Free energy of spherical QCD bubbles

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We discuss the free energy of spherical bubbles of hadronic (quark-gluon plasma) matter in metastable equilibrium in a quark-gluon plasma (hadronic matter) at a fixed temperature $T < T_c$ ($T > T_c$). We derive an expression for the effective interface tension written in terms of the bubble's radius R , namely, $\alpha(R) = \alpha(\infty) / [1 + 2d/R]$, where d is a parameter related to the surface entropy of a planar interface. We argue that this formula should be valid in the case of expanding macroscopic bubbles as well. We also estimate the value of the contribution of curvature to the free energy and explore the consequences of such a radius dependence on the dynamics of the cosmological phase transition.

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Most descriptions of the thermodynamics of QCD matter assume that it can exist in two phases, namely, the hadronic phase (H) and the quark-gluon phase (Q), and that both phases transform into each other at $T = T_c$ through a first-order phase transition. In this case a two-phase configuration in which bulk regions of the H and Q phases are separated by an infinite planar interface at $T = T_c$ is stable both mechanically and thermodynamically (the pressure p and temperature T being equal to p_c and T_c , respectively, on both sides; here we assume that the chemical potential associated with the baryon number is zero, or $\mu = 0$). The interface carries an extra free energy, the interface tension $\alpha(T_c)$, and lattice Monte Carlo computations [1–5] on $N_t = 2, 4$ lattices in quenched QCD have given the values $\alpha(T_c) \approx 0.11 T_c^3$ ($N_t = 2$) and $0.03 T_c^3$ ($N_t = 4$), with roughly 10% statistical errors. The interface is rather thick, about 2–3 fm [2,3]. In a first-order transition one must have $\alpha(T_c) > 0$ for a planar interface. If $\alpha(T_c)$ were to be 0, it would cost no free energy to add an arbitrary number of H - Q interfaces; separate H and Q bulk phases would not exist.

The purpose of this paper is to consider spherical configurations of one phase of QCD matter surrounded by the other and, in particular, to study the free energy and radial dependence of the interface tension. For definiteness, we shall mainly discuss H matter bubbles in a bulk Q phase. We shall also mainly consider configurations in thermal equilibrium, i.e., configurations

for which the temperature T (and $\mu = 0$) is the same throughout the bubble and its environment. We will show that this analysis can be applied to the case of slowly expanding macroscopic bubbles as well. The stable configurations are saddle-point configurations through which the system passes when moving from one local minimum (supercooled Q phase) to another local minimum (stable H phase). In theories for which the effective potential $V(\phi, T)$ is known (ϕ being an order parameter), the free energy of this saddle-point configuration is given by the extremum of the integral:

$$F(T) = \int d^3x \left[\frac{1}{2} (\nabla\phi)^2 + V(\phi, T) \right], \quad (1)$$

$$\phi''(r) + (2/r)\phi'(r) = V'(\phi, T),$$

with the boundary conditions $\phi(\infty) = \phi_1$, $\phi'(0) = 0$. In QCD there is no tree-level effective potential.

In the thin wall approximation to Eq. (1), the free energy of spherical H bubbles of radius R in the Q phase at $T < T_c$ can be expanded in powers of $1/(RT)$ as follows:

$$F(T, R) = -\Delta p \frac{4}{3} \pi R^3 + \alpha(T) 4\pi R^2 + \gamma(T) 8\pi R + \dots, \quad (2)$$

$$\Delta p \equiv p_h(T) - p_q(T) \approx L(1 - T/T_c),$$

where L is the latent heat and γ is the curvature coefficient. Equilibrium bubbles correspond to extrema of F , calculated either from Eq. (1) or from approximation (2). However, the application of Eq. (2) to QCD bubbles featuring a thickness δR of the order of R may be ambiguous. A first problem regards the very definition of a bubble's radius. One can always perform a redefinition of R up to the scale of the interface thickness in such a way that R_{new} approaches R_{old} as $R \rightarrow \infty$. Expanding R_{new} in powers of $1/R$ and including the first three terms gives $R \rightarrow R + D + g/R$ with D and g as constants. The volume term of the free energy in Eq. (2) is then invariant

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while the surface and curvature coefficients transform as

$$\alpha \rightarrow \alpha + d\Delta p, \quad \gamma \rightarrow \gamma + d\alpha + \frac{1}{2}(d^2 + g)\Delta p, \quad (3)$$

and thus are not unique.

