

TRAVELLING WAVES FOR SOLID-GAS REACTION-DIFFUSION SYSTEMS

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Abstract. We study a two-species reaction-diffusion problem described by a system consisting of a semilinear parabolic equation and a first order ordinary differential equation, endowed with suitable conditions. We prove the existing of a unique traveling wave profile and give necessary conditions and sufficient conditions for the occurrence of penetration and conversion fronts.

1. Introduction. Travelling wave solutions of parabolic initial-boundary value problems are often applied to describe interesting phenomena involving chemical reactions, combustion, and population dynamics [9, 2, 3, 5, 8]. In [6, 4, 7] the authors consider gas-solid reactions of different types described by a system of two equations, a semilinear parabolic equation for the gas concentration S and a first order ordinary differential equation for the solid concentration C , endowed with conditions specifying the initial and final concentrations. In all three papers a unique traveling wave profile with constant group velocity was found. Either of the equations of the system studied in [6, 7] contains a nonlinear reaction term which is the product of a power of C and a power of S . Moreover, their parabolic equation contains a second order spatial derivative term (the Laplacian in the case of [6]). In [4] the nonlinear reaction terms are more general products of functions of either concentration only, but the parabolic equation contains a linear first spatial derivative term describing the gas flux.

In this article we study travelling wave solutions of a model describing the conversion of a porous solid as it reacts irreversibly with a gas moving through its pores. The parabolic equation in the system under consideration contains both a first order and a second order spatial derivative term. The reaction is assumed to be proportional to $F(S)G(C)$, where F and G are positive, increasing C^1 -functions such that $F(0) = G(0) = 0$. Typically one has $F(S)G(C) = S^m C^p$, where $m, p > 0$.

In one space dimension, the mass balance for the solid-gas system yields the coupled equations

$$S_t = -\lambda_1 F(S)G(C), \quad (1)$$

$$(\varepsilon C)_t + (H(C))_x - (\Phi(C))_{xx} = -\lambda_2 F(S)G(C), \quad (2)$$

where $x \in \mathbb{R}$ and $t > 0$. Here ε denotes the (variable) porosity of the solid, H describes the gas flux and Φ the gas diffusion as functions of the gas concentration, and $\lambda_1, \lambda_2 > 0$ are the reaction rate parameters. We assume that H and Φ are

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monotonically increasing positive functions such that $H(0) = \Phi(0) = 0$, and that the porosity ε depends linearly on the solid concentration S as follows:

$$\varepsilon = \varepsilon_0 + \varepsilon_1(S^* - S), \tag{3}$$

where $\varepsilon_0 > 0$ and $\varepsilon_1 \geq 0$ are constants and S^* is an upper bound for the solid concentration.

Let us consider the travelling wave solutions $S = S(x - ct)$ and $C = C(x - ct)$ of the system (1)-(2) under the conditions

$$S(-\infty, t) = 0, \quad C(-\infty, t) = C^*, \quad t > 0, \tag{4}$$

$$S(+\infty, t) = S^*, \quad C(+\infty, t) = 0, \quad t > 0, \tag{5}$$

where $S^* > 0$ is the solid concentration at the outlet and $C^* > 0$ is the gas concentration at the inlet. The positive wavespeed c will turn out to be completely determined by the parameters of the reaction-diffusion system.

Let us implement the following rescaling of (1)-(2):

$$\begin{cases} u = \frac{S^* - S}{S^*}, & v = \frac{C}{C^*}, \\ f(y) = \lambda_1 F(yS^*), & g(y) = G(yC^*), \\ h(y) = \frac{H(yC^*)}{C^*}, & \phi(y) = \frac{\Phi(yC^*)}{C^*}. \end{cases} \tag{6}$$

