Self-similar evolution of the A-particle island–semi-infinite B-particle sea reaction-diffusion system

Boris M. Shipilevsky
Institute of Solid State Physics, Chernogolovka, Moscow district, 142432, Russia
(Received 26 March 2013; published 29 July 2013)

We consider diffusion-controlled evolution of the A-particle island–semi-infinite B-particle sea system at propagation of the sharp annihilation front $A + B \to 0$. We show that at a large initial number of island particles the system evolution is described by the universal scaling laws with nonmonotonous front trajectory and a constant velocity of the island center motion. We demonstrate that asymptotically the island moves self-similarly retaining its velocity, shape and width.

DOI: 10.1103/PhysRevE.88.012133 PACS number(s): 05.70.Ln, 82.20.−w

The formation of the localized reaction front $A + B \to 0$, which propagates between domains of unlike diffusing species A and B and occurs as a consequence of their effective dynamical repulsion, is a crucial feature of a broad spectrum of problems in physics, chemistry, biology, and materials science [1,2]. The simplest model of a planar reaction front, introduced by Galfi and Racz (GR) [3], is the quasi-one-dimensional model

$$\partial a/\partial t = D_A \nabla^2 a - R, \quad \partial b/\partial t = D_B \nabla^2 b - R \tag{1}$$

for two initially separated reactants which are uniformly distributed on the left side ($x < 0$) and on the right side ($x > 0$) of the initial boundary. Taking the reaction rate in the mean-field form $R(x,t) = ka(x,t)b(x,t)$ (k being the reaction constant), GR discovered that in the long-time limit $kt \gg 1$ the reaction profile $R(x,t)$ acquires a universal scaling form with the width $w \propto (t/k^2)^{1/6}$ so that on the diffusion length scale $L_D \propto t^{1/2}$ the relative width of the front asymptotically contracts unlimitedly, $w/L_D \sim (kt)^{-1/3} \to 0$ as $kt \to \infty$. Based on this fact, a general concept of the front dynamics, the quasistatic approximation (QSA), was developed [4–8]. The key property of the QSA is that $w(J)$ depends on t only through the time-dependent boundary current, $J_A = |J_B| = J$, the calculation of which is reduced to solving the external diffusion problem with the moving *absorbing boundary* (Stefan problem) $R = J\delta(x - x_f)$. Following this approach, in most subsequent works the use of the QSA was traditionally restricted by the GR *sea-sea* problem with an unlimited number of A and B particles where the stage of monotonous quasistatic front propagation is always reached asymptotically.

Recently, a new line in the study of the $A + B \to 0$ front dynamics has attracted significant attention under the assumption that the particle number of one or both species is finite (island-sea and island-island systems) and, therefore, in the final state one or both islands disappear completely [9–14]. It has been established that in the sharp-front regime these systems exhibit rich scaling behavior, and though in these systems the QSA is always asymptotically violated, at large initial particle numbers and a high-reaction constant the vast majority of particles die in the sharp-front regime over a wide parameter range.

In this paper, we focus on the regularities of the evolution of the *island-sea* system, whose "symmetric" version was first considered in Ref. [9], where it was established that the initial expansion stage is followed by a self-accelerating collapse of the island in a finite time (finite-time collapse). As principally distinct from the "*symmetric*" island-sea problem [9], where the island of A particles with an *immobile* center is surrounded by a symmetric sea of particles B on both sides of the island, in this paper we present the regularities of the "*asymmetric*" island-sea problem, where the island of particles A with a *moving* center is in contact with a semi-infinite sea of particles B. We find that at a large initial number of island particles, the system evolution is described by the universal scaling laws with a nonmonotonous front trajectory and a constant velocity of the island center motion, and we demonstrate that asymptotically, on the exponential relaxation stage, the island moves self-similarly, retaining its velocity, shape, and width.

