Dynamic multiscaling of the reaction-diffusion front for $mA + nB \to 0$

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We consider the reaction zone that grows between separated regions of diffusing species A and B that react according to $mA+nB \to 0$, within the framework of the mean-field-like reaction-diffusion equations. For distances from the center of the reaction zone much smaller than the diffusion length $X_D \equiv \sqrt{Dt}$, the particle density profiles are described by the scaling forms predicted by a quasistatic approximation, whereas they have a diffusive cutoff at a distance of order X_D. This cutoff, and the power-law decay of the quasistatic profiles, give rise to multiscaling behavior, with anomalous values for the exponents describing the moments of the density and reaction profiles. Numerical solutions of the reaction-diffusion equations are in good quantitative agreement with the predictions of this theory.

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I. INTRODUCTION

The problem of a front that grows between initially separate regions of diffusing species A and B that react according to $mA + nB \to 0$ has provoked much recent interest [1–9]. Studies have concentrated on the scaling properties of the reaction rate R per unit volume and particle density profiles a and b, and on the critical dimension above which the mean-field-like reaction-diffusion rate equations are valid. The reaction is concentrated in the region where the densities of the two species are comparable. If the penetration of one species into the other is much shallower than the diffusion length $X_D \equiv \sqrt{Dt}$, the reaction between the two species takes place within a distance $w \ll X_D$ of center x_f of the reaction zone.

Most of the previous studies were devoted to the study of the properties of the reaction front for distances $|x - x_f| \ll X_D$. In this regime the physics is governed by a single length scale w and consequently a simple scaling theory explains the observed behavior. However, if one investigates what is happening for $|x - x_f| \geq X_D$, two length scales w and X_D enter in the description. In this paper, we shall formulate a scaling theory for this system that is valid for all length scales. We shall see that, although the particle densities converge everywhere to the values predicted by the single-length scaling theory, the effects of the second length scale can be seen when measuring the spatial moments.

There are two different, although related, theoretical approaches to the scaling theory. In the first approach, one assumes a scaling ansatz for the differential equations for the densities of the two species. In geometries where the only spatial variation of the densities is along the x axis, these equations take the form [1,5]

$$\partial_t a = D\partial_x^2 a - mka^m b^n, \tag{1}$$

$$\partial_t b = D\partial_x^2 b - nka^m b^n, \tag{2}$$

where k is the reaction constant, and here and subsequently the reagents are assumed to have the same diffusion constant D. The initial conditions appropriate to this problem are

$$a(x,0) = a_0\theta(x), \tag{3}$$

$$b(x,0) = b_0\theta(-x), \tag{4}$$

where a_0 and b_0 are constants and θ is the heavyside function. The quantity $u \equiv (a/m - b/n)$ obeys a simple diffusion equation, with solution [5]

$$u = \frac{1}{2}\left(\frac{a_0}{m} - \frac{b_0}{n}\right) - \frac{1}{2}\left(\frac{a_0}{m} + \frac{b_0}{n}\right)\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right). \tag{5}$$

The center x_f of the reaction zone may be defined as the point where $u = 0$. We therefore have

$$x_f = 2(Dt)^{1/2}\mathrm{erf}^{-1}\left[\frac{(a_0/m - b_0/n)}{(a_0/m + b_0/n)}\right], \tag{6}$$

so if $a_0/m = b_0/n$ we have $x_f = 0$ (note that in Ref. [5], x_f was defined as the point of maximal reaction, which is not necessarily the same point).

One expects that, for $|x - x_f| \ll (Dt)^{1/2}$, the profiles will be described by the single length scale w, leading to the following scaling hypothesis [1,5]:

$$a(x,t) = t^{-\gamma}A\left(\frac{x - x_f}{t^\alpha}\right), \tag{7}$$

$$b(x,t) = t^{-\gamma}B\left(\frac{x - x_f}{t^\alpha}\right), \tag{8}$$

$$R(x,t) = t^{-\beta}\phi\left(\frac{x - x_f}{t^\alpha}\right), \tag{9}$$

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where $w \sim t^{\alpha}$, $\phi = A^m B^n$, and $\beta = (m+n)\gamma$. The number of particles of either species arriving at the reaction front is $\propto t^{-1/2}$, which must equal the total reaction rate, so we must have $\beta - \alpha = 1/2$. Consistency of this scaling ansatz with the equations of motion leads to $\alpha = (1/2)(m+n-1)/(m+n+1)$ [5].

