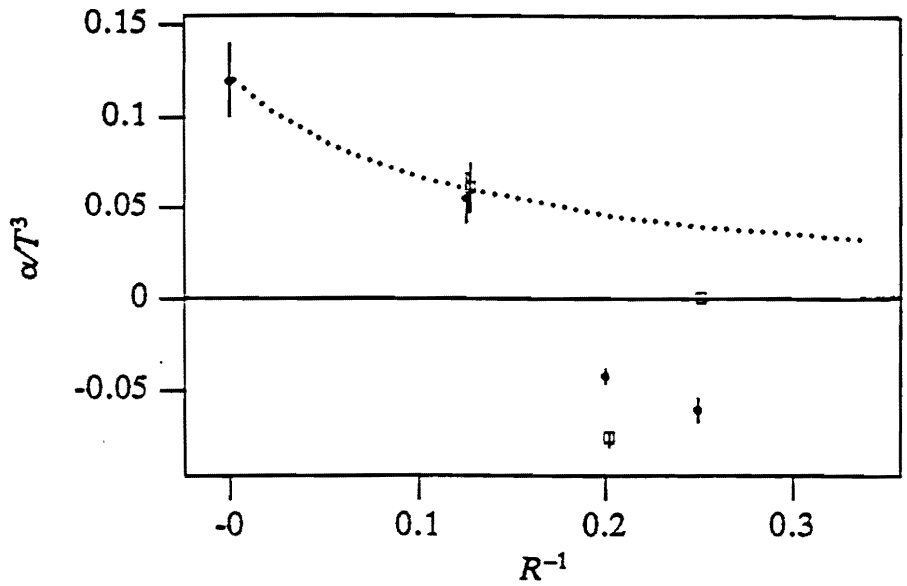

Fig. 3. Radius dependence of the surface tension on hadronic (filled circles) and gluonic (squares) droplets. The data point at R^{-1}=0. corresponds to the wall surface tension (Ref. 4). The dashed curve represents the Tolman-Gibbs equation.

et al. have obtained 0.10(14) and −0.37(80) (in units of T^3) for hadronic and gluonic droplets, values which are consistent with the flat interface studies[4−10] but also consistent with zero surface tension.

Huang et al.[12] have also computed the values of the curvature coefficient, by fitting their data to equation (1). In units of ${T_c}^3$ the fit gave a the following values for the curvature term C: −0.051(9) and −0.077(13) for hadronic and gluonic droplets respectively. There is (some) quantitative agreement between these results and those of reference [13] for the hadronic droplets but *not* for the gluonic droplets. One reason for the discrepency may be in the different extrapolation schemes used, particularly in the computation of the free energy itself.

We note that given the large values of the ratio w/R used so far, one should be suspicious of truncated series such as equation (1), especially when terms in powers of $1/R$ may be important. That the fits may be incorrect can be seen by looking at the fitted value of the wall surface tension (α^{fitted}), which in reference [12] is *twice* the value of α_{oo}, [4−10] instead of being the same.

4. Implications for the Swiss Cheese Instability

Mardor and Svetitsky have studied the surface tension in the Bag Model, [14] using equation (1) as an ansatz. They found a value of the curvature coefficient given by $C = \pm\ (\frac{4}{9})\ T^2$ (− for hadronic droplets and + for gluonic droplets). Moreover, the flat wall surface tension α_{oo} in QCD with NO strange quarks turned out to be zero.

At least for hadronic droplets, the lattice results are consistent with the Bag model calculations at least qualitatively, in that the value of the wall surface tension is small on the scale of the strong interactions, and that the curvature coefficient is negative. Comparisons in the case of gluonic droplets may be premature at this time, given the discrepencies found in different lattice studies regarding the sign of the curvature coefficient (negative in reference [12], positive in reference [13]).

An interesting consequence of Mardor and Svetitsky's results is that the negative value of the curvature term leads to a secondary extremum at small R in the free energy thus generating the so-called "Swiss cheeze" instability. In this scenario, sub-critical hadronic droplets of a certain characteristic size are not destroyed by fluctuations as they would be in classical nucleation theory.[14] At temperatures smaller than T_c, the metastable vacuum would not consist of bulk quark-gluon plasma, but instead of plasma with 'droplets' of hadronic matter.[14] At temperatures larger than T_c, on the other hand, no such 'dirty' metastable hadronic state could exist since the curvature coefficient is positive. Some uncertainties concerning the viability of this scenario remain, however, especially regarding the contribution of $1/R$-terms to the free energy,[19] as well as the inherent (in)stability of these droplets.[20]

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