Let in the infinite interval $x \in (-\infty,\infty)$ particles B with concentration b_0 and particles A with concentration a_0 be initially uniformly distributed in the sea $x \in (-\infty,0)$ and in the island $x \in (0,L)$, respectively. We will assume, as usual, that concentrations $a(x,t)$ and $b(x,t)$ change only in one dimension (flat front). We will also assume for simplicity $D_B = D_A = D$. Then, by measuring the length, time, and concentration in units of L, L^2/D, and b_0, respectively, and defining the ratio $a_0/b_0 = r$, we come from Eq. (1) to the simple diffusion equation for the difference concentration $s = a - b$,

$$\partial s/\partial t = \nabla^2 s, \tag{2}$$

in the interval $x \in (-\infty,\infty)$ with the initial conditions

$$s_0[x \in (-\infty,0)] = -1, \quad s_0[x \in (0,1)] = r, \quad s_0[x \in (1,\infty)] = 0, \tag{3}$$

and the boundary conditions $s(-\infty,t) = -1$ and $s(\infty,t) = 0$. The solution to Eqs. (2) and (3) has the form

$$s = (r/2)\left[\operatorname{erfc}\left(\frac{x-1}{2\sqrt{t}}\right) - \gamma \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right)\right], \tag{4}$$

where $\gamma = (r+1)/r$. According to the QSA, for large $k \to \infty$ at times $t \propto k^{-1} \to 0$ there forms and quasistatically propagates a sharp reaction front, which separates the domains $s < 0 (b = |s|, a = 0)$ and $s > 0 (a = s, b = 0)$ so that the law of the front center motion, $x_f(t)$, is defined by the condition $s(x_f,t) = 0$. Substitution of this condition into Eq. (4) gives

$$\operatorname{erfc}\left(\frac{x_f - 1}{2\sqrt{t}}\right) = \gamma \operatorname{erfc}\left(\frac{x_f}{2\sqrt{t}}\right). \tag{5}$$

Then integrating Eq. (4) for the number of island particles per unit of the initial boundary $N = \int_{x_f}^{\infty} a\,dx = \int_{x_f}^{\infty} s\,dx$, we self-consistently find

$$N/N_0 = \sqrt{t}\left[i\,\mathrm{erfc}\left(\frac{x_f - 1}{2\sqrt{t}}\right) - \gamma i\,\mathrm{erfc}\left(\frac{x_f}{2\sqrt{t}}\right)\right], \qquad (6)$$

where $i\,\mathrm{erfc}(u) = \int_u^{\infty}\mathrm{erfc}(z)dz = e^{-u^2}/\sqrt{\pi} - u\,\mathrm{erfc}(u)$ and (in our units) $N_0 = r$. At small $|x_f|,\sqrt{t} \ll 1$, when the diffusion length remains much less than the island size (GR sea-sea regime) from Eq. (5), in accordance with [3], we find $x_f = c_f\sqrt{t} + \cdots$, where $\mathrm{erf}(c_f/2) = (1-r)/(1+r)$ and, hence, at $r < 1$ the front moves toward the island ($c_f > 0$), whereas at $r > 1$ the front moves toward the sea ($c_f < 0$). As in Ref. [9], here we are mainly interested in the evolution of the system at large times $\sqrt{t} \gg 1$, when the diffusion length becomes much larger than the initial island size. Moreover, as in Ref. [9], here we are mostly interested in the limit of large $r \gg 1$, where, as is shown below, the system demonstrates a universal scaling behavior. Due to the finite number of island particles, it is clear that at $r > 1$ at a certain time t_M the front must change its direction of motion [turning point $\dot{x}_f(t_M) = 0$] reaching its initial position $x_f(t_\star) = 0$ at time $t_\star$ (return point) and moving further in the direction $x_f \to \infty$. From Eq. (5) we find exactly $\mathrm{erf}(1/2\sqrt{t_\star}) = 1/r$, from which at $t,r \gg 1$ it follows that

$$t_\star = r^2/\pi - 1/6 + \cdots. \qquad (7)$$

It is interesting to note that to an accuracy of negligible terms, this time coincides with the island collapse time in the symmetric problem [9] $t_\star \approx t_c \approx r^2/\pi$. Before we proceed to a detailed analysis of the front center motion $x_f(t)$, we focus on the motion law of the island center $x_m(t)$, which, in accordance with [12,13], can be naturally defined as the point where the concentration $a(x,t)$ reaches its maximum $a_m = s_m = \max s(x > x_f)$ and, as a result, the flux changes its sign. From Eq. (4) we easily find

