

The Supercooled Stefan Problem in One Dimension

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Abstract: We study the 1D contracting Stefan problem with two moving boundaries that describes the *freezing* of a supercooled liquid. The problem is borderline ill-posed with a density in excess of unity indicative of the dividing line. We show that if the initial density, $\rho_0(x)$ does not exceed one and is not too close to one in the vicinity of the boundaries, then there is a unique solution for all times which is smooth for all positive times. Conversely if the initial density is too large, singularities may occur. Here the situation is more complex: the solution may suddenly freeze without any hope of continuation or may continue to evolve after a local instant freezing but, sometimes, with the loss of uniqueness.

1 Introduction

The dynamical behavior of certain systems that are out of equilibrium has been described since time immemorial by a free boundary problem known as the *Stefan* equation. In the simplest case, namely $d = 1$ and a single boundary, the classical description consists of a function $\rho(x, t)$ and a boundary $L(t)$: For $x > L(t)$, ρ obeys the diffusion equation, typically with vanishing Dirichlet boundary conditions at $x = L(t)$. Furthermore there is a *Stefan condition* which relates the motion of the (free) boundary to the flux of ρ at $L(t)$ i.e. $\dot{L} = \vartheta \nabla \rho(L, t)$. While it is clear, by scaling that the value of $|\vartheta|$ is unimportant, the sign of ϑ is seminal. Indeed, $\vartheta = -1$ corresponds to a melting – and receding – boundary and is readily handled as a generalized non-linear diffusion problem (c.f. [7]) which is inherently stable. By contrast, $\vartheta = +1$ corresponds to a freezing boundary which encroaches on the interior. In particular, the problem is borderline ill posed: Despite the Dirichlet boundary condition at $L(t)$, if the initial density gets “too large”, there are circumstances where the solutions cannot be interpreted classically.

The problem of a single boundary was studied in [4] (and also [3]) where the pivotal nature of $\rho = 1$ was, to some extent, elucidated. In particular, it was found that for the problem on $[L_0, a]$ with $\rho_0 = \rho(x, 0)$ satisfying $\rho_0 \leq 1$ – and less than some $c_0 < 1$ in a neighborhood of L_0 , there is a unique solution to the weak version of this Stefan equation which, for $t > 0$, is C^∞ . By contrast, in some cases when these conditions are violated, (e.g. the mild circumstances that the average of the density exceed one and that the density at $x = a$ is always as large as the maximum initial value) there is no classical solution: The boundary reaches a particular point

at a particular time and then “disappears”, sometimes with no possibility for a continuation of the solution.

While the one-sided problems were studied in [4], [3], they were actually an auxiliary device to examine a certain two-sided problem. In particular, there was a second boundary $R(t)$ with $R_0 = R(0) > L_0$. In the aforementioned references, where the conditions at the boundaries were motivated by the study of certain 2D interfaces, the boundary condition at $x = R(t)$ was $\rho(R, t) \equiv 1$ and here $\dot{R} = -\nabla\rho(R, t)$. It is noted that, with the initial density in $[0,1]$ this exactly the analog of the condition on the left under the exchange $\rho \rightarrow 1 - \rho$. On occasion this will be referred to as the zero-one Stefan problem. Due to the afore-mentioned symmetry and certain inherent monotonicities, an essentially complete analysis of the zero-one problems was possible in [3] and [4]. However the boundary condition on the right is not pertinent for the study of a single (simple) fluid that has become supercooled. And, it turns out, the zero-one boundary conditions are seminal in the monotonicity based approach of [4]. Thus, an analysis of alternative forms of the two-boundary 1D Stefan problem will require the introduction of additional techniques.

In this note we will study *the* two-sided problem in its own right: the zero-zero Stefan problem. While this problem may be devoid of any immediate applications to 2D interfaces, it is manifestly relevant for the description of a supercooled liquid in a 1D context. The formal description of the problem, at the classical level, is provided by a triple: $\langle \rho(x, t), L(t), R(t) \rangle$ with

$$L_0 = L(0) \leq L(t) \leq R(t) \leq R(0) = R_0, \text{ and } \rho(x, 0) = \rho_0$$

satisfying the free boundary problem

$$\begin{cases} \rho_t - \Delta\rho = 0 & \text{in } \{(x, t) | L(t) < x < R(t), t \geq 0\} \\ \rho(L(t), t) = 0, & \dot{L}(t) = \rho_x(L(t), t) \\ \rho(R(t), t) = 0, & \dot{R}(t) = -\rho_x(R(t), t). \end{cases} \quad (1.1)$$

The weak version of this equation which –formally– accounts for all the conditions at the boundaries is simply

$$\int_{L_0}^{R_0} [a(x, s)G(x, s) - \rho_0(x)G(x, 0)]dx = \int_{L_0}^{R_0} \int_0^s [a(x, t)G_t(x, t) + \rho(x, t)G_{xx}(x, t)] dt dx, \quad (1.2)$$

for any smooth function $G(x, t)$ and, it is tacitly assumed, ρ_0 is supported in $[L_0, R_0]$.

While it may not be apparent from the above formulation, there are, ostensibly, two regions: one where $a \equiv 1$ and where ρ vanishes and another where $a = \rho$. Thus, a moving boundary e.g. $L(t)$ is a dividing point between these the two regions. In this formulation, the region of $a = \rho$ is the (remaining) supercooled fluid while $a \equiv 1$ represents the *equilibrium* crystal or fluid. Since as it turns out, there is overall conservation of a (as is seen by using $G \equiv 1$ in

Eqn.(1.2)) it is already clear from the weak formulation – where $a(x, t)$ has the interpretation of *enthalpy* – that $\rho > 1$ spells a potential for irregular behavior.

It is, perhaps, not surprising that Eqn.(1.2) alone is insufficient to ensure reasonable behavior of the system. In [4], various hypotheses were spelled out which appear to be required. These are, abbreviated for the present purposes:

Hypotheses H.

