

# SELF-PROPAGATING HIGH TEMPERATURE SYNTHESIS (SHS) IN THE HIGH ACTIVATION ENERGY REGIME

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ABSTRACT. We derive the precise limit of SHS in the high activation energy scaling suggested by B. J. Matkowsky and G. I. Sivashinsky in 1978 and by A. Bayliss, B. J. Matkowsky and A. P. Aldushin in 2002. In the time-increasing case the limit turns out to be the Stefan problem for supercooled water with spatially inhomogeneous coefficients.

Although the present paper leaves open mathematical questions concerning the convergence, our precise form of the limit problem suggests a strikingly simple explanation for the numerically observed pulsating waves.

#### 1. INTRODUCTION

The system

(1)

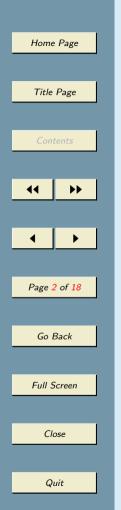
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Key words and phrases. SHS, solid combustion, singular limit, high activation energy, Stefan problem, ill-posed problem, free boundary, hysteresis.

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$$\partial_t u - \Delta u = v f(u)$$
  
 $\partial_t v = -v f(u)$ 



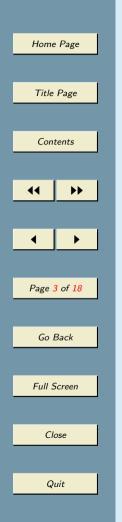
where u is the normalized temperature, v is the normalized concentration of the reactant and the non-negative nonlinearity f describes the reaction kinetics, is a simple but widely used model for solid combustion (i.e. the case of the Lewis number being  $+\infty$ ). In particular it is being used to model the industrial process of Self-propagating High temperature Synthesis (SHS). In the case of high activation energy interesting phenomena like the instability of planar waves, fingering and helical waves are observed.

Since the seventies (and possibly even earlier) it has been argued that the problem is for high activation energy related to a Stefan problem describing the freezing of supercooled water (see [20], [10, p. 57]). In [20] B. J. Matkowsky and G. I. Sivashinsky derived a formal singular limit containing a jump condition for the temperature on the interface. Later the Stefan problem for supercooled water – the intuitive limit – became the basis for numerous papers focusing on stability analysis of (1), fingering, helical waves etc. (see for example [10],[11],[9],[13],[12],[14],[8],[1],[2]).

Surprisingly there are few *mathematical* results on the subject: In [19] E. Logak and V. Loubeau proved existence of a planar wave in one-space dimension and gave a rigorous proof for convergence as the activation energy goes to infinity.

Instability of the planar wave for a special linearization (and high activation energy) is due to [4].

In the present paper we argue that the SHS system converges to the irreversible Stefan problem for supercooled water. As the initial data of the reactant concentration enters the equation as the activation energy goes to infinity, our result also suggests a *surprisingly simple* explanation for the numerically observed pulsating waves (cf. [1] and [2]), namely that they are caused by the spatial inhomogeneity  $v^0$  (or  $Y^0$ , respectively) in the below equation and are therefore mathematically related to the pulsating waves in [3].



In the time-increasing case we give a rigorous convergence proof in higher dimensions. For general initial data in one space-dimension see our forthcoming paper [21].

In the original setting by B. J. Matkowsky and G. I. Sivashinsky [20, equation (2)],

$$\partial_t u_N - \Delta u_N = (1 - \sigma_N) N e^N v_N \exp\left(-\frac{N}{u_N}\right),$$
$$\partial_t v_N = -N e^N v_N \exp\left(-\frac{N}{u_N}\right),$$

each limit  $u_{\infty}$  of  $u_N > 0$  as  $N \to \infty$  satisfies for  $(\sigma_N)_{N \in \mathbb{N}} \subset [0, 1)$  (for  $\sigma_N \uparrow 1, N \to \infty$  the limit in this scaling is the solution of the heat equation; cf. Section 5.1 and Theorem 4.1)

3) 
$$\partial_t u_{\infty} - v^0 \partial_t \chi = \Delta u_{\infty} \text{ in } (0, +\infty) \times \Omega$$

