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LINEAR STABILITY OF PLANAR SOLIDIFICATION FRONTS

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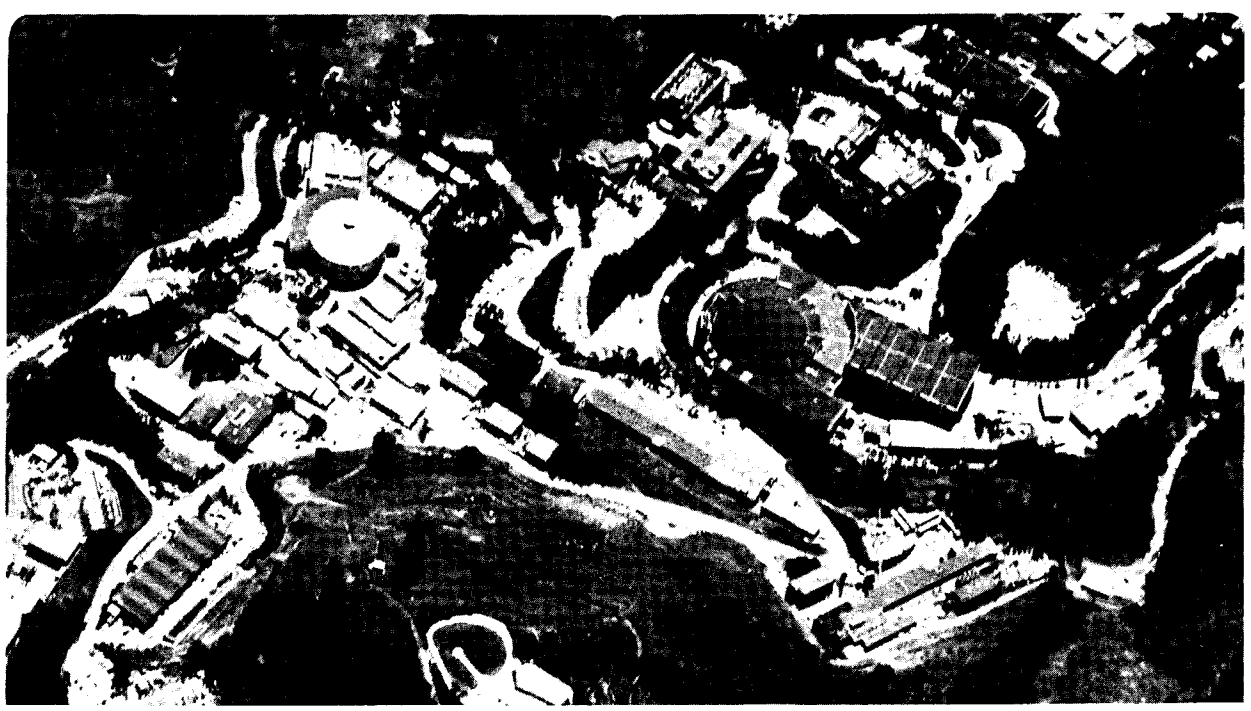
Linear Stability of Planar Solidification Fronts

J. Strain

July 1987

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# LINEAR STABILITY OF PLANAR SOLIDIFICATION FRONTS<sup>1</sup>

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### *ABSTRACT*

We review, extend, and modify the classical linear stability theory of planar solidification fronts due to Langer (Rev. Mod. Phys. 52 (1980), 1) Using a new integral equation for the front position, we compute an exact linear stability equation, and solve it exactly for an important special case. Finally, we extend our analysis to a general planar front by a short-time approximation. Our conclusions differ in several respects from previous analyses. Notably, a catastrophic linear instability occurs.

# Linear Stability of Planar Solidification Fronts\*

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## 1. Introduction

Some time ago, Langer [1,2] introduced the symmetric model of solidification of a pure substance from an undercooled melt. He presented a now-classical approximate analysis of linearized stability of a model planar front. In the course of a recent numerical solution of the model, Sullivan et al. [3] have slightly generalized Langer's analysis. Both studies conclude that zero-capillarity planar fronts are unstable, while nonzero capillarity damps the short-wave instabilities. These predictions are roughly confirmed by the numerical calculations of Sullivan et al., but not by the other numerical analyses described in Chorin [4] and Smith [5]. The latter calculations exhibited persistent oscillations, even within the linearly stable regime.

This report presents an exact linear stability analysis of a planar front which reveals a possible reason for the discrepancy. Our analysis shows that the growth factors of the classical theory are qualitatively correct for short time spans.

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However, for slightly longer times, we predict a catastrophic linear instability of all modes. Such an instability, perhaps overdamped by nonlinear restoring forces, could well account for the observed oscillations.

The paper begins with a review of the symmetric model and the classical stability theory, in a form suitable for comparison with our later results. Then we transform the model into a new integral equation and derive the linear stability equation which governs the evolution of a perturbation to the initial data. Specialization to a planar front with constant speed and unit undercooling yields a fractional differential equation which is solved exactly. After interpreting the solution, we describe a generalization to other planar fronts, and discuss our conclusions.

## 2. Review of Classical Theory

First, we recall the symmetric model [1,2]. Consider a pure substance filling  $\mathbb{R}^n$ , with  $n = 2$  or  $3$ , which has identical thermal properties in its solid and liquid phases. The solid phase is a time-dependent region  $\Omega(t)$ , its boundary -- the phase interface -- will be denoted by  $\Gamma(t)$ , and the temperature field is a continuous function  $u(x, t)$  of  $x \in \mathbb{R}^n$  and  $t \geq 0$ . The temperature field satisfies the heat equation (1) in each phase, and the interface is connected to the temperature field by a heat balance (3) and by the Gibbs-Thomson relation (2) (see also Gurtin's review paper [6] for a discussion).

Thus we work with the following model equations:

$$\frac{\partial u}{\partial t} = \Delta u \quad \text{off } \Gamma(t) \quad (1)$$

$$u = -c \kappa \quad \text{on } \Gamma(t) \quad (2)$$

$$n \cdot [\partial u] = -v \quad \text{on } \Gamma(t) \quad (3)$$

with initial data  $u_0$  and  $\Gamma(0)$  given. Here  $c$  is the capillarity,  $\kappa$  is the curvature of  $\Gamma(t)$  (taken positive if the center of the osculating circle lies in the solid), the outward unit normal to  $\Omega(t)$  is denoted by  $n$ , and  $v$  is the normal velocity of  $\Gamma(t)$ , taken positive if liquid is freezing. Brackets denote the jump in a quantity across  $\Gamma(t)$  :

$$[g](x_0) = \lim_{\substack{x \rightarrow x_0 \\ x \notin \Omega(t)}} g(x) - \lim_{\substack{x \rightarrow x_0 \\ x \in \Omega(t)}} g(x) . \quad (4)$$

$\partial$  is the gradient and  $\Delta$  is the Laplacian. Continuity of  $u$  implies that the initial data  $u_0$  and  $\Gamma(0)$  can be specified independently only up to a compatibility condition

$$u_0 = -c \kappa \quad \text{on } \Gamma(0). \quad (5)$$

This restriction plays an important role in a careful analysis of the problem.