- The function $\rho(x, t) \geq 0$ for a.e. (x, t) .
- The function $\rho_0(x)$ (assumed measurable) satisfies $0 \leq \rho_0 \leq 1$ for a.e. x and is bounded away from one in a neighborhood of L_0 and a neighborhood of R_0
- Whenever $\rho \neq a$, then $a \equiv 1$.
- For all t , the region $\{x \mid \rho(x, t) = a(x, t)\}$ is simply connected.
- There is a specific constant c_0 and an ϵ_0 such that, in the integral sense, the initial data is less than c_0 in all neighborhoods of the points L_0, R_0 that are of size less than ϵ_0 .

We (re)emphasize that the first four items of hypotheses **H** are always satisfied by continuum limits of the Stefan–exclusion process studies in [3]. Moreover, these particle systems *produce* solutions to Eqn.(1.2). The upshot of this and the previous investigation is that under the stated conditions, there are no solutions other than those produced by these particle systems. On the other hand, violation of these conditions most likely will produce other solutions – which in turn could be implemented by other particle systems. There is further discussion of these matters in [4]; research is ongoing.

The final item of Hypotheses **H** is of a more technical nature in that the value c_0 is not optimal. Some condition along these lines is required; it may be presumed that the “ c_0 ” employed in [CK] could be replaced by any constant smaller than unity. Here, for additional technical reasons which will unfold below, the value of c_0 will be smaller still.

The principal result can now be stated:

Theorem 1.1 *Consider the 1D Stefan problem with two free boundaries as described in Eqs.(1.1) – (1.2) and satisfying the hypotheses **H**. Then there is a unique solution to this system. Moreover, the boundary speed is bounded by $C \max(1, t^{-1/2})$ where $C < \infty$ depends on the initial data. For positive times, the boundaries are C^∞ .*

We close this section with an outline of the topics treated:

In Section 2, we define the *separatrix* x^* , and derive a formula for its location; the point x^* is the ideal place to break the two–sided problem into a pair of one–sided problems where some results [4] and [3] may be brought to bear. It is also proved in this section that, if $\rho_0 < 1$, there is no finite-time extinction for the unfrozen phase $\{\rho > 0\}$; indeed a neighborhood of x^* remains unfrozen at all times.

In Section 3, we define a map Φ – taking the set of boundary datum at $x = x^*$ into itself – and demonstrate that, for a reasonable interval of times, Φ is a contraction map. We use the

contraction properties of the map Φ to provide a proof of Theorem 1.1 and also to establish additional results.

In section 4 we discuss the onset of singularities when local averages of ρ_0 are bigger than one. Moreover we discuss possibilities of continuation of the boundary after a jump, sometimes uniquely and sometimes non-uniquely.

We point out that our iteration scheme also applies to the slightly different two-sided problem studied in [CK], to provide existence and uniqueness results. On the other hand the monotone scheme constructed in [CK] is simpler and provides additional stability to the problem in terms of flux order preservation (see Lemma 3.2 in [CK]).

Finally we remark that, in the one-dimensional context, the current work covers any other possibility involving multiple seeding points. Indeed the addition of n additional boundary seeds – intermediate between L_0 and R_0 – simply breaks the system into $n + 1$ decoupled problems of the type treated here.

2 The Separatrix

The model at hand has a well defined *separatrix*, namely an $x^* \in (L_0, R_0)$ with the property (roughly speaking) that all the mass to the left of x^* is transported to the left boundary and the rest goes to the right. (Of course if ρ_0 vanishes identically in a neighborhood of x^* then any other point in this neighborhood shares this property. Otherwise, x^* is uniquely specified.)

We start with some definitions:

Definition For $q \in (L_0, R_0)$ let L_q be defined by

$$L_q = L_0 + \int_{L_0}^q \rho_0(x) dx. \quad (2.1)$$

The quantity L_0 has the interpretation as the location of the left boundary if all the material in $[L_0, q]$ (and nothing else) is transported into the boundary region. Similarly

$$R_q = R_0 - \int_q^{R_0} \rho_0(x) dx \quad (2.2)$$

Next, we define the transports $T_L(q)$ and $T_R(q)$:

$$T_{\mathcal{L}}(q) = \int_{L_0}^q (x - L_x) \rho_0(x) dx = -\frac{1}{2}(L_q^2 - L_0^2) + \int_{L_0}^q x \rho_0(x) dx \quad (2.3)$$

and similarly

$$T_{\mathcal{R}}(q) = \int_q^{R_0} (R_x - x) \rho_0(x) dx = \frac{1}{2}(R_0^2 - R_q^2) - \int_q^{R_0} x \rho_0(x) dx. \quad (2.4)$$

Note that these objects are non-negative and indeed strictly positive unless e.g. ρ_0 vanishes a.e. on $[L_0, q]$. These represent the amount of “transport currency” expended to get the specified masses into the respective boundaries.

The characterization of the separatrix is as follows:

Lemma 2.1 *Let $T_{\mathcal{L}}(q)$, $T_{\mathcal{R}}(q)$ etc. denote the quantities as described above. Then $\exists x^* \in (L_0, R_0)$ that satisfies $T_{\mathcal{L}}(x^*) = T_{\mathcal{R}}(x^*)$; unless ρ_0 vanishes a.e. in a neighborhood of x^* , the point is unique (and otherwise the whole interval serves as the separatrix). Let $\langle \rho, L, R \rangle$ denote a classical solution the the system in Equ.(1.1) and let $L_\star = \lim_{t \rightarrow \infty} L(t)$ and similarly for R_\star . Then x^* has the following properties:*

(i) $L_\star = L_{x^*}$.

(ii) $T_{\mathcal{L}}(x^*) = \lim_{t \rightarrow \infty} \int_{L_0}^{x^*} x[a(x, t) - \rho_0(x)]dx$ and similarly for $T_{\mathcal{R}}(x^*)$.

(iii) $0 = \lim_{T \rightarrow \infty} \int_0^T \nabla \rho(x^*, t)dt$.