The second approach relies on the fact that in the above description, the reaction front is formed quasistatically. Indeed, when $|x - x_f| \gg w$ one of the species is overwhelmingly in the majority, so $|u| \to \max(a/m, b/n)$, and so from Eq. (5) the profile of the majority particle density is $\sim |x - x_f|/t^{1/2}$ for $(Dt)^{1/2} \gg x \gg w$. The diffusion current of particles arriving at x_f is therefore $J \sim t^{-1/2}$, and the characteristic time scale on which this current changes is $(d \ln J/dt)^{-1} \propto t$. The equilibration time of the front is of order Dw^2, so since $\alpha < 1/2$ one would expect that the reaction zone has enough time to reach the steady-state profile it would have if the current J were constant. Thus one can consider the case of a front formed by opposing constant diffusion currents $J_A = mJ$ and $J_B = -nJ$ of A and B particles imposed at $x = -\infty$ and $+\infty$, respectively, which has recently been studied [10–12]. In this case, the system approaches a steady state where the equations

$$(D/m)\partial_x^2 a = k a^m b^n = (D/n)\partial_x^2 b \tag{10}$$

and boundary conditions may be written in dimensionless form, so that the following scaling ansatz is valid for all x [11]:

$$R(x) = \frac{J}{w}\phi_{\rm SS}\left(\frac{x}{w}\right), \tag{11}$$

$$a(x) = JwA_{\rm SS}\left(\frac{x}{w}\right), \tag{12}$$

$$b(x) = JwB_{\rm SS}\left(\frac{x}{w}\right), \tag{13}$$

where $w(J, D, k) \propto J^{-\nu}$ and $\nu = (m+n-1)/(m+n+1)$. From (10), we have $\partial_x^2 u = 0$ [$u \equiv (a/m - b/n)$], whose solution with these boundary conditions is $u = -Jx/D$. For $(x/w) \gg 1$, the B particles are overwhelmingly in the majority, so one has $b = nJx/D + na/m \approx nJx/D$, and hence $A''_{\rm SS}(y) \sim (A_{\rm SS})^m y^n$, leading to

$$A_{\rm SS}(y) \sim \begin{cases} y^{-n/4}\exp(-\sigma y^{1+(n/2)}) & \text{for } m = 1, \\ y^{-(n+2)/(m-1)} & \text{for } m > 1, \end{cases} \tag{14}$$

as $y \to \infty$, where σ is a constant. Similar results hold for $B_{\rm SS}$ by interchanging m and n. Equations (7)–(9) are recovered by simply substituting $J \propto t^{1/2}$ in Eqs. (11)–(13). Within this approach, it is also possible to show [11] that the "mean-field" assumption $R = ka^m b^n$ (assumed in all the above equations) is valid for microscopic stochastic systems in spatial dimension $d > d_c \equiv 2/(m+n-1)$.

For $m = n = 1$ the scaling forms (7)–(9) have been proved rigorously to describe the asymptotic behavior as $t \to \infty$ of the reaction-diffusion equations (1) and (2) [7]. Experiments on real systems, and simulations of microscopic stochastic models, also appear to verify the scaling theory and exponents in dimension $d \geq 2$ [2–4]. For $d = 1$, there has been some controversy as to whether the scaling theory is valid [5,8], but the most recent results [9] appear to show that the steady-state results do indeed apply. However, for $(m, n) \neq (1, 1)$, where rigorous mathematical results are not available, the case is much less clear. Numerical simulations of microscopic stochastic models in $d = 1$ are consistent with a scaling ansatz [6], but they are of low precision, since reaction events are much rarer than for $m = n = 1$.

In this paper, we shall give careful arguments to show that the scaling ansatz is indeed valid for length scales much smaller than $\sim (Dt)^{1/2}$. We shall then show than the two length scales in the problem, w and $(Dt)^{1/2}$, together with the power-law tails of the steady-state profile, give rise to a multiscaling form for the particle density profile, whose moments are described by a spectrum of exponents between α and $1/2$. We then present numerical solutions of the reaction-diffusion equations, and show that the results are in good agreement with the theoretical predictions.