Next, we review the classical linear stability theory of Langer [1,2], following Sullivan et al. [3]. Consider the planar interface in  $\mathbb{R}^2$  parametrized by

$$\Gamma(t) : (x = vt, y = s) \quad s \in \mathbb{R} \quad (6)$$

with temperature field

$$u(x, y, t) = \begin{cases} e^{-v(x-vt)} - 1 & x > vt \\ 0 & x < vt \end{cases} \quad (7)$$

independent of  $y$ . The interface moves into the liquid phase with positive velocity  $v$ , and the temperature field propagates without change of structure.

Perturb this solution by adding temperature fields  $\epsilon u_S$  and  $\epsilon u_L$  in the solid and liquid phases respectively, and let  $\epsilon x_1(t, s)$  be the resulting perturbation of the interface. Thus  $u_S, u_L$ , and  $x_1$  satisfy

$$\begin{aligned} \frac{\partial u_S}{\partial t} &= \Delta u_S & x < vt + \epsilon x_1(t, s) \\ \frac{\partial u_L}{\partial t} &= \Delta u_L & x > vt + \epsilon x_1(t, s) \end{aligned}$$



$$\epsilon u_S = e^{-v \epsilon x_1} - 1 + \epsilon u_L = \frac{c \epsilon x_{1ss}}{(1 + \epsilon^2 x_{1s}^2)^{3/2}} \quad x = vt + \epsilon x_1(t, s)$$

$$-v e^{-v \epsilon x_1} + \epsilon \left( \frac{\partial u_L}{\partial x} - \frac{\partial u_S}{\partial x} \right) = -v - \frac{\epsilon x_{1t}}{(1 + \epsilon^2 x_{1s}^2)^{1/2}} \quad x = vt + \epsilon x_1(t, s)$$

where subscripts denote derivatives.

Linearize these equations by extending  $u_L$  and  $u_S$  up to the unperturbed boundary as solutions of the heat equation, and using Taylor expansion to construct an effective boundary condition there. Drop terms of order  $\epsilon^2$  to get

$$\frac{\partial u_S}{\partial t} = \Delta u_S \quad x < vt \quad (8)$$

$$\frac{\partial u_L}{\partial t} = \Delta u_L \quad x > vt \quad (9)$$

and the effective boundary conditions

$$u_S = -v x_1 + u_L = c x_{1ss} \quad x = vt \quad (10)$$

$$\frac{\partial u_L}{\partial x} - \frac{\partial u_S}{\partial x} = -x_{1t} - v^2 x_1 \quad x = vt \quad (11)$$

Note that the conditions (10) do not preclude continuity of the temperature field across the perturbed interface. The apparent discontinuity arises because extending a solution of the heat equation to a larger domain can be an unstable process, as the exact solution (7) shows: it grows exponentially past  $x = vt$ .

These are linear equations with constant coefficients on a rectangular domain, so we can find exponential solutions of the form

$$\begin{aligned} u_S &= u_0 e^{iky} e^{\sigma t} e^{q(x-vt)} \\ u_L &= u'_0 e^{iky} e^{\sigma t} e^{-q'(x-vt)} \\ x_1 &= x_0 e^{iky} e^{\sigma t} \end{aligned} \quad (12)$$

Furthermore, an arbitrary perturbation of the initial temperature field and

interface can be decomposed into such solutions by means of a Laplace transform in  $x$  and a Fourier transform in  $y$  resp.  $s$ . Thus one could expect to analyze stability by computing the growth factor  $\sigma$  for all positive  $q$  and  $q'$  and real  $k$ .

Unfortunately, the dispersion relations

$$u_0(\sigma - vq - q^2 + k^2) = 0 \quad (13)$$

$$u'_0(\sigma + vq' - q'^2 + k^2) = 0 \quad (14)$$

$$u_0 = -vx_0 + u'_0 = -ck^2x_0 \quad (15)$$

$$q' u'_0 + qu_0 = (\sigma + v^2)x_0, \quad (16)$$

which must be satisfied by solutions of the form (12), fix  $q$  and  $q'$  in terms of  $k$ . To see this, eliminate the amplitudes from (15) and (16) to get three equations

$$\sigma - vq - q^2 + k^2 = 0 \quad (17)$$

$$\sigma + vq' - q'^2 + k^2 = 0 \quad (18)$$

$$\sigma + v^2 + ck^2(q + q') - vq' = 0 \quad (19)$$

in the four unknowns  $\sigma, q, q'$ , and  $k^2$ . These can be solved for  $\sigma, q$  and  $q'$  in terms of  $k$ . But to represent an arbitrary perturbation of the initial temperature field and interface requires three independent parameters,  $q, q'$  and  $k$ . Thus we have too few degrees of freedom to carry out a complete stability analysis. Since the solution is stable if no modes grow, but unstable if any modes grow, we can reliably predict instability by this analysis, but not stability.

Despite this difficulty, we proceed with the classical calculation. First consider the case of capillarity  $c = 0$ . Then (13) becomes vacuous since  $u_0 = 0$  by (15), and a minute or two of algebra gives

$$\sigma = \begin{cases} \pm v |k| & |k| < v \\ v |k| & |k| > v. \end{cases} \quad (20)$$

The choice of sign is forced by the positivity of  $q$  and  $q'$ . Thus the classical

theory predicts instability of all modes, for zero capillarity.

Now suppose  $c > 0$ . Eliminate  $q$  and  $q'$  to get an implicit relation

$$2\sigma + v^2 = (v - 2ck^2)\sqrt{v^2 + 4k^2 + 4\sigma} \quad (21)$$

for the growth factor  $\sigma$ , assuming  $\sigma + k^2 > 0$ . Square (21) and solve for  $\sigma$ , with careful attention to signs. We find

$$\sigma = 2ck^2(ck^2 - v) \pm |k| |v - 2ck^2| \sqrt{1 + c^2k^2 - vc} \quad (22)$$

where the  $\pm$  sign is taken as follows:

$$\pm = \begin{cases} \pm & 2ck^2 < v, \quad 2|k| < v \\ + & 2ck^2 < v, \quad 2|k| > v \\ - & 2ck^2 > v, \quad 2|k| > v. \end{cases} \quad (23)$$

Asymptotically,

$$\sigma \sim \begin{cases} \pm v |k| & \text{as } k \rightarrow 0 \\ -k^2 & \text{as } k \rightarrow \infty. \end{cases} \quad (24)$$

Thus the classical theory predicts the stabilization of short waves by capillarity. Of course, as remarked above, this prediction only applies to those perturbations of the form (12) with  $q$ ,  $q'$ , and  $k$  related by (17-19). Nevertheless, its qualitative features will appear in the exact theory of section 5, at least in the short-time range.

### 3. The integral equation formulation

We convert the moving boundary problem, consisting of partial differential equations, boundary and initial conditions, into an integral equation which involves only the initial data and the geometry of the interface. This will permit a rigorous linearization of the model, and remove the necessity of constructing an effective boundary condition which we faced in section 2. Linearizing the integral

equation will provide a natural linearization of the compatibility condition (5) connecting the initial interface and temperature field. This will supplant the effective boundary conditions (10) and (11).