Proof. We first establish that such an x^* exists. Indeed for $q = L_0$, $T_{\mathcal{L}} = 0$ and similarly for $T_{\mathcal{R}}$ at R_0 while $T_{\mathcal{L}}(R_0)$ and $T_{\mathcal{R}}(L_0)$ are both seen to be positive. Since, manifestly, these are continuous functions, the existence of an x^* is established. Moreover

$$\frac{dT_{\mathcal{L}}}{dq} = -L_q \frac{dL_q}{dq} + q\rho_0(q) = (L_q - q)\rho_0(q) \quad (2.5)$$

and similarly

$$\frac{dT_{\mathcal{R}}}{dq} = (q - R_q)\rho_0(q). \quad (2.6)$$

The first of these is non-negative and the second non-positive – with everything strict unless $\rho_0(q)$ vanishes. Thus x^* is unique modulo the possibility that ρ_0 vanishes in an interval containing x^* – in which case anywhere in the interval suffices.

Next we note, after a small calculation, that

$$\frac{d}{dt} \int_{L_0}^{R_0} -xa(x, t)dx = -\frac{d}{dt} [\frac{1}{2}L^2 - \frac{1}{2}L_0^2 + \int_L^R x\rho(x, t)dx + \frac{1}{2}R_0^2 - \frac{1}{2}R^2] = 0 \quad (2.7)$$

due to the Stefan conditions and boundary conditions at $x = L$ and $x = R$. Thence

$$-\frac{1}{2}(L_\star^2 - L_0^2) + \frac{1}{2}(R_0^2 - R_\star^2) = \lim_{t \rightarrow \infty} \int_{L_0}^{R_0} -xa(x, t)dx = -\int_{L_0}^{R_0} x\rho_0(x)dx. \quad (2.8)$$

Moreover as mentioned earlier, there is mass conservation:

$$0 = \frac{d}{dt} \int_{L_0}^{R_0} a(x, t)dx \quad (2.9)$$

i.e.

$$(L(t) - L_0) + (R_0 - R(t)) + \int_{L(t)}^{R(t)} \rho(x, t)dx = \int_{L_0}^{R_0} \rho_0(x)dx. \quad (2.10)$$

In particular, $(L_\star - L_0) + (R_0 - R_\star) = \int_{L_0}^{R_0} \rho_0 dx$.

Now let q^* satisfy $L_\star = L_{q^*}$. Then, with the preceding in mind,

$$L_\star - L_0 - \int_{L_0}^{q^*} \rho_0(x) dx = 0 = R_\star - R_0 + \int_{q^*}^{R_0} \rho_0(x) dx \quad (2.11)$$

so it follows that $R_{q^*} = R_\star$ as well. Similarly splitting the integral on the right hand side of Equ.(2.8) at q^* we find

$$T_{\mathcal{L}}(q^*) = -\frac{1}{2}(L_\star^2 - L_0^2) + \int_{L_0}^{q^*} x \rho_0 dx = \frac{1}{2}(R_0^2 - R_\star^2) - \int_{q^*}^{R_0} x \rho_0 dx = T_{\mathcal{R}}(q^*) \quad (2.12)$$

Evidently $q^* = x^*$ (or belongs to the appropriate interval if ρ_0 vanishes in a neighborhood of q^*) and we have proved item (i). Item (ii) follows immediatly from Equ.(2.12). To obtain item (iii), we note that by mass conservation,

$$L(t) - L_0 + \int_L^{x^*} \rho(x, t) dx - \int_L^{x^*} \rho_0(x) dx = \int_0^t \nabla \rho(x^*, t') dt'. \quad (2.13)$$

Taking $t \rightarrow \infty$ forces $\rho(x, t) \rightarrow 0$ and $L(t)$ to L_\star . Using $L_\star = L_{x^*} = L_0 - \int_{L_0}^{x^*} \rho_0 dx$ we conclude that

$$0 = \int_0^\infty \nabla \rho(x^*, t) dt. \quad (2.14)$$

□

Remark 1. We remark (since $L_\star = L_{x^*}$ and ρ_0 is not identically one) that $R_\star - L_\star > 0$. I.e. there is always a gap between the boundaries with the separatrix lying strictly between. It is not difficult to see that, if the solution stays regular, it will persist for all time. The situation is therefore in sharp contrast to the one-side problems where, usually, the solution extinguishes in finite time.

3 A contraction principle

Let x^* (as defined in Lemma 2.1) be the separatrix; it is emphasized that if the classical solution exists for all times then x^* is the “actual” spot with all the properties described; in particular, the moving boundaries are always a finite distance from x^* . Below we will show that, under the hypotheses **H** this is indeed the case and, in fact the classical solution is the unique weak solution of (1.2). In greater generality, we show that the solution is unique as long as it is regular e.g. with a finite propagation speed. All of this will be accomplished by the construction of a contraction map Φ which is described as follows:

Consider the one-sided problem with fixed density at $x = x^*$ given by $\rho_F(t)$. It is assumed that ρ_F is non-negative and, temporarily, $\rho_F(t) \leq 1$. Formally, this one-sided Stefan problem reads

$$\begin{cases} \rho_t - \Delta \rho = 0 & \text{in } \{(x, t) | L(t) < x < x^*, t \geq 0\} \\ \rho(L(t), t) = 0, \quad \dot{L}(t) = \rho_x(L(t), t) \\ \rho(x^*, t) = \rho_F(t) \end{cases} \quad (3.1)$$

and, from our perspective, *generates* the left boundary $L(t)$. A right boundary $R(t)$ is produced independently in the same fashion with the same $\rho_F(t)$. We remark [3], [4] that (depending on the large t behavior of $\int_0^t \rho_F(s) ds$) both problems “survive” up to particular times at which the boundaries coincide with x^* ; c.f. Eqn.(3). This is most likely to be of secondary importance since, ostensibly, we shall only be concerned with short times. However, for future technical convenience we shall always restrict to time intervals $t < T$ with T small enough so that on the left, the boundaries never get further, then $\frac{1}{2}[x^* + L_\star]$ and similarly on the right.

