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Dynamical growth rate of a diffuse interface in first-order phase transitions

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We compute the dynamical prefactor in the nucleation rate of bubbles or droplets in first-order phase transitions for the case where both viscous damping and thermal dissipation are significant. This result, which generalizes previous work on nucleation, may be applied to study the growth of bubbles or droplets in condensed matter systems as well as in heavy ion collisions and in the expansion of the early universe.

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When matter in a certain phase is metastable, localized fluctuations in the state variables may activate the nucleation of bubbles (a term we use below to represent either bubbles or droplets) of a more stable phase of matter. If these bubbles have a radius larger than some critical value, they begin to grow exponentially. The nucleation and growth of these critical bubbles has historically been of great interest in the physics of liquid-gas phase transitions and in condensed matter physics [1]. More recently, they have been studied in the context of first-order phase transitions in the early universe [2–4] and in high energy heavy ion collisions [5].

A general kinetic theory of homogeneous nucleation was developed by Langer [6]. In the neighborhood of a first-order phase transition, when the critical radii of the bubbles exceed the correlation length, a reduced description of nucleation in terms of a coarse-grained free energy is appropriate. Langer and Turski [7] used such a phenomenological approach to show that the nucleation rate of bubbles could be written as a product of three terms

$$I = \frac{\kappa}{2\pi}\Omega_0 \exp(-\Delta F/T)\,. \tag{1}$$

If the bubbles have a radius smaller than a certain critical radius R_*, they are unstable and will collapse. On the other hand, if the bubble radius exceeds R_*, they will begin to grow exponentially. The dynamical prefactor κ determines the initial exponential rate of growth of bubbles of radii larger than the critical radius. For the bubbles to grow beyond the critical radius, latent heat must be carried away from the surface of the bubble. This is achieved through thermal dissipation and/or viscous damping. Kawasaki [8] and Turski and Langer [9], neglecting viscous damping, show that κ for the condensation of a supersaturated vapor is linearly proportional to the thermal conductivity of the vapor. The statistical prefactor Ω_0 is a measure of the phase space volume of the saddle point region of the free energy functional and ΔF is the change in the free energy required to activate the formation of a critical bubble.

Recently, the theory of Langer and Turski has been used by Csernai and Kapusta to study nucleation in relativistic first-order phase transitions [3]. The baryon density in the systems studied is negligible. In the absence of a net conserved charge, the thermal conductivity vanishes and the expression of Langer and Turski for the dynamical prefactor is no longer applicable. It was shown in Ref. [3] that, for the systems studied, the latent heat could be transported from the growing bubble by viscous damping instead of thermal dissipation; the new expression for the dynamical prefactor depends linearly on the shear viscosity of the surrounding medium. The resulting expression for the preexponential factor differs significantly from earlier estimates where, on dimensional grounds, the prefactor was taken to be T^4 or T_c^4. Here T is the temperature and T_c is the critical temperature of the first-order phase transition.

In this work, we derive a general expression for the dynamical prefactor in the nucleation rate of critical sized bubbles in first-order phase transitions. The results of Langer and Turski and Csernai and Kapusta are obtained as extreme limits of our general formula. This formula may be used to study nucleation in liquids and gases and in condensed matter systems where both the viscosity and thermal conductivity are significant. It may also

be used to estimate the probability of formation of superheated quark-gluon droplets or supercooled hadronic bubbles in the baryon-rich matter produced in high energy heavy ion collisions [10]. Further applications also include the expansion of the early universe and the formation of neutron stars.

Consider two phases of matter, phase A and phase B, where phase A is a metastable state which decays into the more stable phase B. Phase A, for instance, may be a supersaturated vapor which when supercooled nucleates bubbles of a liquid phase B. When the radius R_* of the critical bubble of phase B is greater than the correlation length ξ in phase A, the behavior of the system can be described in terms of a coarse-grained energy functional F. This functional depends on the fluid density $n(\vec{r})$, the local fluid velocity $U(\vec{r})$, and the temperature $T(\vec{r})$. Following Ref. [7], we make the ansatz that $F = F_K + F_I$ where F_K is the kinetic energy. The interaction term F_I is the sum of the Helmholtz free energy and the van der Waals–Cahn–Hilliard gradient energy [11]. The formalism for the coarse-grained free energy functional is also valid for relativistic systems where the pressure is comparable to the energy density and the fluid velocity $U(\vec{r})$ in the local rest frame is small compared to the speed of light.

In addition to the homogeneous phases A and B, the free energy is also stationary for a configuration whose solution is a generalization of the van der Waals soliton. If the critical radius is much larger than the correlation length, the stationary solution has a hyperbolic tangent-like density profile. To determine the expansion of the bubble about this stationary configuration, we linearize the hydrodynamic equations around the stationary configuration: $n(\vec{r}) = \bar{n}(\vec{r}) + \nu(\vec{r})$, $\vec{U}(\vec{r}) = \vec{0} + \vec{U}(\vec{r})$, and $T(\vec{r}) = T_0 + \theta(\vec{r})$, where the quantities ν, $\vec{U}$, and θ correspond to small deviations in the density, velocity, and temperature, respectively, from their stationary values. They approach constant values away from the interface. We derive below a general expression for κ which does not depend on any specific parametrization of the free energy.

