PHYSICAL REVIEW E VOLUME 60, NUMBER 6 DECEMBER 1999

Dynamical renormalization group calculation of a two-phase sharp interface model

G. Caginalp
University of Pittsburgh, Pittsburgh, Pennsylvania 15260
(Received 28 May 1999)

The temporal evolution of an interface separating two phases is studied using renormalization group and scaling theory and exact calculation of a sharp interface model incorporating surface tension and kinetic undercooling. Under conditions favoring rapid solidification the characteristic length, $R(t)$, varies as $t^{1/2}$ while the total surface area of the interface, $S(t)$, varies as $t^{(d-1)/2}$. This complements the results of Jasnow and Vinals who found $R(t)\sim t$ in the quasistatic regime. The transition in exponents from $R(t)\sim t$ to $R(t)\sim t^{1/2}$, as solidification proceeds from the quasistatic to the rapid solidification regime, suggests a complex evolution toward a self-similar late stage growth. [S1063-651X(99)50612-0]

PACS number(s): 47.20.−k, 47.55.−Kf, 68.10.−m

I. INTRODUCTION

The study of spatial pattern formation arising from nonequilibrium growth has involved several avenues including large scale computations, linear perturbation, and analytical methods [1,2]. In many cases, pattern formation arises through the motion of an interface separating two phases or fluids [2]. The material satisfies a differential equation such as the heat equation on either side of the interface and a condition on the interface itself [1]. Various features have been of interest historically: the onset of instability for fluids (Saffman and Taylor [3]), for alloys (Mullins and Sekerka [4]), and for Stefan-like supercooled solidification [5] have been treated through linear stability methods.

Late stage evolution has been of great interest in dendritic growth (see [6] and references therein), directional solidification in alloys as well as in fluids [2]. In many problems, this is the key issue (see [7,8] for further references and discussion).

A key goal is the development of analytic methodology, analogous to linear stability theory, that would characterize the length scale of self-similar growth. Significant progress toward this end was made by Jasnow and Vinals [7,8] (see references contained therein) who implemented a renormalization group approach to study approximations to a one-phase interface problem.

Using a quasistatic approximation, i.e., the heat equation $u_t=\nabla^2 u$ is replaced by Laplace's equation, $\nabla^2 u=0$, in one of the phases, they found that the characteristic length, $R(t)$, of a self-similar system evolves linearly in time so that $R(t)\sim t$. In this paper, we consider the full two-phase and dynamical problem in arbitrary spatial dimension in a highly supercooled environment so that rapid solidification occurs.

The main results are that the characteristic length in the system, $R(t)$, evolves as $t^{1/2}$, and that the capillarity length is (once again) not relevant to the scaling of the large scale behavior. The difference in exponents in the two regimes indicates a complex transition between the two.

II. GREEN'S REPRESENTATION OF THE INTERFACE

A. Model and traveling wave solutions

We consider a very fundamental problem that can easily be generalized to include many physical phenomena. For convenience, we utilize thermodynamic terminology. A material occupying a spatial region $\Omega\subset\mathbb{R}^d$ can be in either of two phases, which we call liquid $(+)$ and solid $(-)$ phases. A (sharp) interface problem describing the thermal properties of this system involves solving for the temperature, T, and the interface, $\Gamma(t)$ in

$$C_v T_t = K\Delta T, \quad \text{in } \Omega\backslash\Gamma, \tag{2.1}$$

$$l v_n = -K[\nabla T\cdot\hat{n}]_-^+ \quad \text{on } \Gamma, \tag{2.2}$$

$$T-T_{eq}=\frac{-\sigma}{[s]_{eq}}(\kappa+\alpha v) \quad \text{on } \Gamma. \tag{2.3}$$

Here, $[\cdots]_-^+$ denotes the difference in the limiting values between the two sides of the interface, T_{eq} is the melting temperature which we assume, without loss of generality, is zero, C_v is specific heat, K is thermal conductivity, l is latent heat, σ is surface tension and $[s]_{eq}$ is the entropy difference between phases. The variables κ and v_n are curvature and normal velocity at the point on the interface, respectively.

