Asymptotics of Solutions in a A+B→C Reaction–Diffusion System

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Abstract. We analyze the long time behavior of an initial value problem that models a chemical reaction–diffusion process $A + B \to C$. The problem has previously been studied by Gálfi and Rácz [1], who predicted the critical indices associated with the reaction by using a scaling ansatz motivated by numerical simulations. In this paper we point out some difficulties which appear in problems of this type due to the non–uniform convergence of the solution towards the scaling limit, and solve them by giving an explicit description of the corrections to scaling that have to be included to prove bounds on the solution that are uniform in space and time. This allows us to relate rigorously the critical exponents as computed from the scaling ansatz to the exponents of the reaction.

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1. Introduction and Main Results

In this paper we consider the reaction–diffusion system

$$\begin{aligned} \partial_t a(x,t) &= \partial_x^2 a(x,t) - 2a(x,t)b(x,t), \\ \partial_t b(x,t) &= \partial_x^2 b(x,t) - 2a(x,t)b(x,t), \end{aligned} \tag{1.1}$$

for $x \in \mathbb{R}$, $t \in [0,\infty)$, with initial conditions

$$\begin{aligned} a(-x,0) = b(x,0) &= 1, \qquad x > 0, \\ a(-x,0) = b(x,0) &= 0, \qquad x < 0, \\ a(0,0) = b(0,0) &= \frac{1}{2}. \end{aligned} \tag{1.2}$$

This initial value problem models the time evolution of a chemical system of two initially separated substances A and B that diffuse in some substratum and which react according to $A + B \to C$. The substance C is supposed not to participate in the reaction anymore. The quantities a and b are proportional to the concentrations of the substances A and B, respectively. The product

$$F(x,t) = a(x,t)b(x,t) \tag{1.3}$$

is called the reaction term, and one is interested in describing the behavior of this term for large times. The following figures are produced by solving the system (1.1) numerically. They show graphs of the reaction term and of its scaled version F_s,

$$F_s(x,t) = t^{2\gamma} F(xt^{\alpha}, t), \tag{1.4}$$

with $\alpha = \frac{1}{6}$ and $\gamma = \frac{1}{3}$, for several fixed times. The sequence of graphs for F_s seems to converge to a fixed shape.

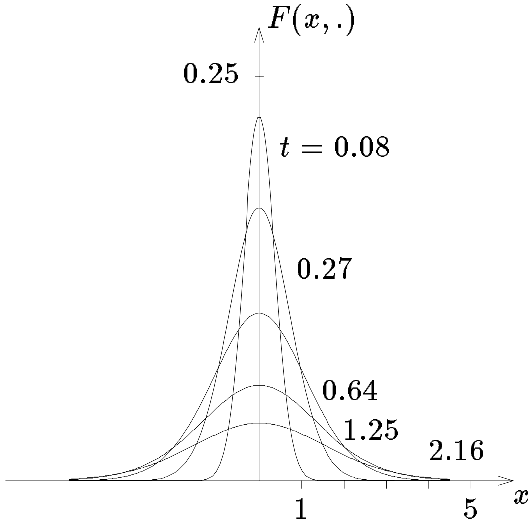

Fig. 1: The Reaction Term F

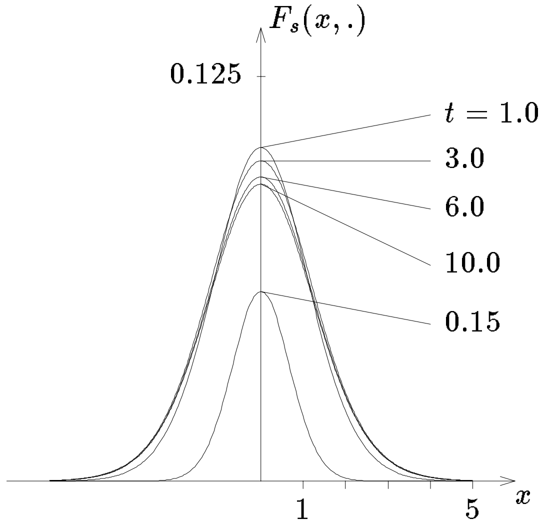

Fig. 2: The Scaled Reaction Term F_s

The numbers α and γ in (1.4) are the critical indices associated with the reaction term and are defined by the equations

$$\begin{aligned} \alpha &= \lim_{t\to\infty} \frac{\log \omega(t)}{\log t}, \\ \gamma &= -\frac{1}{2} \lim_{t\to\infty} \frac{\log F(0,t)}{\log t}, \end{aligned} \tag{1.5}$$

where ω is the variance of the reaction peak,

$$\omega(t)^2 = \frac{\int_{-\infty}^{+\infty} x^2 F(x,t)dx}{\int_{-\infty}^{+\infty} F(x,t)dx}. \tag{1.6}$$

In this paper we give a detailed and mathematically rigorous analysis of the numerical findings described above.