A second problem concerns the terms omitted in Eq. (2). They are clearly important when R approaches δR , but the expansion in powers of $1/(RT)$ has only a finite radius of convergence around $R = \infty$ and cannot be used for $R \rightarrow 0$.

To define R uniquely, we consider H bubbles both in thermal and mechanical equilibrium. To each temperature $T < T_c$ there corresponds one and only one configuration defined by the radial free-energy density profile $f(r, T) = -V(\phi(r), T)$, where $\phi(r)$ is the solution of the differential equation in Eq. (1). The closer T is to T_c , the larger is the radius (to be defined) of the configuration. We know that

$$f(0, T) \approx -p_h(T) < f(\infty, T) = -p_q(T).$$

Since $f(r, T)$ does not return to the same value when crossing the interface, a unique interface free energy can only be defined after specifying the position of the interface (cf. Eq. (5) below and Ref. [6]). Only for a planar interface, which can be regarded as the $R \rightarrow \infty$ limit of a spherical configuration, is $p_h(T_c) = p_q(T_c)$ and $\alpha(T = T_c) \equiv \alpha(R = \infty)$ unique. An H bubble is also only a saddle point if $T < T_c$: any perturbation will make it grow indefinitely or disappear completely. Only the planar configuration is absolutely stable at $T = T_c$.

To define the radius uniquely, we write the free energy $F(T)$ as

$$F(T) = -[p_h(T) - p_q(T)] \frac{4}{3} \pi R^3(T) + \alpha[R(T)] 4\pi R^2(T), \quad (4)$$

where the interior and exterior pressures $p_h(T)$ and $p_q(T)$ are known and $R(T)$ is the radius corresponding to the saddle point. The free energy of a configuration with a diffuse surface is thus written as a sum of volume and surface terms corresponding to a sharp radius $R(T)$. The notation $\alpha[R(T)]$ implies that the T dependence of α arises most naturally through $R(T)$, as shown below. A second relation between R and α is given by the condition of mechanical (meta)stability:

$$p_h(T) - p_q(T) = \frac{2\alpha[R(T)]}{R(T)}. \quad (5)$$

This is the usual Laplace condition for a bubble in hydrostatic equilibrium (the difference of pressure inside and outside the bubble being compensated by the surface tension), and is, in this context of a diffuse or thick surface, the definition of $R(T)$ as suggested by Gibbs [6].

From Eqs. (4) and (5) we obtain

$$R = \left[\frac{3}{2\pi} \frac{F}{\Delta p} \right]^{1/3}, \quad \alpha = \left[\frac{3}{16\pi} F (\Delta p)^2 \right]^{1/3}. \quad (6)$$

In theories featuring a known effective potential, $F(T)$ can be computed from Eq. (1); moreover, $\Delta p \equiv p_h(T) - p_q(T)$ is also known and these equations define $R(T)$ and $\alpha(T)$ uniquely. A numerical computation of $F(T)$ in the full parameter space with a quartic

$V(\phi, T)$ is given in Ref. [7].

