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Effects of a changing temperature on the nucleation rate

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In recent calculations of the nucleation rate I for a metastable material whose temperature is changing in time, an expression for I, derived under the assumption of constant temperature, is used. It is argued here that for a rapidly changing temperature the static temperature expression for I does not hold and that a full time dependent treatment of nucleation is necessary. The case of pion bubbles forming in quark-gluon plasma is considered as an example. [S1063-651X(96)12209-1]

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I. INTRODUCTION

There have been a number of recent calculations of phase transition rates [1,3,4] involving the nucleation rate $I(T)$ of critical size drops or bubbles of stable material in a metastable medium whose temperature T is changing with time. These calculations make use of expressions for $I(T)$, each of which are derived assuming the temperature and the distribution of bubble sizes is independent of time [5,6]. In the calculations of phase transition rates $I(T)$ is evaluated at the instantaneous time t using the corresponding value of $T(t)$. No information about $\dot{T}$ is included in the expression for I. In this report we refer to this approach as the adiabatic method, by which we mean that the nucleation rate is calculated as if the system were at the instantaneous temperature indefinitely. The term adiabatic here does not imply that the entropy is being held constant. In Sec. II a brief summary of the formalism used to calculate the adiabatic nucleation rate is presented.

In the case of a changing temperature the distribution of bubble or drop sizes of stable material in the metastable medium $f(g)$ the size of the critical bubble, and also the nucleation rate are affected. In this report we investigate the effects of a changing temperature and discuss the need for a different approach than the adiabatic method, to obtain $I(T)$, for the case of a rapidly changing temperature. We suggest that in the case of a rapidly changing temperature the distribution of bubble sizes $f(g)$ can be quite different from $f^0(g)$, its adiabatic value. In addition, the nucleation rate may also be changed significantly. For the case that $\dot{T}$ is small, $f(g)$ should be altered slightly from $f^0(g)$. A simple expression for this modification is obtained in Sec. III. On the other hand, if $\dot{T}$ is large a full time dependent approach to nucleation, including the effects of a changing bubble distribution, is necessary. An outline of this approach is given in Sec. III. Finally, a short numerical calculation of the effects of a changing temperature on the nucleation rate is made using the model of [1] which describes the nucleation of pion bubbles in an initially cooling quark-gluon vapor.

II. ADIABATIC NUCLEATION

We first give a brief description of nucleation theory for a constant temperature (adiabatic) system in order to present the formalism which we will later apply to the nonadiabatic case. We follow the work of Becker, Doring, and Zeldovich described in [5] instead of the more complicated model of Langer [6]. The conclusions reached in this report, however, should apply to both as the latter is a generalization of the former. The nucleation rate is given by

$$I(g)=-D(g)N(g)\frac{\partial}{\partial g}\left[\frac{f(g)}{N(g)}\right], \tag{1}$$

where $D(g)$ is a diffusion constant, $N(g)$ an equilibrium distribution of drop sizes, and $f(g)$ the actual nonequilibrium distribution of drop sizes. Here g is the number of consituent particles in a drop. $I(g)$ denotes the difference in the rate of growth of $g-1$ size drops into g size drops and the rate of evaporation of g drops into $g-1$ drops. A positive $I(g)$ at $g\approx g_*$, the critical size, is necessary for nucleation to occur and implies a probability flow toward larger size drops. One should note that I, D, N, and f are functions of temperature in addition to drop size g. In particular,

$$N(g)\propto\exp[-\Delta F(g,T)/T]. \tag{2}$$

ΔF is the difference in free energy between a system with a drop plus vapor and one with vapor alone. The time dependence of $f(g)$ is governed by

$$\frac{\partial f(g)}{\partial t}=-\frac{\partial I(g)}{\partial g}. \tag{3}$$

For the case of a time independent $f(g)$, an assumption used in the adiabatic case, $I(g)$ is independent of g, i.e., is a constant. One may integrate (1) from g to G to obtain an expression for $f^0(g)$, where the superscript 0 of f indicates that the system is at constant temperature (adiabatic). G is a particular value for g, slightly larger than the critical size (in practice about 20%) for which the boundary condition $f(G)=0$ is imposed. This boundary condition is a requirement of the picture of nucleation used in the literature in which bubbles of size G are removed from the system and replaced with an equal amount of vapor material. After integration of (1) one finds