II. VALIDITY OF THE SCALING ANSATZ

The scaling ansatz can be shown to be exact for the case of a steady-state front formed between balancing opposing currents, and so its applicability to the time-dependent case relies on the front being formed quasistatically [11]. Naively, one would expect that the time for a diffusive system to equilibrate within a region of size $\sim t^{\nu}$ would be $\propto t^{2\nu}$, whereas the time scale upon which the current $J \propto t^{-1/2}$ changes is $(d \ln J/dt)^{-1} \propto t$, which predicts that quasistatic approximation would be valid for length scales with $\nu < 1/2$. However, since some of the density profiles decay algebraically, one might wonder whether the flow of particles towards $|x| \to \infty$ necessary to sustain these steady-state profiles might be too great for the quasistatic approximation to be valid.

In this section, we shall show that the quasistatic approximation is internally consistent for length scales smaller than $t^{1/2}$, in that it predicts that (i) the number of particles up to a distance $\sim t^{1/2}$ is always much less than the total particles that have reacted, so that the number of particles in the tails is never too much to have a feedback effect on the profiles at distances of order $t^{1/2}$; (ii) the time taken for each part of the particle density tail to equilibrate at its quasistatic value is always much less that the characteristic time scale on which this value changes.

Consider the part of the tail of the A-particle profile $a(x,t) \sim t^{-\gamma}(x/t^{\alpha})^{-\lambda}$, where $\lambda = [n+2]/[m-1]$ [see Eq. (14)], in the region $x_1 < x < x_2$, with $x_1 \propto t^{\epsilon_1}$ and $x_2 \propto t^{\epsilon_2}$ ($\alpha < \epsilon_1 < \epsilon_2 < 1/2$). The current of A particles at x is

$$J_A = -D\partial_x a \sim \frac{a(x,t)}{x}, \tag{15}$$

so the ratio $J_A(x_2)/J_A(x_1) = t^{-(\epsilon_2 - \epsilon_1)(1+\lambda)} \to 0$ as $t \to \infty$. Almost all of the particles that enter at x_1 are therefore removed by the reaction, rather than by dif-

fusing out at x_2. The number of particles in the region is

$$N_A \equiv \int_{x_1}^{x_2} a\,dx \sim \begin{cases} a(x_1)x_1 & \text{for } \lambda > 1 \\ t^{\alpha-\gamma}\ln\left(\frac{x_2}{x_1}\right) & \text{for } \lambda = 1 \\ a(x_2)x_2 & \text{for } \lambda < 1. \end{cases} \quad (16)$$

The number of particles in the tail can diverge for certain values of λ. This could invalidate the assumption that the total reaction rate equals the number of particles arriving at the origin if this number was found to be larger than the total number of particles $\propto t^{1/2}$ that have reacted. However, the total number of particles in the tail up to a length scale $t^{1/2}$, found by substituting $\epsilon_2 = 1/2$, is found in each of the above cases to be of order less than $t^{1/2}$. The time taken for N_A particles to enter the region $x_1 < x < x_2$ is

$$N_A/J_A(x_1) \sim \begin{cases} t^{2\epsilon_1} & \text{for } \lambda > 1 \\ t^{2\epsilon_1}\ln t & \text{for } \lambda = 1 \\ t^{\epsilon_1+\epsilon_2-(\epsilon_2-\epsilon_1)(1-\lambda)} & \text{for } \lambda < 1, \end{cases} \quad (17)$$

which is always $\ll t$ since $\epsilon_1 < \epsilon_2 < 1/2$. The front therefore has enough time to reach its steady-state value for length scales smaller than $t^{1/2}$.

III. MULTISCALING THEORY

The arguments of the preceding section show that the scaling ansatz (7)–(9) should be consistent for all length scales $\sim t^{\epsilon}$, with $\epsilon < 1/2$. However, the quasistatic approximation, and hence the scaling forms (7)–(9), cannot be valid on length scales of order the diffusion length. To see this, consider the solutions to Eqs. (1) and (2) in the case where no reaction is permitted ($k = 0$). In this case, the solutions for a and b are error functions, and so the tails of the densities have an exponential decay of characteristic length $(Dt)^{1/2}$. If we consider the case of finite k, it is clear that the particles cannot penetrate further than when there is no reaction, and so the densities in the tails must be smaller than for $k = 0$. The algebraic decay of the tails of the steady-state profiles must therefore be superseded by an exponential cutoff at a length scale of order $(Dt)^{1/2}$, which represents the fact that on such length scales the particle densities are limited by diffusion. The shape of this cutoff is in fact irrelevant to the following discussion—all that is required is that all spatial moments are defined, which is guaranteed by the fact that the profiles all have an exponential upper bound.