The next step is to solve the heat equation in the domain

$$(L, R) := \bigcup_{0 < t < T} (L(t), R(t)) \times \{t\}$$

with Dirchlet conditions at the boundaries and ρ_0 as the initial condition. Denoting this solution by $P(x, t)$, the mapping Φ is defined by

$$\Phi(\rho_F(t)) = P(x^*, t).$$

It is re-emphasized that the initial data $\rho_0(x)$ will be kept fixed throughout the construction and iteration of the map Φ . The key result is as follows:

Proposition 3.1 *Suppose that the initial data satisfies the relevant properties in hypotheses **H**. Then there is a $T_0 > 0$ such that Φ is a contraction map in $L^\infty([0, T_0])$. The quantity T_0 only depends only on $c_0, \epsilon_0, |L_0 - R_0|$ and $\sup \rho_0$.*

For the proof, we shall borrow a result from [1]

Lemma 3.2 *Let $\Sigma = \{(x, t) : x \geq f(t)\}$, where f is Lipschitz with Lipschitz norm M and with $f(0) = 0$. Suppose $\rho(x, t)$ is a positive solution of the heat equation in $\Sigma \cap Q_1$, where $Q_r = B_r(0) \times (-r, r)$, which vanishes on the boundary $\{x = f(t)\}$ and further that $\rho(1/2, 0) = 1$. Then there exist positive constants $0 < \epsilon, \delta < 1$, depending only on M and the supremum of ρ in Q_2 , such that*

$$\rho + \rho^{1+\epsilon} \text{ is convex and } \rho - \rho^{1-\epsilon} \text{ is concave in } Q_\delta.$$

Proof. This is the 1D version of Lemma 5 in [1]. □

Proof of Proposition 3.1. For what is to follow, we shall let C denote a constant of order unity whose value may evolve as the equations progress. Let $\sigma(t), \theta(t)$ be functions in $[0, 1]$. We would like to show that

$$\sup_{0 \leq t \leq s} |\Phi(\theta)(s) - \Phi(\sigma)(s)| \leq m(t) \sup_{0 \leq t \leq s} |\theta(s) - \sigma(s)| \quad (3.2)$$

where $m(t) \rightarrow 0$ as $t \rightarrow 0$.

Let $\langle \rho_\sigma, L_\sigma \rangle, \langle \rho_\theta, L_\theta \rangle$ solve the one-sided Stefan problems on $[L_0, x^*]$ with initial value ρ_0 and, respectively, lateral boundary data $\sigma(t)$ and $\theta(t)$ at $x = x^*$. As a consequence of [4], Lemma 3.7, the boundaries are smooth, except at $t = 0$ and for all t , have boundary speed bounded above by $Ct^{-1/2}$. (Here C depends on c_0, ϵ_0 and, in general on the supremum of ρ_0 which here can be taken as unity. Obviously, C only diminishes with c_0 – and, also, as ϵ_0 increases). In other words the domains under consideration are Lipschitz in time with the parabolic scaling.

Suppose $L_\sigma(t) \leq L_\theta(t)$. Then due to Lemma 3.2 we have

$$\rho_\sigma(L_\theta(t), t) \leq C \frac{L_\theta(t) - L_\sigma(t)}{t^{1/2}} \rho_\sigma(L_\sigma(t) + bt^{1/2}, t) \leq Cc_0 \frac{L_2(t) - L_1(t)}{t^{1/2}}. \quad (3.3)$$

where b is an intermediate constant. A parallel argument for the case $L_\sigma \geq L_\theta$ therefore gives us

$$\max\{\rho_\sigma, \rho_\theta\}(\max\{L_\sigma, L_\theta\}) \leq Cc_0 \frac{|L_\sigma(t) - L_\theta(t)|}{t^{1/2}} \quad (3.4)$$

We now let

$$K(t) := \sup_{0 \leq s \leq t} (|L_\sigma(s) - L_\theta(s)|), \quad K_2(t) := \sup_{0 \leq s \leq t} |\sigma(s) - \theta(s)|.$$

and let

$$u(x, t) := |\rho_\sigma - \rho_\theta|$$

First it is noted that u is a subsolution of the heat equation in the contracting domain $\Sigma := (L_\sigma, x^*) \cap (L_\theta, x^*)$ with zero initial data and data on the left side lateral boundary which, by Eqn.(3.3) is less than

$$Cc_0 t^{-1/2} |L_\sigma(t) - L_\theta(t)|$$

and data at $x = x^*$ given by $|\sigma(t) - \theta(t)|$. Hence $u(x, t)$ is less than any nonnegative solution $v(x, t)$ of the heat equation in the domain Σ with these boundary conditions.

Next, we will use the explicit well-known formula for the Green's function (see for example p 87 in [E]):

$$w(x, t) := \frac{x}{\sqrt{4\pi}} \int_0^t \frac{1}{(t-s)^{3/2}} \exp^{-\frac{x^2}{4(t-s)}} g(s) ds \quad (3.5)$$

so that $w(x, t)$ solves the boundary Dirichlet problem in $\mathbb{R}^+ \times [0, \infty)$:

$$\begin{cases} w_t - w_{xx} = 0 & \text{in } \mathbb{R}^+ \times (0, \infty) \\ w(0, t) = g(t) & \text{in } \{x = 0\} \times [0, \infty) \\ w(x, 0) = 0. \end{cases}$$

For our purposes, we shall actually use two functions based on Eqn.(3.5) – one to account for the data on the left and the other on the right. The two functions will be denoted by w_D and w_{x^*} respectively; w_{x^*} is just (the reflection of) the formula in Eqn.(3.5) with g given by K_2 . As for w_D , let $D(\tau) := \max\{L_\sigma(\tau), L_\theta(\tau)\}$. Then, in the domain

$$\{x > D(\tau)\} \times [0, \tau]$$

we use Eqn.(3.5) as though all the data, $c_0 C t^{-1/2} K(t)$ occurred on the line $x = D(\tau)$. On the basis of straightforward monotonicity/positivity considerations

$$v(x, t) \leq w_D(x, t) + w_{x^*}(x, t) \quad \text{in} \quad (D(\tau), x^*) \times [0, \tau].$$