Let  $u$  be a temperature field satisfying the model equations (1-3), with initial data  $u_0$ . Fix a time  $T > 0$ , and let  $K$  be the Gauss kernel (see [8], Chap. 1 or [9])

$$K(x, t) = \begin{cases} \frac{e^{-\|x\|^2/4t}}{(4\pi t)^{n/2}} & t > 0 \\ 0 & t \leq 0. \end{cases} \quad (25)$$

For a fixed  $x$  in  $\Omega(T)$  and  $\delta > 0$ , let

$$f(y, t) = K(x - y, T - t + \delta) \quad (26)$$

Let

$$n_t = \begin{cases} 1 & t = T & x \in \Omega(T) \\ -1 & t = 0 & x \in \Omega(0) \\ \frac{-v}{\sqrt{1+v^2}} & 0 < t < T & x \in \Gamma(t) \end{cases} \quad (27)$$

denote the time component of the outward unit normal to the product set

$$\Omega_T = \prod_0^T \Omega(t). \quad (28)$$

Add the divergence theorem ([9], p. 79)

$$\int_{\Omega_T} \frac{\partial}{\partial t}(f u) = \int_{\partial\Omega_T} (f u) n_t \quad (29)$$

to the Green identity ([9], p. 80)

$$\int_{\Omega_T} u \Delta f - f \Delta u = \int_0^T \int_{\Gamma(t)} u \frac{\partial f}{\partial n} - f \frac{\partial u}{\partial n}, \quad (30)$$

use the backward heat equation satisfied by  $f$  in  $\Omega_T$ , and take the limit  $\delta \rightarrow 0$ .

The result is

$$u(x, T) = \int_{\Omega(0)} f u - \int_0^T \int_{\Gamma(t)} (f u) n_t - f \frac{\partial u}{\partial n} + u \frac{\partial f}{\partial n} \quad (31)$$

for  $x$  in  $\Omega(T)$ . Similarly,

$$u(x, T) = \int_{\mathbb{R}^n \sim \Omega(0)} f u + \int_0^T \int_{\Gamma(t)} (f u) n_t - f \frac{\partial u}{\partial n} + u \frac{\partial f}{\partial n} \quad (32)$$

for  $x$  outside  $\Omega(T)$ .

The last two terms in (31) and (32) are single and double layer heat potentials [10]

$$S(x, T) = \int_0^T \int_{\Gamma(t)} \mu(y, t) K(x-y, T-t) dy dt \quad (33)$$

$$D(x, T) = \int_0^T \int_{\Gamma(t)} \mu(y, t) \frac{\partial}{\partial n_y} K(x-y, T-t) dy dt. \quad (34)$$

with densities  $\mu = \frac{\partial u}{\partial n}$  and  $\mu = u$  respectively. To construct an integral equation for the interface, we need to evaluate (31) and (32) on  $\Gamma(T)$ . Since the integrands are singular if  $x \in \Gamma(T)$ , this requires jump formulae for  $S$  and  $D$ ; analogous to the well-known jump formulae for the Newtonian potential [11]. The relevant formulae are derived in the Appendix. They read

$$[S](x_0, T) = 0 \quad (35)$$

$$[D](x_0, T) = \mu(x_0, T), \quad (36)$$

for  $x_0 \in \Gamma(T)$ . The jump is defined in equation (4). Thus evaluation of (31) and (32) on  $\Gamma(T)$  yields

$$\frac{1}{2} u(x, T) = \int_{\Omega(0)} f u - \int_0^T \int_{\Gamma(t)} (f u) n_t - f \frac{\partial u}{\partial n} + u \frac{\partial f}{\partial n} \quad (37)$$

$$= \int_{\mathbb{R}^n \sim \Omega(0)} f u + \int_0^T \int_{\Gamma(t)} (f u) n_t - f \frac{\partial u}{\partial n} + u \frac{\partial f}{\partial n} \quad (38)$$

for  $x$  on  $\Gamma(T)$ . Add these formulae and apply the boundary conditions (2) and (3); the result is an integral equation

$$-c \kappa(x, T) = \int_{\mathbb{R}^n} K(x-y, T) u_0(y) dy + \int_0^T \int_{\Gamma(t)} K(x-y, T-t) v(y, t) dy dt. \quad (39)$$

for the interface  $\Gamma(T)$ .

Observe that a smooth solution  $\Gamma(t)$  is determined at  $t = 0$  by the initial temperature field  $u_0$ , via a compatibility condition

$$-c \kappa(x, 0) = u_0(x) \quad \text{on } \Gamma(0), \quad (40)$$

just as in section 2.

The integral equation (39) has a simple physical interpretation; the temperature at a point  $x$  on the interface is the sum of the temperature field induced by the initial distribution, plus the single layer heat potential produced by the release of latent heat of phase change by the moving boundary.

Langer [1,2] has presented a similar formulation of the symmetric model as an integral equation. His equation can be derived by our method, if we first begin at an initial time  $t = t_0$ , instead of  $t = 0$  as we did. Then (39) becomes

$$-c \kappa(x, T) = \iint K(x-y, T-t_0) u(y, t_0) dy + \int_{t_0}^T \int_{\Gamma(t)} K(x-y, T-t) v(y, t) dy dt.$$

Assume that  $u(x, t_0)$  approaches a constant as  $t_0 \rightarrow -\infty$ , and take the limit  $t_0 \rightarrow -\infty$ . Langer's equation ([2], equation 5.13 with  $l_T^{-1} = v = 0$ ) results.

However, this derivation points up an imperfection in his formulation. Namely, the same equation results for any temperature field  $u \rightarrow -1$ , say, as  $t_0 \rightarrow -\infty$ . Thus Langer's equation must be satisfied by any such solution, but it

cannot determine the solution uniquely. (More precisely, the solution of Langer's equation can be unique only if every solution is completely determined by its undercooling alone.) Since our formulation retains the initial temperature field as a datum, it should determine its solution uniquely.

#### 4. The Linear Stability Equation

Consider a solution  $\Gamma_0(t)$  of the integral equation in two space dimensions, with initial data  $u_0$  and  $\Gamma_0$  satisfying the compatibility condition

$$-c \kappa_0(x, 0) = u_0(x) \quad \text{on } \Gamma_0(0). \quad (41)$$

Any (continuous) perturbed solution must also satisfy this condition. This restricts the allowable perturbations of the initial field and interface to those which satisfy (41), at least to first order in the perturbation parameter  $\epsilon$ . However, we need not derive a first-order approximation to this condition explicitly. The beauty of the integral equation approach is that the linearized integral equation will contain a natural linearization of (41), just as (39) contains (41). The integral equation (39) is an uncountable family of equations, one for each time  $T$ , and (41) is just the  $T = 0$  member of the family. Similarly, the linearized equation will contain a linearized version of (41), obtainable by evaluation at  $T = 0$ .