Then the system (1)-(2) reduces to the dimensionless equations

$$u_t = \frac{1}{S^*} f(1 - u)g(v), \tag{7}$$

$$(\varepsilon v)_t + (h(v))_x - (\phi(v))_{xx} = -\frac{\lambda}{C^*} f(1 - u)g(v), \tag{8}$$

where $\lambda = \lambda_2/\lambda_1$ is the Thiele modulus. The conditions (4)-(5) become

$$u(-\infty, t) = 1, \quad v(-\infty, t) = 1, \quad t > 0, \tag{9}$$

$$u(+\infty, t) = 0, \quad v(+\infty, t) = 0, \quad t > 0. \tag{10}$$

Let us now make the travelling wave Ansatz

$$u = u(\eta), \quad v = v(\eta), \quad \eta = x - ct. \tag{11}$$

Then the system (7)-(8) with conditions (9)-(10) is converted into the problem

$$-cu' = \frac{1}{S^*} f(1 - u)g(v), \tag{12}$$

$$-c(\varepsilon v)' + (h(v))' - (\phi(v))'' = -\frac{\lambda}{C^*} f(1 - u)g(v), \tag{13}$$

$$u(-\infty) = v(-\infty) = 1, \quad u(+\infty) = v(+\infty) = 0. \tag{14}$$

Eliminating the nonlinear terms in the right-hand sides of (12) and (13) and integrating with respect to η , we see that the expression

$$-c\varepsilon v + h(v) - (\phi(v))' - \frac{\lambda S^* c}{C^*} u \tag{15}$$

is constant, while all four terms have finite limits as $\eta \rightarrow \pm\infty$. Because $\phi(v)$ also has finite limits as $\eta \rightarrow \pm\infty$, we see that $(\phi(v))' \rightarrow 0$ as $\eta \rightarrow \pm\infty$. Using (3), (9) and (10) as well as the equality $f(0) = g(0) = h(0) = 0$ and the relation $(\phi(y))' \rightarrow 0$ as $y \rightarrow 0^+$ to take the limits as $\eta \rightarrow \pm\infty$, we find for the constant given by (15)

$$-c(\varepsilon_0 + \varepsilon_1^*) + h(1) - \frac{\lambda S^* c}{C^*} = 0,$$

where $\varepsilon_1^* = \varepsilon_1 S^*$, and hence the travelling wave speed is given by

$$c = \frac{h(1)C^*}{(\varepsilon_0 + \varepsilon_1^*)C^* + \lambda S^*}. \tag{16}$$

Finally, we employ (15) and (16) to write (12)-(13) in the form

$$u' = -C_1 f(1-u)g(v), \tag{17}$$

$$(\phi(v))' = C_2(v-u) + C_3(1-u)v + h(v) - h(1)v, \tag{18}$$

where $C_1 = 1/cS^*$, $C_2 = (\lambda S^*c)/C^*$, and $C_3 = c\varepsilon_1^*$ are positive constants. In the sequel we will restrict ourselves to the special case where

$$h(v) = H(v) = qv, \quad \phi(v) = D^*v^k, \tag{19}$$

where q is the constant gas flux and $D = D^*(C^*)^{1-k}$ is the constant effective diffusivity. In this special case (18) is replaced by

$$(v^k)' = C_4(v-u) + C_5(1-u)v, \tag{20}$$

where $C_4 = C_2/D^*$ and $C_5 = C_3/D^*$ are positive constants.

2. Travelling Wave Profiles. In this section we prove the existence and, under certain hypotheses, the uniqueness of a travelling wave profile. First we confine ourselves to the system (17) and (20). At the end of this section we list the assumptions of ϕ and g required to extend the result to the more general system (17)-(18).

Theorem 1. *There exists at least one solution (u, v) of (17)-(20) such that u and v are both decreasing in η . This solution is unique if $0 < k \leq 1$ and $w \mapsto g(w^{1/k})$ is Lipschitz continuous in $[0, \delta]$ for some $\delta > 0$.*

Proof. By the change of variable $\eta \mapsto -\eta$ one converts the system (17) and (20) with boundary conditions (14) into the following system:

$$u' = C_1 f(1-u)g(v), \tag{21}$$

$$(v^k)' = C_4(u-v) - C_5(1-u)v, \tag{22}$$

$$u(-\infty) = v(-\infty) = 0, \quad u(+\infty) = v(+\infty) = 1. \tag{23}$$

Let us consider (u, v) as points of the closed square $\{(u, v) : 0 \leq u \leq 1, 0 \leq v \leq 1\}$. Then the points (u, v) in the square for which the right-hand side of (22) vanishes, form a hyperbolic arc connecting $(0, 0)$ to $(1, 1)$. Now consider the open subregion \mathcal{D} bounded by the union of the sets

$$\partial S_1 = \{(u, 0) : 0 < u < 1\},$$

$$\partial S_2 = \{(1, v) : 0 < v < 1\},$$

$$\partial S_3 = \{(u, v) : 0 < u < 1 \text{ and } C_4(u-v) - C_5(1-u)v = 0\},$$

together with the points $(0, 0)$, $(1, 0)$ and $(1, 1)$. Then the right-hand sides of (21) and (22) are positive for all $(u, v) \in \mathcal{D}$.