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$$f^0[g,T(t)]=\frac{I}{D}\exp(-\Delta F/T+\Delta F_*/T)\times\int_{g-g_*}^{G-g_*}\exp\left(-\frac{\gamma x^2}{2T}\right)dx, \tag{4}$$

where

$$\gamma\equiv-\left(\frac{\partial^2\Delta F}{\partial g^2}\right)\bigg|_{g=g_*}. \tag{5}$$

In order to obtain (4) $\Delta F(g)$ appearing in $N(g)$ in the numerator of (1) is expanded about $\Delta F(g_*)$. Finally one may solve for I by making use of (4) and the condition that $f(g)/N(g)\approx 1$ for $g \ll g_*$.

The distribution $f^0(g)$ is almost identical to the equilibrium distribution N for small g. For $g=g_*$ $f^0(g_*)\approx 0.5N(g_*)$. N then increases for $g>g_*$ while $f(g)$ decreases to 0 at $g=G$. In the above calculations $G-g_*$ is assumed to be greater than

$$1\bigg/\left(\frac{\partial\Delta F}{\partial g^2}\frac{1}{2T}\right)^{1/2} \tag{6}$$

to allow for the Gaussian integral in (4) to be evaluated analytically.

III. EFFECT OF TEMPERATURE ON THE DISTRIBUTION OF DROP SIZES

In the case that the temperature is changing,

$$\frac{\partial f[g,T(t)]}{\partial t}=\dot{T}\frac{\partial f(g)}{\partial T}\neq 0, \tag{7}$$

and so, according to (3), I is not independent of g as it is in the adiabatic case. For a system whose temperature is changing rapidly $f(g)$ may be found from

$$\frac{\partial f(g)}{\partial t}=\frac{\partial}{\partial g}\left[D\frac{\partial f(g)}{\partial g}\right]+\frac{1}{T}\frac{\partial}{\partial g}\left[Df(g)\frac{\partial\Delta F}{\partial g}\right], \tag{8}$$

which is obtained by combining (1) and (3). $I(g)$ can then be found using (1). We now consider how $f(g)$ is modified from its adiabatic value $f^0(g)$ in the case that the effects of the changing temperature are small. The modification gives an expression for a first order change to $f(g)$ for the case of a slowly changing temperature. If the modification term is large a full time dependent treatment of nucleation is necessary and $f(g)$ must be obtained from (8).

In the case of small temperature effects one may write

$$f(g)=f^0(g)+q(g), \tag{9}$$

where $q(g)$ is presumed to be small in magnitude relative to $f^0(g)$. The boundary conditions $f(G)=0$ and $f^0(G)$ are imposed to be consistent with the picture [5] in which drops of size G are removed from the system for both the adiabatic and nonadiabatic cases. We use the approximation

$$\frac{\partial}{\partial t}f(g)\approx\partial_t f^0(g)=\dot{T}\frac{\partial}{\partial T}f^0(g) \tag{10}$$

in (8). This is equivalent to assuming that the time derivative of q relative to $\partial_t f^0(g)$ is small. Such an assumption is necessary to ensure that q remains small relative to $f^0(g)$ for long periods of time. One may note that inserting $f^0(g)$ in place of $f(g)$ on the right-hand side (RHS) of (8) gives zero by the definition of $f^0(g)$. Thus

$$\dot{T}\frac{\partial}{\partial T}f^0(g)=\frac{\partial}{\partial g}\left(D\frac{\partial q}{\partial g}\right)+\frac{1}{T}\frac{\partial}{\partial g}\left(Dq\frac{\partial\Delta F}{\partial g}\right). \tag{11}$$