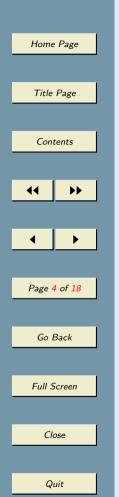
where  $v^0$  are the initial data of  $v_{\infty}$  and

$$\chi(t,x) \begin{cases} \in [0,1], & \text{esssup}_{(0,t)} u_{\infty}(\cdot,x) \leq 1, \\ = 1, & \text{esssup}_{(0,t)} u_{\infty}(\cdot,x) > 1, \end{cases}$$

and in the time-increasing case,

(2)

$$\chi(t,x) \begin{cases} = 0, & u_{\infty}(t,x) < 1 ,\\ \in [0,1], & u_{\infty}(t,x) = 1 ,\\ = 1, & u_{\infty}(t,x) > 1 . \end{cases}$$



In the SHS system with another scaling and a temperature threshold (see [2, p. 109–110]),

$$\partial_t \theta_N - \Delta \theta_N = (1 - \sigma_N) N Y_N \exp\left(\frac{N(1 - \sigma_N)(\theta_N - 1)}{\sigma_N + (1 - \sigma_N)\theta_N}\right) \chi_{\{\theta_N > \bar{\theta}\}},$$
$$\partial_t Y_N = -(1 - \sigma_N) N Y_N \exp\left(\frac{N(1 - \sigma_N)(\theta_N - 1)}{\sigma_N + (1 - \sigma_N)\theta_N}\right) \chi_{\{\theta_N > \bar{\theta}\}}.$$

where  $N(1 - \sigma_N) >> 1, \sigma_N \in (0, 1)$  and  $\bar{\theta} \in (0, 1)$ , each limit  $\theta_{\infty}$  of  $\theta_N$  satisfies (cf. Section 5.2 and Theorem 4.1)

$$\partial_t \theta_{\infty} - Y^0 \partial_t \chi = \Delta \theta_{\infty} \qquad \text{in } (0, +\infty) \times \Omega,$$

where  $Y^0$  are the initial data of  $Y_{\infty}$  and

$$\chi(t,x) \begin{cases} \in [0,1], & \text{esssup}_{(0,t)} \theta_{\infty}(\cdot,x) \leq 1 , \\ = 1, & \text{esssup}_{(0,t)} \theta_{\infty}(\cdot,x) > 1 , \end{cases}$$

and in the time-increasing case,

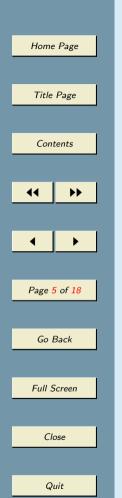
(4)

(5)

$$\chi(t,x) \begin{cases} = 0, & \theta_{\infty}(t,x) < 1, \\ \in [0,1], & \theta_{\infty}(t,x) = 1, \\ = 1, & \theta_{\infty}(t,x) > 1. \end{cases}$$

To our knowledge this precise form of the limit problem, i.e. the equation with the discontinuous hysteresis term, has not been known. Even in the time-increasing case it does not coincide with the formal result in [20].

In the case that  $\theta_{\infty}$  (or  $u_{\infty}$ , respectively) is increasing in time and  $v^0$  (or  $Y^0$ , respectively) is constant, our limit problem coincides with the Stefan problem for supercooled water, an extensively studied ill-posed problem (for a survey see [5]). As it is a forward-backward



parabolic equation it is not clear whether one should expect uniqueness (see [6, Remark 7.2] for an example of non-uniqueness in a related problem).

On the positive side, much more is known about the Stefan problem for supercooled water than the SHS system, e.g. existence of a finger ([15]), instability of the finger ([18]), one-phase solutions ([6]); those results, when combined with our convergence result, suggest that similar properties should be true for the SHS system.

It is interesting to observe that even in the time-increasing case our singular limit selects certain solutions of the Stefan problem for supercooled water. For example,  $u(t) = (\kappa - 1)\chi_{\{t<1\}} + \kappa\chi_{\{t>1\}}$  is for each  $\kappa \in (0, 1)$  a perfectly valid solution of the Stefan problem for supercooled water, but, as easily verified, it cannot be obtained from the ODE

$$\partial_t u_{\varepsilon}(t) = -\partial_t \exp\left(-\frac{1}{\varepsilon} \int_0^t \exp\left(\frac{1 - \frac{1}{(u_{\varepsilon}(s) + 1)}}{\varepsilon}\right) \,\mathrm{d}s\right) \,\,\mathrm{as}\,\,\varepsilon \to 0$$

### 2. NOTATION

Throughout this article  $\mathbb{R}^n$  will be equipped with the Euclidean inner product  $x \cdot y$  and the induced norm  $|x| \cdot B_r(x)$  will denote the open *n*-dimensional ball of center x, radius r and volume  $r^n \omega_n$ . When the center is not specified, it is assumed to be 0.