Note, that the factor of two which multiplies the reaction term in (1.1) is just a normalization, and has been chosen for convenience later on. In fact, any system of equations of the form

$$\begin{aligned} \partial_t a &= D_a \partial_x^2 a - k_a ab, \\ \partial_t b &= D_b \partial_x^2 b - k_b ab, \end{aligned} \tag{1.7}$$

with positive D_a, D_b, k_a, and k_b and with initial conditions

$$\begin{aligned} &a(x,0) = a_0 > 0, \qquad x < 0, \\ &b(x,0) = b_0 > 0, \qquad x > 0, \\ &a(x,0) = b(-x,0) = 0, \qquad x > 0, \end{aligned} \tag{1.8}$$

can be reduced, by scaling space and time and the amplitudes, to

$$\begin{aligned} \partial_t a &= \partial_x^2 a - 2ab, \\ \partial_t b &= D\partial_x^2 b - 2ab, \end{aligned} \tag{1.9}$$

$D > 0$, and with initial conditions

$$\begin{aligned} &a(x,0) = 1, \qquad x < 0, \\ &b(x,0) = k > 0, \qquad x > 0, \\ &a(x,0) = b(-x,0) = 0, \qquad x > 0. \end{aligned} \tag{1.10}$$

Here, we restrict ourselves to the case $k = 1$, and $D = 1$. Choosing $k = 1$ makes the initial conditions to be symmetric with respect to the origin $x = 0$, a symmetry which is preserved under the time evolution. The case $k \neq 1$ leads to a moving reaction front. Changing coordinates to the moving frame complicates the analysis but could as well be handled with the methods presented here. Choosing $D = 1$ makes the equations mathematically simpler. As a consequence, as we show below, the two equations for a and b can be reduced to just one equation for the sum $v = a+b$, since the equation for the difference $u = a-b$ can be solved explicitly. Even though one does not expect on physical grounds the solution to change in any relevant way for the case $D \neq 1$, i.e. the critical exponents are not supposed to change, the strategy of proof would have to be changed considerably, since the equations can not be decoupled in that case.

For completeness we note that the solution to (1.1) is not expected to change in any relevant way neither if the initial conditions (1.2) are slightly changed locally. The methods of proof presented here could in principle be adapted to such cases as well if needed, but this is not the topic of this paper.

We now express (1.1) in terms of the sum $v = a + b$ and the difference $u = a - b$. Subtracting the two equations in (1.1) we find that u satisfies the linear diffusion equation

$$\partial_t u(x,t) = \partial_x^2 u(x,t), \tag{1.11}$$

with initial condition

$$u(x,0) = -\mathrm{sign}(x), \tag{1.12}$$

and this initial value problem is explicitly solvable, namely

$$\begin{aligned} u(x,t) =& \hat{u}(\frac{x}{\sqrt{t}}) = -\frac{2}{\sqrt{\pi}} \int_0^{\frac{x}{2\sqrt{t}}} \mathrm{e}^{-\sigma^2}\, d\sigma \\ \equiv& -\mathrm{erf}(\frac{x}{2\sqrt{t}}). \end{aligned} \tag{1.13}$$

From now on u and $\hat{u}$ will always denote the functions defined by (1.13). Adding the two equations in (1.1) we find that v satisfies the equation

$$\partial_t v(x,t) = \partial_x^2 v(x,t) - v^2(x,t) + u^2(x,t), \tag{1.14}$$

with initial condition

$$v(x,0) = 1, \qquad x \in \mathbb{R}. \tag{1.15}$$

In terms of u and v, the reaction term F becomes

$$F(x,t) = \frac{1}{4}\big(v^2(x,t) - u^2(x,t)\big). \tag{1.16}$$

Based on the numerical findings described above, Gálfi and Rácz [1] proposed for large times t a scaling solution v_s to (1.14) of the form

$$v_s(x,t) = t^{-\gamma'} e(\frac{x}{t^{\alpha'}}). \tag{1.17}$$

By inserting v_s into (1.14), and matching powers of t for t large, they found $\alpha' = \alpha = \frac{1}{6}$, $\gamma' = \gamma = \frac{1}{3}$, with the scaling function e the (unique) solution of the boundary value problem

$$\begin{aligned} \eta''(x) &= \eta^2(x) - \kappa^2 x^2, \\ \eta'(0) &= 0, \\ \lim_{|x|\to\infty} (\eta(x) - \kappa|x|) &= 0, \end{aligned} \tag{1.18}$$

where $\kappa = |\hat{u}'(0)| = \frac{1}{\sqrt{\pi}}$. However, in view of the behavior of v_s for large x — $v(x,t)$ is bounded by 1 for all x and t whereas v_s diverges linearly as a function of x for t fixed — one cannot expect the convergence of the solution v towards the scaling solution v_s to be uniform in x. Indeed, as a consequence of our main estimate below, for any fixed x

$$\lim_{t\to\infty} t^{\frac{1}{3}} v(xt^{\frac{1}{6}},t) = e(x). \tag{1.19}$$

This means that the scaling solution v_s, as defined in (1.17), does approximates the solution v but, for any fixed t, only in a range of x of the order of $t^{\frac{1}{6}}$. Now, since the definition of the critical index α as given by (1.5) involves the solution v for fixed t on the whole real line, it is not clear that the exponent α' as computed from the scaling ansatz (1.17) is equal to the exponent α defined through (1.5), as Gálfi and Rácz implicitly assume in their work. Here, we prove that the two exponents are indeed equal.

The following theorem describes the corrections to scaling mentioned above. It is our main estimate from which all further results are derived.