Consider a perturbed initial temperature field  $u_0 + \epsilon u_1$ , let  $\Gamma_\epsilon(t)$  be the perturbed interface, and take a family of parametrizations

$$\Gamma_\epsilon(t) : (x(t, s) + \epsilon x_1(t, s) + O(\epsilon^2), y(t, s) + \epsilon y_1(t, s) + O(\epsilon^2)).$$

The curvature and velocity  $\times$  element of length have expansions

$$\kappa_\epsilon = \kappa_0 + \epsilon \kappa_1 + O(\epsilon^2) \quad (42)$$

$$v_\epsilon dy_\epsilon = v_0 dy_0 + \epsilon v_1 dy_1 + O(\epsilon^2), \quad (43)$$

where

$$\kappa_1 = (a(x, y) \frac{\partial}{\partial s} + b(x, y) \frac{\partial^2}{\partial s^2}) x_1 - (a(y, x) \frac{\partial}{\partial s} + b(y, x) \frac{\partial^2}{\partial s^2}) y_1 \quad (44)$$

with

$$a(x, y) = (x_s^2 + y_s^2)^{-5/2} [(y_s^2 - 2x_s^2) y_{ss} + 3x_s y_s x_{ss}] \quad (45)$$

$$b(x, y) = -(x_s^2 + y_s^2)^{-3/2} y_{ss}, \quad (46)$$

and

$$v_1 dy_1 = (x_t y_{1s} + y_s x_{1t} - x_s y_{1t} - y_t x_{1s}) ds. \quad (47)$$

To derive these expressions, differentiate the standard expressions (see [13]) for curvature and velocity  $\times$  element of length with respect to  $\epsilon$  and evaluate at  $\epsilon = 0$ . The calculations are straightforward but tedious, and are therefore omitted. Substitute the expansions (42) and (43) into the integral equation (39), use the assumption that the zero-order terms satisfy (39), and drop terms of second or higher orders in  $\epsilon$ . After integration by parts, the result is the linear stability equation

$$\begin{aligned} -c \kappa_1 = & x_1 \iint K(x-y, t) \partial u_0(y) d^2 y + \iint K(x-y, t) u_1(y) d^2 y \quad (48) \\ & + \int_0^t \iint (x_1 - x'_1) \cdot \partial K(x-x', t-t') v'_0 ds' dt' + \int_0^t \iint K(x-x', t-t') v'_1 ds' dt' \end{aligned}$$

where  $\partial$  is the gradient,  $x = x(t, s)$ ,  $x' = x(t', s')$ , and so forth.

If  $x_1$  is a smooth solution to this equation, then evaluation at  $t = 0$  gives the linearized compatibility condition

$$-c \kappa_1 = x_1 \cdot \frac{1}{2} [\partial u_0(x_0^+) + \partial u_0(x_0^-)] + \frac{1}{2} (u_1(x_0^+) + u_1(x_0^-)) \quad \text{on } \Gamma_0(0). \quad (49)$$

(Note that  $\partial u_0$  is discontinuous at  $x \in \Gamma_0$ , so its convolution with the Gauss kernel converges to the average of its values on the two sides of the discontinuity; see [8].) For the special perturbation



$$u_1(x, y) = \begin{cases} u_0 e^{iky} e^{qx} & x < 0 \\ u'_0 e^{iky} e^{-q'x} & x > 0 \end{cases} \quad (50)$$

to the solution (7) discussed in section 2, the condition (49) follows from the effective boundary conditions (15), but does not imply them.

## 5. Stability of the special planar interface

Recall the special planar interface discussed in section 2, with

$$\Gamma(t) : (x = vt, y = s) \quad (51)$$

$$u_0(x) = \begin{cases} e^{-vx} - 1 & x > 0 \\ 0 & x < 0. \end{cases} \quad (52)$$

Since a line has zero curvature and

$$\iint K(vT - x, s - y, T) u_0(x) dx dy + \int_0^T \int_{\Gamma(t)} K(vT - vt, s - \sigma; T - t) v d\sigma dt = \quad (53)$$

$$= \frac{1}{\sqrt{\pi}} \int_{\sqrt{v^2 t/4}}^{\infty} e^{-x^2} dx - \frac{1}{\sqrt{\pi}} \int_{-\sqrt{v^2 t/4}}^{\infty} e^{-x^2} dx + \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{v^2 t/4}} e^{-x^2} dx$$

$$= 0,$$

this is an exact solution of the integral equation for any capillarity  $c$ , as of course it should be. For a perturbation with

$$\Gamma_\epsilon(t) : (x = vt + \epsilon x_1(t, s), y = s) \quad (54)$$

$$u_0(x, y) = u_0(x) + \epsilon u_1(x, y), \quad (55)$$

the linearized curvature and velocity simplify to

$$\kappa_1 = -x_{1ss} \quad (56)$$

$$v_1 dy_1 = x_{1t} ds. \quad (57)$$

Thus the linearized stability equation is

$$\begin{aligned}
 cx_{1ss}(T, s) &= x_1(T, s) \int_{-\infty}^{\infty} \frac{e^{-(vt-y)^2/4T}}{\sqrt{4\pi T}} u'_0(y) dy \\
 &+ \int \int K(vT-y, s-\sigma; T) u_1(y, \sigma) dy d\sigma \\
 &+ \frac{v^2}{2} \int_0^{\infty} \int_{-\infty}^{\infty} (x_1(T, s) - x_1(t, \sigma)) K(vT-vt, s-\sigma; T-t) d\sigma dt \\
 &+ \int_0^{\infty} \int_{-\infty}^{\infty} K(vT-vt, s-\sigma; T-t) x_{1t}(t, \sigma) d\sigma dt.
 \end{aligned} \tag{58}$$

Because of the simple  $s$ -dependence of the kernel  $K$ , we can Fourier analyze an arbitrary perturbation into solutions with

$$u_1(x, y) = f(x) e^{iky} \tag{59}$$

$$x_1(t, s) = g(t) e^{iks}. \tag{60}$$

Then  $g$  satisfies the reduced equation

$$(2ck^2 - v)g(t) + \int_0^t \frac{e^{-(\lambda+k^2)s}}{\sqrt{\pi(t-s)}} (g'(s) + 2\lambda g(s)) ds = e^{-(\lambda+k^2)t} F(t) \tag{61}$$

where  $\lambda = v^2/4$  and

$$F(t) = -2e^{\lambda t} \int_{-\infty}^{\infty} \frac{e^{-(vt-y)^2/4t}}{\sqrt{4\pi t}} f(y) dy. \tag{62}$$

The new unknown

$$G(t) = e^{(\lambda+k^2)t} g(t) \tag{63}$$

then satisfies a fractional differential equation

$$[D^{1/2} + (2ck^2 - v) + (\lambda - k^2)D^{-1/2}]G(t) = \frac{G(0)}{\sqrt{\pi t}} + F(t) \tag{64}$$

where  $D^{1/2}$  and  $D^{-1/2}$  are the Riemann-Liouville fractional derivative and

integral defined by (see [14] for background on fractional calculus)

$$D^{1/2}G(t) = DD^{-1/2}G(t) \quad (65)$$

$$\begin{aligned} &= D \int_0^t \frac{G(s)ds}{\sqrt{\pi(t-s)}} \\ &= \frac{G(0)}{\sqrt{\pi t}} + \int_0^t \frac{DG(s)ds}{\sqrt{\pi(t-s)}} \end{aligned} \quad (66)$$

and  $D$  denotes differentiation.