We therefore propose the following ansatz for a and b in the limit $t \to \infty$:

$$a(x,t) = a_{\rm SS}(x,t)G_A\left(\frac{x}{t^{1/2}}\right), \quad (18)$$

$$b(x,t) = b_{\rm SS}(x,t)G_B\left(\frac{x}{t^{1/2}}\right), \quad (19)$$

where $a_{\rm SS} = t^{-\gamma}A_{\rm SS}(x/t^{\alpha})$ and $b_{\rm SS} = t^{-\gamma}B_{\rm SS}(x/t^{\alpha})$ are the solutions to the steady-state equations (12) and (13), and $G_A(y)$ and $G_B(-y)$ are functions that provide a cutoff at $y = O(1)$, and ensure that $a(x,t)$ and $b(x,t)$ satisfy (5) away from the reaction zone. All positive moments of the tail of $G_A(y)$ and $G_B(-y)$ for $y > 0$ are defined, and there is no power-law behavior for $y \to 0$.

This form leads to multiscaling behavior for the moments of the particle profiles, by virtue of the power-law tails of a and/or b when $(m,n) \neq (1,1)$. Consider a function F of the form $F(x,t) = t^{-\delta}\phi(x/t^{\alpha})G(x/t^{1/2})$, where $\phi(y) \to y^{-\mu}$ as $y \to \infty$, $\phi \to 1$ as $y \to 0$, $G(y) \to 1$ as $y \to 0$, and all positive moments of G are defined. Then the qth moment of F is of the form

$$\int_0^{\infty} x^q F(x,t)\,dx = \int_0^{\infty} x^q t^{-\delta}\phi\left(\frac{x}{t^{\alpha}}\right) G\left(\frac{x}{t^{1/2}}\right) dx \sim \begin{cases} t^{\alpha(q+1)-\delta} & \text{for } \mu > q+1 \\ t^{\alpha(q+1)-\delta}\ln t & \text{for } \mu = q+1 \\ t^{\alpha\mu-\delta+\frac{1}{2}(q-\mu+1)} & \text{for } \mu < q+1. \end{cases}$$

When $\mu > q+1$, the qth moment of ϕ is finite, whereas, for $\mu < q+1$, the dominant contribution comes from $(x/t^{1/2}) = O(1)$. Defining $X^{(q)} \equiv [\int x^q F\,dx/\int F\,dx]^{1/q}$, we find that, for $\mu \leq 1$, $X^{(q)} \sim t^{1/2}$ (with logarithmic corrections for $\mu = 1$). For $\mu > 1$, we find the multiscaling behavior $X^{(q)} \sim t^{\zeta_q}$, where

$$\zeta_q = \begin{cases} \alpha & \text{for } q < \mu - 1 \\ \frac{1}{2} - \frac{1}{q}\left(\frac{1}{2} - \alpha\right)(\mu - 1) & \text{for } q > \mu - 1, \end{cases} \quad (20)$$

and $X^{(q)} \sim t^{\alpha}\ln^{1/(\mu-1)} t$ when $q = \mu - 1$. Notice that ζ_q increases monotonically as a function of q from α to $1/2$.