Let us proceed with some estimates: Suppose $g(s)$ increases in time. Then, by a straightforward computation,

$$\begin{aligned} w(x, t) &\leq g(t) \int_0^t \frac{x}{(t-s)^{3/2}} e^{-\frac{x^2}{(t-s)}} ds \\ (z = \frac{x^2}{4(t-s)}) &\leq g(t) \int_{x^2/4t}^\infty z^{-1/2} e^{-z} dz \\ &\leq g(t) e^{-x^2/4t}. \end{aligned}$$

Therefore

$$w_{x^*}(x, t) \leq K_2(t) e^{-\frac{(x-x^*)^2}{4t}}$$

and

$$\int_{L_0}^{x^*} (x^* - x) w_{x^*}(x, t) dx \leq K_2(t) \int_0^{x^*-L_0} z e^{-z^2/4t} dz \leq t C K_2(t).$$

On the other hand, using $t = \tau$ (and $D = D(t)$ as in the previous display) we have

$$\begin{aligned} \int_{\Sigma(t)} w_D(x, t) dx &\leq C c_0 \int_D^{x^*} \int_0^t \frac{x-D}{(t-s)^{3/2}} e^{-\frac{(x-D)^2}{4(t-s)}} s^{-1/2} K(s) ds dx \\ (z = \frac{x-D}{4(t-s)^{1/2}}) &\leq C c_0 \int_0^t (\int_0^\infty z e^{-z^2} dz) (t-s)^{-1/2} s^{-1/2} K(s) ds \\ &\leq C c_0 K(t) (\int_0^\infty z e^{-z^2} dz) (\int_0^t (t-s)^{-1/2} s^{-1/2} ds) \\ &\leq c_0 C K(t), \end{aligned}$$

where in the last step, having pulled out the $K(t)$, what remains of the integral is of order unity and independent of t .

Assume, temporarily for convenience, that the initial position of the left boundary was $L_0 = 0$. Due to above computations it follows that

$$\begin{aligned} \int_0^{x^*} (x^* - x) u(x, t) dx &\leq x^* \int_{\Sigma(t)} w_D(x, t) dx + \int_0^{x^*} (x^* - x) w_{x^*}(x, t) dx \\ &\leq x^* C c_0 K(t) + t K_2(t) \end{aligned}$$

On the other hand, $\rho_\sigma(x, t)$ and $\rho_\theta(x, t)$ satisfy the transport equations, e.g.

$$x^* L_\sigma(t) - \frac{1}{2} L_\sigma^2(t) + \int_0^{x^*} (x^* - x) \rho_\sigma(x, t_0) = \int_0^t \sigma(s) ds + \int_0^{x^*} (x^* - x) \rho_0(x) dx.$$

(which may be obtained by plugging $G(x, t) = (x^* - x)$ into the weak formulation of the one-phase Stefan problem). Therefore, by taking differences between these equations for ρ_σ and ρ_θ , and recalling that $L_\sigma, L_\theta \leq \frac{1}{2}[x^* + L_\star]$ we have

$$\frac{1}{2}[x^* - L_\star] |L_\sigma(t) - L_\theta(t)| \leq \int_0^{x^*} (x^* - x) u(x, t) dx + \int_0^t |\sigma(s) - \theta(s)| ds.$$

Taking the supremum for the left hand side and using above estimate on $\int_0^{x^*} (x^* - x) u(x, t) dx$, we have

$$\frac{1}{2}[x^* - L_\star - c_0 C x^*] K(t) \leq 2t K_2(t)$$

We now insist that, all along, c_0 was small enough so that the coefficient of K is positive and of order unity. We run a parallel argument for the right and redesignate K to mean the maximum of the objects from the left and right. Thus, all in all we now have

$$K(t) \leq Ct K_2(t). \tag{3.6}$$

Lastly, let P_σ and P_θ respectively solve the heat equation in (L_σ, R_σ) and (L_θ, R_θ) with zero lateral boundary data. Once again using (3.5) we obtain

$$|P_\sigma(x^*, t) - P_\theta(x^*, t)| \leq C e^{-\frac{d^2}{t}} K(t) \tag{3.7}$$

where

$$d = \min(|R_\star - x^*|, |L_\star - x^*|).$$

Equations (3.6) and (3.7) yields our claim, (3.2), with

$$m(t) = Ct$$

for sufficiently small t . □

Next will use Proposition 3.1 to construct the unique solution of Eqn.(1.1) – or Eqn.(1.2) for the initial data etc. satisfying hypotheses **H**.

Proof of Theorem 1.1. We start by fixing a T_0 which, certainly, is small enough so that even with $\rho_F(t) \equiv 1$, for the problem described in Eqn.(3.1), and its analog on the right, the boundaries stay well away from x^* as discussed earlier. Then, making T_0 smaller still (if necessary) we can guarantee that Φ is a contraction mapping in $L^\infty([0, T_0])$. Starting then with some arbitrary initial lateral data e.g. positive and not in excess of unity, we converge to some limiting density and, as is clear from the fixed point property, and the estimates (e.g. Eqn.(3.6)) that have

preceded, this represents the density at $x = x^*$ of what is evidently the unique solution of Eqn.(1.1) and/or Eqn.(1.2) for the interval $[0, T_0]$.

Now we iterate above process to extend the time interval during which the unique solution exists. Let (L, R) denote the Stefan boundary of the unique solution for the time interval $0 \leq t \leq T$. In [CK] a bound of the form

$$\sup_{0 \leq t \leq T} (|\dot{L}|, |\dot{R}|) \leq C \max\{1, t^{-1/2}\}. \quad (3.8)$$

was established in the context of the “zero-one” two-sided problem described in the introduction. (C.f. [4] Lemmas 3.10 – 3.11 and the formula following Eqn.(3.50).) For this problem, the boundaries ultimately collide at a finite time \tilde{T} and $T < \tilde{T}$ was introduced to ensure a finite distance between the boundaries and thus $C = C(T)$. (Indeed, the boundary velocities again become singular at the moment of collision.) Here, since the boundaries are always well apart, we may take over the arguments of [CK] directly with no T -dependence in the constant; we shall omit the details.