$$\partial_x s = (r/2\sqrt{\pi t})e^{-x^2/4t}[\gamma - e^{(2x-1)/4t}],$$

from which, with regard to condition $(\partial_x s)_m = 0$, we immediately obtain the remarkable result

$$x_m = 2t\ln\gamma + 1/2, \qquad (8)$$

from which it follows that at *any* t and r the island center moves with a constant velocity $v_m = 2\ln\gamma$, which, at large r, drops with increasing the initial number of island particles by the law

$$v_m = 2\ln\gamma \approx 2/r.$$

From Eq. (5), it is easy to check that at $t \gg t_\star$ the front velocity increases monotonously, so, due to the condition $x_f < x_m$, it is clear that v_m defines the asymptotic limit of the front velocity at $t/r^2 \to \infty$. Indeed, assuming that $x_f/\sqrt{t} \gg 1, t \gg r^2 \gg 1$, from Eq. (5) we find $x_f = 2t\ln\gamma + 1/2 - 2t/x_f + 8t^2/x_f^3 + \cdots$, from which we obtain asymptotically

$$\begin{aligned} x_f &= 2t\ln\gamma + 1/2 - 1/\ln\gamma + 1/2t\ln^3\gamma + \cdots, \\ x_m - x_f &= 1/\ln\gamma - 1/2t\ln^3\gamma + \cdots \qquad (9)\\ &= r + 1/2 - r^3/2t + \cdots, \end{aligned}$$

and therefore

$$x_m - x_f \approx r + 1/2, \quad (v_m - v_f)/v_m \approx r^4/4t^2 \to 0$$

as $t/r^2 \to \infty$. According to Eq. (8), at large $r,t \gg 1$, in the vicinity of the island center the value $x/t \sim O(1/t,1/r) \ll 1$. Since outward from the island center $x \gg x_m$ the concentration drops exponentially fast, $s/s_m \propto e^{(x_m^2 - x^2)/4t}$, it is clear that in a considerable region of change s the condition $x/t \ll 1$ should remain valid. Transforming Eq. (4) with consideration of this fact, we find

$$s = (r/2\sqrt{\pi t})e^{-x^2/4t}(1+\phi) - \mathrm{erfc}(x/2\sqrt{t})/2, \qquad (10)$$

where $\phi(x,t) = x/4t - 1/12t + \cdots$. Thus, neglecting the term $|\phi(x,t)| \ll 1$ in Eq. (10) and introducing the scaling variables $\xi = x/r$ and $\tau = t/r^2$, we conclude that at large $t,r \gg 1$ the evolution of the island-sea system is described by the universal scaling law

$$s(\xi,\tau) = (1/2\sqrt{\pi\tau})e^{-\zeta^2} - \mathrm{erfc}(\zeta)/2, \qquad (11)$$

where $\zeta = x/2\sqrt{t} = \xi/2\sqrt{\tau}$. From Eq. (11) there immediately follows (a) an equation describing the universal front trajectory $\xi_f(\tau)$,

$$e^{-\zeta_f^2} = \sqrt{\pi\tau}\,\mathrm{erfc}(\zeta_f), \qquad (12)$$

and (b) the universal scaling law of island particle death,

$$N/N_0 = \mathcal{G}(\tau) = \mathrm{erfc}(\zeta_f)/2 - \sqrt{\tau}i\,\mathrm{erfc}(\zeta_f). \qquad (13)$$

According to Eq. (12), in the front turning point $(\dot{\xi_f})_M = 0$ we have $\xi_f^M = \tau_M - (\tau_M^2 + 2\tau_M)^{1/2}$, from which, using Eqs. (11)–(13), we find $\xi_f^M = -0.294\,528, \tau_M = 0.061\,481\,5, N_M/N_0 = 0.455\,18$, and $s_m^M = 0.706\,93$. Correspondingly, in the front return point $\xi_f^\star = 0$ we find $\tau_\star = 1/\pi, N_\star/N_0 = 0.181\,69$, and $s_m^\star = 0.151\,22$. In the most interesting asymptotic limit of large τ, where, in accordance with Eqs. (9) the front and island centers move with the same constant velocity and, as a consequence, the half-width of island $\xi_m - \xi_f$ remains *constant*, for the leading terms of $\xi_{m,f}(\tau)$ from Eqs. (11) and (12) we find