Theorem 1.1. *Let e be the unique solution of the boundary value problem (1.18), and let*

$$\bar{e}(x) = |\hat{u}|(x) - \kappa|x|. \tag{1.20}$$

Let v be the solution of (1.14) with initial condition (1.15), and let

$$v_a(x,t) = \frac{1}{t^{\frac{1}{3}}}\mathrm{e}(\frac{x}{t^{\frac{1}{6}}}) - \bar{e}(\frac{x}{\sqrt{t}}). \tag{1.21}$$

Then, there exist positive constants t_0, A, b, such that

$$|v(x,t) - v_a(x,t)| \le \frac{A}{t}\cosh^{-1}(\frac{bx}{t^{\frac{1}{6}}}), \tag{1.22}$$

for all $x \in \mathbb{R}$, $t \ge t_0$.

The paper is organized as follows. In Section 2 we prove the existence and uniqueness of a solution to the boundary value problem (1.18) and derive some of its properties that we need in later chapters. In Section 3 we prove Theorem 1.1 by constructing explicit upper and lower bounds on the solution v using a comparison theorem for parabolic operators [2]. In Section 4, finally, we use our main estimate to discuss the reaction term and to compute the critical indices.

2. Existence and Properties of the Scaling Function

In this section we prove the existence and uniqueness of a solution to the boundary value problem (1.18). In view of the invariance of the equations under $x \to -x$, it is sufficient to prove the existence and uniqueness of a solution on the positive real axis, and we therefore restrict ourselves to $x \geq 0$ in this section. Next, since it is easier to work with zero boundary conditions at infinity than with linearly divergent ones, we study instead of (1.18) the boundary value problem

$$\begin{aligned} \varphi''(x) &= \varphi^2(x) + 2x\varphi(x), \\ \varphi'(0) &= -1, \\ \lim_{x\to+\infty} \varphi(x) &= 0. \end{aligned} \tag{2.1}$$

Any solution e of (1.18) is of the form

$$e(x) = \kappa^{\frac{2}{3}}\phi(\kappa^{\frac{1}{3}}x) + \kappa x, \tag{2.2}$$

with ϕ a solution of (2.1), and $\kappa = |\hat{u}'(0)| = \frac{1}{\sqrt{\pi}}$ as above. The results of this section are summarized in the following theorem.

Theorem 2.1. *The boundary value problem (2.1) has a unique positive solution ϕ and one has the bounds*

$$0.84 \leq \phi(0) \leq 0.91 \tag{2.3}$$

and

$$\frac{w'_{\phi(0)}(x)}{w_{\phi(0)}(x)} \leq \frac{\phi'(x)}{\phi(x)} \leq \frac{w'_0(x)}{w_0(x)}, \tag{2.4}$$

where for any $a \in \mathbb{R}$ the function w_a is defined by

$$w_a(x) = \mathrm{Ai}(2^{\frac{1}{3}}(x + \frac{a}{2})). \tag{2.5}$$

Remark. The Airy function Ai in Theorem 2.1 is the unique solution of the second order linear differential equation

$$w''(x) = xw(x) \tag{2.6}$$

which satisfies $w(x) > 0$ for $x \geq 0$ and $\lim_{x\to+\infty} w(x) = \lim_{x\to+\infty} w'(x) = 0$. See [3].

Proof. We first prove the uniqueness of a positive solution ϕ. Assume the contrary, then there are two positive solutions ψ_1 and ψ_2, and we can choose $\psi_1(0) > \psi_2(0)$. We show first that $\psi_1(x) > \psi_2(x)$ for all x. Assume the contrary, then there is a first x_0 such that $\psi_1(x_0) = \psi_2(x_0)$. The difference $\psi_{12} = \psi_1 - \psi_2$ has a positive second derivative on $[0, x_0)$ because it satisfies the equation

$$\psi''_{12}(x) = (\psi_1(x) + \psi_2(x) + 2x)\psi_{12}(x). \tag{2.7}$$

So, after integrating twice and using $\psi_{12}(0) > 0$ and $\psi'_{12}(0) = 0$ we find that $\psi_{12}(x_0) > 0$, a contradiction. Using (2.7) again, we conclude that $\psi''_{12}(x) > 0$ for all x, and that implies that ψ_{12} diverges as x goes to infinity, in contradiction with ψ_1 and ψ_2 both being solutions of (2.1). So, there is at most one positive solution ϕ.

To prove the existence of a solution ϕ we use the so called shooting method, i.e. we replace the boundary value problem (2.1) by the initial value problem

$$\begin{aligned} &\varphi''(x) = \varphi^2(x) + 2x\varphi(x), \\ &\varphi'(0) = -1, \\ &\varphi(0) = \rho > 0, \end{aligned} \tag{2.8}$$

and prove that there is a value of $\rho > 0$ for which the solution to (2.8) goes to zero as x goes to infinity. The initial value problem (2.8) has for all $\rho > 0$ a unique local solution ϕ_ρ on $[0, x_\rho)$, for some positive (and possibly infinite) x_ρ. Since by definition the derivative $\phi'_\rho(0) = -1$, all the local solutions are decreasing for x small enough. The idea is now to prove that for ρ too small the solution ϕ_ρ intersects the real axis and becomes negative, whereas for ρ too large it has a minimum and then diverges to plus infinity. The "correct" ρ is obtained as the (only) point "between" these two sets. To implement this idea we define two sets I_1 and I_2.