In Ref. [9] relations were derived between the velocity potential and the density and temperature functions on either side of a diffuse interface. These relations, the Kotchine conditions [12], are generalizations of the well-known Rankine-Hugoniot discontinuity conditions for shocks. For instance, in the former case, the velocity of matter diffusing through the interface is a function of position and falls off away from the interface. In the latter case, the velocity of the matter is a constant. It was shown in Ref. [9] that these Kotchine conditions give the correct dispersion spectrum for capillary waves.

We now use the Kotchine conditions for a spherically growing bubble to derive an expression for the dynamical prefactor κ. Our derivation is similar to that of Turski and Langer but differs from theirs in some key aspects. The Kotchine conditions for a spherical bubble are

$$[nU_R] = [n]\frac{dR}{dt}\,, \tag{2}$$

$$[P] = -\frac{2\sigma}{R}\,, \tag{3}$$

$$[\mu] = 0\,, \tag{4}$$

$$\frac{ln_an_b[U_R]}{[n]} = -\lambda(\nabla T)_R - \left(\frac{4}{3}\eta + \zeta\right) U_R \left(\frac{dU}{dr}\right)_R . \tag{5}$$

In the above, the brackets denote the difference in the bracketed quantity across the interface. For instance, $[n] \equiv n_b - n_a = \Delta n$, where the subscripts denote phase B and phase A, respectively. Also, U_R is the velocity of matter through the interface, dR/dt is the velocity of the bubble wall, P is the pressure, and μ the chemical potential. The latent heat per particle is given by l, λ is the thermal conductivity, and η and ζ are the shear and bulk viscosities, respectively.

The first Kotchine condition, Eq. (2), is the matter continuity relation across the interface. The second Kotchine condition is the well-known Laplace formula for the surface tension. The third denotes the continuity of chemical potentials between the two phases at T_c. The final Kotchine condition equates the latent heat produced per unit area per unit time at the interface to the energy dissipated per unit area per unit time.

Combining Eq. (2) and Eq. (5), the total energy flux transported outwards is given by

$$\Delta w \frac{dR}{dt} = -\lambda \frac{dT}{dr} - \left(\frac{4}{3}\eta + \zeta\right) U_R \frac{dU_R}{dr}\,. \tag{6}$$

Here Δw is the difference in the enthalpy densities of the two phases. From the continuity relation $\partial_t \nu = -\vec{\nabla} \cdot (\bar{n}\vec{U}_R)$, one may show [see the discussion preceding Eq. (77) in Ref. [3]] on very general grounds that the radial dependence of the velocity at the interface $U_R \propto 1/r^2$. Hence, $dU(r)/dr|_{r=R} = -2U_R(r)/R$. Substituting this relation in the above equation, we obtain

$$\Delta w \frac{dR}{dt} = -\lambda \frac{dT}{dr} + 2\left(\frac{4}{3}\eta + \zeta\right) \frac{U_R^2}{R}\,. \tag{7}$$

We wish to obtain a similarly simple expression for the gradient in the temperature dT/dr. For the systems we consider, we may assume that the temperature varies slowly across the bubble wall. If we represent the temperatures in the two phases by T_a and T_b, we can define an average temperature T and the variation θ_0 by $T_a = T + \theta_0$ and $T_b = T - \theta_0$. In the quasistationary approximation $\nabla^2\theta \approx 0$. The solution to the Laplacian is then [13]

$$\begin{aligned} \theta_b &= \theta_0\ , \forall\, r \le R\,, \\ \theta_a &= \frac{\theta_0 R}{r}\ , \forall\, r > R\,, \end{aligned} \tag{8}$$

where θ_0 is a constant. Hence,

$$\left.\frac{dT}{dr}\right|_{r=R} = -\frac{\theta_0}{R}\,. \tag{9}$$

To determine θ_0, we use the continuity of chemical potentials $\mu_a = \mu_b$ across the interface of the critical bubble (the third Kotchine condition). Then, using the first law of thermodynamics and assuming a large latent heat (strong first-order transition), we arrive at the relation

$$\frac{P_b}{n_b} - \frac{P_a}{n_a} \approx -\frac{l\theta_0}{T} . \tag{10}$$

Now from the second Kotchine condition, Eq. (3),

$$P_b = P_a + \frac{2\sigma}{R} . \tag{11}$$

Substituting this equation in Eq. (10), we obtain, after a little algebra,

$$P_a = \frac{n_a}{\Delta n}\left(\frac{2\sigma}{R} + \frac{n_b l\theta_0}{T}\right) . \tag{12}$$