$$\xi_f = 2\tau - 1 + \cdots, \quad \xi_m - \xi_f = 1 - 1/2\tau + \cdots, \qquad (14)$$

from which, following substitution of $\xi_{m,f}$ into Eqs. (11) and (13) for the leading terms of the universal long-time relaxation of the reduced particle number in the island, N/N_0, and its amplitude, s_m, we obtain

$$N/N_0 \sim c_+ e^{-\tau}/\tau^{3/2}, \quad s_m \sim (c_+/e)e^{-\tau}/\tau^{3/2}, \qquad (15)$$

where $c_+ = e/4\sqrt{\pi}$. It should be emphasized, however, that, in accordance with Eqs. (9), at any large but finite $r \gg 1$, the deviation of the $\xi_{m,f}(r,\tau)$ trajectories from the universal ones increases with time by the law $|\delta\xi_{m,f}(r,\tau)| \sim \tau/r (\xi_f = 2\tau - 1 - \tau/r + \cdots)$ and, therefore, although at any τ the ratio $|\delta\xi_{m,f}(r,\tau)|/\xi_{m,f}(\tau) \sim 1/r \ll 1$, the ratio $|\delta\xi_{m,f}(r,t)|/(\xi_m - \xi_f) \sim \tau/r$ remains small only in the interval $\tau/r \ll 1$. Moreover, from Eqs. (4) and (6) it is easy to check that with growing τ, the corresponding deviations in the relaxation laws of the particle number and amplitude of the island $|\delta N(r,\tau)|/N(\tau) \sim |\delta s_m(r,\tau)/s_m(\tau)| \sim \tau/r$ remain small only at $\tau/r \ll 1$. Yet it is clear that at sufficiently large r, deviations from the universality become noticeable only when the fraction

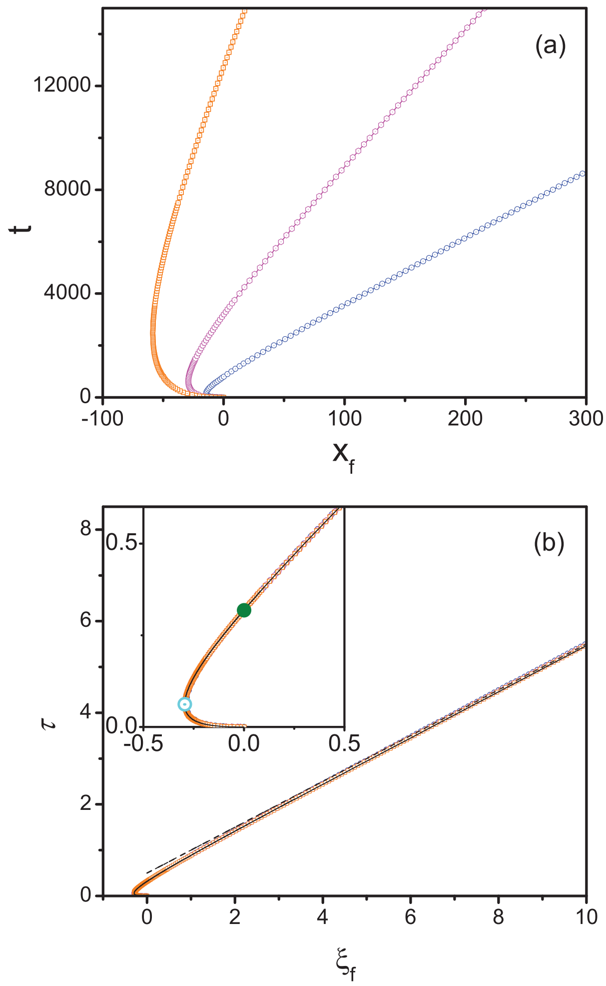

FIG. 1. (Color online) (a) Trajectories of the front center $x_f(t)$ calculated from Eq. (5) for $r = 50$ (circles), $r = 100$ (hexagons), and $r = 200$ (squares). (b) Collapse of the presented trajectories to the scaling law Eq. (12) (line) in the rescaled coordinates $\xi_f = x_f/r$ vs $\tau = t/r^2$. Dashed line shows long-time asymptote $\xi_f = 2\tau - 1$. Circles denote turning ($\xi_f^M = -0.294\,528, \tau_M = 0.061\,481\,5$) and return ($\xi_f^\star = 0, \tau_\star = 1/\pi$) front points.

