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Coating of moving domain boundaries by a diffusive ordered phase

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Abstract
Domain boundaries in a solid can be wetted by the layer of a new phase of the host material. The formation of such a layer is considered for the case where the defect moves under an external force, and where the order parameter of the wetting film is a conserved quantity.

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The nucleation of a new phase at a moving extended defect [1] generates, via energy dissipation into the nucleus, a viscous friction force acting on the defect [2]. Above some (temperature-dependent) velocity threshold this can lead to an unexpected self-acceleration and, as a consequence, to a morphological instability of the defect [3]. The origin of these phenomena is a delicate interplay between the defect motion and the formation process of the nucleus. This has recently been discussed for the model of a simple domain boundary, dressed by the nucleus of a non-conserved Ginzburg–Landau order parameter [4]. For the case of a conserved order parameter the overall behaviour turns out to be similar, but shows some notable peculiarities, which have been worked out in the present paper. The problem is related to that of grain-boundary dragging by particle diffusion [5], reviewed in [6]. Whereas these treatments crucially depend on the assumption of a smoothly-varying internal structure of the grain boundary [7], a sharp-interface approximation is sufficient in the present analysis.

The configurations of the domain boundary at time t will accordingly be described in the purely geometric form $z = Z(x, t)$ where x are two-dimensional Cartesian coordinates

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vertical to z. In terms of $Z(x,t)$ and the order-parameter field $\varphi(\boldsymbol{r},t)$ with $\boldsymbol{r} \equiv (x,z)$, the effective Hamiltonian of the system reads

$$H = \int \mathrm{d}^2x \left[\frac{\sigma}{2}(\partial Z)^2 - kZ\right] + \int \mathrm{d}^3r \left[\frac{1}{2}(\nabla\varphi)^2 + \frac{\varepsilon}{2}\varphi^2 + \frac{u}{4}\varphi^4 - \frac{\kappa}{2}\delta(z-Z)\,\varphi^2\right]. \tag{1}$$

Here, σ is the stiffness of the defect, ∂ is the two-dimensional nabla operator and k is a driving force in the z-direction. Furthermore, $\varepsilon = \alpha(T - T_c)$ measures the temperature distance from the bulk critical point of φ, and κ quantifies a local reduction of the transition temperature at the defect.

The dynamics of the system will be modelled by the Edwards–Wilkinson [8] and model-B-type [9] equations

$$\partial_t Z = -\Gamma\delta H/\delta Z \qquad \partial_t\varphi = D\nabla^2\delta H/\delta\varphi \tag{2}$$

where Γ is the defect mobility and D the diffusion coefficient of the order parameter. Additional Langevin forces have not been included in (2) since presently we are only interested in the mean-field behaviour of the system.

At sufficiently high temperatures or velocities a nucleus cannot build up, so that the mean-field solutions of (2) are $Z(x,t) = Vt$ with a constant defect velocity $V = \Gamma k \equiv F$, and $\varphi(\boldsymbol{r},t) = 0$. A non-trivial solution of the form $\varphi(\boldsymbol{r},t) = \Phi(z - Vt)$ branches off from the trivial one at the nucleation threshold $T = T_0(V)$ close to which the second equation (2) can be treated by the bifurcation theory [10]. With the notation $\zeta \equiv z - Vt$, one finds the low-amplitude behaviour

$$\Phi(\zeta) = X\psi_0^+(\zeta) + O(X^3) \qquad X \equiv \left(\mathrm{d}^2\psi_0^-, \Phi\right) \tag{3}$$

where the scalar product means integration along the ζ-axis. Moreover, $\psi_0^+(\zeta;V)$ and $\psi_0^-(\zeta;V)$ are the lowest right and left bound-state eigenfunctions of the linearized equation for Φ. In the case of a non-conserved order parameter this equation has the form of a Schrödinger equation with the scalar potential $-\kappa\delta(\zeta)$ and an imaginary vector potential $\mathrm{i}v \equiv \mathrm{i}D^{-1}V$ [4].

For a conserved order parameter one instead is led to the eigenvalue problem

$$\left(\psi_\alpha^-, [\mathrm{d}^4 + \kappa\,\mathrm{d}^2\delta - v\,\mathrm{d}]\psi_\beta^+\right) = \varepsilon_\alpha\left(\psi_\alpha^-,\ \mathrm{d}^2\psi_\beta^+\right) = \varepsilon_\alpha\delta_{\alpha\beta}. \tag{4}$$

Here, α, β label the eigenfunctions and eigenvalues, and d denotes the derivative with respect to ζ. Compared to the non-conserved case, one notes that the gauge symmetry of the fictitious Schrödinger problem is missing. Nevertheless, the lowest eigenvalue $\varepsilon_0(v)$ and its eigenfunctions $\psi_0^\pm(v)$ again can be calculated exactly.