A first integration of (11) gives

$$\frac{\dot{T}}{D}\int_g^G\frac{\partial}{\partial T}f^0dg=\left(\frac{\partial}{\partial g}q+\frac{1}{T}q\frac{\partial\Delta F}{\partial g}\right)\bigg|_g^G. \tag{12}$$

When the RHS of (12) is evaluated at G only the first term survives because $q(G)=0$. We assume that this first term, the derivative of q with respect to g, is small at G and may be neglected. The RHS of (12) can be expressed as the g derivative of a single term if one uses

$$q\equiv Q(g,T)N(g,T), \tag{13}$$

where N is given by (2) and Q is to be determined . Equation (12) can then be solved for Q. This leads to

$$q=-N(g)\dot{T}\int_g^G dg\left[\frac{1}{DN(g)}\int_g^G\frac{\partial}{\partial T}f^0(g')dg'\right]. \tag{14}$$

Thus one may obtain an approximation for $q(g)$ and, hence, the correction to $f^0(g)$, for the case that the effects of the changing temperature are small. If q is not small, relative to $f^0(g)$, one is alerted to the fact that the full time dependent equation (8) must be solved.

IV. NUMERICAL CONSIDERATIONS

In this section we examine the extent to which a changing temperature affects the results of a calculation of the nucleation of pion bubbles in a cooling quark-gluon plasma. Such an example is considered in Ref. [1] where an expression for I, derived under the assumption of a constant temperature, is evaluated at the instantaneous temperature of the cooling quark-gluon plasma. The work of [1] is interesting to study because of the large change of 25% in ΔF for a critical size drop when T changes by 1 MeV at $T=160.5$ MeV $=0.95T_c$. Here T_c is the temperature at which the critical radius becomes infinite. One should note that $f(g)$ is proportional to $\exp(-\Delta F/T)$ among other factors. For $T=152$ MeV $(0.9T_c)$ ΔF changes by 11%. Thus it is possible that for temperatures of about $0.95T_c$ the effects of the changing temperature may be important.

In an adiabatic situation I is independent of g because $\partial f(g)/\partial t=0$. For a rapidly changing temperature this is not the case. We assume, however, that the effects of the changing temperature are very small, i.e., that $f(g)$ is only changed slightly from its constant temperature value. We then test if

$$[I(g_*)-I(G)]/I(G) \tag{15}$$

is small. This is a test of the dependence of I on g rather than a test of the modification of $f^0(g)$ due to a rapidly changing temperature. Expression (15) is simpler to evaluate than the correction (14) to $f^0(g)$. Expression (15) and that for q (14), however, are closely related as will be shown. If (15) is small then the effects of temperature are insignificant and the adiabatic approach can be used. Otherwise a full time dependent approach to nucleation, using (1) and (8), is needed. To calculate $[I(g_*)-I(G)]/I(G)$ one may integrate (3) to obtain

$$\int_{g_*}^{G}\frac{\partial f}{\partial t}dg=-I(G)+I(g_*). \tag{16}$$

Both sides of (16) can be divided by I to give a per cent change in the nucleation rate. One may note that the integral on the left-hand side (LHS) of (16) is present in the expression for q (14). It can be shown that if (15) is large this implies q is large relative to $f^0(g)$. Assuming that the effects due to the changing temperature are small one can replace $f(g)$ in (16) with $f^0(g)$ given by (4). We now consider the numerical inputs needed to evaluate (15). The temperature of the vapor drops, in a Bjorken model (see [1]), according to

$$T(t)=2T_c\left(\frac{t}{3/8}\right)^{-1/3}, \tag{17}$$

where t, measured in fm/c, represents the proper time, i.e., the time measured in a frame moving with the expanding vapor, and $T_c=169$ MeV. To evaluate (16) using (4) we make use of expressions for quantities such as R_*, ΔF, and I provided in [1,2]. Here R is the bubble radius and R_* the radius of the critical size bubble. References [1,2] do not provide a value for the diffusion constant D. An expression for D, however, can be obtained, following the work of Langer [6]:

$$D=T\kappa/\gamma. \tag{18}$$

To evaluate κ we use the expression given in [2]

$$\kappa=\frac{16\sigma\eta}{3R_*^3(\Delta w)^2}. \tag{19}$$

(A different result for κ has been proposed in [7] but this additional result does not affect the final conclusions of this report.) When dealing with pion bubbles it is convenient to express g as a product of the pion density and the bubble volume. The pion density then cancels from expression (16) and all derivatives and integrals can be expressed in terms of the variable volume. The volume associated with G is taken to be 1.2 times that of g_*, Fig. 1.