By substituting from (14) the appropriate power-law tails of $A_{\rm SS}$ and $B_{\rm SS}$, the multiscaling forms predict the following behavior for the following quantities (without loss of generality, we have assumed $m \geq n$):

$$w^2 \equiv \frac{\int_{-\infty}^{\infty} x^2 R(x,t)dx}{\int_{-\infty}^{\infty} R(x,t)dx} \sim \begin{cases} t^{2\alpha} & \text{for } m-n < 3 \\ t^{2\alpha}\ln t & \text{for } m-n = 3 \\ t^{1-\left(\frac{1}{2}-\alpha\right)(\nu-1)} & \text{for } m-n > 3, \end{cases} \quad (21)$$

$$w_a^2 \equiv \frac{\int_{-\infty}^{x_f} x^2 a(x,t)dx}{\int_{-\infty}^{x_f} a(x,t)dx} \sim \begin{cases} t^{2\alpha} & \text{for } 3m-n < 5 \\ t^{2\alpha}\ln t & \text{for } 3m-n = 5 \\ t^{1-\left(\frac{1}{2}-\alpha\right)(\lambda-1)} & \text{for } 3m > n+5 > m+2 \\ \frac{t}{\ln t} & \text{for } m-n = 3 \\ t & \text{for } m-n > 3, \end{cases} \quad (22)$$

$$w_b^2 \equiv \frac{\int_{x_f}^{\infty} x^2 b(x,t)dx}{\int_{x_f}^{\infty} b(x,t)dx} \sim \begin{cases} t^{2\alpha} & \text{for } m+5 > 3n \\ t^{2\alpha}\ln t & \text{for } m+5 = 3n \\ t^{1-\left(\frac{1}{2}-\alpha\right)(\kappa-1)} & \text{for } m+5 < 3n, \end{cases} \quad (23)$$

where $\lambda = (n+2)/(m-1)$, $\nu = 2+\lambda$, and $\kappa = (m+2)/(n-1)$. If these quantities were described by a one-length scaling theory, all of these quantities would behave

as $\sim t^{2\alpha}$, so we describe departure from this behavior as "anomalous."

Defining

$$x_c \equiv \frac{\int_{-\infty}^{\infty} xR(x,t)dx}{\int_{-\infty}^{\infty} R(x,t)dx}, \tag{24}$$

a similar procedure may be used to find the scaling behavior for x_c. Notice, however, that the contribution to x_c coming from the scaling term is identically zero, since $mR_{SS} = D\partial_x^2 a$ implies $\int_{-\infty}^{\infty} xR_{SS}\,dx = 0$. The behavior of x_c is therefore determined wholly by the corrections to scaling. From (1) and (2), one has

$$\int_{-\infty}^{\infty} xR\,dx = \int_{-\infty}^{0} \frac{D}{m} x\partial_x^2 a\,dx + \int_{0}^{\infty} \frac{D}{n} x\partial_x^2 b\,dx - \int_{-\infty}^{0} x\partial_t a\,dx - \int_{0}^{\infty} x\partial_t b\,dx. \tag{25}$$

The first two terms may be integrated by parts, yielding $D[a(0,t)/m - b(0,t)/n]$, which is zero by virtue of (5) for the initial conditions $u(0,0) = 0$. The final two terms are of opposite sign, and cancel identically for $m = n$ by symmetry. For $m \neq n$, they typically have different scaling behaviors, and so the scaling behavior is determined by the largest term. Substituting the forms (18) and (19) for a and b, and differentiating, one finds the following scaling behavior for x_c:

$$x_c \sim \begin{cases} t^{3\alpha-1} & \text{for } 2m-n<4 \\ t^{\frac{1}{2}-\frac{1}{m-1}} \ln t & \text{for } 2m-n=4 \\ t^{\alpha-(\frac{1}{2}-\alpha)\lambda} & \text{for } 2m-n>4. \end{cases} \tag{26}$$

IV. NUMERICAL SIMULATIONS

In order to verify the scaling ansatz (7)–(9), we have solved the reaction-diffusion equations (1) and (2) numerically. We approximated (1) and (2) with a finite-difference method, with Δt, Δx satisfying $k\Delta t = 0.01$, $D\Delta t/(\Delta x)^2 = 0.04$, and a lattice of $N = 12\,001$ sites, which was sufficient for finite-size effects to be unimportant. Henceforth we will choose the reference system in which $\Delta x = \Delta t = 1$, so that our numerical results will correspond to the case $k = 0.01$ and $D = 0.04$. The initial condition satisfied $a_0/m = b_0/n$, so that $x_f = 0$ from (6). The reaction rate R thus obtained for times $t = 10^3$–10^7 and $n = 1$, $2 \leq m \leq 4$ are presented in Figs. 1–3, rescaled by $t^{\alpha+\frac{1}{2}}$ and plotted as a function of x/t^α. The solid curve in each figure is a numerical solution of the steady-state equation (10), for the same values of D and k, and using the time-dependent current as a boundary condition. We see that the data appear to converge to the solid line as $t \to \infty$, so that the scaling ansatz (7)–(9) is valid in the sense that

$$t^{\alpha+\frac{1}{2}} R(x,t) \to F(x/t^\alpha) \qquad \text{as } t \to \infty, \tag{27}$$

where $F(x/t^\alpha)$ is a function of x/t^α. Notice that the convergence appears to be slower for larger values of m.