In QCD, which has no effective potential, one can nevertheless proceed by studying Eq. (5) near $T = T_c$. For the bulk quantities one has the standard relations

$$p_h(T) = p_c - T_c s_H \left[1 - \frac{T}{T_c} \right], \quad (7)$$

$$p_q(T) = p_c - T_c s_Q \left[1 - \frac{T}{T_c} \right],$$

and for the interface tension $\alpha(T)$ we write

$$\alpha(T) = \alpha(T_c) - T_c \alpha'(T_c) \left[1 - \frac{T}{T_c} \right] = \alpha(T_c) - d\Delta p, \quad (8)$$

where we have introduced the quantity

$$d = \frac{T_c \alpha'(T_c)}{L} = \frac{-s_s}{s_Q - s_H}. \quad (9)$$

d is related to the surface entropy density as $s_s = S_s/A = -\alpha'(T_c)$ of a planar interface.

Equation (8) describes how $\alpha(T)$ behaves as a function of T . Since $R(T)$ is uniquely defined by Eq. (5), we can convert this T dependence to an R dependence. The result is

$$\alpha[R(T)] = \frac{\alpha(\infty)}{1 + 2d/R(T)}, \quad H \text{ in } Q. \quad (10)$$

Similar results for the liquid drops are well known in classical nucleation theory [6,8]. For Q droplets in H matter the sign of the left-hand side in Eq. (5) is changed due to the interchange of the inside and outside of the bubble. Although the T -dependent equations (8) and (9) are unchanged, as they have to be since they refer to a planar interface, we now have

$$R(T) = 2\alpha(T_c)/(-\Delta p) + 2d$$

and the R -dependent form becomes

$$\alpha[R(T)] = \frac{\alpha(\infty)}{1 - 2d/R(T)}, \quad Q \text{ in } H. \quad (11)$$

Since Eq. (8) is simply a Taylor expansion, Eqs. (8), (10), and (11) are valid if $d\Delta p \ll \alpha(T_c)$, $2d/R \ll 1$.

Equations (10) and (11) give the surface tension of a metastable equilibrium bubble. Now we would like to argue that they apply (at least in form) to a macroscopic nonequilibrium bubble as well. These bubbles are those configurations in classical nucleation theory which have a radius larger than $R(T)$ and continue growing indefinitely. We assume here that latent heat is small and that the bubbles are macroscopic in size and grow at a slow rate compared to the time scale of the microscopic interactions so that internal pressure, temperature and energy can be defined in a nonambiguous manner.

We use the first law of thermodynamics,

$$dE = T dS - p dV + \alpha(R, T) dA,$$

and write the variation of the bubble's internal energy E and entropy S in terms of the volume change dV as $dE = L_b dV$ and $dS = s_b dV$, L_b and s_b being the latent heat and latent entropy (per unit volume) released due to bubble's expansion. These equations yield a generalized

Laplace equation,

$$L_b - Ts_b + p = 2\alpha(R, T)/R, \quad (12)$$

which expresses the fact that the pressure difference across the bubble's surface is no longer balanced by the surface tension (the relation $L = Ts$ usually valid in the bulk would no longer apply in a bubble because of the surface's own energy and entropy).

In similarity with Eq. (9), we assume the existence of a length d' related to the derivative of α as

$$d' \Delta(L_b - Ts_b + p) = \Delta[\alpha(R, T)]. \quad (13)$$

Integrating (13) using (12) we obtain Eq. (10) again, with the difference that R and T are now independent.

Returning to Eqs. (10) and (11), let us point out that for consistency they should be expanded in powers of $2d/R$ (or $2d'/R$), keeping only the first correction (see below). A comparison with Eq. (2) gives the following value for the curvature coefficient:

$$\gamma(T_c) = -d\alpha(T_c) = s_s \frac{T_c \alpha(T_c)}{L} \quad (14)$$

for H bubbles in Q . We notice that in Eq. (9) the difference of entropy across the surface of stable bubbles is given by the latent heat since $s_Q - s_H = L/T_c$. No direct information exists so far about the surface entropy s_s of H - Q (order-disorder) interfaces. Note that only $f_s = \alpha - \epsilon_s - Ts_s$ has to be positive; all surface contributions corresponding to quantities which change when crossing the interface will also depend on its location. To illustrate this, assume that the entropy density varies according to