Let T_∞ be the maximum time extension one can obtain via the iteration process. If $T_\infty = \infty$ then we are done, so suppose T_∞ is finite. Due to Eqn.(3.8) we have $u(\cdot, T_\infty)$ continuously vanish on the boundary $x = L(T_\infty), R(T_\infty)$. This enables us to iterate the process yet once more to extend the solution on a slightly longer interval, contradicting the definition of T_∞ . \square

We now turn to some auxiliary problems where the hypothesis $\rho_0 \leq 1$ is relaxed. We shall still assume bounded data and, for technical reasons previously discussed, that $\rho_0 \leq c_0$ in the neighborhood of the boundaries L_0 and R_0 . However, it is worth mentioning that here c_0 must be adjusted “smaller still” to account for a larger $\sup \rho_0$. With this in mind:

Theorem 3.3 *Suppose $u(x, t)$ and $v(x, t)$ are both solutions of (1.1) for $0 \leq t \leq T$ with ρ_0 satisfying all the conditions stated in **H** except the condition $\rho_0 \leq 1$ replaced by $\rho_0 \leq C_0$, and with c_0 adjusted accordingly. Further suppose that $u(x, t)$ and $v(x, t)$ have continuous boundaries with vanishing lateral boundary value. Then $u = v$ for $0 \leq t \leq T$.*

Proof. We start with the remark that, going all the way back to [3], the use of the condition $\rho_F \leq 1$ was for the *constructive* purpose of producing a solution. In the present context, the existence of the solutions comes with the statement of the theorem. Using the fact that u and v are fixed points of the mapping Φ and applying Proposition 3.1 over time intervals short enough to guarantee the contraction property we realize, starting from $t = 0$, that $u = v$ over the whole time interval under consideration. \square

The above is used in conjunction with our final observation of this section:

Theorem 3.4 *Let ρ_0 be as in Theorem 3.3. Then there exists a unique continuous solution ρ of (1.1) in the time interval $[0, t_2)$, where $t_2 \geq t_1(c_0, \epsilon_0, C_0)$. Moreover*

$$t_2 = \sup\{t : \limsup_{x \rightarrow L(t^-), s \rightarrow t^-} \rho(x, s) < c_0\}.$$

Sketch of the proof. Consider points close to the initial boundary points L_0 and R_0 i.e. at $x = L_0 + \ell$ and $R_0 - r$. By comparison with the solution of heat equation in $[L_0, R_0] \times [0, \infty)$ with initial data ρ_0 we can guarantee that for a short time interval $0 \leq t \leq t_0$, where $t_0 = t_0(c_0, \epsilon_0, C_0)$, the solution of the heat equation in any domain with contracting boundaries is less than one at points at $x = L_0 + 2\ell$ and $R_0 - 2r$, if ℓ and r is chosen small enough depending on c_0, ϵ_0 and C_0 . We now apply a double-barrel version of the map Φ described earlier with updates of the fixed boundary data at $x = L_0 + 2\ell$ and $x = R_0 - 2r$.

By comparison with the $\rho \equiv 1$ at $x = L_0 + 2\ell$ and $x = R_0 - 2r$, we know that the amount of time it takes for the boundaries to reach half-way (e.g. $x = L_0 + \ell$ and $x = R_0 - r$) is uniformly bounded from below throughout the iteration, depending on c_0, ϵ_0 and C_0 . Our stopping time t_1 is the earliest time the boundaries reach $x = \ell$ or $x = r$. The proof that, for some time $0 < \tilde{t}_1 \leq t_1$, there is a contraction follows, mutatis mutandis the proof of Lemma 3.1 and the rest follows. Indeed via iteration process one can continue the solution up to the time that the boundary jumps. Lastly, due to Theorem 1.1 the boundary will never jump up to $t = t_2$: indeed the density vanishes at the boundary. \square

Obviously at $t = t_2$ the system is exhibiting some form of irregular behavior: these matters will be discussed in the next section.

4 Irregular behavior

In this final section, we will provide illustrations (and stratagem) for circumstances where the initial density is allowed to exceed the critical value of one. As illustrated in the preceding results, these singularities are neither immediate nor inevitable – they come about if the density gets large in the vicinity of the boundary. Indeed because of the Dirichlet condition at the boundary, it is often enough the case that a certain excess of density can be processed which will ward off the jump. Evidently it is a finite (i.e. sufficiently strong) excess that causes the singularities and thus the situation is “complicated”: beyond the criterion of unit density, it is unlikely that substantial progress towards characterization will be made.

4.1 Blow-up with an overloaded initial data

To demonstrate the borderline ill-posedness of the problem (1.1), here we discuss the cases where the Stefan boundary disappears instantly (or the liquid instantly freezes) at some finite time. This happens when the initial data has high density; in the current context, it is sufficient that the average initial density exceeds unity, a situation that we call *overloaded*.

Lemma 4.1 *Consider the problem as described in Eqn.(1.1) with initial density $\rho_0 \in L^1$ a function with strictly positive overload, namely,*

$$\int_{L_0}^{R_0} \rho_0 dx - (R_0 - L_0) = \Delta > 0$$

Then any solution of Eqn.(1.2) will exhibit non-classical behavior at a finite time.

Proof. Let $\rho(x, t)$ denote the purported solution and let $\varphi(x, t)$ denote the solution of the diffusion equation with the same initial conditions but with fixed boundaries $L \equiv L_0$, $R \equiv R_0$ at which φ vanishes. Then, $\varphi \geq \rho$ and, moreover, $\int_{L_0}^{R_0} \varphi(x, t) dx \rightarrow 0$ at large times. By material conservation,

$$\int_L^R \rho(x, t) dx - (R(t) - L(t)) = \int_{L_0}^{R_0} \rho_0(x) dx - (R_0 - L_0) = \Delta > 0 \quad (4.1)$$

Thence

$$\Delta + (R(t) - L(t)) = \int_L^R \rho(x, t) dx \leq \int_L^R \varphi(x, t) dx \rightarrow 0 \quad (4.2)$$

which is obviously impossible. Thus, at some finite time there will be an exhibition of non-classical behavior. \square

4.2 Local overload without global overload.

Here we construct an example where $\int_{L_0}^{R_0} \rho_0 dx < R_0 - L_0$ but the solution has a jump. This demonstrates that the phenomena under discussion is genuinely an immediate response to stress and not caused by some sort of “violation” of global constraints.