Definition 2.2. *We define the sets I_1 and I_2,*

$$I_1 = \big\{\rho > 0 | \exists x_1 < \infty, \phi_\rho(x_1) = 0, \text{ and } \phi_\rho(x) \neq 0, \text{ for } x \in (0, x_1)\big\}, \tag{2.9}$$

$$I_2 = \big\{\rho > 0 | \exists x_2 < \infty, \phi'_\rho(x_2) = 0, \text{ and } \phi'_\rho(x) \neq 0, \phi_\rho(x) \neq 0, \text{ for } x \in (0, x_2)\big\}, \tag{2.10}$$

with ϕ_ρ the (local) solutions of (2.8) defined above.

By definition, $I_1 \cap I_2 = \emptyset$. As a consequence of the continuity of the solution ϕ_ρ as a function of the initial data ρ, the two sets I_1 and I_2 are open and in addition I_1 is nonempty and bounded as we will prove below. $\bar\rho = \sup I_1$ is neither in I_1 nor in I_2 and therefore the solution $\phi_{\bar\rho}$ is decreasing and stays positive for all x which implies that the limit $\lim_{x\to\infty} \phi_{\bar\rho}(x)$ exists. This limit is zero because otherwise by (2.8) $\phi''_{\bar\rho}$ diverges which after integration contradicts the boundedness of $\phi_{\bar\rho}$. This proves that $\phi_{\bar\rho}$ is a positive solution to the boundary value problem (2.1).

To prove that I_1 is nonempty we fix any ρ_1 positive. Choose $\varepsilon > 0$ small enough such that on $[0, \varepsilon]$ the solution $\psi_1 \equiv \phi_{\rho_1}$ exists and is strictly decreasing. Choose now $\rho_2 < \rho_1 - \psi_1(\varepsilon)$, let $\psi_2 \equiv \phi_{\rho_2}$ be the corresponding solution and define $\psi_{12} = \psi_1 - \psi_2$. Then, since $\psi''_{12} > 0$ by (2.7), we find after integrating twice that ψ_2 becomes negative for some $x \leq \varepsilon$. So I_1 is not empty. To prove that the interval I_1 is bounded we analyze the "energy functional" E associated with equation (2.8),

$$E[\varphi](x) = \frac{1}{2}\varphi'(x)^2 - \frac{1}{3}\varphi^3(x) - x\varphi^2(x).$$

For any solution ϕ_ρ of (2.8), $E[\phi_\rho]$ is a nonincreasing function since $E[\phi_\rho]'(x) = -\phi_\rho^2(x) \leq 0$, and therefore $E[\phi_\rho](x) \leq E[\phi_\rho](0) = \frac{1}{2} - \frac{1}{3}\rho^3$. So assume $\rho \in I_1$, and $\rho > (\frac{3}{2})^{\frac{1}{3}}$. Then, $E[\phi_\rho](x) < 0$ for all x, but at the zero x_1 of ϕ_ρ, $E[\phi_\rho](x_1) = \frac{1}{2}{\phi'_\rho}^2(x_1) \geq 0$, a contradiction. So, I_1 is bounded. This completes the proof of the existence and uniqueness of a solution to (2.1).

We now proceed to prove the remaining statements in Theorem 2.1. By definition the function w_a as defined in (2.5) satisfies the linear differential equation

$$w_a''(x) = (a + 2x)w_a(x). \tag{2.11}$$

To prove the inequality (2.4) we study the Wronskian of w_a and the solution ϕ, i.e., we define

$$W_a(x) = \phi'(x)w_a(x) - \phi(x)w_a'(x). \tag{2.12}$$

We have $W_a' = \phi w_a(\phi - a)$. Thus, W_0 is an increasing function and $W_{\phi(0)}$ is a decreasing function. Moreover, since $\lim_{x\to\infty} W_a(x) = 0$ ($\lim_{x\to\infty} \phi'(x) = 0$ since $\phi''(x) > 0$ and $\lim_{x\to\infty} \phi(x) = 0$) we find by integrating from plus infinity to x that $W_0(x) \leq 0$ and $W_{\phi(0)}(x) \geq 0$, which implies (2.4). We are left with proving the estimates (2.3). Integrating the differential equation $E[\phi]'(x) = -\phi^2(x)$ from zero to infinity we find

$$1 = \frac{2}{3}\phi(0)^3 + 2\int_0^\infty \phi^2(x)\, dx. \tag{2.13}$$

Similarly one finds the following virial identity for w_a

$$2\int_0^\infty w_a^2(x)\, dx = w_a'(0)^2 - aw_a(0)^2. \tag{2.14}$$

If we integrate the inequality (2.4) we find after exponentiating and squaring that

$$\phi^2(x) \leq \Big(\frac{\phi(0)}{w_0(0)}\Big)^2 w_0^2(x). \tag{2.15}$$

Inserting this estimate in (2.13) and using the identity (2.14) for $a = 0$, we obtain

$$0 \leq \frac{2}{3}\phi(0)^3 + \Big(\frac{w_0'(0)}{w_0(0)}\Big)^2 \phi(0)^2 - 1, \tag{2.16}$$

which implies that $\phi(0)$ is larger than the only real zero of the polynomial

$$p(t) = \frac{2}{3}t^3 + \Big(\frac{w_0'(0)}{w_0(0)}\Big)^2 t^2 - 1. \tag{2.17}$$

Using that $w_0(0) > 0.35$, and $-w_0'(0) < 0.26$, (see [3]), we easily see that $p(0.84) < 0$, which proves the lower bound in (2.3). We have already proved above that $\phi(0) < (\frac{3}{2})^{\frac{1}{3}}$. A better upper bound is obtained from the function θ

$$\theta(x) = \frac{4}{3}\phi^3(x) + 2x\phi^2(x) - \phi'^2(x). \tag{2.18}$$

Inequality (2.4) implies that $\lim_{x\to\infty} \theta(x) = 0$. Moreover $\theta'(x) = 2\phi^2(x)(1 + \phi'(x)) \geq 0$. Therefore $\theta(0) = \frac{4}{3}\phi(0)^3 - 1 \leq 0$, i.e. $\phi(0) \leq (\frac{3}{4})^{\frac{1}{3}} < 0.91$.