Another interesting feature of Figs. 1–3 is that the point at which R reaches its maximal value differs from 0. As the x axes of these figures have been rescaled by

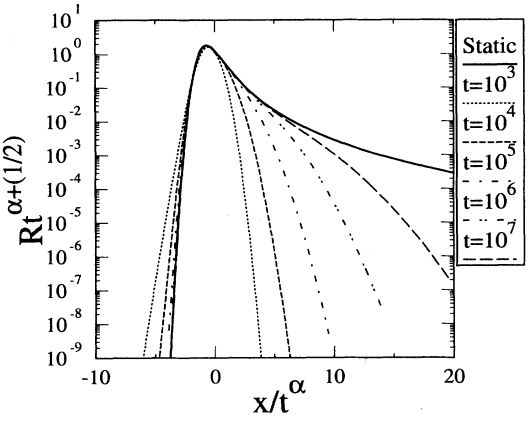

FIG. 2. Rt^β vs x/t^α for $n = 1$ and $m = 3$ and $t = 10^3, 10^4, \ldots, 10^7$.

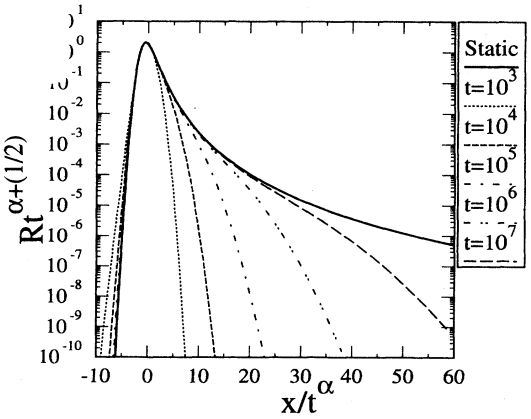

FIG. 1. Rt^β vs x/t^α for $n = 1$ and $m = 2$ and $t = 10^3, 10^4, \ldots, 10^7$.

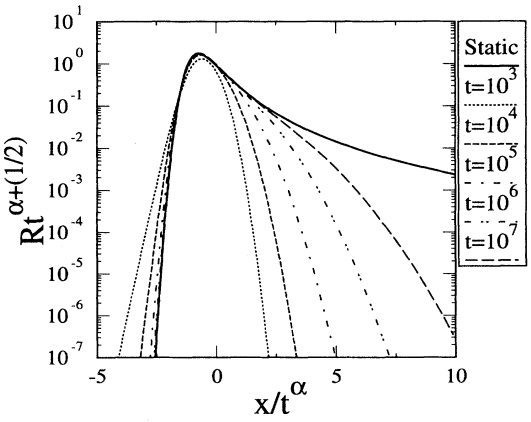

FIG. 3. Rt^β vs x/t^α for $n = 1$ and $m = 4$ and $t = 10^3, 10^4, \ldots, 10^7$.

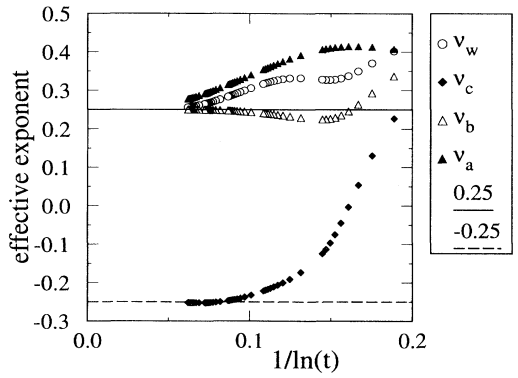

FIG. 4. Effective exponents for $(m,n) = (2,1)$. The horizontal lines represent the theoretical asymptotic values from Table I.