A traveling wave solution, $\{T(t,z,c^*\}$ in the $\hat{z}$ direction with velocity c^* can be written subject to the condition $T(t,\infty)=T_{\text{cool}}$ at $z=\infty$ as (see Caginalp and Nishiura [9])

$$T^0(t,z)=\begin{cases} T_{\text{cool}}+l/C_v e^{-[c^*(C_v/K)](z-c^*t)} & z>c^*t \\ T_{\text{cool}}+l/C_v & z\leqslant c^*t, \end{cases} \tag{2.4}$$

$$c^*=\frac{-[s]_{eq}}{\alpha\sigma}(T_{\text{cool}}+l/C_v). \tag{2.5}$$

By subtracting out the planar solution $T^0(t,z)$ from the full solution to Eqs. (2.1)–(2.3) which we denote $T(t,\vec{x},z)$ with $\vec{x}\in\mathbb{R}^{d-1}$ describing the remaining spatial coordinates, we let

$$w(t,\vec{x},z)=T(t,\vec{x},z)-T^0(t,z). \tag{2.6}$$

Following Jasnow and Vinals [7,8], we write $z=h(t,\vec{x})$ as the displacement of the interface from $z=0$ (i.e., the original stationary units). Then dh/dt measures movement in the $\hat{z}$

direction (with unit vector $\hat{k}$), so that the normal velocity can be written as $v_n=(dh/dt)\hat{k}\cdot\hat{n}$ with $\hat{n}$ in the direction from solid to liquid.

Substitution of Eqs. (2.5) and (2.6) and v_n into Eqs. (2.1)–(2.3) leads to the following system of equations for *w*:

$$C_v w_t = K\Delta w, \tag{2.7}$$

$$-K[\nabla w\cdot\hat{n}]_-^+ = l\frac{d}{dt}(h-c^*t)\hat{k}\cdot\hat{n} \quad \text{on } \Gamma, \tag{2.8}$$

$$w=\frac{-\sigma}{[s]_{eq}}\left\{\kappa+\alpha\frac{d}{dt}(h-c^*t)\hat{k}\cdot\hat{n}\right\} \quad \text{on } \Gamma, \tag{2.9}$$

where Eq. (2.4) for $z=c^*t$ has been used in the last equation.

B. Representation using Green's theorem

We consider Eqs. (2.7)–(2.9) in a domain, $\mathcal{D}$, in $\mathbb{R}^d$ which is infinite in the $\hat{z}$ direction and large in the remaining $d-1$ dimensions. We impose periodic boundary conditions in these $(d-1)$ dimensions and initial conditions $w(0,\vec{x},z)=g(\vec{x},z)$. The first two equations, (2.7) and (2.8), can be written as a single equation (Oleinik [10]) by defining locally a signed distance, r (defined a sufficiently small distance from the interface), that is positive on the liquid side, and a discontinuous function $\varphi(r,t)$ that is $+1$ in the liquid phase and -1 in the solid phase. One has then

$$C_v w_t - K\Delta w = \frac{-l}{2}\varphi_t, \tag{2.10}$$

where φ depends upon r and t in the form

$$\varphi(t,\vec{x},z)=F\left(r-\frac{\partial}{\partial t}(h-c^*t)\hat{k}\cdot\hat{n}\right). \tag{2.11}$$

Here φ is interpreted in the sense of distributions, or equivalently, as a limit of functions $\varphi^{(\epsilon)}(z)=\tanh(z/\epsilon)$ as $\epsilon\to 0+$.

Treating the sharp "phase" function φ, as a source term in the parabolic differential equation, one can use the Green's formulation to write, with $\vec{X}$ denoting $(\vec{x},z)\in\mathbb{R}^d$,

$$w(\vec{X},t)=\int_0^t ds\int_{\mathcal{D}} d^d y\, G(\vec{X}-\vec{y},t-s)\left(\frac{-l}{2C_v}\varphi_s(s,\vec{y})\right), + \int_{\mathcal{D}} d^d y\, G(\vec{X}-\vec{y},t)g(\vec{y}),$$

$$\text{with } G(\vec{y},t):=(4\pi Dt)^{-d/2}e^{-(4Dt)^{-1}|\vec{y}|^2}, \quad D:=K/C_v. \tag{2.12}$$