As a background, we recapitulate a result from [4] Lemma A.3:

Suppose we have the one-phase Stefan problem on $[0, 1] \times [0, \infty]$ with $L_0 = 0$, fixed boundary data $\rho_F(t)$ at $x = 1$ and $\int_0^1 \rho_0(x) dx > 1$. Then, it turns out, that if $\nabla \rho(1, t) \geq 0$ for all $t > 0$ (which is easily arranged) then, at some finite time before the boundary reaches $x = 1$, the solution “vanishes”.

Consider then an initial density ρ_0 supported in $[0, R_0]$, where

$$\rho_0(x) = \begin{cases} M(9 - (x - 3)^2); & \text{for } 0 \leq x \leq 3, \\ \max[M(9 - (x - 3)^2), \epsilon_0]; & \text{for } 3 \leq x \leq R_0 \end{cases}$$

with a sufficiently small constant ϵ_0 .

Lemma 4.2 *If M and R_0 are chosen sufficiently large then the left Stefan boundary, associated with the initial data ρ_0 given above, jumps before it reaches $x = 1$.*

Proof. Let $\rho(x, t)$ be the corresponding solution of Eqn.(1.1) with initial data ρ_0 . Also let (L, R) denote the Stefan boundary. Set $R_0 \geq 6$ large enough that L reaches $x = 1$ before R reaches $x = 3$.

Let $T = T(M, R_0)$ be the time that L reaches $x = 1$. Note that $T \rightarrow 0$ as $M \rightarrow \infty$ and T stays bounded as $R_0 \rightarrow \infty$. Also observe, by fiat, that $(1, 3) \subset (L(t), R(t))$ for $0 \leq t \leq T$.

Now suppose that the boundary moves continuously up to $t = T$. If M is large enough such that T is sufficiently small, then we claim that

$$\nabla\rho(2, t) \geq 0 \text{ for } 0 \leq t \leq T. \quad (4.3)$$

To prove the claim, first note that, due to interior regularity estimate for solutions of heat equation (for example see Theorem 9 in Chapter 2.3 of [E]),

$$|\nabla\rho|(x, t) \leq CMt^{-1/2} \text{ in } \Sigma := \left(\frac{3}{2}, \frac{5}{2}\right) \times [0, T].$$

Hence $\nabla\rho$ solves the heat equation in Σ with initial data $-2M(x-3) \geq M$ and lateral boundary data of size less than $Mt^{-1/2}$. Considering the heat kernel formula using the fact that $x = 2$ is a fixed distance away from the lateral boundaries of Σ , we conclude that if T is sufficiently small then (4.3) holds.

Now, of course $\nabla\rho$ also satisfies the heat equation in the larger (moving) domain

$$\bigcup_{0 \leq t \leq T} (L(t), 2) \times \{t\}.$$

Moreover it is positive at $t = 0$ and cannot be negative at $x = L(t)$ so it follows from Eqn.(4.3) that $\nabla\rho(1, t) \geq 0$ for all $t \in [0, T]$. But now, assuming that M is already large enough so that $\int_0^1 \rho_0 dx > 1$, we are in the domain of Lemma A.3 in [4] which takes us to the desired result.

Finally, it is noted that R_0 can be chosen as *large* as we want. So, in particular we can choose R_0 so that there is no global overload: $\int_0^{R_0} \rho_0(x) < R_0$. \square

4.3 Continuation of the solution after a jump.

Here we show that the Stefan boundary may continue to evolve after a finite jump. Let us further discuss the example from the previous subsection. Keep in mind that M and R_0 can be chosen as large as we want, and the upper bound of T only depends on M (once R_0 is large). For this example, consider the weak equation, Eqn.(1.2) at time s_1 subtracted from that at time $s_2 > s_1$

$$\int_{L_0}^{R_0} [a(x, s_2)G(x, s_2) - a(x, s_1)G(x, s_1)] dx = \int_{L_0}^{R_0} \int_{s_1}^{s_2} [a(x, t)G_t(x, t) + \rho(x, t)G_{xx}(x, t)] dt dx.$$

In the example from the previous subsection suppose the left boundary jumps from $\mathbf{A} = L(t_0^-)$ to $\mathbf{B} = L(t_0^+) > \mathbf{A}$ at $t = t_0$. From the above equation, it is not hard to see that $\rho(x, t)$ needs to satisfy

$$\int_{\mathbf{A}}^{\mathbf{B}} \rho(x, t_0^-) dx = \mathbf{B} - \mathbf{A}. \quad (4.4)$$

Indeed, assuming for simplicity that ρ is classical before and after the jump. Then $a(x, t)$ and $\rho(x, t)$ satisfy Eqn.(1.2) iff ρ satisfies Eqn.(1.1) for $0 \leq t < T$ and $t > T$ with the additional

condition in Eq.(4.4). So, the problem of resolving the jumps boils down to the question of whether or not we can find a spot $B > A$ at which Eqn.(4.4) holds. It is not hard to see that in the cases with *global* overload, (or the example Lemma A.3 of [4]) no such A exists.

Going back to our example, via a barrier argument we see that $\rho(\cdot, T) < 2\epsilon_0$ at the time of jump $t = T$ in $[\frac{1}{2}R_0, R_0]$ if R_0 is large enough compared to M . Also we showed that the boundary jump occurs before the left boundary hits $x = 1$. Next, via comparison with solution of heat equation in the cylindrical domain in $[1, 4] \times [0, T]$ with initial data $M(x - 1)$, it can be deduced that $\rho(x, T) \geq b_0 M(x - 1)$ in $[2, 3]$ where b_0 is a universal constant. Therefore then $\int_2^3 \rho(x, t) \geq b_0 M$ at $t = T$.

The following lemma, whose proof we postpone to the end of the section, gives us a better idea for the profile of ρ at $t = T$: in fact the lemma yields that there is a unique spot where the boundary may jump and continue itself.

Lemma 4.3 $\nabla \rho \leq 0$ in the region $[4, \infty) \times [0 \leq t \leq T]$.