Further, on $\partial S_1 \cup \partial S_2$, the right-hand side of (21) vanishes, while the right-hand side of (22) is positive. Finally, on ∂S_3 the right-hand side of (21) is positive, while the right-hand side of (22) vanishes. Further, the right-hand sides of (u, v) are Lipschitz continuous in (u, v) on $\mathcal{D} \cup \partial S_3$. As a result, solution curves of (21)-(23) which enter \mathcal{D} through $\partial S_1 \cup \partial S_3$ remain inside \mathcal{D} and proceed in the right-upper direction until they reach a point of ∂S_2 for $\eta = \bar{\eta} < +\infty$ (after which they proceed

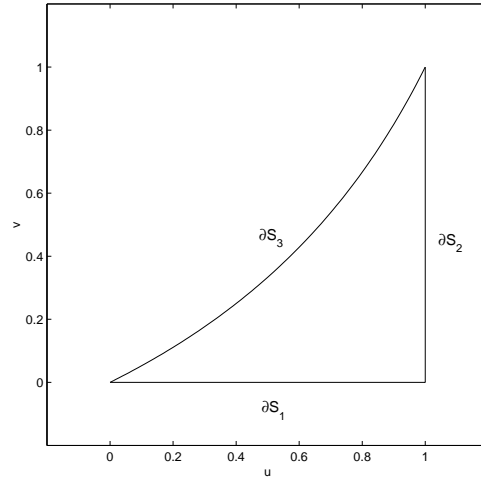


FIGURE 1. The parts ∂S_1 , ∂S_2 and ∂S_3 of the boundary of the open region \mathcal{D} in the (u, v) -plane for $C_4 = C_5 = 1$.

towards $(1, 1)$ along ∂S_2) or $(1, 1)$ for $\eta \leq +\infty$. Different solution curves cannot meet within $\mathcal{D} \cup \partial S_3$.

To prove the existence part of Theorem 1, it is sufficient to prove the existence of a unique C^1 -curve in $\mathcal{D} \cup \{(0, 0), (1, 1)\}$ which connects $(0, 0)$ and $(1, 1)$ and on which (21) and (22) hold. An elementary translation $\eta \mapsto \eta - \eta_0$ then converts one solution into another.

Let \mathcal{D}^* be the set of all points of \mathcal{D} that belong to a solution curve entering \mathcal{D} from a point of ∂S_3 . Similarly, let \mathcal{D}_* be the set of all points of \mathcal{D} that belong to a solution curve entering \mathcal{D} from a point of ∂S_1 . Then, obviously, \mathcal{D}^* and \mathcal{D}_* are open subsets of \mathcal{D} , while $(u_0, v^*) \in \mathcal{D}^*$ and $(u_0, v_*) \in \mathcal{D}_*$ imply that $0 < v_* < v^* < C_4 u / [C_4 + C_5(1 - u)]$. For every $u \in (0, 1)$ we now define

$$\alpha^*(u) = \inf\{v : (u, v) \in \mathcal{D}^*\}, \quad \alpha_*(u) = \sup\{v : (u, v) \in \mathcal{D}_*\}.$$

Then

$$0 < \alpha_*(u) \leq \alpha^*(u) < \frac{C_4 u}{C_4 + C_5(1 - u)},$$

so that

$$\lim_{u \downarrow 0} \alpha^*(u) = \lim_{u \downarrow 0} \alpha_*(u) = 0.$$

Moreover, $\alpha^*(1^-)$ and $\alpha_*(1^-)$ exist and $0 < \alpha_*(1^-) \leq \alpha^*(1^-) \leq 1$. We therefore put $\alpha^*(0) = \alpha_*(0) = 0$ and extend α^* and α_* to functions that are continuous on $[0, 1]$ and C^1 on $(0, 1)$; this one easily obtains by proving that α^* and α_* are solution curves.