$$s(x) = \frac{1}{2}(s_Q + s_H) - \frac{1}{2}(s_Q - s_H) \tanh(x/\lambda)$$

when crossing across the interface. If the position of the interface is at x_s , s_s is given by

$$s_s = \int_{-\infty}^{x_s} dx [s(x) - s_H] + \int_{x_s}^{\infty} dx [s(x) - s_Q] \\ = (s_Q - s_H)x_s. \quad (15)$$

From Eqs. (9) and (14), one sees that s_s is negative and d is positive when the position of the interface is closer to the inside hadron matter. For H - Q interfaces one cannot say *a priori* what d is; Eqs. (9) and (10) rather offer a way of determining it. Preliminary lattice Monte Carlo data on $N_t = 2$ pure SU(3) gauge theory [9,10] have given value $\gamma/T_c^2 = -0.48 \pm 0.16$ in the case of H bubbles; the data for Q droplets may be consistent with the opposite sign [9] but is still controversial [10]. This should yield the numerical value $d = 4.5/T_c$, $s_s = -4.5L/T_c^2$, a rather large negative surface entropy and a parameter d of the order of interface thickness. Also, on (Polyakov lines) ordered-ordered interfaces in $N_t = 2$ SU(3) gauge theory, a lattice calculation has given $s_s = -24.0T_c^2$ at T a few % above T_c [4]. Counting eight massless gluons, one has $L = 7.0T_c^4$ and thus $d = 3.4/T_c$. Thus s_s is roughly the same for ordered-disordered and for ordered-ordered interfaces, but one must remember that the latter are much simpler since $s(x)$ returns to the same value s_Q when crossing the interface, implying that s_s is independent of the interface position.

We now use Eq. (2) together with Eq. (10) to study the

free energy of stable and (slowly) growing bubbles as a function of R and T :

$$F(R, T) = -\Delta p \frac{4}{3} \pi R^3 + \frac{\alpha 4\pi R^3}{R + 2d} \\ \approx -\Delta p \frac{4}{3} \pi R^3 + \alpha 4\pi R^2 - d\alpha 8\pi R + \dots \quad (16)$$

Comparing Eqs. (16) and (2) shows that all the terms omitted in Eq. (2) are essential to keep $F(R, T)$ positive for all R (for $d > 0$) near T_c . Figs. 1 and 2 show the total free energy $F(R)$ for $dT_c = 0, 4, 8$ as a function of R and $1 - T/T_c$, respectively, using parameter values relevant to the cosmological $Q \rightarrow H$ phase transition (to be discussed below). At $T > T_c$, Δp is negative and $F(R, T)$ grows monotonically from its minimum at $R = 0$; no stable H bubbles exist in the Q phase. At $T < T_c$, one has $\Delta p > 0$ and $F(R, T)$ is positive for values of the radius such that $R < R_0 = 3\alpha/\Delta p - 2d$, and has a maximum at

$$R = R_{\max} = \frac{\alpha}{\Delta p} - 2d + \left[\frac{\alpha}{\Delta p} \left(\frac{\alpha}{\Delta p} + 2d \right) \right]^{1/2} \leq R_0. \quad (17)$$

The extremal free energy is obtained by inserting Eq. (17) into Eq. (16); for small $d\Delta p/\alpha$ it behaves as

$$F(R_{\max}, T) = \frac{16\pi\alpha^3}{3\Delta p^2} \left[1 - 3 \frac{d\Delta p}{\alpha} + \frac{15}{4} \left(\frac{d\Delta p}{\alpha} \right)^2 - \dots \right] \quad (18)$$

and vanishes for $d\Delta p/\alpha = 3/2$ ($R_0 = 0$). In other words, the maximal supercooling the system can support is $1 - T/T_c = 3\alpha/(2Ld)$.