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3. Proof of the Main Theorem

The proof of Theorem 1.1 is based on a comparison principle for the parabolic operator

$$L[v] = \partial_t v - \partial_x^2 v + v^2 - u^2 \tag{3.1}$$

where u is given by (1.13). In terms of L, (1.14) becomes $L[v] = 0$. The following proposition is our main technical tool.

Proposition 3.1. *(Comparison Principle) Let $0 \le \tau < T$, and v_1, v_2 two bounded functions of x and t, such that*

$$v_1(x, \tau) \le v_2(x, \tau) \quad \forall x \in \mathbb{R} \tag{3.2}$$

and

$$L[v_1] \le L[v_2] \qquad \forall x \in \mathbb{R}, \qquad t \in [\tau, T], \tag{3.3}$$

then

$$v_1(x, t) \le v_2(x, t) \qquad \forall x \in \mathbb{R}, \qquad t \in [\tau, T]. \tag{3.4}$$

Proof. For a proof of this theorem see [2].

Theorem 1.1 will follow by comparing v with the functions v_1 and v_2 defined below and which are chosen in such a way that $L[v_1] \le 0 = L[v] \le L[v_2]$.

Since the asymptotic solution v_a defined by (1.21) is a good approximation to v only for $t \ge t_0$, for some $t_0 \ge 1$, we get good bounds on v from v_a only on the time interval $[t_0, \infty)$. On the time interval $[0, t_0]$, we have to use different comparison functions.

Proposition 3.2. *For all $t \ge 0$ one has the inequalities*

$$\max\{|\hat{u}|(x/\sqrt{t}), \frac{1}{1+t}\} \le v(x, t) \le 1. \tag{3.5}$$

Proof. The idea is to apply Proposition 3.1 with $\tau = 0$ and $T = \infty$ to the pair v and the constant function $v_2 \equiv 1$ to get the upper bound, and to v and $v_1 = \hat{u}$, $v_1 = -\hat{u}$ and $v_1 = \frac{1}{1+t}$, respectively, to get the lower bound. However, for a correct application of Proposition 3.1 we have to prove that v stays bounded. For this purpose one splits the time interval $[0, \infty)$ into a sequence of intervals $I_n = [\varepsilon n, \varepsilon(n + 1)]$, $n = 0, 1, 2 \ldots$, and uses the local (in time) existence of a solution to (1.14) to prove inductively the boundedness of v. Namely, since $|v|(x, 0) \le 1$, local existence guarantees that $|v|(x, t) < 2$ for $t \in I_0$ for ε small enough. Using Proposition 3.1 with the just mentioned comparison functions, it then follows that $|v|(x, t) \le 1$ for $t \in I_0$, and the argument can be repeated for $n > 0$.

■

To prove Theorem 1.1 we apply Proposition 3.1 for some $\tau = t_0$, and $T = \infty$, and use (3.5) to bound the values of v at $t = \tau = t_0$. As comparison functions we use

$$v_j(x, t) = \frac{1}{t^{\frac{1}{3}}} \mathrm{e}(z) - \bar{e}(y) + \frac{1}{t} h_j(z), \tag{3.6}$$

$j = 1, 2$, where

$$h_j(x) = A_j \cosh^{-1}(b_j x), \tag{3.7}$$

for some constants A_j, b_j to be chosen below, and where we have put, once and for all, $z = t^{-\frac{1}{6}} x$, $y = \frac{x}{\sqrt{t}}$. For later use we give the expression for $L[v_j]$.

$$\begin{aligned} L[v_j](x,t) =& t^{-2}\left[-h_j(z) - \frac{1}{6} z h_j'(z) + h_j^2(z)\right] \\ &+ t^{-\frac{4}{3}}\left[-h_j''(z) + 2(e(z) - \kappa|z|) h_j(z) - \frac{1}{3}(e(z) + \frac{1}{2} z e'(z) - \frac{3}{2}\kappa|z|)\right] \\ &+ t^{-1}\left[2|\hat{u}|(y) h_j(z)\right] \\ &+ t^{-\frac{1}{3}}\left[2(e(z) - \kappa|z|)\bar{e}(y)\right]. \end{aligned} \tag{3.8}$$

In the following two subsections we show that there are constants $A_1 < 0$ and $b_1 > 0$ and $A_2 > 0$ and $b_2 > 0$, respectively, such that $L[v_1] \leq 0 \leq L[v_2]$, which implies Theorem 1.1 with $A = \max\{-A_1, A_2\}$, and $b = \min\{b_1, b_2\}$.

3.1. Lower Bound

In this subsection we prove the lower bound of Theorem 1.1. In what follows, the sentence "for t_0 big enough and b_1 small enough ..." should be read as "there is a positive constant C such that for all $t_0 > C$ there is a constant D (that depends on the choice of t_0) such that for all $b_1 < D$ ...".