To settle the uniqueness part of Theorem 1, it suffices to exploit the Lipschitzianity of the map

$$(u, w) \mapsto \left(C_1 f(1 - u)g(w^{1/k}), C_4(u - w^{1/k}) - C_5(1 - u)w^{1/k} \right)$$

in a neighborhood of $(0, 0)$. This is obviously the case if $(1/k) \geq 1$ and g is Lipschitz continuous in $[0, \delta]$ for some $\delta > 0$. □

If $k = 1$, it is impossible to reach the point $(1, 1)$ in finite time¹ along solution curves. Indeed, let us assume the existence of a solution curve $\eta \mapsto (u(\eta), v(\eta))$ such that $v(\bar{\eta}) = 1$. Then (22) with $k = 1$ can be written in the form

$$\left(e^{(C_4+C_5)\eta} v(\eta) \right)' = e^{(C_4+C_5)\eta} [C_4 + C_5 v] u,$$

and hence

$$\begin{aligned} e^{(C_4+C_5)\bar{\eta}} - v(0) &= \int_0^{\bar{\eta}} e^{(C_4+C_5)\eta} [C_4 + C_5 v(\eta)] u(\eta) d\eta \\ &< \int_0^{\bar{\eta}} e^{(C_4+C_5)\eta} [C_4 + C_5] d\eta = e^{(C_4+C_5)\bar{\eta}} - 1, \end{aligned}$$

which implies that $v(0) > 1$ and hence leads to a contradiction. Unfortunately, we do not know if the same statement holds for $k \neq 1$.

Theorem 1 is easily generalized to the more general system (17)-(18). Letting ϕ be a monotonically strictly increasing function mapping $(0, \infty)$ onto itself whose inverse function ϕ^{-1} is Lipschitz continuous on each compact subset of $(0, \infty)$, we put $w = \phi(v)$. Changing the variable $\eta \mapsto -\eta$, (17)-(18) then take the form

$$u' = C_1 f(1 - u)g(\phi^{-1}(w)), \tag{24}$$

$$w' = C_2(\phi^{-1}(w) - u) - C_3(1 - u)\phi^{-1}(w) - h(\phi^{-1}(w)) + h(1)\phi^{-1}(w). \tag{25}$$

If we also assume h to be a monotonically strictly increasing function mapping $(0, \infty)$ onto itself such that $0 < h(v) \leq h(1)v$ for every $v \in (0, 1]$, we can repeat the proof of Theorem 1 almost verbatim and derive the following result.

Theorem 2. *There exists at least one solution (u, v) of (24)-(25), with $v = \phi^{-1}(w)$, such that u and v are both decreasing in η . This solution is unique if ϕ^{-1} and $w \mapsto g(\phi^{-1}(w))$ are both Lipschitz continuous in $[0, \delta]$ for some $\delta > 0$.*

3. Conversion and Penetration Fronts. In this final section we restriction ourselves to the system consisting of (17) and (20).

A travelling wave $u = u(x - ct)$ is said to have a *conversion front* if

$$a := \inf\{\eta : u(\eta) < 1\} > -\infty \tag{26}$$

and to have a *penetration front* if

$$b := \sup\{\eta : u(\eta) > 0\} < +\infty. \tag{27}$$

Defining

$$\tilde{b} := \sup\{\eta : v(\eta) > 0\}, \tag{28}$$

we easily show (as in [4]) that b and \tilde{b} coincide.

The following result can be proved in the same way as in [4].

Theorem 3. *There is a conversion front if and only if $(1/f) \in L^1(0, \delta)$ for some $\delta > 0$.*

Proof. Suppose a conversion front exists and hence (26) holds. From (17) we obtain

$$u' = -C_1 f(1 - u)g(v) \geq -C_1 f(1 - u)g(1),$$

¹Here we adopt the change of variable $\eta \mapsto -\eta$ made in the proof of Theorem 1.

and hence for any $a < \eta_1 < \eta_2$ we get

$$\int_{1-u(\eta_1)}^{1-u(\eta_2)} \frac{1}{f(z)} dz = \int_{\eta_1}^{\eta_2} \frac{-u'}{f(1-u)} d\eta \leq C_1 g(1)(\eta_2 - \eta_1).$$

Letting $\eta_1 \downarrow a$ yields

$$\int_0^{1-u(\eta_2)} \frac{1}{f(z)} dz \leq C_1 g(1)(\eta_2 - a) < +\infty,$$

thus implying that $(1/f) \in L^1(0, \delta)$ for some $\delta > 0$.