The singular term  $\frac{G(0)}{\sqrt{\pi t}}$  on the right-hand side of (64) suggests that we should carefully consider the smoothness to be expected of  $F$  and  $G$ . Consider for example the initial temperature field perturbation from the theory of section 2:

$$f(x) = \begin{cases} u'_0 e^{-q' x} & x > 0 \\ u_0 e^{qx} & x < 0 \end{cases} \quad (67)$$

with  $q, q' \geq 0$ . A change of variables of the form

$$x = \sqrt{(y^2 - vty - q' y)/4t} \quad (68)$$

in each half of the range of integration puts  $F$  in the more transparent form

$$\begin{aligned} F(t) &= -u'_0 e^{(q' - v/2)^2 t} \Phi((q' - v/2)\sqrt{t}) \\ &\quad - u_0 e^{(q + v/2)^2 t} \Phi((q + v/2)\sqrt{t}) \end{aligned} \quad (69)$$

where

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-x^2} dx. \quad (70)$$

Differentiation shows that  $F$  has the short-time asymptotic behavior

$$F(t) \sim F_0 + 2F_1 \sqrt{t/\pi} \quad \text{as } t \rightarrow 0, \quad (71)$$

with constants

$$F_0 = -f(0^+) - f(0^-) \quad (72)$$

$$F_1 = -Df(0^+) + Df(0^-) - \frac{v}{2}(f(0^+) - f(0^-)). \quad (73)$$

Unless  $f$  is  $C^1$  at  $x = 0$ , there is a singularity in the first derivative of  $F$  at  $t = 0$ . By a Laplace transform (or direct calculation), this behavior of  $F$  is easily seen to be characteristic of piecewise smooth  $f$ 's decaying at  $\infty$  and having possible jump discontinuities at  $x = 0$ . Thus we assume that  $F$  belongs to the class  $C^{1/2}[0, \infty) \cap C^1(0, \infty)$ , and ask in what class the solution  $G$  of

$$[D^{1/2} + (2ck^2 - v) + (\lambda - k^2)D^{-1/2}]G(t) = \frac{G(0)}{\sqrt{\pi t}} + F(t) \quad (74)$$

should be sought.

It is tempting to assume that  $G$  behaves like  $F$ . But if

$$G(t) \sim G_0 + 2G_1\sqrt{t/\pi} \quad (75)$$

as  $t \rightarrow 0$ , the equation becomes to lowest order in  $t$

$$G_1 + (2ck^2 - v)G_0 = F_0. \quad (76)$$

This determines the unknown constant  $G_0$  only in terms of the equally unknown constant  $G_1$ . More generally, assuming  $F$  and  $G$  are power series in  $\sqrt{t}$  and equating terms in (74) gives an infinite set of equations for the coefficients  $G_n$  which does not determine  $G_0$  at all. This suggests, as does the physically unreasonable infinite initial velocity implied by (75), that we should assume  $G$  is  $C^1$  up to  $t = 0$ . Of course, we must check the consistency of this assumption afterwards. Then apply the operator

$$L = D^{1/2} - (2ck^2 - v) + (\lambda - k^2)D^{-1/2} \quad (77)$$

and some careful interchange of integrals (cf. [15], p. 76) to the equation (74) for

$G$ . A second order constant coefficient ordinary differential equation

$$[D^2 + (2(\lambda - k^2) - (2ck^2 - v)^2)D + (\lambda - k^2)^2]D^{-1}G(t) = L\left[\frac{G(0)}{\sqrt{\pi t}} + F(t)\right] \quad (78)$$

results, for the new unknown  $D^{-1}G(t)$ . Here  $D^{-1}$  denotes indefinite integration;

$$D^{-1}G(t) = \int_0^t G(s)ds. \quad (79)$$

Let  $\xi_1$  and  $\xi_2$  be the roots of

$$\xi^2 + (2(\lambda - k^2) - (2ck^2 - v)^2)\xi + (\lambda - k^2)^2 = 0, \quad (80)$$

and put

$$S(t) = \frac{\xi_1 e^{t\xi_1} - \xi_2 e^{t\xi_2}}{\xi_1 - \xi_2} \quad (81)$$

to save writing. Apply variation of parameters [16] to equation (78); the result is

$$G(t) = G(0)S(t) + S * \left[ L\left(\frac{G(0)}{\sqrt{\pi t}} + F(t)\right) \right] \quad (82)$$

where  $*$  is the convolution product

$$f * g(t) = \int_0^t f(t-s)g(s)ds. \quad (83)$$

This expression simplifies somewhat if we evaluate the fractional differential equation (74) at  $t = 0$ . Assume  $DG(0)$  is finite. Then (65) and (66) imply

$$D^{1/2}G(t) \sim \frac{G(0)}{\sqrt{\pi t}} + O(\sqrt{t}) \quad (84)$$

$$D^{-1/2}G(t) \sim O(\sqrt{t}) \quad (85)$$

as  $t \rightarrow 0$ . Consequently (74) reads

$$(2ck^2 - v)G(0) = F(0). \quad (86)$$

at  $t = 0$ . This and the formula (66) with  $G$  replaced by  $F$  result in a fortunate

cancellation of singular terms in the expression for  $G$ . We find

$$G(t) = G(0)(D + \lambda - k^2)D^{-1}S(t) \quad (87)$$

$$+ S * [D^{-1/2}(D + \lambda - k^2)F(t) - (2ck^2 - v)F(t)].$$

(87) implies that

$$DG(0) = G(0)[\xi_1 + \xi_2 + (\lambda - k^2) - (2ck^2 - v)^2] + F_1 \quad (88)$$

$$= F_1 - (\lambda - k^2)G(0)$$

is finite, so the assumption that  $G$  is  $C^1$  is consistent.

Now we can determine linear stability of the interface. Its stability will depend on the sign of the growth factor  $\sigma$ , which we define here by

$$\sigma = \frac{Dg(0)}{g(0)}. \quad (89)$$

This is a reasonable definition of  $\sigma$  for times so short that  $e^{\sigma t}$  is well approximated by the first two terms in its Taylor series. The definition (63) implies that

$$Dg(0) = -(\lambda + k^2)G(0) + DG(0). \quad (90)$$

Substitute (86) and (88) in (90). Then (89) becomes

$$\sigma = \frac{F_1}{F_0}(2ck^2 - v) - \frac{v^2}{2}. \quad (91)$$

With the values (72) and (73), we find

$$\sigma = \frac{Df(0^+) - Df(0^-) + \frac{v}{2}(f(0^+) - f(0^-))}{f(0^+) + f(0^-)} - (2ck^2 - v) - \frac{v^2}{2}. \quad (92)$$

By a Laplace transform, it suffices (for smooth  $f$ ) to discuss  $f$  of the form

$$f(x) = \begin{cases} u_0' e^{-q' x} & x > 0 \\ u_0 e^{qx} & x < 0 \end{cases} \quad (93)$$

considered in section 2. Then  $\sigma$  is given by

$$\sigma = (v - 2ck^2) \frac{q' u'_0 + qu_0 + \frac{v}{2}(u_0 - u'_0)}{u'_0 + u_0} - \frac{v^2}{2}. \quad (94)$$

We can take this as the growth factor, or we can put additional restrictions on the allowable perturbations  $f$ . The virtue of this whole calculation is that it can handle any or no additional compatibility conditions on  $f$ . This is important, because it is not clear what additional restrictions, if any, should be imposed on  $f$ . However, we consider two possibilities, the first for the sake of comparison with the classical theory, the second for mathematical appeal.