When considering a set A,  $\chi_A$  shall stand for the characteristic function of A, while  $\nu$  shall typically denote the outward normal to a given boundary. The operator  $\partial_t$  will mean the partial derivative of a function in the time direction,  $\Delta$  the Laplacian in the space variables and  $\mathcal{L}^n$  the *n*-dimensional Lebesgue measure.

Finally  $\mathbf{W}_{p}^{2,1}$  denotes the parabolic Sobolev space as defined in [17].

## 3. Preliminaries



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In what follows,  $\Omega$  is a bounded  $C^1$ -domain in  $\mathbb{R}^n$  and

 $u_{\varepsilon} \in \bigcap_{T \in (0, +\infty)} \mathbf{W}_2^{2, 1}((0, T) \times \Omega)$ 

is a strong solution of the equation

(6)

$$\partial_t u_{\varepsilon}(t,x) - \Delta u_{\varepsilon}(t,x) = -v_{\varepsilon}^0(x)\partial_t \exp\left(-\frac{1}{\varepsilon}\int_0^t g_{\varepsilon}(u_{\varepsilon}(s,x)) \, \mathrm{d}s\right)$$
$$u_{\varepsilon}(0,\cdot) = u_{\varepsilon}^0 \qquad \text{in } \Omega,$$
$$\nabla u_{\varepsilon} \cdot \nu = 0 \qquad \text{on } (0,+\infty) \times \partial\Omega;$$

here  $g_{\varepsilon}$  is a non-negative function on  $\mathbb{R}$  satisfying:

- 0)  $g_{\varepsilon}$  is for each  $\varepsilon \in (0,1)$  piecewise continuous with only one possible jump at  $z_0$ ,  $g_{\varepsilon}(z_0-) = g_{\varepsilon}(z_0) = 0$  in case of a jump, and  $g_{\varepsilon}$  satisfies for each  $\varepsilon \in (0,1)$  and for every  $z \in \mathbb{R}$  the bound  $g_{\varepsilon}(z) \leq C_{\varepsilon}(1+|z|)$ .
- 1)  $g_{\varepsilon}/\varepsilon \to 0$  as  $\varepsilon \to 0$  on each compact subset of  $(-\infty, 0)$ .
- 2) for each compact subset K of  $(0, +\infty)$  there is  $c_K > 0$  such that  $\min(g_{\varepsilon}, c_K) \to c_K$  uniformly on K as  $\varepsilon \to 0$ .

The initial data satisfy  $0 \le v_{\varepsilon}^0 \le C < +\infty$ ,  $v_{\varepsilon}^0$  converges in  $L^1(\Omega)$  to  $v^0$  as  $\varepsilon \to 0$ ,  $(u_{\varepsilon}^0)_{\varepsilon \in (0,1)}$  is bounded in  $L^2(\Omega)$ , it is uniformly bounded from below by a constant  $u_{\min}$ , and it converges in  $L^1(\Omega)$  to  $u^0$  as  $\varepsilon \to 0$ .

**Remark 3.1.** Assumption 0) guarantees existence of a global strong solution for each  $\varepsilon \in (0, 1)$ .

# 4. The High Activation Energy Limit

**Theorem 4.1.** The family  $(u_{\varepsilon})_{\varepsilon \in (0,1)}$  is for each  $T \in (0, +\infty)$  precompact in  $L^1((0,T) \times \Omega)$ , and each limit u of  $(u_{\varepsilon})_{\varepsilon \in (0,1)}$  as a sequence  $\varepsilon_m \to 0$ , satisfies in the sense of distributions the initial-boundary value problem

$$\partial_t u - v^0 \partial_t \chi = \Delta u \qquad in \ (0, +\infty) \times \Omega,$$
$$u(0, \cdot) = u^0 + v^0 H(u^0) \qquad in \ \Omega,$$
$$\nabla u \cdot \nu = 0 \qquad on \ (0, +\infty) \times \partial\Omega,$$