Using local coordinates $(\vec{r},\vec{\sigma})$ that are normal and tangential, to the interface, respectively, one can integrate across the interface (i.e., $\int d\vec{r}$) leaving only the surface area or arc length integral

$$w(\vec{X},t)=\int_0^t ds\int_\Gamma d\sigma_y G(\vec{X}-\vec{y},t-s)\left[\frac{-l}{C_v}\left(\frac{\partial h}{\partial s}-c^*\right)\hat{k}\cdot\hat{n}\right] + \int_{\mathcal{D}} G(\vec{X}-\vec{y},t)g(\vec{y})dy. \tag{2.13}$$

For points $(\vec{X},t)$ on the interface one can substitute Eq. (2.9) for the left-hand side of Eq. (2.13) and write

$$\frac{\sigma}{[s]_{\rm eq}}\left\{\kappa+\alpha\frac{\partial}{\partial t}(h-c^*t)\hat{k}\cdot\hat{n}\right\} = \frac{l}{C_v}\int_0^t ds\int_\Gamma d\sigma_y G(\vec{X}-\vec{y},t-s)\left(\frac{\partial h}{\partial s}-c^*\right)\hat{k}\cdot\hat{n} + \int_{\mathcal{D}} G(\vec{X}-\vec{y},t)g(\vec{y})d\vec{y}. \tag{2.14}$$

III. RENORMALIZATION GROUP ANALYSIS OF THE INTERFACE EQUATION

We define the reduced dimensional quantities $u_{\rm cool}:=T_{\rm cool}/(l/C_v)$, $u_0(\vec{y}):=g(\vec{y})/(l/C_v)$, $d_0:=(\sigma/[s]_{eq})/(l/C_r)$ and rewrite Eq. (2.14) with $\xi:=h-c^*t$ as

$$d_0\left\{\kappa+\alpha\frac{\partial\xi}{\partial t}\hat{k}\cdot\hat{n}\right\}=\int_0^t ds\int_\Gamma d\sigma_y G(\vec{X}-\vec{y},t-s)\frac{\partial\xi}{\partial s}\hat{k}\cdot\hat{n} + \int_{\mathcal{D}} G(\vec{X}-\vec{y},t)u_0(\vec{y})d\vec{y} \tag{3.1}$$

Following Jasnow and Vinals [7,8] we write Eq. (3.1) entirely in dimensionless variables by choosing $\mathcal{L}$ as a reference length (e.g., some fixed d_0) and letting $d_0':=d_0/\mathcal{L}$ and $\kappa'=\kappa/(1/\mathcal{L})$. With $\mathcal{T}$ as a reference time scale so that $t'=t/\mathcal{T}$ and the dimensionless velocities are $v_n'=v_n/(\mathcal{L}/\mathcal{T})$, $c^{*\prime}=c^*/(\mathcal{L}/\mathcal{T})$, etc., and the diffusivity in dimensionless form is

$$D':=(K/C_v)/(\mathcal{L}^2/\mathcal{T}).$$

Unlike the elliptic Green's function with dimensions of $(\text{length})^{2-d}$ used by Jasnow and Vinals [7,8], the (parabolic) Green's function has dimensions of $(\text{length})^{-d}$, and has the dimensionless counterpart

$$G'(\vec{y},t)=G(\vec{y}',t')/\mathcal{L}^{-d}=(4\pi D't')^{-d/2}e^{-(4D't')^{-1}|\vec{y}'|^2}. \tag{3.2}$$

Using the dimensionless units, with primes omitted, using $\bar{\zeta}\in\mathbb{R}^{d-1}$ for points on the interface, suppressing $\hat{k}\cdot\hat{n}$ and omitting the initial condition term (which does not influence the calculations) we write

$$d_0\left\{\kappa(\vec{\zeta},t)+\alpha\frac{d}{d\tilde{t}}\xi(\vec{\zeta},\tilde{t})|_{\tilde{t}=t}\right\}$$

$$=\int_0^t ds\int_\Gamma d^{d-1}\sigma G(\vec{\zeta}-\vec{\sigma},t-s)\frac{\partial}{\partial\tilde{t}}\xi(\vec{\sigma},\tilde{t})|_{\tilde{t}=s}. \tag{3.3}$$