First, to satisfy (3.2) we need that $v_1(x, t_0) \leq \max\{|\hat{u}|(\frac{x}{\sqrt{t_0}}), \frac{1}{1+t_0}\}$, which follows from

$$t_0{}^{-\frac{1}{3}} e(\frac{x}{t_0{}^{\frac{1}{6}}}) - \kappa\frac{|x|}{\sqrt{t_0}} + \frac{1}{t_0} A_1 \cosh^{-1}(\frac{b_1 x}{t_0{}^{\frac{1}{6}}}) \leq \max\{\frac{1}{1+t_0} - \kappa\frac{|x|}{\sqrt{t_0}}, 0\}, \tag{3.9}$$

using that $-\kappa|y| \leq -|\hat{u}|(y)$. Consider first b_1 equal zero, and let $z_0 = \frac{\sqrt{t_0}}{\kappa(1+t_0)}$. On $[z_0, \infty]$ we can bound the left hand side in (3.9) by its value at z_0 since the function f,

$$f(z) = e(z) - \kappa|z| \equiv \kappa^{\frac{2}{3}} \phi(\kappa^{\frac{1}{3}} z), \tag{3.10}$$

is decreasing, and on $[0, z_0]$ we can bound it by its value at z_0, since the function e is increasing since $e''(z) = f''(z) \geq 0$ and $e'(0) = 0$. Therefore, by continuity, (3.9) is satisfied for

$$|A_1| > t_0{}^{\frac{2}{3}} f(\frac{t_0{}^{\frac{1}{3}}}{\kappa(1+t_0)}), \tag{3.11}$$

and b_1 small enough. For convenience, we choose in the following

$$A_1 = -\frac{5}{4}\, t_0{}^{\frac{2}{3}} f(\frac{t_0{}^{\frac{1}{3}}}{\kappa(1+t_0)}), \tag{3.12}$$

and show that for t_0 big enough and b_1 small enough the function $L[v_1]$ is negative for $t \geq t_0$. The term proportional to $t^{-\frac{1}{3}}$ in (3.8) is negative, as well as the term $-t^{-2}\frac{1}{6} z h'(z)$, and we bound them by zero. The remaining terms proportional to t^{-2} are positive and we can therefore replace the factor t^{-2} by ${t_0}^{-\frac{2}{3}}t^{-\frac{4}{3}}$. Furthermore, for $t \geq t_0 \geq 1$, $|\hat{u}|(y) \geq t^{-\frac{1}{3}}|\hat{u}|(z)$, and hence

$$L[v_1] \leq t^{-\frac{4}{3}} g(z, -A_1, b_1), \tag{3.13}$$

where

$$\begin{aligned} g(z,A,b) =& {t_0}^{-\frac{2}{3}}\left[A^2\cosh^{-2}(bz) + A\cosh^{-1}(bz)\right] + Ab^2\cosh^{-1}(bz) - 2Ab^2\cosh^{-3}(bz) \\ & - 2A\left[e(z) - \kappa|z| + |\hat{u}|(z)\right]\cosh^{-1}(bz) \\ & - \frac{1}{3}\left[e(z) + \frac{1}{2}ze'(z) - \frac{3}{2}\kappa|z|\right]. \end{aligned} \tag{3.14}$$

We show that for $b = 0$, g is negative for t_0 big enough, which by continuity implies that g is negative for b small enough. For $b = 0$ (3.14) becomes

$$g(z, A, 0) = {t_0}^{-\frac{2}{3}}(A^2 + A) - 2A(f(z) + |\hat{u}|(z)) - \frac{1}{3}(f(z) + \frac{1}{2}zf'(z)). \tag{3.15}$$

To estimate the last term we note that the function $\bar{f}$, $\bar{f}(z) = f(z) - zf'(z)$, is positive since $\lim_{z\to\infty}\bar{f}(z) = 0$ and since by (2.8) $\bar{f}' = -zf'' \leq 0$. Therefore, $-\frac{1}{3}(f(z)+\frac{1}{2}zf'(z)) \leq \frac{1}{6}f(0)$. Next, using that $f(z) \geq f(0) - \kappa|z|$ and that $|\hat{u}|(z) \geq \kappa|z|(1 - \frac{z^2}{12})$ for $|z| < 2$, we find that $f(z) + |\hat{u}|(z) \geq f(0)(1 - \frac{1}{12}(\frac{f(0)}{\kappa})^2)$, since on the interval $[0, \frac{f(0)}{\kappa}]$ we can use that $f(z) + |\hat{u}|(z) \geq f(0) - \frac{\kappa}{12}z^3$, which is smallest at the right endpoint, and on $[\frac{f(0)}{\kappa}, \infty]$ we can use that $f(z) + |\hat{u}|(z) \geq |\hat{u}|(z)$, which is smallest at the left endpoint. Therefore,

$$g(z, A, 0) \leq {t_0}^{-\frac{2}{3}}(A^2 + A) - 2Af(0)(1 - \tfrac{1}{12}(\tfrac{f(0)}{\kappa})^2) + \frac{1}{6}f(0). \tag{3.16}$$

For $A = -A_1$, with A_1 as defined in (3.11) we get

$$g(z, -A_1, 0) \leq \frac{5}{4}f(x_0) + \frac{1}{6}f(0) - \frac{5}{4}{t_0}^{\frac{2}{3}}f(x_0)\left[2f(0)(1 - \tfrac{1}{12}(\tfrac{f(0)}{\kappa})^2) - \frac{5}{4}f(x_0)\right], \tag{3.17}$$

where $x_0 = \frac{{t_0}^{\frac{1}{3}}}{\kappa(1+t_0)}$. From (3.17) and (2.3) and using that $f(0) = \kappa^{\frac{2}{3}}\phi(0)$, it follows that $g < 0$ for t_0 big enough, and therefore $L[v_1] < 0$ for t_0 big enough and b_1 small enough.