where

(7)

$$\chi(t,x) \left\{ \begin{array}{ll} \in [0,1], & \mathrm{esssup}_{\ (0,t)} u(\cdot,x) \leq 0 \;, \\ & = 1, & \mathrm{esssup}_{\ (0,t)} u(\cdot,x) > 0 \;, \end{array} \right.$$

and H is the maximal monotone graph

$$H(z) \begin{cases} = 0, & z < 0, \\ \in [0, 1], & z = 0, \\ = 1, & z > 0. \end{cases}$$

Moreover,  $\chi$  is increasing in time and u is a supercaloric function.

If  $(u_{\varepsilon})_{\varepsilon \in (0,1)}$  satisfies  $\partial_t u_{\varepsilon} \geq 0$  in  $(0,T) \times \Omega$ , then u is a solution of the Stefan problem for supercooled water, i.e.

$$\partial_t u - v^0 \partial_t H(u) = \Delta u \qquad in \ (0, +\infty) \times \Omega \ .$$

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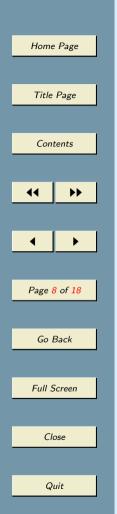
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**Remark 4.2.** Note that assumption 1) is only needed to prove the second statement "If ....".

Proof. <u>Step 0.</u> (Uniform Bound from below): Since  $u_{\varepsilon}$  is supercaloric, it is bounded from below by the constant  $u_{\min}$ . <u>Step 1.</u>  $(L^2((0,T) \times \Omega)$ -Bound):

The time-integrated function  $v_{\varepsilon}(t,x) := \int_0^t u_{\varepsilon}(s,x) \, \mathrm{d}s$ , satisfies

(8) 
$$\partial_t v_{\varepsilon}(t,x) - \Delta v_{\varepsilon}(t,x) = w_{\varepsilon}(t,x) + u_{\varepsilon}^0(x)$$

where  $w_{\varepsilon}$  is a measurable function satisfying  $0 \leq w_{\varepsilon} \leq C$ . Consequently

$$\int_0^T \int_\Omega (\partial_t v_{\varepsilon})^2 + \frac{1}{2} \int_\Omega |\nabla v_{\varepsilon}|^2 (T) = \int_0^T \int_\Omega (w_{\varepsilon} + u_{\varepsilon}^0) \partial_t v_{\varepsilon}$$
$$\leq \frac{1}{2} \int_0^T \int_\Omega (\partial_t v_{\varepsilon})^2 + \frac{T}{2} \int_\Omega (C + |u_{\varepsilon}^0|)^2,$$

implying

(9) 
$$\int_0^T \int_\Omega u_{\varepsilon}^2 \leq T \int_\Omega (C + |u_{\varepsilon}^0|)^2$$

Step 2.  $(L^2((0,T) \times \Omega))$ -Bound for  $\nabla \min(u_{\varepsilon}, M)$ : For

$$G_M(z) := \begin{cases} \frac{z^2}{2}, & z < M, \\ Mz - \frac{M^2}{2}, & z \ge M, \end{cases}$$



and any  $M \in \mathbb{N}$ ,

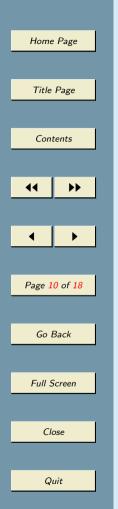
$$\int_{\Omega} G_M(u_{\varepsilon}) - G_M(u_{\varepsilon}^0) + \int_0^T \int_{\Omega} |\nabla \min(u_{\varepsilon}, M)|^2$$
$$= \int_0^T \int_{\Omega} -v_{\varepsilon}^0 \min(u_{\varepsilon}, M) \partial_t \exp\left(-\frac{1}{\varepsilon} \int_0^t g_{\varepsilon}(u_{\varepsilon}(s, x)) \, \mathrm{d}s\right).$$