The ideas discussed above can be used in the study of bubble nucleation in the cosmological $Q \rightarrow H$ phase transition [7,11]. The probability of nucleation is given by (regarding the preexponential factor, see Ref. [12])

$$p(t) = T_c^4 e^{-S(t)}, \quad S(t) = F(R_{\max}(T), T)/T, \quad (19)$$

where F is given by Eqs. (16) and (18) and where $tT^2 = 0.301 M_{\text{Planck}}/\sqrt{g_*}$, in standard notation. The temperature $T_f < T_c$ at which the nucleation effectively takes place is determined by the equation

FIG. 1. The free energy $F(R, T)/T$ in the parametrization of Eq. (5) plotted as a function of the radius R (in units of $1/T_c$) for $dT_c = 0, 4$, and 8 (maxima from the left). The fixed parameters are $L = 10T_c^4$, $\alpha = 0.1T_c^3$ and the degree of supercooling is chosen so that the maximum is at 182 [Eq. (20)]: for $dT_c = 0, 4, 8$ one has $1 - T/T_c = 0.000959, 0.000636, 0.000493$, respectively.

FIG. 2. The extremal free energy $F(R_{\max}(T), T)/T$ given by the Eqs. (5) and (7) plotted as a function of the degree of supercooling $1 - T/T_c$ for $dT_c = 0, 4, 8$ (from top to bottom) and for $L = 10T_c^4$, $\alpha = 0.1T_c^3$.

$$\ln \frac{M_{\text{Planck}}^4}{T_c^4} = 182 = \frac{F(R_{\max}(T_f), T_f)}{T_f}. \quad (20)$$

As is evident from Figs. 1 and 2, when d increases the amount of supercooling decreases and the radius of the critical bubble increases. Quantitatively, if $L = 10T_c^4$, $\alpha = 0.1T_c^3$, and d increases from 0 to $8/T_c$, $1 - T_f/T_c$ decreases from 0.00096 to 0.00049 and R_{cr} increases from $20.8/T_c$ to $31.4/T_c$. An even more important parameter is the distance between nucleation centers [11,13]. For $d = 0$ it is approximately

$$R_{\text{nuc}} = 7.0m[\alpha^{3/2}/(L\sqrt{T_c})](200 \text{ MeV}/T_c)^2;$$

to first order in d this is decreased by the possibly significant factor

$$1 - 12d \left[\frac{\pi\alpha}{3T_c} \right]^{1/2} \frac{1}{\sqrt{182}} \approx 1 - 0.29dT_c. \quad (21)$$

Finally, we note that spherical bubbles in the bag mod-

el have been discussed in Ref. [14] (see also Ref. [15]). In this model one can compute $F(T)$ to arbitrary numerical accuracy [cf. Eq. (1)] or apply the approximation in Eq. (2). Defining $R(T)$ to be R_{bag} one now has $\alpha(T_c) = 0$ (for gluons and massless quarks) and $\gamma/T^2 = -4/9$ for gluons. The former property is in contradiction with the assumption of a first-order phase transition and it is ultimately not surprising that one finds paradoxical instabilities, although they also appear for $m_s \neq 0$, $\alpha(T_c) \neq 0$ but are small. Interestingly, however, the negative curvature coefficient is in agreement with the preliminary lattice results [9,10]. In electroweak theories with a quartic $V(\phi, T)$, the curvature coefficient, as computed from Eqs. (1) and (6) and using the Gibbs definition of $R(T)$, is positive.

Summarizing, we have considered the free energy of spherical configurations of H matter in Q plasma in thermal equilibrium ($T < T_c$). Basically the issue is to determine corrections to the thin wall approximation to Eq. (1). We have discussed the unique definition of the radius and determined the curvature contribution to the free energy in terms of the surface entropy and interface tension of a planar interface and of the latent heat of the bulk transition.

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