First, it is interesting to see what we get if we impose the effective boundary conditions (10) and (11) of the theory of section 2, evaluated at  $t = 0$ . These read

$$u_0 = -ck^2 g(0) \quad (95a)$$

$$u'_0 = (v - ck^2)g(0) \quad (95b)$$

$$q' u'_0 + qu_0 = Dg(0) + g(0)v^2. \quad (95c)$$

Here  $g(0)$  and  $Dg(0)$  are given by

$$(2ck^2 - v)g(0) = -(u_0 + u'_0) \quad (96a)$$

$$Dg(0) = q' u'_0 + qu_0 + \frac{v}{2}(u_0 - u'_0) - \frac{v^2}{2}g(0), \quad (96b)$$

from (90), (86), (88), and the definition (93), with some tedious algebra. Substitute these values in the effective boundary conditions. After some more tedious algebra, only one requirement on  $f$  results; it is the obvious one

$$(v - ck^2)u_0 + ck^2 u'_0 = 0. \quad (97)$$

Note that this precludes continuity of the initial temperature field, for  $v \neq 0$ .

Then the growth factor is given by

$$\sigma = v(q' - v) - ck^2(q + q') \quad (98)$$

just as in equation (19) of the classical theory. Thus we recover the growth factors of the classical theory if we restrict ourselves to consideration of its initial perturbations. Since our calculation proceeds from a completely different formulation of the model, this rather surprising agreement is an excellent check on the correctness of our calculation. Note also that we recover the classical result in greater generality, without the restrictions (17) and (18) which  $q$  and  $q'$  had to satisfy in section 2. Hence we have a true extension of the classical theory.

On the other hand, we may enforce continuity of the initial data. This requires -- as it did not in section 2 -- continuity of  $f$ . Set  $u_0 = u'_0$ . Then (94) becomes

$$\sigma = \frac{1}{2}v(q' + q - v) - ck^2(q' + q). \quad (99)$$

This result is qualitatively similar to the conclusion of section 2, but nonetheless differs in detail. We see that large- $k$  modes are stable, while modes with small  $k$  and sufficiently large temperature gradients in either solid or liquid phases are unstable. This is more in accord with intuition than the previous result, which is independent of temperature gradients in the solid phase.

Thus our analysis confirms, qualitatively and for short times, the classical predictions. However, this picture of linear stability theory is valid only for very short times, because of the definition (89) of  $\sigma$ . This definition would assign the growth factor 0 to the function  $g(t) = \cosh(\sigma t)$ , even though  $g$  grows quite rapidly. This is reasonable only for times so short that the third term in a power series expansion of  $g$  is negligible;

$$(\sigma t)^2 \ll 1. \quad (100)$$

For slightly longer times, direct examination of  $g$  paints a completely different



picture. From (63) and (87), we have

$$\begin{aligned}
 g(t) &= e^{-(\lambda+k^2)t} G(t) \\
 &= g(0) \frac{(\xi_1+\lambda-k^2)e^{(\xi_1-\lambda-k^2)t} - (\xi_2+\lambda-k^2)e^{(\xi_2-\lambda-k^2)t}}{\xi_1-\xi_2} \quad (101)
 \end{aligned}$$

$$+ e^{-(\lambda+k^2)t} S * [D^{-1/2}(D+\lambda-k^2)F(t) - (2ck^2-v)F(t)]$$

where  $F$  and  $D^{-1/2}(D+\lambda-k^2)F$  are bounded. Clearly for slightly longer times, the relevant growth factors are

$$\begin{aligned}
 \sigma &= \xi - \lambda - k^2 \quad (102) \\
 &= 2ck^2(ck^2-v) \pm |k| |2ck^2-v| \sqrt{1+c^2k^2-vc}.
 \end{aligned}$$

The second equality comes from solving (80). These growth rates are given by the same formula (22) as in section 2, but now both signs are allowed. This agreement is quite surprising, because our calculation proceeds along lines completely different from the classical theory. Note also that this result is independent of the conditions imposed on  $f$  and of temperature gradients.

Thus we expect that for  $(\sigma(k)t)^2 \cong 1$ , the associated modes  $k$  will grow catastrophically. Since (102) implies

$$\sigma \sim 2c^2k^4 \quad \text{as } k \rightarrow \infty, \quad (103)$$

there will always be unstable modes no matter how short the time span. (However, we should observe that the domain of applicability of linearized stability theory itself decreases as  $\sigma$  increases.) Large- $k$  modes are stabilized by capillarity only for times so short that  $e^{\sigma t} \cong 1 + \sigma t$ . This contrasts sharply with the classical theory.

## 6. The general planar interface

A general planar interface is given by

$$\Gamma_0(t) : ( x = x(t) , y = s ) \quad (104)$$

where  $x$  is the solution of

$$0 = \int_{-\infty}^{\infty} \frac{e^{-(x(t)-y)^2/4t}}{\sqrt{4\pi t}} u_0(y) dy + \int_0^t \frac{e^{-(x(t)-x(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} x_\tau(\tau) d\tau. \quad (105)$$

The initial temperature field  $u_0$  must depend only on the coordinate  $y$  normal to the interface.

A perturbation  $\epsilon u_1(x, y)$  of the initial temperature field produces an interface perturbation  $\epsilon x(t, s)$  satisfying the exact linear stability equation

$$\begin{aligned} \epsilon x_{ss}(t, s) = & \epsilon x(t, s) \int_{-\infty}^{\infty} \frac{e^{-(x(t)-y)^2/4t}}{\sqrt{4\pi t}} u_0'(y) dy \\ & + \int \int K(x(t)-y, s-\sigma; t) u_1(y, \sigma) dy d\sigma \\ & + \int_0^t \int_{-\infty}^{\infty} (x(t, s) - x(\tau, \sigma)) \frac{x(t) - x(\tau)}{2(t-\tau)} K(x(t) - x(\tau), s - \sigma; t - \tau) x_\tau(\tau) d\sigma d\tau \\ & + \int_0^t \int_{-\infty}^{\infty} K(x(t) - x(\tau), s - \sigma; t - \tau) x_\tau(\tau, \sigma) d\sigma d\tau. \end{aligned} \quad (106)$$

Again, it suffices to consider temperature field perturbations

$$u_1(x, y) = f(x) e^{iky} \quad (107)$$

with resulting interfacial perturbations

$$x(t, s) = g(t) e^{iks}. \quad (108)$$

The reduced equation for  $g$  is

$$\begin{aligned}
 -ck^2g(t) &= g(t) \int_{-\infty}^{\infty} \frac{e^{-(x(t)-y)^2/4t}}{\sqrt{4\pi t}} u'_0(y) dy \\
 &+ e^{-k^2t} \int_{-\infty}^{\infty} \frac{e^{-(x(t)-y)^2/4t}}{\sqrt{4\pi t}} f(y) dy \\
 &+ \int_0^t [e^{-k^2(t-\tau)}g(\tau) - g(t)] \frac{x(t)-x(\tau)}{2(t-\tau)} x'(\tau) \frac{e^{-(x(t)-x(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} d\tau \\
 &+ \int_0^t \frac{e^{-(x(t)-x(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} e^{-k^2(t-\tau)} g'(\tau) d\tau.
 \end{aligned} \tag{109}$$