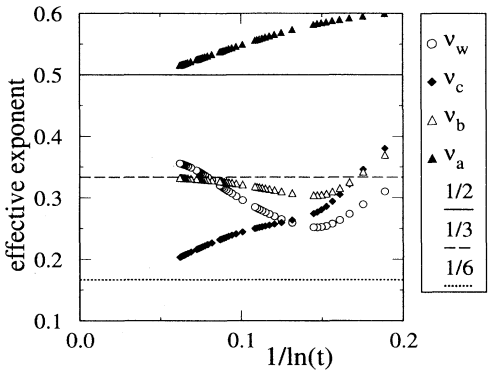

FIG. 6. Effective exponents for $(m,n) = (4,1)$. The horizontal lines represent the theoretical asymptotic values from Table I.

a factor t^α, the location of this point changes with time like t^α. This shows that the definition of x_f as the point of maximal reaction is not equivalent to the definition in this paper as the point where $u = 0$.

To verify the multiscaling properties of the reaction zone, we investigated the behavior of the functions w, w_a, w_b, and x_c. According to (21)–(24), they should diverge as $t^\nu \ln^\kappa(t)$, with ν and κ being some exponents dependent on m and n. In Figs. 4–6 we have plotted effective values of ν_w, ν_a, ν_b, and ν_c (corresponding to the behavior of the properties w, w_a, w_b, and x_c, respectively), defined as successive gradients from a log-log plot, as a function of $1/\ln(t)$. The quantities were first normalized by the logarithmic prefactor $\ln^{-\kappa}(t)$ so as to give quicker convergence to the theoretical values of ν. It can be seen that ν_a and ν_b converge satisfactorily to the theoretical values, even though the values for ν_a are anomalous. The convergence for ν_c is slower, but the data are consistent with the theoretical predictions. The convergence for ν_w is also slow, and in fact the trend for $m = 4$ is in the wrong direction; however, it is plausible that the trend may change at later times, as is seen for $m = 3$ in Fig. 5. The values of the effective exponents at the last value of time (10^7) are compared with the theoretical values in Table I.

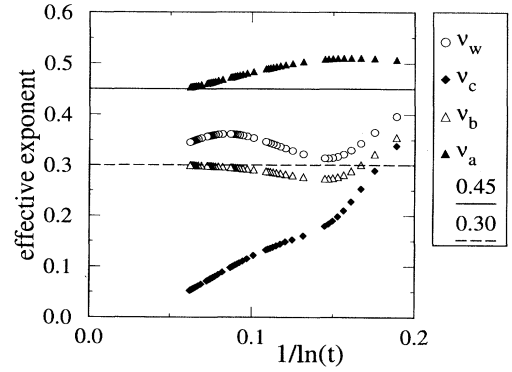

FIG. 5. Effective exponents for $(m,n) = (3,1)$. The horizontal lines represent the theoretical asymptotic values from Table I. The theoretical value for ν_c is 0.

The reason why some of the exponents deviate from the theoretical values may be understood from Figs. 1–3. The convergence to the solid curve for $x < 0$, where Eq. (14) predicts an exponential decay, is very rapid—semilogarithmic plots of $R(-x)$ were found to be in very good agreement with these predictions for up to 10 decades. However, the convergence of the profiles to the steady-state profiles is much slower for $x > 0$ (where the asymptotic behavior is algebraic). In fact, numerical investigation of the steady-state profiles showed that the regime for which the power-law behavior predicted by (14) appears is beyond the point at which the diffusive cutoff is already active in the data. This means that the asymptotic regime has not yet been reached. In view of this fact, the agreement between the measured exponents and the theory is surprisingly good.

V. CONCLUSIONS

The multiscaling theory predicts that the reaction profile of the system is described asymptotically by a scaling form, in the sense that Eq. (27) holds, but that the moments of the reaction and density profiles may have anomalous behavior. Numerical solutions of the reaction-diffusion equations verify the asymptotic scaling behavior, and also give values for the anomalous exponents

TABLE I. The measured values of the exponents ν_w, ν_a, and ν_b describing w, w_a, w_b, and x_c, respectively, together with the nonanomalous exponent α, for three values of the duple (m,n). The values in square brackets are the predictions of the multiscaling theory; the presence of a value for κ indicates the presence of a logarithmic correction of the form $\ln^\kappa(t)$, account of which has been taken in calculating the ν.