of the remaining particles in the island becomes negligibly small and, hence, within the limits of applicability of the sharp front approximation (see below) the vast majority of particles die in the universal regime. As an illustration, Fig. 1 shows the $x_f(t)$ dependencies calculated from Eq. (5) at $r = 50$, 100, and 200 [Fig. 1(a)] and replotted in Fig. 1(b) in the scaling coordinates ξ_f versus τ. It is seen that with growing r, the dependencies presented converge fast to the universal dependence $\xi_f(\tau)$ calculated from Eq. (12). In addition, it is seen that the asymptotics $\xi_f = 2\tau - 1$ is reached with a good accuracy even at $\tau \sim 3$. Figure 2 shows the dependencies $N(\tau)/N_0$ calculated from Eqs. (5) and (6) at $r = 100$, 200, and 400. It is seen that with growing r, the dependencies presented converge fast to the scaling function $\mathcal{G}(\tau)$ calculated from Eqs. (12) and (13). Here the above-calculated front turning and return points are marked and the exponential asymptotics of Eq. (15) is shown. It is seen that although $\mathcal{G}(\tau)$ converges to its long-time asymptotics slower than $\xi_f(\tau)$, at $\tau > 10$ the deviation from the exponential asymptotics becomes less than

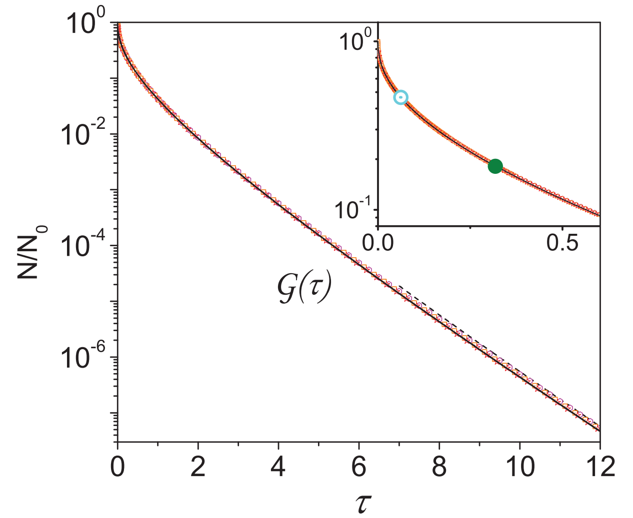

FIG. 2. (Color online) Collapse of the time dependencies calculated from Eqs. (5) and (6), N/N_0 vs τ, to the universal scaling function $\mathcal{G}(\tau)$ (line) with growing r: $r = 100$ (hexagons), $r = 200$ (squares), and $r = 400$ (stars). Dashed line shows long-time exponential asymptotics Eq. (15). Circles denote turning ($N_M/N_0 = 0.455\,18, \tau_M = 0.061\,481\,5$) and return ($N\star/N_0 = 0.181\,69, \tau_\star = 1/\pi$) front points.

20%. Figure 3 (main panel) shows the $|s(\xi,r)|$ dependencies calculated from Eq. (4) for $r = 100$, 200, and 400 at $\tau = 3$. It is seen that with growing r, the dependencies presented converge fast to the corresponding universal distribution $|s(\xi)|$ calculated by Eq. (11).

