Death of an A-particle island in the B-particle sea: Propagation and evolution of the reaction front $A+B\leftrightarrow C$

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We present a systematic theory of propagation and evolution of the reaction front $A+B\leftrightarrow C$ in the reaction-diffusion system where an island of particles A is surrounded by the uniform sea of particles B. In the first part of the work we give a systematic analysis of the crossover from the irreversible to reversible regime of front propagation in terms of the quasistatic approximation (QSA) and derive the key condition for the island death in the quasiequilibrium front regime. We show that the same as in the case of pure annihilation $A+B\to 0$ the QSA enables the description of the quasiequilibrium front propagation only to a critical point t_c on approaching to which the QSA is violated. In the second part of the work under the assumption of a sufficiently large forward reaction constant k we derive the perturbative expansion in powers of $1/k$ which gives the asymptotically exact description of the quasiequilibrium front evolution up to $t\to\infty$. We demonstrate that below some critical value of the reduced backward reaction constant $g<g_c$ there appear *two turning points* on the front trajectory, the first of which arises at the sharp localized front stage and is due to the finite number of island particles whereas the second is a consequence of radical transformation of the front structure at the passage through the critical point (delocalization of the front). We find a remarkable property of *self-similarity* of the passage through the critical point, we derive scaling laws for such passage and show that in the limit $g\to 0$ these laws lead to a striking phenomenon of an *abrupt delocalization* of the front.

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I. INTRODUCTION

The reaction-diffusion system $A+B\to C$, where unlike species A and B diffuse and irreversibly react in a d-dimensional medium, has attracted great interest in the last decades. This fundamentally simple system, depending on the initial conditions, displays a rich variety of phenomena and, depending on the interpretation of A and B (chemical reagents, quasiparticles, topological defects, etc.), it provides a model for a broad spectrum of problems [1–4]. A crucial feature of many such problems is the dynamical reaction front—a localized reaction zone which propagates between domains of unlike species.

The simplest model of a reaction front, introduced almost two decades ago by Galfi and Racz (GR) [5], is a quasi-one-dimensional model for two initially separated reactants which are uniformly distributed on the left-hand side ($x<0$) and on the right-hand 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 $kt\to\infty$ the reaction profile $R(x,t)$ acquires the universal scaling form

$$R=R_f\mathcal{Q}\left(\frac{x-x_f}{w}\right), \tag{1}$$

where $x_f\propto t^{1/2}$ denotes the position of the reaction front center, $R_f\propto t^{-\beta}$ is the height, and $w\propto t^{\alpha}$ is the width of the reaction zone. Subsequently, it has been shown [6–13] that the mean-field approximation can be adopted at $d>d_c=2$, whereas in one-dimensional (1D) systems fluctuations play the dominant role. Nevertheless, the scaling law (1) takes place at all dimensions with $\alpha=1/6$ at $d>d_c=2$ and $\alpha=1/4$ at $d=1$, so that at any d the system demonstrates a remarkable property of the effective "dynamical repulsion" of A and B: On the diffusion length scale $L_D\propto t^{1/2}$ the width of the reaction front asymptotically contracts unlimitedly

$$w/L_D\to 0 \quad \text{as } t\to\infty.$$

Based on this property a general concept of the front dynamics for nonzero diffusivities, the quasistatic approxmation (QSA), has been developed [6,8,12,14]. The QSA consists in the assumption that for sufficiently long times the kinetics of the front is governed by two characteristic time scales. One time scale $t_J=-(d\ln J/dt)^{-1}$ controls the rate of change in the diffusive current $J=J_A=|J_B|$ of particles arriving at the reaction zone. The second time scale $t_f\propto w^2/D$ is the equilibration time of the reaction front. Assuming $t_f/t_J\ll 1$ from the QSA in the mean-field case with $D_{A,B}=D$ it follows that [6,8,14]

$$R_f\sim J/w,\quad w\sim(D^2/Jk)^{1/3}, \tag{2}$$

whereas in the 1D case w acquires the k-independent form $w\sim(D/J)^{1/2}$ [6,8].

The most important feature of the QSA is that w and R_f depend on t only through the time-dependent boundary current $J(t)$, which can be calculated analytically representing the reaction zone on the scale L_D in the form $R(x,t)=J\delta(x-x_f)$. On the basis of the QSA a general description of spatiotemporal behavior of the system $A+B\to C$ has been obtained for arbitrary nonzero diffusivities [15] which was then generalized to the cases of anomalous diffusion [16], diffusion in disordered systems [17,18], diffusion in systems with inhomogeneous initial conditions [19], and to several more complex reactions. Following the simplest GR model [5] the main attention has been traditionally focused on the systems with A and B domains having an unlimited extension, i.e., with unlimited number of A's and B's particles, where, after a more or less rich transient stage [20–23], asymptotically the stage of monotonous quasistatic front propagation is always reached, $t_f/t_J \to 0$ as $t \to \infty$.