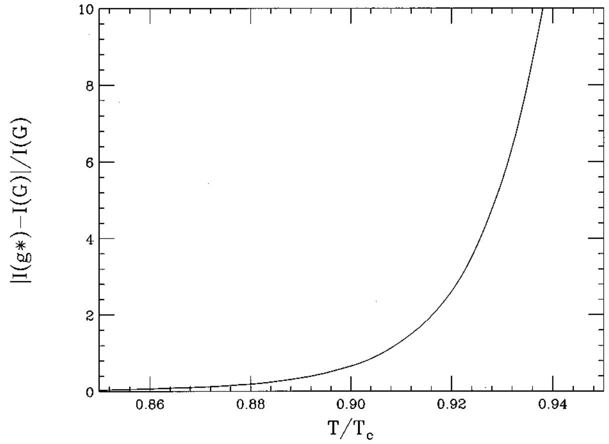

FIG. 1. The dependence of I on g due to the effects of a decreasing temperature.

In the model of [1] the quark-gluon medium cools to $0.95T_c$ before the nucleation rate becomes appreciable. The medium then continues to cool to $0.8T_c$ before beginning to warm due to the energy released in the phase transition from quark-gluon matter to growing pion bubbles. The large value for $T=0.95T_c$ is due to a large $\dot{T}$, namely, -15 MeV/(fm/c), and a large change in $\exp(-\Delta F/T)$ of about 50%. A large change in $[I(g_*)-I(G)]/I(G)$ indicates that the effect of the cooling temperature of the quark-gluon medium, is large. Thus for high temperatures, near $0.95T_c$, the constant temperature approximation breaks down completely and a time dependent calculation of $f(g)$ (8) is needed. I is then evaluated using (1). One should note that the adiabatic result for $f(g)$, i.e., $f^0(g)$, is obtained under the assumption that $I(g)$ is independent of g. This condition does not hold at $0.95T_c$. For $T=0.87T_c$ the value of $|I(g_*)-I(G)|/I(G)$ has fallen to about 10%. For low temperatures, e.g., $0.85T_c$, the effects of a changing temperature become negligible. At this low temperature, however, the critical size of the pion bubble is so small that it is questionable, as pointed out in [2], whether there is nucleation at all.

The fact that the integral on the LHS of (16) is large relative to $I(G)$, for T near $0.95T_c$, implies that q, given by (14), is large relative to $f^0(g)$. Thus not only is $I(g)$ strongly dependent on g but $f(g)$ is significantly changed from $f^0(g)$. We should point out that we have considered the case of f close to f^0 in our numerical example and found large effects due to the changing temperature. It is necessary, however, to calculate the actual f from (8) to find the exact effect of the changing temperature.

V. CONCLUSION

It is necessary to consider a full time dependent treatment of nucleation in a metastable medium whose temperature is changing rapidly in time. For the case of small $\dot{T}$ it is possible to find a correction to $I(T)$, due to the changing temperature, using (14) and (1). We have examined the case of pion bubbles forming in a quark-gluon vapor and find that the small temperature change modification is not enough for T near $0.95T_c$. Thus it appears that one cannot evaluate an expression for the nucleation rate, derived under the assumption of constant temperature, at each instantaneous temperature of the cooling quark-gluon plasma. Rather the very different approach of solving for the drop size distribution $f(g)$ from the time dependent differential equation (8) should be used. The nucleation rate may then be obtained from (1).

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