On the other hand, if no conversion front exists and therefore $u(\eta) < 1$ for all $\eta \in \mathbb{R}$, we have

$$\int_{1-u(\eta_1)}^{1-u(\eta_2)} \frac{1}{f(z)} dz = \int_{\eta_1}^{\eta_2} \frac{-u'}{f(1-u)} d\eta \geq C_1 g(v(\eta_2))(\eta_2 - \eta_1),$$

where $g(v(\eta_2)) > 0$. Thus $(1/f) \notin L^1(0, \delta)$ for all $\delta > 0$. □

Theorem 4. *Let $G_k(v) = \int_0^v \hat{v}^{k-1} g(\hat{v}) d\hat{v}$. Then the following is true:*

1. *If there is a penetration front, then $v^{k-1}/\sqrt{G_k(v)}$ belongs to $L^1(0, \delta)$ for some $\delta > 0$.*
2. *If $k = 1$ and g is a concave function on $(0, \delta)$ for some $\delta > 0$ such that $(v/g(v)) \rightarrow 0$ as $v \downarrow 0$, there exists a penetration front if and only if $G_1(v)^{-1/2}$ belongs to $L^1(0, \delta)$.*
3. *If $0 < k < 1$ and g is a concave function on $(0, \delta)$ for some $\delta > 0$, there exists a penetration front if and only if $v^{k-1}G_k(v)^{-1/2}$ belongs to $L^1(0, \delta)$.*

Proof. Using that $v' \leq 0$ we obtain from (17) and (20)

$$\begin{aligned} \frac{d}{d\eta} [(v^k)']^2 &\geq 2kv^{k-1}v' \cdot C_1[C_4 + C_5v]f(1-u)g(v) \\ &\geq 2kv^{k-1}v' \cdot C_1C_6f(1-u)g(v) \geq 2kC_1C_6f(1)v^{k-1}v'g(v), \end{aligned} \tag{29}$$

where $C_6 = C_4 + C_5$, so that

$$[(v^k)']^2 \leq 2kC_1C_6f(1) \int_0^v \hat{v}^{k-1}g(\hat{v}) d\hat{v}.$$

Therefore,

$$v' \geq -\sqrt{\frac{2C_1C_6f(1)}{k}} v^{1-k} \sqrt{G_k(v)}, \tag{30}$$

where $G_k(v) = \int_0^v \hat{v}^{k-1}g(\hat{v}) d\hat{v}$.

Suppose there is a penetration front. Then (30) implies that

$$\int_{v(\eta_2)}^{v(\eta_1)} \frac{v^{k-1}}{\sqrt{G_k(v)}} dv = \int_{\eta_1}^{\eta_2} \frac{-v^{k-1}v'}{\sqrt{G_k(v)}} d\eta \leq \sqrt{\frac{2C_1C_6f(1)}{k}} (\eta_2 - \eta_1).$$

Letting $\eta_2 \uparrow b$ and using (28) with $\tilde{b} = b$, we get

$$\int_0^{v(\eta_1)} \frac{v^{k-1}}{\sqrt{G_k(v)}} dv \leq \sqrt{\frac{2C_1C_6f(1)}{k}} (b - \eta_1) < +\infty,$$

which proves that $((\cdot)^{k-1}/\sqrt{G_k(\cdot)}) \in L^1(0, \delta)$ for some $\delta > 0$ if there is a penetration front.

To prove the second and third parts of Theorem 4, we substitute (30) in the first line of (29) to get

$$\begin{aligned} \frac{d}{d\eta} [(v^k)']^2 &= 2kv^{k-1}v' [C_4v' + C_1(C_4 + C_5v)f(1-u)g(v) + C_5(1-u)v'] \\ &\leq 2kC_6v^{k-1}v' \left[-\sqrt{\frac{2C_1C_6f(1)}{k}} v^{1-k} \sqrt{G_k(v)} + C_1f(1-u)g(v) \right]. \end{aligned}$$