The result for the latter reads

$$\psi_0^\pm(\zeta) = \left(\frac{\kappa}{2\varepsilon_0}\right)^{(1/2)} [\Theta(\zeta)\psi_>^\pm(\zeta) + \Theta(-\zeta)\psi_<^\pm(\zeta)] \tag{5}$$

where

$$\begin{aligned}\psi_>^+(\zeta) &= q_1\frac{q_2 - q_0}{q_1 - q_2}\exp(-q_1\zeta) - q_2\frac{q_1 - q_0}{q_1 - q_2}\exp(-q_2\zeta)\\ \psi_<^+(\zeta) &= -q_0\exp(-q_0\zeta)\end{aligned} \tag{6}$$

and

$$\mathrm{d}^2\psi_>^-(\zeta) = \psi_<^+(-\zeta) \qquad \mathrm{d}^2\psi_<^-(\zeta) = \psi_>^+(-\zeta). \tag{7}$$

In (6) q_0, q_1, q_2 are the roots of the cubic characteristic equations

$$q_i^3 - \varepsilon_0 q_i + v = 0 \qquad i = 0,1,2 \tag{8}$$

arising from (4), with q_0 identified as the always existing real negative solution of (10).

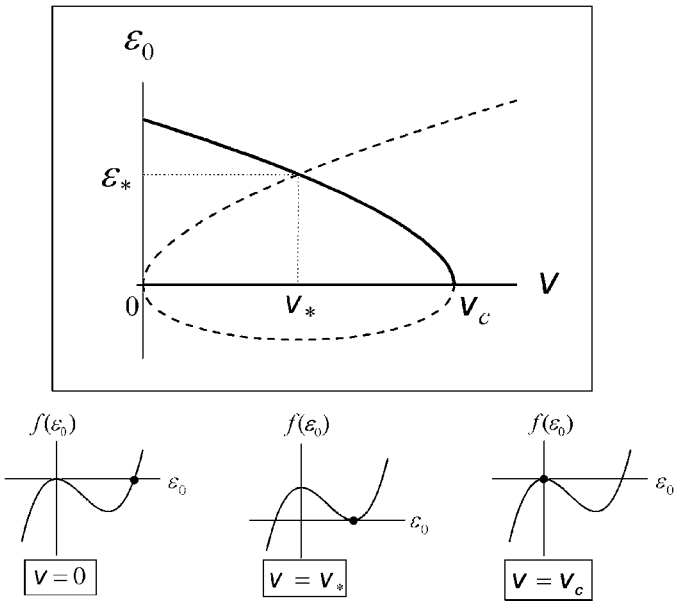

Figure 1. Branches of solutions of equation (11). Whereas the dotted lines are unphysical branches, the full line represents the physical solution (13), illustrated in (*a*), (*b*), (*c*) for $v = 0$, $v = v_*$, and $v = v_c$.

The right eigenfunctions (6) determine the profile of the nucleus, attached to the defect. In the static case $v = 0$ one of the roots of (8), say q_1, vanishes, so that $\psi_>^+$ in (6) reduces to a single exponential. For $v > 0$, however, $\psi_>^+$ consists, contrary to the non-conserved case, of two modes. Above some critical velocity $v_0 \equiv \left(2[\varepsilon_0(v_0)/3]^{3/2}\right)$ the parameters q_1, q_2 form a pair of complex quantities. As a consequence $\psi_>^+$ displays (strongly) damped oscillations, corresponding to alternating order-parameter domains of the nucleus in the direction of propagation.

In order to determine the eigenvalue $\varepsilon_0(v)$, one has to use the jump condition $\mathrm{d}\psi_>^+(0) - \mathrm{d}\psi_<^+(0) = -\kappa\psi_<^+(0)$ which implies

$$2q_0^2 + q_1q_2 = -\kappa q_0. \tag{9}$$

If this is combined with the equations

$$q_0 + q_1 + q_2 = 0 \qquad q_0q_1 + q_1q_2 + q_2q_0 = -\varepsilon_0 \qquad q_0q_1q_2 = -v \tag{10}$$

equivalent to (8), one finds for $\varepsilon_0(v)$ the cubic equation

$$\varepsilon_0^3 - \frac{\kappa^2}{4}\varepsilon_0^2 + \frac{v}{4}(\kappa^3 - 27v) \equiv f(\varepsilon_0) = 0. \tag{11}$$