We implement a renormalization procedure that is similar to that used by Jasnow and Vinals [7,8]. The first step is to make an algebraic substitution into Eq. (3.3) of $b\vec{\zeta}$ for $\vec{\zeta}$ and $b^{-\lambda}t$ for t, where $b\in\mathbb{R}^+$ and $\lambda\in\mathbb{R}$ are arbitrary,

$$d_0\left\{\kappa(b\vec{\zeta},b^{-\lambda}t)+\alpha\frac{\partial\xi}{\partial\tilde{t}}(b\vec{\zeta},\tilde{t})|_{\tilde{t}=b^{-\lambda}t}\right\}$$

$$=\int_0^{b^{-\lambda}t} ds\int_\Gamma d^{d-1}\sigma G(b\vec{\zeta}-\vec{\sigma},b^{-\lambda}t-s)\frac{\partial}{\partial\tilde{t}}\xi(\vec{\sigma},\tilde{t})|_{\tilde{t}=s}. \tag{3.4}$$

Defining new variables $s' := s/b^{-\lambda}$ and $\vec{\sigma}' := \vec{\sigma}/b$ in order to rescale time and space, we can rewrite the right-hand side of Eq. (3.4) as

$$\int_0^t b^{-\lambda}ds'\int_\Gamma b^{d-1}d^{d-1}\sigma'$$

$$=G(b\vec{\zeta}-b\vec{\sigma}',b^{-\lambda}t-b^{-\lambda}s')\frac{\partial}{\partial\tilde{t}}\xi(b\vec{\sigma}',\tilde{t})|_{\tilde{t}=b^{-\lambda}s'}, \tag{3.5}$$

so that Eq. (3.4) now has the form

$$d_0\left\{\kappa(b\vec{\zeta},b^{-\lambda}t)+\frac{\alpha}{b^{-\lambda}}\frac{\partial\xi}{\partial t}(b\vec{\zeta},b^{-\lambda}t)\right\}$$

$$\times\int_0^t b^{-\lambda}ds'\int_\Gamma b^{d-1}d^{d-1}\sigma'$$

$$\times G(b\vec{\zeta}-b\vec{\sigma}',b^{-\lambda}t-b^{-\lambda}s')$$

$$\times\frac{1}{b^{-\lambda}}\frac{\partial}{\partial s'}\xi(b\vec{\sigma}',b^{-\lambda}s'). \tag{3.6}$$

Recalling that the Green's function, G, [see Eq. (2.12)] incorporates the diffusivity, D, we write the identity

$$G(b(\vec{\zeta}-\vec{\sigma}'),b^{-\lambda}(t-s');D)$$

$$=b^{-d}G(\vec{\zeta}-\vec{\sigma}',t-s';D/b^{2+\lambda}). \tag{3.7}$$

At this point we assume *self-similarity* (see Jasnow and Vinals [8]), i.e.,

$$\xi(b\vec{\sigma},b^{-\lambda}t)=b\xi(\vec{\sigma},t),\quad b\kappa(b\vec{\sigma},b^{-\lambda}t)=\kappa(\vec{\sigma},t). \tag{3.8}$$

This is simply the statement that if we rescale the position on the interface by b and time by $b^{-\lambda}$, then the position in the $\hat{z}$ direction, ξ, also changes by a factor b. Similarly, the sum of principal curvatures, κ, has units of 1/(length) and scales as b^{-1}. In other words, if $\xi(\vec{\sigma},t)$ and $\kappa(\vec{\sigma},t)$ are the values for the height ($\hat{z}$ coordinate) and curvature at time t, then we can obtain the values at time $b^{-\lambda}t$ by multiplying all length scales in the problem by b.

Substitution of Eqs. (3.7) and (3.8) into Eq. (3.6) yields the interface equation

$$\frac{d_0}{b}\left\{\kappa(\vec{\sigma},t)+\frac{\alpha}{b^{-\lambda-2}}\frac{\partial}{\partial t}\xi(\vec{\sigma},t)\right\}$$

$$=\int_0^t ds'\int_\Gamma d^{d-1}\sigma' G(\vec{\zeta}-\vec{\sigma}',t-s';D/b^{2+\lambda})$$

$$\times\frac{\partial\xi}{\partial s'}(\vec{\sigma}',s'). \tag{3.9}$$

The second step in the renormalization process is to rescale the physical parameters so that Eq. (3.9) has the same form as that of the original system, namely, Eq. (3.3). Thus, the process of rescaling spatial coordinates $b\vec{r}\to\vec{r}$ and time, $b^{-\lambda}t\to t$, as done in Eqs. (3.6)–(3.9), under the self-similarity assumption (3.8), together with the rescalings

$$d_0\to d_0/b,\quad \alpha\to\alpha/b^{-\lambda-2},\quad D\to D/b^{2+\lambda} \tag{3.10}$$

allows us to transform the interface equation back into the original form.