Now choose $\bar{f} \in (0, f(1))$ and fix η_1 such that $f(1-u(\eta)) > \bar{f}$ for $\eta > \eta_1$. Then we can improve the above inequality to obtain for $\eta > \eta_1$

$$\frac{d}{d\eta} [(v^k)']^2 \leq 2kC_6v^{k-1}v' \left[-\sqrt{\frac{2C_1C_6f(1)}{k}} v^{1-k} \sqrt{G_k(v)} + C_1\bar{f}g(v) \right].$$

Integrating from η_1 to $+\infty$ we find

$$\begin{aligned} [(v^k)']^2(\eta_1) &\geq C_6 \left[2\sqrt{2kC_1C_6f(1)} \int_{\eta_1}^{\infty} \sqrt{G_k(v)}v' d\eta \right. \\ &\quad \left. - 2kC_1\bar{f} \int_{\eta_1}^{\infty} v^{k-1}g(v)v' d\eta \right] \end{aligned}$$

and hence

$$[(v^k)']^2(\eta_1) \geq C_6 \left[-2\sqrt{2kC_1C_6f(1)} \int_0^{v_1} \sqrt{G_k(v)}dv + 2kC_1\bar{f} \int_0^{v_1} v^{k-1}g(v)dv \right], \tag{31}$$

where $v_1 = v(\eta_1)$.

Let us now assume g to be concave in $(0, \delta)$, where $\delta \in (0, 1)$, and let us choose η_2 such that $v(\eta_2) = \delta$. We then have

$$0 \leq v(\eta) \leq \frac{\delta}{g(\delta)} g(v(\eta)), \quad \eta \geq \eta_2,$$

and hence

$$G_k(v) = \int_0^v \hat{v}^{k-1}g(\hat{v}) d\hat{v} \leq v^k g(v) \leq \left(\frac{\delta}{g(\delta)}\right)^k g(v)^{k+1}, \quad \eta \geq \eta_2. \tag{32}$$

Using (31) and (32), we now obtain for $\eta \geq \bar{\eta} = \max(\eta_1, \eta_2)$

$$\begin{aligned} [(v^k)']^2(\eta_1) &\geq C_6 \left[-2\sqrt{2kC_1C_6f(1)} \left(\frac{\delta}{g(\delta)}\right)^{k/2} \int_0^{v_1} g(v)^{\frac{k+1}{2}} dv \right. \\ &\quad \left. + 2kC_1\bar{f}G_k(v_1) \right]. \end{aligned} \tag{33}$$

For $k = 1$ we get from (33)

$$[v']^2(\eta_1) \geq C_6 \left[-2\sqrt{2C_1C_6f(1)} \left(\frac{\delta}{g(\delta)}\right)^{1/2} + 2C_1\bar{f} \right] G_1(v_1).$$

Then, if $(v/g(v)) \rightarrow 0$ as $v \downarrow 0$, we get

$$v' \leq -\text{const.} \sqrt{G_1(v)}$$

for small enough positive v . The divergence of the integral $\int_0^v G_1(\hat{v})^{-1/2} d\hat{v}$ then implies the nonexistence of a penetration front, as claimed.

For $0 < k < 1$ we see that $g(v)^{\frac{k+1}{2}} = o(v^{k-1}g(v))$ as $v \downarrow 0$, if and only if $v^2 = o(g(v))$ as $v \downarrow 0$. In this case the first term in the right-hand side of (33) can

be neglected with respect to the second term, especially since $(\delta/g(\delta)) \geq 1$ as a result of the concavity of g . Thus there exists a positive constant C_7 such that

$$(v^k)'(\eta) \leq -C_7\sqrt{G_k(v)}$$

for v_1 small enough. If we integrate with respect to $\eta \in (\eta_1, \eta_2)$ and put $v_i = v(\eta_i)$ ($i = 1, 2$), then

$$\int_{v_2}^{v_1} \frac{v^{k-1}}{\sqrt{G_k(v)}} dv \geq \frac{C_7}{k}(\eta_2 - \eta_1).$$

Hence, if there is no penetration front and hence $\eta_2 \rightarrow +\infty$ corresponds to $v_2 \downarrow 0$, we obviously get

$$\int_0^{v_1} \frac{v^{k-1}}{\sqrt{G_k(v)}} dv = +\infty,$$

whence $v^{k-1}/\sqrt{G_k(v)}$ does not belong to $L^1(0, \delta)$ for any $\delta > 0$. □

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