One of the most remarkable consequences of Eqs. (15) is the fact that at the long-time exponential relaxation stage, the particle number and amplitude of the island decay

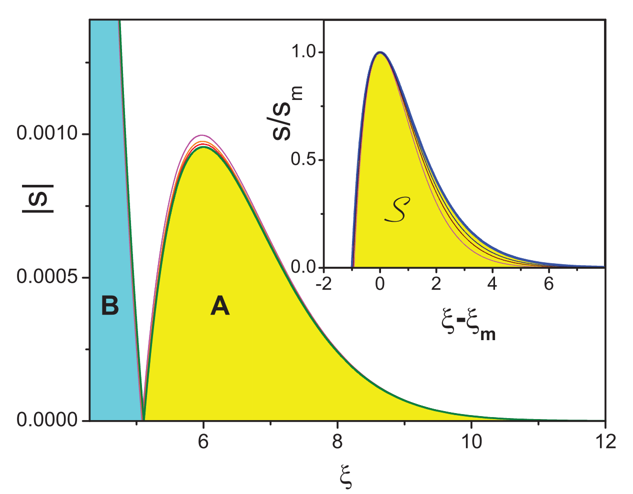

FIG. 3. (Color online) Main panel: Collapse of $|s(\xi,r)|$ dependencies calculated from Eq. (4) for $r = 100$, 200, and 400 (thin lines) at $\tau = 3$ to universal distribution $|s(\xi)|$ (thick line) calculated from Eq. (11). Areas under curves $b(\xi) = |s(\xi < \xi_f)|$ and $a(\xi) = s(\xi > \xi_f)$ are colored. Inset: Collapse of s/s_m vs $\xi - \xi_m$ dependencies calculated in accordance with Eq. (11) for $\tau = 5$, 10, and 20 (thin lines) to the universal scaling function $\mathcal{S}(\xi - \xi_m)$ [Eq. (17)] (thick line). Area under the scaling function $\mathcal{S}$ is colored.

"synchronously,"

$$N(\tau)/s_m(\tau) = N_0 e = \text{const.} \tag{16}$$

This fact indicates that at the exponential relaxation stage, the island moves *self-similarly* retaining its velocity, shape, and width. Let us show that these remarkable properties of long-time relaxation actually occur. From Eqs. (11) at $\tau,\xi_m \gg 1$, it follows that [15]

$$s/s_m = e^{(\xi_m^2-\xi^2)/2\xi_m}(\xi_m/\xi)[\xi - \xi_m + (\xi_m/\xi)^2 + \cdots],$$

from which, assuming $|\Delta\xi| = |\xi - \xi_m| \ll \sqrt{\xi_m}$ and neglecting the terms $O[(\Delta\xi)^2/\xi_m]$, i.e., "cutting off" the distribution at distances $1 \ll \Delta\xi_c \ll \sqrt{\xi_m}$, where the contribution into the particle number becomes exponentially small, we find asymptotically

$$s/s_m = \mathcal{S}(\xi - \xi_m) = e^{(\xi_m-\xi)}(1 + \xi - \xi_m). \tag{17}$$

Integration of Eq. (17) immediately leads to the result (16). When fixing the right island "boundary" by the condition $s(\Delta\xi_c)/s_m = \epsilon \ll 1$, we find from Eq. (17) $\Delta\xi_c(\epsilon) \sim \ln(\Delta\xi_c/\epsilon)$ and come to the announced conclusion about self-similar evolution of the moving island with a constant width and an exponentially decaying amplitude. In the inset to Fig. 3 shown are the s/s_m versus $\xi - \xi_m$ dependencies calculated from Eq. (11) for $\tau = 5$, 10, and 20. It is seen that with growing τ, the dependencies presented converge to the scaling function $\mathcal{S}(\xi - \xi_m)$, reaching it rapidly on the left side of the island ($\Delta\xi < 0$) and relatively slower on the right side ($\Delta\xi > 0$). Summarizing, it should be noted that although the regime of self-similar island evolution is reached only asymptotically when the reduced particle number in the island becomes exponentially small, the existence of such a regime with a constant velocity of the island motion as a whole is observed for the first time and is of principal significance [16].