If the system is described by a characteristic length, R, then it is also governed by the self-similarity relation of the form (3.11), i.e.,

$$bR(b^{\lambda}t;d_0/b,D/b^{2+\lambda},\alpha/b^{-\lambda-2})=R(t;d_0,D,\alpha). \tag{3.11}$$

The scaling equation for the characteristic length, Eq. (3.11), then describes the required change in the physical parameters (d_0,D,α) under the RG transformation. Since b is arbitrary, we can choose $b=t^{-1/\lambda}$ and rewrite Eq. (3.11) as

$$R(t;d_0,D,\alpha)=t^{-1/\lambda}R(1;d_0/t^{-1/\lambda},D/t^{-2/\lambda-1},\alpha/t^{1+2/\lambda}). \tag{3.12}$$

The value of λ clearly determines the large time characteristics of the characteristic length, R. The identity (3.12) distinguishes the value $\lambda=-2$ since either $\lambda>-2$ or $\lambda<-2$ imply that the arguments $D/t^{-2/\lambda-1}$ and $\alpha/t^{2/\lambda+1}$ on the right-hand side of Eq. (3.12) either diverge or vanish for $t\to\infty$. Each of these is physically irrelevant since $\alpha\to 0$ or $\alpha\to\infty$ implies the velocity of the plane wave given by Eqs. (2.4) and (2.5) is then infinity or zero.

Hence, the only possibility for a fixed point is for $\lambda=-2$, for which

$$d_0\to\frac{d_0}{t^{1/2}}\to 0,\quad D\to D,\quad \alpha\to\alpha, \tag{3.13}$$

so that any values of D and α are fixed points while d_0 iterates to zero.

Hence, $\lambda=-2$ is the physically relevant exponent so that Eq. (3.12) can now be written as

$$R(t;d_0,D,\alpha)=t^{1/2}R(1;d_0/t^{1/2},D,\alpha)\approx t^{1/2}R(1;0,D,\alpha). \tag{3.14}$$

The scaling relation (3.14) for this high undercooling regime results in a growth rate of $t^{1/2}$ which differs from the $R\sim t$ found for the regime considered by Jasnow and Vinals [7,8].

IV. CONCLUSIONS

For the fully dynamic rapid solidification regime characterized by large undercooling [$T_{\mathrm{cool}}<-l/C_V$ in Eq. (2.5)], one has the key relation $R\sim t^{1/2}$, i.e., that the characteristic length increases as the square root of the time elapsed. Hence, the exponent in $t^{1/2}$ differs from that found for the quasistatic problem (Jasnow and Vinals [7,8]). Similarly, one calculates the large time total surface area, $S(t)$, of the interface as $S\sim t^{(d-1)/2}$ that differs from the quasistatic regime. This Green's function approach also offers the potential for understanding this transition between the two very different regimes, and for developing a formation that can interpolate between static and dynamic scaling.

ACKNOWLEDGMENT

G.C. was supported by NSF Grant No. DMS-9703530.

[1] J. Crank, *Free and Moving Boundary Problems* (Clarendon Press, Oxford, 1984).
[2] M. Cross and P. C. Hohenberg, Rev. Mod. Phys. **65**, 851 (1993).
[3] P. G. Saffman and G. I. Taylor, Proc. R. Soc. London, Ser. A **245**, 312 (1958).
[4] W. W. Mullins and R. Sekerka, J. Appl. Phys. **35**, 445 (1964).
[5] J. R. Ockendon, in *Free Boundary Problems*, edited by E. Magenes (Technoprint, Bologna, 1980), pp. 444–478.
[6] M. Ben Amar and Y. Pomeau, in *Physiochemical Hydrodynamics and Interfaces Phenomena*, edited by M. E. Velarde (Plenum, New York, 1989).
[7] D. Jasnow and J. Vinals, Phys. Rev. A **40**, 3864 (1989).
[8] D. Jasnow and J. Vinals, Phys. Rev. A **41**, 6910 (1990).
[9] G. Caginalp and Y. Nishiura, Q. Appl. Math. **49**, 147 (1991).
[10] O. A. Oleinik, Sov. Math. Dokl. **1**, 1350 (1960).