3.2. Upper Bound

In this subsection we prove the upper bound of Theorem 1.1. In what follows, the sentence "for A_2 big enough and b_2 small enough ..." should be read as "there is a positive constant C such that for all $A_2 > C$ there is a constant D (that depends on the choice of A_2) such that for all $b_2 < D$ ...".

We choose $t_0 = 1$. To satisfy (3.2) we then need that $v_2(x,1) \geq 1$. But

$$\begin{aligned} v_2(x,1) &= e(x) + \bar{e}(x) + A_2 \cosh^{-1}(b_2 x) \\ &= (e(x) - \kappa|x|) + |\hat{u}|(x) + A_2 \cosh^{-1}(b_2 x) \\ &\geq |\hat{u}|(x) + A_2 \cosh^{-1}(b_2 x) \geq 1, \end{aligned} \tag{3.18}$$

for A_2 big enough and b_2 small enough. In the last inequality we have used that $|\hat{u}(x)| \geq 1 - \exp(-\frac{x^2}{4})$ and that $\cosh^{-1}(x) \geq \exp(-x)$ for $x \geq 0$.

Next we bound the function $L[v_2]$ for $t \geq 1$. First we prove the positiveness of the term proportional to t^{-2}, i.e. we prove that

$$A_2 \cosh^{-2}(b_2 z)\big[A_2 - \cosh(b_2 z) + \frac{1}{6}(b_2 z)\sinh(b_2 z)\big] \geq 0.$$

Since the function $-\cosh(b_2 z) + \frac{1}{6}(b_2 z)\sinh(b_2 z)$ has a global minimum independent of b_2, this inequality is satisfied for A_2 big enough.

Next we show that the combination of the second term in (3.8) with one half the third term in (3.8) is positive. Since, for $t \geq 1$, one has that $|\hat{u}|(y) \geq t^{-1/3}|\hat{u}|(z)$, we can factor $t^{-\frac{4}{3}}$, and we are left with showing that

$$\begin{aligned} &-\frac{1}{3}(e(z) + \frac{1}{2}ze'(z) - \frac{3}{2}\kappa|z|) \\ &+ 2(e(z) - \kappa|z|)A_2 \cosh^{-1}(b_2 z) \\ &+ A_2 \cosh^{-1}(b_2 z)|\hat{u}|(z) + 2A_2 {b_2}^2 \cosh^{-3}(b_2 z) - A_2 {b_2}^2 \cosh^{-1}(b_2 z) \geq 0. \end{aligned} \tag{3.19}$$

Since $|\hat{u}|(z) + 2{b_2}^2\cosh^{-2}(b_2 z) - {b_2}^2 = |\hat{u}|(z) + {b_2}^2 - 2{b_2}^2\tanh^2(b_2 z)$ is positive for b_2 small enough and since $e(z) - \kappa|z|$ is strictly positive, it is sufficient to show that

$$-\frac{1}{3} - \frac{1}{6}\frac{ze'(z) - \kappa|z|}{e(z) - \kappa|z|} + 2A_2 \cosh^{-1}(b_2 z) \geq 0. \tag{3.20}$$

But, the function $f(z) = e(z) - \kappa|z|$ is logarithmically convex since $\big(ff'' - f'^2\big)' \geq 0$ and $\lim_{z\to\pm\infty}\big(ff'' - f'^2\big)(z) = 0$, and therefore

$$-\frac{1}{6}|z|\frac{|e'|(z) - \kappa}{e(z) - \kappa|z|} \geq \frac{1}{6}|z|\frac{\kappa}{e(0)}. \tag{3.21}$$

Inequality (3.20) therefore follows if

$$-\frac{1}{3} + \frac{\kappa}{e(0)b_2}|b_2 z| + 2A_2 \cosh^{-1}(b_2 z) \geq 0, \tag{3.22}$$

which is easily seen to be true because the left hand side in (3.22) is positive at zero for A_2 big enough and increasing in $b_2 z$ for b_2 small enough.

Finally we show that the combination of one half the third term in (3.8) plus the forth term in (3.8) is positive. Since $y \equiv t^{-\frac{1}{3}}z$, it suffices to show that

$$\frac{\bar{e}(y)}{y^2}\left[2(e(z)-\kappa|z|)z^2\cosh(b_2 z)\right] + A_2|\hat{u}|(y) \geq 0. \tag{3.23}$$

Inequality (2.15) implies that $e(z)-\kappa|z|$ decays roughly like $\exp(-|z|^{\frac{3}{2}})$ for large $|z|$, and therefore the function $(e(z)-\kappa|z|)z^2\cosh(b_2 z)$ is smaller than some constant for all b_2 sufficiently small. Since, by definition, $\bar{e}(y) \geq \max\{-\kappa|y|, -|y|^3\}$, (3.23) is satisfied for A_2 big enough and b_2 small enough. This completes the proof of Theorem 1.1.