This equation describes the exact evolution of  $g$ , and seems intractable in this generality. However, linear theory can only be expected to be valid for short times. Thus it is reasonable to simplify the variable coefficients by short-time Taylor expansions. Hence we make the approximation

$$\frac{x(t)-x(\tau)}{2(t-\tau)} \cong \frac{1}{2}v \tag{110}$$

where

$$x'(\tau) \cong x'(0) \equiv v \tag{111}$$

and replace all variable coefficients multiplying  $g$  by their values at  $t = 0$ . Then (109) simplifies to

$$(U_0 - ck^2)g(t) = e^{-k^2t} F(t) + \int_0^t \frac{e^{-(\lambda+k^2)(t-\tau)}}{\sqrt{\pi(t-\tau)}} [g'(\tau) + 2\lambda g(\tau)] d\tau \tag{112}$$

with  $\lambda = v^2/4$ ,

$$U_0 = -\frac{1}{2}[u'_0(x(0)^+) + u'_0(x(0)^-)], \tag{113}$$

and  $F$  defined by

$$F(t) = \int_{-\infty}^{\infty} \frac{e^{-(x(t)-y)^2/4t}}{\sqrt{4\pi t}} f(y) dy. \tag{114}$$

This reduces the general planar interface to the special case treated in section 2.

Thus the conclusions of that section can be expected to hold for short times.

As an application, consider the classical Neumann solution defined by [17]

$$x(t) = 2p \sqrt{t+t_0} - 2p \sqrt{t_0} \quad (115)$$

$$u_0(x) = \begin{cases} -2p \int_0^{x/\sqrt{4t_0}} e^{-(\lambda^2+2p\lambda)} d\lambda & x > 0 \\ 0 & x < 0. \end{cases} \quad (116)$$

Here  $p$  is a parameter fixed by the undercooling at  $\infty$ . The exact temperature field has the similarity form

$$u(x,t) = \begin{cases} -2p \int_0^{(x-x(t))/\sqrt{4(t+t_0)}} e^{-(\lambda^2+2p\lambda)} d\lambda & x > x(t) \\ 0 & x < x(t). \end{cases} \quad (117)$$

Note the square root singularity at  $t = 0$  if we put  $t_0 = 0$ . For this example, we have

$$v = x'(0) = \frac{p}{\sqrt{t_0}} \quad (118)$$

$$U_0 = \frac{-p}{2\sqrt{t_0}}, \quad (119)$$

so the growth factor  $\sigma$  is given by

$$\sigma = (q' + q) \left( \frac{p}{2\sqrt{t_0}} - ck^2 \right) - \frac{p^2}{2t_0}. \quad (120)$$

The interest in this example is that the singular solution with  $t_0 = 0$  is stable (at  $t = 0$ ) to perturbations of all wavenumbers. Of course, it becomes unstable as soon as  $t$  becomes positive.

## 7. Conclusions

The classical linear stability theory is incomplete in two ways. First, it does not consider a complete set of normal modes for the initial perturbation. This is because it treats the initial data as consisting only of the interface, when actually the initial temperature field is also an important datum. Second, our analysis suggests that the classical theory can be valid only for times so short and  $c^2 k^4$  so small that  $e^{\sigma t} \cong 1 + \sigma t$ . For longer times, linear theory predicts a catastrophic instability.

Our analysis attempts to remedy these deficiencies, by treating general perturbations of the initial data for arbitrary time spans. The key is our integral equation formulation, which clearly displays the following unusual feature of the model. In most initial-value problems, the initial data is given in a space, say  $X$ , and the solution is then a trajectory in  $X$ . Here, however, the initial data consists primarily of the temperature field, while the solution is the family of interfaces  $\Gamma(t)$ . The initial temperature plays more the role of a forcing term than of initial data. This feature is a source of some conceptual difficulty in the classical theory.

Linearization is straightforward and rigorous in this formulation, with no effective boundary conditions required. Because the integral equation contains the compatibility conditions, appropriate linearized compatibility conditions follow automatically from the linearized stability equation. We use these as initial conditions for the interfacial perturbation, so we can handle a complete set of perturbations of the full initial data. The integral equation approach is suitable for studying the effect of additional compatibility conditions as well, because it can deliver  $g$  for any  $f$ . It is unclear whether any additional restrictions on  $f$  need be imposed, or what they should be.

The linear stability equation is exactly solvable for the important special case of an interface with constant speed and unit undercooling. This special case is important not only as an example, but because it approximates the general interface. Thus our conclusions extend immediately to the general planar interface.

Our analysis reveals two modifications of the classical theory. First, even for short times, continuity of the perturbed initial temperature field requires that the classical growth factor

$$\sigma = v(q' - v) - ck^2(q' + q) \quad (121)$$

be replaced by

$$\sigma = \frac{1}{2}v(q + q' - v) - ck^2(q' + q) \quad (122)$$

in the exact linear theory. A sufficiently careful numerical solution of the model could presumably determine which growth factor actually applies in general, and help decide the question of the correct additional conditions (if any) to be imposed on  $f$ .

Second, if the domain of applicability of linearized stability theory itself is long enough, we expect a catastrophic instability to appear. (Note that since  $\sigma$  given by (102) becomes infinite with  $k$ , there can be no time so short that  $e^{\sigma t} \cong 1 + \sigma t$  for every wavenumber  $k$ . Thus only a short-wave cutoff could prevent this instability from surfacing in a numerical analysis of the model.) Numerical analyses of the model do not unambiguously exhibit this instability. But Chorin's results [4] display a morphological oscillation which does not decay, even though the classical theory predicts it should. Perhaps the interaction of our instability with a nonlinear restoring force might explain the observed oscillations.