Thanks to above lemma, $\rho(\cdot, T)$ is large in $[2, 3]$ but decreases in $[4, R_0]$ and stays near ϵ_0 in $[6, R_0]$. Therefore if R_0 is sufficiently large compared to M and if $\epsilon_0 > 0$ is small, there exists a unique point $x_0 \in [3, R(t)]$ such that

$$(x_0 - A)^{-1} \int_A^{x_0} \rho(x, T) dx = 1.$$

Note that $0 \leq A \leq 1$ and thus

$$1 = (x_0 - A)^{-1} \int_A^{x_0} \rho(x, T) dx \geq (x_0 - A)^{-1} \int_1^3 \rho(x, T) dx \geq \frac{2c_0}{3(x_0 - A)} M$$

we obtain that $\frac{2}{3}c_0 M + A \leq \frac{2}{3}c_0 M \leq x_0$.

Now, via comparison with the global solution with initial data ρ_0 , we obtain that

$$\rho(x_0, T) \sim M \exp^{-M/T}.$$

Hence if M is sufficiently large, one can continue this solution.

Remark 2. Note that there may be more than one way to continue the left boundary, generate non-uniqueness of solutions; for example imagine that we attach additional initial mass $\rho_0 = M$ for $R_0 \leq x \leq R_0 + 2$ and $\rho_0 = \epsilon_0$ for $2R_0 \leq x \leq 4R_0$ and so on (See Figure above) to create a bumpy initial data. Then there will be multiple points x_0 at which (4.4) holds and where the solution can be continued. Moreover, in the present context, extra work has to be done to ensure that the c_0 -condition is satisfied when/where the classical solution is ready to recommence. This technical condition could presumably be removed and, as a consequence, non-uniqueness in these systems is generic. The problem of a natural selection principle for this problem is currently under investigation by the authors.

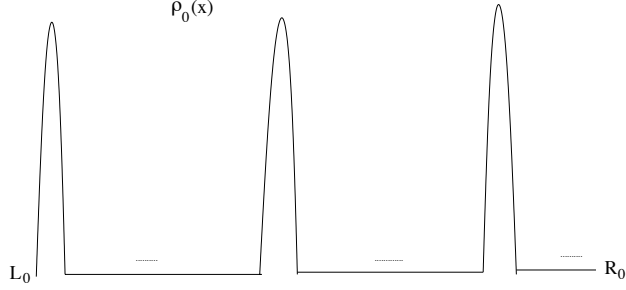


Figure: Initial data with non-unique, discontinuous Stefan boundaries in near future

Proof of Lemma 4.3 Note that $\nabla\rho$ solves the heat equation in $\Sigma := \cup_{0 < t \leq T} [4, R(t)] \times \{t\}$ with

$$\nabla\rho_0 \leq -M \text{ for } 7/2 \leq x \leq 6 - o(\epsilon_0) \text{ and } \nabla\rho_0 = 0 \text{ for } x \geq 6 - o(\epsilon_0).$$

Since ϵ_0 is chosen sufficiently small and C_1 is sufficiently large, the right Stefan boundary $R(t)$ moves continuously at least for $0 \leq t \leq T$; in fact $R(t) - R(0) = \epsilon_0 O(t^{1/2})$. Therefore $\rho(R(t), t) = 0$ and $\nabla\rho(R(t), t) \leq 0$ for $0 \leq t \leq T$. Consequently it suffices to prove that

$$\nabla\rho(x, t) \leq 0 \text{ at } \{x = 4\} \times [0, T]. \quad (4.5)$$

To prove (4.5), note that, via integration by part using Stefan boundary condition,

$$\int_0^t \nabla\rho(7/2, s) ds \leq \int_{7/2}^\infty (\rho_0(x) - \rho(x, t)) dx + R(0) - R(t) \leq MO(t^{1/2}) + \epsilon_0 O(t^{1/2}) \quad (4.6)$$

(In the last inequality, the term $MO(t^{1/2})$ bounds the diffusion of the solution, and the second term bounds $R(0) - R(t)$.)

Now let us write $\nabla\rho = u_1 + u_2$, where u_1 solves the heat equation in Σ with initial data zero and lateral boundary data $u_1 = \nabla\rho$ at $x = 2$, $x = R_0$. Since R_0 is large, using (3.5) and (4.6) a straightforward computation yields that

$$u_1(4, t) \leq MO(t^{-1} \exp^{-1/2t}).$$

On the other hand, by comparing u_2 with solutions of the heat equation in $[5/2, C_1] \times [0, T]$ with initial data $-M\chi_{2 \leq x \leq 7/2}$ and lateral boundary data zero one obtains

$$u_2(3, t) \leq -M + MO(t^{1/2}).$$

Putting above estimates together, we conclude that $\nabla\rho(3, t)$ stays negative for $0 \leq t \leq T$ if T is sufficiently small. This concludes the lemma. \square

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References

- [1] I. Athanasopoulos, L. Caffarelli and S. Salsa, *Caloric Functions in Lipschitz Domains and the Regularity of Solutions to Phase Transition Problems*, The Annals of Mathematics, **143** no. 3, 413–434 (1996)
- [2] E. Di Benedetto and A. Friedma, *The Ill-Posed Hele-Shaw Model and The Stefan Problem for Supercooled Water*, Trans. Amer. Math. Soc. **282** no. 1 183–204 (1984).
- [3] L. Chayes and G. Swindle, *Hydrodynamic Limits for OneDimensional Particle Systems with Moving Boundaries*, Ann. Probab. **24**, no.1, 559–598 (1996).
- [4] L. Chayes and I.C. Kim, *A Two-Sided Contracting Stefan Problem*, submitted for publication.
- [5] C. Evans, *Partial Differential Equations*, Graduate Studies in Mathematics, Volume 19, AMS (1998).
- [6] A. Fasano, and M. Primicerio, *General Free–Boundary Problems for the Heat Equation*, J. Math. Anal. Appl. **57** 694–723 (1977).
- [7] H. Ishii, *On a Certain Estimate of the Free Boundary in the Stefan Problem*, J. Differential Equations **42** 106–115 (1981).