As  $\partial_t \exp(-\frac{1}{\varepsilon} \int_0^t g_{\varepsilon}(u_{\varepsilon}(s,x)) \, \mathrm{d}s) \leq 0$ , we know that  $\partial_t \exp(-\frac{1}{\varepsilon} \int_0^t g_{\varepsilon}(u_{\varepsilon}(s,x)) \, \mathrm{d}s)$  is bounded in  $L^{\infty}(\Omega; L^1((0,T)))$ , and

$$\begin{split} \int_{0}^{T} \int_{\Omega} -v_{\varepsilon}^{0} \min(u_{\varepsilon}, M) \partial_{t} \exp\left(-\frac{1}{\varepsilon} \int_{0}^{t} g_{\varepsilon}(u_{\varepsilon}(s, x)) \, \mathrm{d}s\right) \\ & \leq C \int_{\Omega} \sup_{(0, T)} \max(\min(u_{\varepsilon}, M), 0) \leq CM\mathcal{L}^{n}(\Omega) \end{split}$$

Step 3. (Compactness):

Let  $\chi_M : \mathbb{R} \to \mathbb{R}$  be a smooth non-increasing function satisfying  $\chi_{(-\infty,M-1)} \leq \chi_M \leq \chi_{(-\infty,M)}$ and let  $\Phi_M$  be the primitive such that  $\Phi_M(z) = z$  for  $z \leq M - 1$  and  $\Phi_M \leq M$ . Moreover, let  $(\phi_{\delta})_{\delta \in (0,1)}$  be a family of mollifiers, i.e.  $\phi_{\delta} \in C_0^{0,1}(\mathbb{R}^n; [0, +\infty))$  such that  $\int \phi_{\delta} = 1$  and supp  $\phi_{\delta} \subset B_{\delta}(0)$ . Then, if we extend  $u_{\varepsilon}$  and  $v_{\varepsilon}^0$  by the value 0 to the whole of  $(0, +\infty) \times \mathbb{R}^n$ ,



we obtain by the homogeneous Neumann data of  $u_{\varepsilon}$  that

$$\begin{pmatrix} \Phi_{M}(u_{\varepsilon}) * \phi_{\delta} \rangle (t, x) \\ = \left( \left( \chi_{M}(u_{\varepsilon}) \left( \chi_{\Omega} \Delta u_{\varepsilon} - v_{\varepsilon}^{0} \partial_{t} \exp\left( -\frac{1}{\varepsilon} \int_{0}^{t} g_{\varepsilon}(u_{\varepsilon}(s, x)) \, \mathrm{d}s \right) \right) \right) * \phi_{\delta} \right) (t, x) \\ = \int_{\mathbb{R}^{n}} \chi_{M}(u_{\varepsilon})(t, y) \left( \chi_{\Omega}(y) \Delta u_{\varepsilon}(t, y) \right) \\ - \left( v_{\varepsilon}^{0}(y) \partial_{t} \exp\left( -\frac{1}{\varepsilon} \int_{0}^{t} g_{\varepsilon}(u_{\varepsilon}(s, y)) \, \mathrm{d}s \right) \right) \phi_{\delta}(x - y) \, \mathrm{d}y \\ = \int_{\mathbb{R}^{n}} \phi_{\delta}(x - y) \left( - \chi'_{M}(u_{\varepsilon}(t, y)) \chi_{\Omega}(y) |\nabla u_{\varepsilon}(t, y)|^{2} \\ - \chi_{M}(u_{\varepsilon}(t, y)) v_{\varepsilon}^{0}(y) \partial_{t} \exp\left( -\frac{1}{\varepsilon} \int_{0}^{t} g_{\varepsilon}(u_{\varepsilon}(s, y)) \, \mathrm{d}s \right) \right) \\ + \chi_{M}(u_{\varepsilon}(t, y)) \chi_{\Omega}(y) \nabla u_{\varepsilon}(t, y) \cdot \nabla \phi_{\delta}(x - y) \, \mathrm{d}y.$$

Consequently

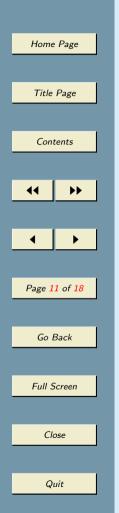
 $\partial_t$ 

$$\int_0^T \int_{\mathbb{R}^n} |\partial_t \left( \Phi_M(u_\varepsilon) * \phi_\delta \right)| \leq C_1(\Omega, C, M, \delta, T)$$

and

$$\int_0^T \int_{\mathbb{R}^n} |\nabla \left( \Phi_M(u_\varepsilon) * \phi_\delta \right)| \leq C_2(\Omega, M, \delta, T) .$$

It follows that  $(\Phi_M(u_{\varepsilon}) * \phi_{\delta})_{\varepsilon \in (0,1)}$  is for each  $(M, \delta, T)$  precompact in  $L^1((0, T) \times \mathbb{R}^n)$ .