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**Appendix: Jump formulae for the heat potentials  $S$  and  $D$**

First we guess the correct formulae, by reducing heat potentials to classical Newtonian potentials in the limit  $T \rightarrow \infty$ . This is physically reasonable, since Laplace's equation is the steady-state form of the heat equation. Let  $\Gamma(t) \equiv \Gamma$  and  $\mu(y, t) \equiv \mu(y)$  be constant in time. Interchange the order of integration in (33) and (34) and put

$$s = \frac{\|x-y\|^2}{4t}$$

in the time integral; then  $S$  and  $D$  become

$$S(x, T) = \int_{\Gamma} \mu(y) \frac{\|x-y\|^{2-n}}{4 \pi^n / 2} \int_{\|x-y\|^2/4T}^{\infty} e^{-s} s^{n/2-2} ds dy$$

$$D(x, T) = \int_{\Gamma} \mu(y) \cos(n, x-y) \frac{\|x-y\|^{1-n}}{2 \pi^n / 2} \int_{\|x-y\|^2/4T}^{\infty} e^{-s} s^{n/2-1} ds dy$$

where  $\cos(a, b) = a \cdot b / \|a\| \|b\|$ . Take the limit  $T \rightarrow \infty$ . Except for the single layer potential in dimension  $n = 2$ , we find

$$S(x, \infty) = \frac{\Gamma(n/2-1)}{4 \pi^n / 2} \int_{\Gamma} \frac{\mu(y) dy}{\|x-y\|^{n-2}}$$

$$D(x, \infty) = \frac{\Gamma(n/2)}{2 \pi^n / 2} \int_{\Gamma} \frac{\mu(y) \cos(n, x-y) dy}{\|x-y\|^{n-1}},$$

the familiar Newtonian single and double layer potentials. For  $n = 2$ , a preliminary integration by parts shows that

$$S(x, T) \sim \frac{\log(4T)}{4\pi} \int_{\Gamma} \mu(y) dy - \frac{1}{2\pi} \int_{\Gamma} \mu(y) \log \|x-y\| dy.$$

Thus we recover the single layer logarithmic potential only modulo an infinite constant.



At any rate, the well-known jump relations (see [11]) of Newtonian potential theory now suggest that

$$[S](x_0, T) = 0$$

$$[D](x_0, T) = \mu(x_0, T)$$

for  $x_0 \in \Gamma(T)$ . A formal proof might proceed along the following lines.

First consider the single layer

$$S(x, T) = \int_0^T \int_{\Gamma(t)} \mu(y, t) K(x-y, T-t) dy dt.$$

Write ( after Pogorzelski [10])

$$\begin{aligned} K(x-y, T-t) &= \frac{e^{-\|x-y\|^2/4(T-t)}}{(4\pi(T-t))^{n/2}} \\ &= \frac{2^{-2\theta}}{\pi^{n/2}} \frac{1}{(T-t)^\theta} \frac{1}{\|x-y\|^{n-2\theta}} \left( \frac{\|x-y\|^2}{4(T-t)} \right)^{n/2-\theta} e^{-\|x-y\|^2/4(T-t)} \end{aligned}$$

and apply the inequality

$$q^m e^{-q} \leq m^m e^{-m}$$

valid for positive  $m$  and nonnegative  $q$ . The result is an estimate

$$K(x-y, T-t) \leq C_\theta \frac{1}{(T-t)^\theta} \frac{1}{\|x-y\|^{n-2\theta}}, \quad (*)$$

for  $C_\theta$  a constant depending on  $1/2 < \theta < 1$ . This dominates  $K$  by an integrable function, so the dominated convergence theorem [18] implies that  $S$  is continuous; thus  $[S] = 0$ .

Now consider the double layer  $D$ . First, we show that  $[D](x_0, T) = 0$  if  $\mu$  vanishes in a neighborhood of  $x_0 \in \Gamma(T)$ . It suffices then to calculate  $[D]$  for a density  $\mu$  which is nonzero only near  $x_0$ . For such a density, the double integral (34) can be approximated by integrating over the tangent plane to  $\Gamma(T)$  instead.

Then the jump yields to explicit calculation.

First suppose that

$$\mu(y, t) = 0 \quad \text{for } \|y - x_0\| + |T - t| \leq 2\epsilon.$$

An argument exactly like the one preceding (\*) establishes the inequality

$$\left| \frac{\partial}{\partial n_y} K(x - y, T - t) \right| \leq C_\theta \frac{1}{(T - t)^\theta} \frac{1}{\|x - y\|^{n+1-2\theta}}$$

for  $1/2 < \theta < 1$ , with a constant  $C_\theta$ . It follows that on the set where  $\mu$  is nonzero,

$$\left| \frac{\partial}{\partial n_y} K(x - y, T - t) \right| \leq \begin{cases} \text{constant} & \text{for } \|y - x_0\| \leq \epsilon \\ \frac{\text{constant}}{(T - t)^\theta} & \text{for } \|y - x_0\| \geq \epsilon. \end{cases}$$

Hence such a density induces a continuous  $D$ .

Next consider a general density  $\mu$ . Let  $\phi$  be a smooth function on  $\mathbb{R}^n \times [0, \infty)$  which is identically 1 for  $\|x - x_0\| + |T - t| \leq \epsilon$  and identically 0 for  $\|x - x_0\| + |T - t| \geq 2\epsilon$ , and put  $\mu = \phi\mu + (1 - \phi)\mu$ . This exhibits  $\mu$  as the sum of a density  $(1 - \phi)\mu$  of the type treated in the previous paragraph, and a density  $\phi\mu$  which vanishes everywhere except near  $x_0$ . Since  $(1 - \phi)\mu$  contributes nothing to  $[D](x_0, T)$ , we can assume  $\mu = \phi\mu$ . Then for  $\epsilon$  sufficiently small,  $\Gamma(t)$  is nearly flat and nearly constant in time in the range where  $\mu$  is nonzero. Thus we can replace  $\Gamma(t)$  in the integral by the tangent hyperplane to  $\Gamma(T)$  at  $x_0$ , with an error which vanishes with  $\epsilon$ . It remains only to calculate  $[D]$  when  $\Gamma(t) \equiv \Gamma$  is a hyperplane. By a rigid motion, we can assume that  $\Gamma$  is the hyperplane  $\{x_1 = 0\}$  in  $\mathbb{R}^n$ . Write  $x = (x_1, y)$ ,  $y \in \mathbb{R}^{n-1}$ , and make the change of variables  $t \leftarrow T - t$  to get

$$\begin{aligned}
 D(x, T) &= D(x_1, y; T) \\
 &= \int_0^T \int_{\mathbb{R}^{n-1}} \mu(s, t) \frac{x_1 e^{-x_1^2/4(T-t)}}{4\sqrt{\pi}(T-t)^{3/2}} \frac{e^{-\|y-s\|^2/4(T-t)}}{(4\pi(T-t))^{(n-1)/2}} ds dt \\
 &= \int_0^T \frac{x_1 e^{-x_1^2/4t}}{4\sqrt{\pi}t^{3/2}} g(y, t) dt
 \end{aligned}$$

where

$$\begin{aligned}
 g(y, t) &= \int_{\mathbb{R}^{n-1}} \mu(s, T-t) \frac{e^{-\|y-s\|^2/4t}}{(4\pi t)^{(n-1)/2}} ds \\
 &\rightarrow \mu(y, T) \quad \text{as } t \rightarrow 0.
 \end{aligned}$$

By a change of variables and the dominated convergence theorem,

$$\begin{aligned}
 D(x_1, y; T) &= \frac{\text{sgn}(x_1)}{2\sqrt{\pi}} \int_{x_1^2/4T}^{\infty} g(y, x_1^2/4\sigma) e^{-\sigma} \frac{d\sigma}{\sqrt{\sigma}} \\
 &\rightarrow \pm \frac{1}{2} \mu(y, T) \quad \text{as } x_1 \rightarrow 0^\pm.
 \end{aligned}$$

Thus  $D$  has a jump across  $\Gamma(T)$  given by

$$[D](x_0, T) = \mu(x_0, T).$$

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