To complete the picture outlined, we have to reveal the applicability limits for the key condition of the sharp annihilation front [10,12],

$$\eta = w/(x_m - x_f) \ll 1. \tag{18}$$

According to the QSA, the width of the mean-field reaction front (in our units) is defined by the expression $w \sim (kJ)^{-1/3}$ [9]. Calculation of the boundary current $J = |\nabla s|_{x=x_f} = -\dot{N}$ at large $\tau \gg 1$ in accordance with Eqs. (11) and (15) yields $J \sim e^{-\tau}/\tau^{3/2}r$. Substituting this result into Eq. (18) and considering that $x_m - x_f \sim r$, we find that at the exponential evolution stage, the relative front width increases by the law $\eta \sim (e^\tau\tau^{3/2}/kr^2)^{1/3}$. Thus, defining the time boundary of the sharp front regime by the condition $\eta \sim 0.1$ [10], we obtain $\tau|_{\eta=0.1} \sim \ln(\eta^3 kr^2/\tau_\eta^{3/2})$. Following [10,12], we shall estimate the applicability limit of the sharp front approximation for a perfect 3D diffusion-controlled reaction with dimensionless (in units of D/L^2b_0) constant $k \sim r_a L^2 b_0$, where r_a is the reaction radius. Substituting here $r_a \sim 10^{-8}$ cm, $L \sim 0.1$ cm, and $b_0 \sim 10^{20}$ cm^{-3}, we obtain $k \sim 10^{10}$ and find $\tau|_{\eta=0.1} \sim \ln(10^7 r^2/\tau_\eta^{3/2})$, from which we conclude that at a sufficiently large r the exponential relaxation stage is reached in the sharp-front regime.

In conclusion, it should be emphasized that although the evolutions of the "symmetric" and "asymmetric" planar island-sea systems are radically different, in both systems the scaling laws of island death have the form $N = N_0 F(t/N_0^2)$.

This research was financially supported by the RFBR through Grant No. 08-03-00054.

[1] P. L. Krapivsky, E. Ben-Naim, and S. Redner, *A Kinetic View of Statistical Physics* (Cambridge University Press, Cambridge, 2010).
[2] B. Chopard and M. Droz, *Cellular Automata Modeling of Physical Systems* (Cambridge University Press, Cambridge, 1998).
[3] L. Galfi and Z. Racz, Phys. Rev. A **38**, 3151 (1988).
[4] E. Ben-Naim and S. Redner, J. Phys. A **28**, L575 (1992).
[5] S. Cornell and M. Droz, Phys. Rev. Lett. **70**, 3824 (1993).
[6] B. P. Lee and J. Cardy, Phys. Rev. E **50**, R3287 (1994).
[7] G. T. Barkema, M. J. Howard, and J. L. Cardy, Phys. Rev. E **53**, R2017 (1996).
[8] Z. Koza, J. Stat. Phys. **85**, 179 (1996).
[9] B. M. Shipilevsky, Phys. Rev. E **67**, 060101(R) (2003).
[10] B. M. Shipilevsky, Phys. Rev. E **77**, 030101(R) (2008).
[11] S. Kisilevich, M. Sinder, J. Pelleg, and V. Sokolovsky, Phys. Rev. E **77**, 046103 (2008).
[12] B. M. Shipilevsky, Phys. Rev. E **79**, 061114 (2009).
[13] B. M. Shipilevsky, Phys. Rev. E **82**, 011119 (2010).
[14] C. P. Haynes, R. Voituriez, and O. Benichou, J. Phys. A **45**, 415001 (2012).
[15] Considering the fact that at $\xi_m = 2\tau \gg 1$ within the island the value $\zeta = \xi/\sqrt{2\xi_m} \gg 1$, from Eq. (11) we find $s/s_m = e^{(\xi_m^2-\xi^2)/2\xi_m}(\xi_m/\xi)[\xi - \xi_m + (\xi_m/\xi)^2 - 3(\xi_m/\xi)^4/\xi_m + \cdots]/(1 - 3/\xi_m + \cdots)$, from which, taking into account that $\xi_m/\xi < \xi_m/\xi_f \sim 1$ and neglecting the terms $O(1/\xi_m)$, we arrive at the expression given in the text.
[16] Note that asymptotic front and island center motion at a constant velocity was first discovered in Ref. [12] as one of the three characteristic scaling relaxation regimes of the island-island system in the limit of nearly equal initial particle numbers. However, Ref. [12] presented no systematic analysis of the evolution of the smaller island as a whole.