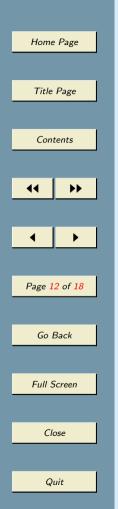
On the other hand

$$\int_{0}^{T} \int_{\mathbb{R}^{n}} |\Phi_{M}(u_{\varepsilon}) * \phi_{\delta} - \Phi_{M}(u_{\varepsilon})| \\ \leq C_{3} \left( \delta^{2} \int_{0}^{T} \int_{\Omega} |\nabla \Phi_{M}(u_{\varepsilon})|^{2} \right)^{\frac{1}{2}} + 2(M - u_{\min})T\mathcal{L}^{n}(B_{\delta}(\partial\Omega)) \\ \leq C_{4}(C, \Omega, u_{\min}, M, T) \delta.$$

Combining this estimate with the precompactness of  $(\Phi_M(u_{\varepsilon}) * \phi_{\delta})_{\varepsilon \in (0,1)}$  we obtain that  $\Phi_M(u_{\varepsilon})$  is for each (M,T) precompact in  $L^1((0,T) \times \mathbb{R}^n)$ . Thus, by a diagonal sequence argument, we may take a sequence  $\varepsilon_m \to 0$  such that  $\Phi_M(u_{\varepsilon_m}) \to z_M$  a.e. in  $(0, +\infty) \times \mathbb{R}^n$  as  $m \to \infty$ , for every  $M \in \mathbb{N}$ . At a.e. point of the set  $\{z_M < M - 1\}, u_{\varepsilon_m}$  converges to  $z_M$ . At each point (t,x) of the remainder  $\bigcap_{M \in \mathbb{N}} \{z_M \ge M - 1\}$ , the value  $u_{\varepsilon_m}(t,x)$  must for large m (depending on (M,t,x)) be larger than M-2. But that means that on the set  $\bigcap_{M \in \mathbb{N}} \{z_M \ge M - 1\}$ , the sequence  $(u_{\varepsilon_m})_{m \in \mathbb{N}}$  converges a.e. to  $+\infty$ . It follows that  $(u_{\varepsilon_m})_{m \in \mathbb{N}}$  so for each  $T \in (0, +\infty)$  bounded in  $L^2((0,T) \times \Omega)$ ,  $(u_{\varepsilon_m})_{m \in \mathbb{N}}$  converges by Vitali's theorem (stating that a.e. convergence and a non-concentration condition in  $L^p$  imply in bounded domains  $L^p$ -convergence) for each  $p \in [1, 2)$  in  $L^p((0,T) \times \Omega)$  to the weak  $L^2$ -limit u of  $(u_{\varepsilon_m})_{m \in \mathbb{N}}$ . It follows that

$$\mathcal{L}^{n+1}(\bigcap_{M \in \mathbb{N}} \{ z_M \ge M - 1 \}) = \mathcal{L}^{n+1}(\{ u = +\infty \}) = 0.$$

<u>Step 4.</u> (Identification of the Limit Equation in esssup  $_{(0,t)}u > 0$ ): Let us consider  $(t, x) \in (0, +\infty) \times \Omega$  such that  $u_{\varepsilon_m}(s, x) \to u(s, x)$  for a.e.  $s \in (0, t)$  and



 $u(\cdot, x) \in L^2((0, t))$ . In the case esssup  $_{(0,t)}u(\cdot, x) > 0$ , we obtain by Egorov's theorem and assumption 2) that

$$\exp\left(-\frac{1}{\varepsilon_m}\int_0^t g_{\varepsilon_m}(u_{\varepsilon_m}(s,x)) \, \mathrm{d}s\right) \to 0 \qquad \text{as} \qquad m \to \infty.$$