As illustrated in figure 1, equation (11) has a set of three real solutions in the interval $0 < v < v_c = (\kappa/3)^3$ which is symmetric with respect to the line $v = v_c/2 \equiv v_*$. One of these solutions can directly be excluded, since it is negative and therefore corresponds to temperatures below the bulk transition temperature. The other two branches are positive, monotonically increasing and decreasing, respectively, and intersect each other at $v_*, \varepsilon(v_*) \equiv \varepsilon_*$. The increasing branch again can be excluded, since it is only compatible with a positive, i.e. unphysical, value of q_0. This follows from relations (9) and (10) which imply

$$q_0 = \frac{9(v - v_*) - \kappa(\varepsilon_0 - \varepsilon_*)}{\kappa^2 - 6(\varepsilon_0 - \varepsilon_*)}. \tag{12}$$

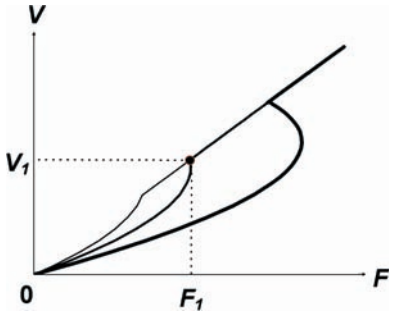

Figure 2. Isotherms in the force–velocity plane, showing hysteresis above the critical point F_1, V_1, T_1.

If, e.g., (12) is evaluated at the singular point $v = v_*$, $\varepsilon = \varepsilon_*$, one finds $q_0 > 0$ for the branch with the positive slope which consequently can be ruled out.

The remaining solution is conveniently represented by the parametric form

$$\begin{aligned} \varepsilon_0 &= \frac{\kappa^2}{12} + \frac{\kappa^2}{6}\left[\Theta(v_* - v)\cos\frac{\phi}{3} + \Theta(v - v_*)\cos\frac{\phi + 4\pi}{3}\right] \\ \cos\phi &= 1 - 8\,\frac{v}{v_c}\left(1 - \frac{v}{v_c}\right). \end{aligned} \tag{13}$$

In accordance with figure 1 it decreases monotonically from $\varepsilon_0(0) = \kappa^2/4$ via $\varepsilon_0(v_*) = \kappa^2/6$ to $\varepsilon_0(v_c) = 0$, and determines the nucleation threshold $T_0(V) \equiv T_c + \alpha^{-1}\varepsilon_0(D^{-1}V)$ which qualitatively looks similar to that in the conserved case [4].

Since in (6) q_1, q_2 can, via (10), be eliminated in favour of q_0 which in turn follows from (12), the mean-field behaviour of (2) close to the nucleation threshold can now be evaluated explicitly. To lowest order in the expansion (3) the first equation (2) assumes the form $V = F + \Gamma\kappa[\psi_0^+ \,\mathrm{d}\psi_0^+]_{\zeta=0}X^2$, and, after insertion of the result for ψ_0^+,

$$V = F - \rho(V)\frac{\kappa^2}{4}X^2(T, V). \tag{14}$$

This looks identical to the corresponding result for the non-conserved case, except for the redefinition of the ratio of timescales $\rho(V) \equiv \Gamma\big/\big[D\varepsilon_0(D^{-1}V)\big]$.

In view of (4), the same approximation for the second equation (2) yields $\big[(\varepsilon - \varepsilon_0)\psi_0^+ + u\,(\psi_0^+)^3X^2\big]X = 0$. From this an equation for X, consistent with (3), can be projected out by forming the scalar product with $\mathrm{d}^2\psi_0^-$. The result

$$\left[\tau(T, V) + u\frac{\kappa}{4}X^2(T, V)\right]X(T, V) = 0 \tag{15}$$

again has the appearance of the previous one [4], now, however, with the new pre-factor $\alpha(V) \equiv \alpha\,(\kappa/4)\big/\big(\mathrm{d}^2\psi_0^-, [\psi_0^+]^3\big)$ in $\tau(T, V) \equiv \alpha(V)[T - T_0(V)]$.

Evaluation of the scalar products in $\alpha(V)$, and elimination of the amplitude X from (14) and (15) leads, in the F–V plane, to the set of isotherms shown in figure 2. Above some critical point $F_1, V_1, T_1 \equiv T_0(V_1)$ the isotherms show hysteresis, generated by a regime where $\partial V/\partial F < 0$. At the low-velocity limit of this regime the defect experiences a long-wavelength morphological instability which can be analysed in the way described in [4]. Here we only point out that the results of the present paper support our belief in the universal character of these phenomena.

As a final remark we point out that a new non-equilibrium critical exponent arises in our scenario which presumably is universal in the strict sense of the renormalization group. It is

defined by $\varepsilon_0 \propto (v_c - v)^y$ and, correspondingly, describes the way in which the nucleation threshold $T_0(V)$ approaches the critical point T_c. From (13) one can extract the mean-field value $y = 1/2$, visible in figure 1, whereas in the non-conserved case one finds $y = 1$ [4]. In both cases anomalies of these exponents are expected to arise from order-parameter fluctuations of the bulk as well as of the nucleus.

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