Quantity	(2,1)		(3,1)		(4,1)	
α	$\frac{1}{4}$		$\frac{3}{10}$		$\frac{1}{3}$	
ν_w	0.26	$[\frac{1}{4}]$	0.35	$[\frac{3}{10}]$	0.36	$[\frac{1}{3}, \kappa = \frac{1}{2}]$
ν_a	0.28	$[\frac{1}{4}, \kappa = \frac{1}{2}]$	0.45	[0.45]	0.52	$[\frac{1}{2}, \kappa = -\frac{1}{2}]$
ν_b	0.25	$[\frac{1}{4}]$	0.30	$[\frac{3}{10}]$	0.33	$[\frac{1}{3}]$
ν_c	−0.25	$[-\frac{1}{4}]$	0.05	[0]	0.20	$[\frac{1}{6}]$

close to those predicted by the theory. Longer times would have to be simulated to find better values for the exponents.

The convergence to the asymptotic behavior becomes progressively slower as the order of the reaction is increased. This means that simulations probing the asymptotic behavior also become more difficult. Nevertheless, Eq. (21) suggests that it would be worthwhile to look at at least one case where $m - n > 3$.

In the steady-state problem, it has been shown [11] that the critical dimension is $d_c = 2/(m + n - 1)$. This means that the reaction-diffusion equations correctly describe the scaling behavior of "real" stochastic realizations for all physical dimensions, except for $(m, n) = (2, 1)$ in dimension 1, where logarithmic corrections to the steady-state behavior are expected. Because of the strong link between the steady-state problem and the time-dependent problem studied in the present paper, we expect the critical dimensions to be the same. The only microscopic simulation results available [6] agree broadly with the picture in the present paper, though they are not of sufficiently high quality to give a thorough test.

For the case $m = n = 1$, the solutions to the steady-state differential equations (10) have exponential tails, and so all moments are described by the length scale w and not by the diffusion length $(Dt)^{1/2}$. These equations do not apply beneath the critical dimension $d_c = 2$ [11], but simulations show that the steady-state reaction profile for $d = 1$ is Gaussian in shape [13], so we again have exponential tails for the particle profiles. This predicts that the case $m = n = 1$ should display simple dynamical scaling independently of spatial dimension. However, Araujo *et al.* have reported simulation results in one dimension that violate dynamical scaling [8], supporting instead a multiscaling form. The authors of that paper argued that the two competing length scales in the problem are the separation $l \sim t^{1/4}$ and midpoint fluctuations $m \sim t^{3/8}$ of the neighboring A-B particle pair (the diffusion length did not appear in this theory), and that the large fluctuations in m make the steady-state results inapplicable to the problem. This multiscaling theory predicts that the quantities $X^{(q)}$ for the reaction profile should be of the form $X^{(q)} \sim t^{\zeta}$, with ζ increasing with q from 1/4 to 3/8, which was in apparent agreement with their measurements. However, more extensive simulations [9] appear to show that m scales like t^{θ}, with $\theta \sim 0.30$ apparently decreasing in time, and that apparent departures from simple dynamical scaling behavior are more likely to be due to transient effects. The point remains controversial, however, as a recent field-theoretic treatment by Howard and Cardy [14] has predicted algebraic correction terms to the steady-state profiles in this problem, which would lead to multiscaling behavior of the type described in the present paper. These predictions are nevertheless very different from those of Araujo *et al.* because the two length scales are w and the diffusion length $(Dt)^{1/2}$. Howard and Cardy predict that the algebraic corrections would only be seen at distances and times currently out of the range of simulations, and suggest that they might not be present at all for the models used so far, where reactions occur whenever an A-B pair meet.

The theory outlined in this paper is based on heuristic arguments and numerical results only, so a first-principles analytical justification is needed. It would be possible to write the equation of motion for the corrections to the multiscaling terms, and then investigate whether they are truly small and do not contribute to the behavior of the moments. Although no conclusive results have been found, a preliminary attempt at this procedure suggests that there may be values for m and n where the assumption may break down that the interpenetration of the species is smaller than the number of particles that have reacted [15]. The multiscaling theory presented in this paper might therefore have to be revised in those cases.

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