 $\underbrace{ Step 5.}_{\text{Let }(t,x)} \text{ for ease } \partial_t u_{\varepsilon} \geq 0 \text{ ):} \\ \text{Let } (t,x) \text{ be such that } u_{\varepsilon_m}(t,x) \to u(t,x) = \lambda < 0 \text{: Then by assumption 1} \text{ ),} \\ \end{cases}$ 

$$\exp\left(-\frac{1}{\varepsilon_m}\int_0^t g_{\varepsilon_m}(u_{\varepsilon_m}(s,x)) \, \mathrm{d}s\right) \geq \exp\left(-t\frac{\max_{[u_{\min},\lambda/2]}g_{\varepsilon_m}}{\varepsilon_m}\right) \to 1 \text{ as } m \to \infty.$$

# Remark 4.3.

- 1) For a more general result in one space-dimension see the forthcoming paper [21].
- 2) We also obtain a rigorous convergence result in the case of (higher dimensional) traveling waves with suitable conditions at infinity. In this case our  $L^2(W^{1,2})$ -estimate (Step 2) implies a no-concentration property of the time-derivative.

### 5. Applications

Although the limit equation is an ill-posed problem, the convergence to the limit seems to be robust with respect to perturbations of the  $\varepsilon$ -system and the scaling: here we mention two examples of different systems leading to the same limit. Other examples can be found in mathematical biology (see [16] and [22]).

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## 5.1. The Matkowsky-Sivashinsky scaling

We apply our result to the scaling in [20, equation (2)], i.e.

$$\partial_t u_N - \Delta u_N = (1 - \sigma_N) N v_N \exp\left(N\left(1 - \frac{1}{u_N}\right)\right),$$
$$\partial_t v_N = -N v_N \exp\left(N\left(1 - \frac{1}{u_N}\right)\right),$$

where the normalized temperature  $u_N$  and the normalized concentration  $v_N$  are non-negative,  $(\sigma_N)_{N \in \mathbb{N}} \subset [0,1)$  (in the case  $\sigma_N \uparrow 1, N \to \infty$  the limit equation in the scaling as it is would be the heat equation, but we could still apply our result to  $u_N/(1-\sigma_N)$ ) and the activation energy  $N \to \infty$ .

Setting  $u_{\min} := -1$ ,  $\varepsilon := 1/N$ ,  $u_{\varepsilon} := u_N - 1$  and

$$g_{\varepsilon}(z) := \begin{cases} \exp\left(\frac{1-\frac{1}{z+1}}{\varepsilon}\right), & z > -1\\ 0, & z \le -1 \end{cases}$$

and integrating the equation for  $v_N$  in time, we see that the assumptions of Theorem 4.1 are satisfied and we obtain that each limit  $u_{\infty}, \sigma_{\infty}$  of  $u_N, \sigma_N$  satisfies

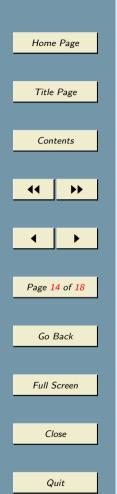
.) 
$$\partial_t u_{\infty} - (1 - \sigma_{\infty}) v^0 \partial_t \chi = \Delta u_{\infty} \text{ in } (0, +\infty) \times \Omega,$$

where

(11)

(10)

$$\chi(t,x) \begin{cases} \in [0,1], & \text{esssup}_{(0,t)} u_{\infty}(\cdot,x) \leq 1, \\ & = 1, & \text{esssup}_{(0,t)} u_{\infty}(\cdot,x) > 1, \end{cases}$$



and in the time-increasing case,

(12)

(13)

$$\partial_t u_{\infty} - (1 - \sigma_{\infty}) v^0 \partial_t H(u_{\infty}) = \Delta u_{\infty} \qquad \text{in } (0, +\infty) \times \Omega,$$
$$u_{\infty}(0, \cdot) = u^0 + v^0 H(u^0) \qquad \text{in } \Omega,$$
$$\nabla u_{\infty} \cdot \nu = 0 \qquad \text{on } (0, +\infty) \times \partial\Omega,$$

where  $v^0$  are the initial data of  $v_{\infty}$ . Moreover,  $\chi$  is increasing in time and  $u_{\infty}$  is a supercaloric function.