4. Reaction Front

In this section we discuss the asymptotic shape of the reaction front (1.4) and compute the critical indices (1.5).

Proposition 4.1. *Let α and γ be the critical indices as defined in (1.5), let F_s be the scaled reaction term as defined in (1.4) and let ω^2 be the variance of the reaction peak as defined in (1.6). Then,*

$$\alpha = \frac{1}{6}, \qquad \gamma = \frac{1}{3}. \tag{4.1}$$

Furthermore,

$$\lim_{t\to\infty} F_s(x,t) = e''(x) \equiv r(x), \tag{4.2}$$

where e is the unique solution of (1.18), and

$$\lim_{t\to\infty} t^{-2\alpha}\omega^2(t) = \frac{\int_{-\infty}^{+\infty} x^2 r(x)}{\int_{-\infty}^{+\infty} r(x)}. \tag{4.3}$$

Remark. Equation (4.3) expresses the fact that the integration over x and the limit $t\to\infty$ can be exchanged, at least for the computation of the asymptotics of the second moment of F. We conjecture, based on work in progress [4], that for the case of reaction terms of the form $a^n b^m$, with $|n-m| \geq 3$, this exchange of limits is wrong. Indeed, on a formal level it is easy to see that the corresponding scaling functions r_{nm} do not have a second moment, even though the reaction peaks F_{nm} do.

Proof. Let F be as defined in (1.3), and v_a as in (1.21), and let for $j = 1, 2$,

$$v_j(x,t) = v_a(x,t) + \frac{(-1)^j}{t} h\left(\frac{x}{t^{\frac{1}{6}}}\right), \tag{4.4}$$

where $h(x) = A\cosh^{-1}(bx)$, with A, b as in Theorem 1.1. Then, we define the lower bound F_1 and the upper bound F_2 of F by the equations

$$F_1(x,t) \equiv \frac{1}{4}\big(v_1^2(x,t) - u^2(x,t)\big) \le F(x,t) \le \frac{1}{4}\big(v_2^2(x,t) - u^2(x,t)\big) \equiv F_2(x,t). \tag{4.5}$$

In terms of $z = xt^{-\frac{1}{6}}$, $y = xt^{-\frac{1}{2}}$ we get that

$$F_j(x,t) = \frac{1}{t^{\frac{2}{3}}}e''(z) + \frac{2}{t^{\frac{1}{3}}}\bar{e}(y)\big[e(z) - \kappa|z|\big] + v_a(x,t)\frac{(-1)^j}{t}h(z) + \frac{1}{t^2}h(z)^2, \tag{4.6}$$

$j = 1, 2$, since

$$\begin{aligned} v_a^2(x,t) - u^2(x,t) =& \frac{1}{t^{\frac{2}{3}}}e^2(z) + \bar{e}^2(y) + \frac{2}{t^{\frac{1}{3}}}e(z)\bar{e}(y) - \hat{u}^2(y) \\ =& \frac{1}{t^{\frac{2}{3}}}e''(z) + \frac{2}{t^{\frac{1}{3}}}\bar{e}(y)\big[e(z) - \kappa|z|\big]. \end{aligned} \tag{4.7}$$

Using that $y \equiv t^{-\frac{1}{3}}z$ and that $\bar{e}(0) = \bar{e}'(0) = \bar{e}''(0) = 0$ one easily verifies (4.2), and $\gamma = \frac{1}{3}$. To prove (4.3) we note that for $t \ge t_0$

$$\frac{\int_{-\infty}^{+\infty} x^2 F_1(x,t)dx}{\int_{-\infty}^{+\infty} F_2(x,t)dx} \le w^2(t) \le \frac{\int_{-\infty}^{+\infty} x^2 F_2(x,t)dx}{\int_{-\infty}^{+\infty} F_1(x,t)dx}. \tag{4.8}$$

By a change of variables from x to $zt^{\frac{1}{6}}$, one computes with (4.6) that for any $n \ge 0$, $j = 1, 2$,

$$\begin{aligned} t^{(3-n)/6}\int_{-\infty}^{+\infty} |x|^n\big(v_j^2(x,t) - u^2(x,t)\big)\,dx =& \int_{-\infty}^{+\infty} |z|^n e''(z)dz \\ &+ 2t^{\frac{1}{3}}\int_{-\infty}^{+\infty} |z|^n\bar{e}(\frac{z}{t^{\frac{1}{3}}})\big[e(z) - \kappa|z|\big]\,dz \\ &+ (-1)^j A^2 t^{-\frac{4}{3}}\int_{-\infty}^{+\infty} \frac{|z|^n}{\cosh^2(bz)}dz \\ &+ 2(-1)^j A t^{-\frac{1}{3}}\int_{-\infty}^{\infty} |z|^n\frac{e(z)}{\cosh(bz)}dz \\ &+ 2(-1)^j A t^{-\frac{1}{3}}\int_{-\infty}^{\infty} |z|^n\bar{e}(\frac{z}{t^{\frac{1}{3}}})\frac{1}{\cosh(bz)}dz. \end{aligned} \tag{4.9}$$

Since $0 \ge \bar{e}(z/t^{\frac{1}{3}}) \ge -\big(|z|/t^{\frac{1}{3}}\big)^3$, one easily verifies that all the terms in (4.9) except the first one go to zero as t goes to infinity, which proves (4.3), and $\alpha = \frac{1}{6}$. This completes the proof of Proposition 4.1.

■

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