The temperature difference between the two phases, $2\theta_0$, is due to the dissipation of latent heat. For the critical bubble, $\theta_0 = 0$, which implies that

$$P_a = \frac{2n_a\sigma}{\Delta n R_*} . \tag{13}$$

Replacing P_a in Eq. (12) with the above expression, we obtain finally for θ_0 the relation

$$\theta_0 = \frac{2\sigma T}{\Delta w R}\left(\frac{1}{R_*} - \frac{1}{R}\right) . \tag{14}$$

Substituting this result for θ_0 in Eq. (9), we have

$$\left.\frac{dT}{dr}\right|_R = -\frac{2\sigma T}{\Delta w R}\left(\frac{1}{R_*} - \frac{1}{R}\right) . \tag{15}$$

We have one further unknown—the velocity $U_R(r)$ of matter diffusing through the surface of the growing bubble. If there exists a net momentum flux through the interface, then from Laplace's formula

$$\Delta w\, U_R^2 = 2\sigma\left(\frac{1}{R_*} - \frac{1}{R}\right) . \tag{16}$$

We have omitted the shear term in the above equation since it represents a higher order contribution to the linearized hydrodynamic equations.

Combining our results in Eq. (15) and Eq. (16) with Eq. (7), we obtain the expression

$$\frac{dR}{dt} = \frac{2\sigma}{(\Delta w)^2 R}\left(\frac{1}{R_*} - \frac{1}{R}\right)\left[\lambda T + 2\left(\frac{4}{3}\eta + \zeta\right)\right] . \tag{17}$$

If $R - R_* \propto \exp(\kappa t) << R$, we obtain finally our result for the dynamical prefactor when both the viscosity and the thermal conductivity of the surrounding medium are significant:

$$\kappa = \frac{2\sigma}{(\Delta w)^2 R_*^3}\left[\lambda T + 2\left(\frac{4}{3}\eta + \zeta\right)\right] . \tag{18}$$

In the limit of zero baryon number, $\lambda \to 0$, and we obtain the result of Csernai and Kapusta. If the matter is baryon rich but viscous damping is negligible, $\eta, \zeta \to 0$, we obtain the result of Kawasaki, and Turski and Langer. Indeed, our broader interpretation (compared to Turski and Langer) of the Kotchine condition in Eq. (5) suggests that the dynamical prefactor in the nucleation rate of a system undergoing a first-order phase transition is linearly proportional to the sum of the transport coefficients of the various dissipative processes occurring in the medium outside the nucleated bubble. The particular dependence on the transport coefficients is a consequence of linearized hydrodynamics. However, we should stress that the Kotchine conditions have a generality which extends beyond linearized hydrodynamics and may in principle be applied to systems where the energy dissipated is not linear in the transport coefficients. In such situations, additional physical assumptions may be required. The Kotchine conditions are necessary but not sufficient to obtain an expression for the dynamical prefactor.

We should point out that there are several assumptions that have been made in our derivation of the dynamical prefactor. As discussed above, our result is strictly valid when nonlinear effects can be ignored and the linearized hydrodynamic equations are applicable. Further, for the coarse-graining description to hold, the radii of the bubbles must be larger than the correlation length. We have also assumed that heating due to dissipation is slow, causing the temperature to vary slowly across the bubble wall. Finally, we have assumed in our derivation that the phase transition is strongly first order, releasing considerable latent heat.

To summarize, we have derived above an expression for the dynamical prefactor which governs the initial growth of critically sized bubbles nucleated in first-order phase transitions. Our derivation emphasizes the importance of the generalized conservation laws for diffuse interfaces and suggests that their validity extends beyond the specific assumptions discussed above. Our results are applicable to the wide range of phenomena where both viscous damping and thermal dissipation effects are important. In the future [10] we will discuss one such application—the nucleation of quark-gluon droplets in baryon-rich hadronic matter created in high energy heavy ion collisions.

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[1] J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8.
[2] A. D. Linde, *Particle Physics and Inflationary Cosmology* (Harwood Academic Publishers, Chur, Switzerland, 1990).
[3] L. P. Csernai and J. I. Kapusta, Phys. Rev. D **46**, 1379 (1992).
[4] M. Carrington and J. I. Kapusta, Phys. Rev. D **47**, 5304 (1993).
[5] L. P. Csernai and J. I. Kapusta, Phys. Rev. Lett. **69**, 737 (1992); L. P. Csernai, J. I. Kapusta, G. Kluge, and E. E. Zabrodin, Z. Phys. C **58**, 453 (1993).
[6] J. S. Langer, Ann. Phys. (N.Y.) **54**, 258 (1969).
[7] J. S. Langer and L. A. Turski, Phys. Rev. A **8**, 3230 (1973).
[8] K. Kawasaki, J. Stat. Phys. **12**, 365 (1975).
[9] L. A. Turski and J. S. Langer, Phys. Rev. A **22**, 2189 (1980).
[10] J. I. Kapusta, R. Venugopalan, and A. Vischer (unpublished).
[11] J. W. Cahn and J. E. Hilliard, J. Chem. Phys. **28**, 258 (1958).
[12] R. Ghez, Surf. Sci. **4**, 125 (1966).
[13] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Pergamon, London, 1959), pp. 201–202.