# 5.2. SHS in another scaling with temperature threshold Here we consider (cf. [2, p. 109–110]), i.e.

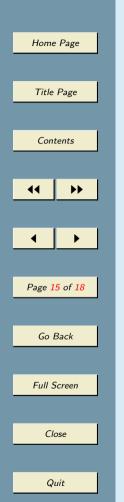
 $(N(1-\sigma_N)(\theta_N-1))$ 

$$\partial_t \theta_N - \Delta \theta_N = (1 - \sigma_N) N Y_N \exp\left(\frac{N (1 - \sigma_N) \theta_N}{\sigma_N + (1 - \sigma_N) \theta_N}\right) \chi_{\{\theta_N > \bar{\theta}\}},$$
$$\partial_t Y_N = -(1 - \sigma_N) N Y_N \exp\left(\frac{N(1 - \sigma_N) (\theta_N - 1)}{\sigma_N + (1 - \sigma_N) \theta_N}\right) \chi_{\{\theta_N > \bar{\theta}\}}.$$

where  $N(1 - \sigma_N) >> 1, \sigma_N \in (0, 1)$  and the constant  $\bar{\theta} \in (0, 1)$  is a threshold parameter at which the reaction sets in.

Setting  $u_{\min} = -1$ ,  $\varepsilon := 1/(N(1 - \sigma_N))$ ,  $\kappa(\varepsilon) := 1 - \sigma_N$ ,  $u_{\varepsilon} := \theta_N - 1$ ,

$$g_{\varepsilon}(z) := \begin{cases} \exp\left(\frac{z}{\overline{\kappa(\varepsilon)z+1}}{\varepsilon}\right), & z > \overline{\theta} - 1\\ 0, & z \le \overline{\theta} - 1 \end{cases}$$



and integrating the equation for  $Y_N$  in time, we see that the assumptions of Theorem 4.1 are satisfied and we obtain that each limit  $u_{\infty}$  of  $u_N$  satisfies

(14)

$$\partial_t u_{\infty} - v^0 \partial_t \chi = \Delta u_{\infty} \qquad \text{in } (0, +\infty) \times \Omega,$$
  
$$\chi(t, x) \begin{cases} \in [0, 1], & \text{esssup } _{(0,t)} u_{\infty}(\cdot, x) \le 1, \\ = 1, & \text{esssup } _{(0,t)} u_{\infty}(\cdot, x) > 1, \end{cases}$$

and in the time-increasing case,  

$$\partial_t u_{\infty} - v^0 \partial_t H(u_{\infty}) = \Delta u_{\infty} \qquad \text{in } (0, +\infty) \times \Omega,$$
(15)  

$$u_{\infty}(0, \cdot) = u^0 + v^0 H(u^0) \qquad \text{in } \Omega,$$

$$\nabla u_{\infty} \cdot \nu = 0 \qquad \text{on } (0, +\infty) \times \partial\Omega,$$

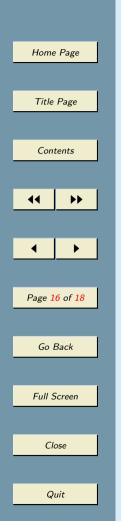
(15)

where  $v^0$  are the initial data of  $v_{\infty}$ . Moreover,  $\chi$  is increasing in time and  $u_{\infty}$  is a supercaloric function.

## 6. Open questions

The most pressing task is of course to study the existence or non-existence of "peaking" (cf. Figure 1) of the solution in the negative phase (for the case of one space dimension see the for the formula paper [21]). A related question is whether  $(u_{\varepsilon})_{\varepsilon \in (0,1)}$  is bounded in  $L^{\infty}$  in the case of uniformly bounded initial data. Although this seems obvious, it is not obvious how to prevent concentration close to the interface.

Uniqueness for the limit problem (the irreversible Stefan problem for supercooled water) in general seems unlikely. One might however ask whether time-global uniqueness holds in the case that u is strictly increasing in the  $x_1$ -direction. By the result in [7] for the ill-posed Hele-Shaw problem, time-local uniqueness is likely to be true here, too.



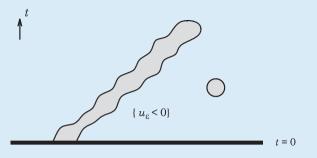


Figure 1. Is it possible for the solution to have a tiny peak traveling at high speed?.

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