Recently, in the work [24] a new line in the study of the $A+B\to C$ dynamics has been developed under the assumption that the particle number of one of the species is finite, i.e., an A-particle island is surrounded by the uniform sea of particles B. It has been established, that at sufficiently large initial number of A particles, N_0, and a sufficiently high reaction rate constant k the death of the majority of island particles $N(t)$ proceeds in the universal scaling regime

$$N = N_0 \mathcal{G}(t/t_c), \tag{3}$$

where $t_c \propto N_0^2$ is the lifetime of the island in the limit k, $N_0 \to \infty$. This result was obtained for the quasi-one-dimensional geometry (flat front) under the assumption that the reaction front propagates quasistatically and is sustained to be quite sharp, $w/x_f \ll 1$ until the collapse time $t \approx t_c$, so that the law of the motion of the front center $x_f(t)$ governs the island width evolution. It has been shown that while dying, the island first expands to a certain maximal amplitude $x_f^M \propto N_0$ and then begins to contract by the law

$$x_f = x_f^M \zeta_f(t/t_c), \tag{4}$$

so that on reaching the maximal expansion amplitude x_f^M (the turning point of the front),

$$t_M/t_c = 1/e, \quad N_M/N_0 = 0.19886\cdots, \tag{5}$$

and, therefore, irrespective of the initial particle number and dimensionality of the system, $\approx 4/5$ of the particles die at the stage of the island expansion and the remaining $\approx 1/5$ at the stage of its subsequent contraction. According to (2) the rapid island contraction is accompanied by the rapid growth of the front width w and, therefore, in some vicinity of the critical point $|\mathcal{T}| = |(t-t_c)/t_c| \sim \mathcal{T}_Q$ the reaction front becomes "blurred" ($w/x_f \sim 1$) and the QSA is no longer applicable. In the work [24] it has been shown that at small $|\mathcal{T}|$,

$$w/x_f \propto \sqrt{t_f/t_J} \propto |\mathcal{T}_Q/\mathcal{T}|^{\mu}, \tag{6}$$

where for the mean-field front ($d>2$) $\mu_{\rm MF}=2/3$ and

$$\mathcal{T}_Q^{\rm MF} \propto 1/N_0\sqrt{k},$$

whereas for the fluctuation front ($d=1$) $\mu_{\rm F}=3/4$ and

$$\mathcal{T}_Q^{\rm F} \propto 1/N_0^{2/3},$$

so that $\mathcal{T}_Q \to 0$ at large k, $N_0 \to \infty$.

The goal of the present paper is to generalize the results of the work [24] for a broader class of reversible reactions $A+B\leftrightarrow C$ with mobile particles A, B, and C. The first to analyze the propagation of the "reversible" $A+B\leftrightarrow C$ front were Chopard *et al.* [25]. Following the simplest GR model they numerically demonstrated a crossover from the irreversible to the reversible regime of front propagation and based on the scaling arguments showed that independently of the system's dimensionality d the width of the "reversible" front grows by the law $w \propto \sqrt{t}$. The next important step was made by Sinder and Pelleg who presented a detailed analysis of the "reversible" front propagation in the limit of small backward reaction constant $g\to 0$ [26,27]. They showed that in the $g\to 0$ limit the mean-field "reversible" front propagates quasistatically ($t_f/t_J \propto g \to 0$), and obtained the exact asymptotic law of the front amplitude decay $R_f \propto t^{-1}$. The presented analysis allowed the conclusion that the crossover irreversible regime–reversible regime radically changes only the local dynamic in the vicinity of the front without changing the particles distribution beyond it and, as a consequence, leaving unchanged the law of the front motion. The most consistent asymptotic theory of the reversible regime has been proposed recently by Koza [28]. He obtained a systematic expansion of the solution in powers of $1/t$ and showed that at equal diffusivities of all species the main terms of the expansion give the asymptotically exact description for arbitrary values of g. Moreover, he showed that in the limit $g\to 0$ the obtained solution converges to the singular quasistatic limit. So, Koza has clearly demonstrated that in contrast to the quasistatic description of the irreversible regime, in the reversible regime the GR problem admits the asymptotically exact description at any front shape. In the present work we will show that this remarkable property of the reversible regime holds valid for the much more general (nonmonotonous) law of the front propagation. We will present a systematic theory of death of an A-particle island in the B-particle sea in the reversible reaction regime and, based on it, we will give a detailed description of all consecutive stages of the front evolution up to $t\to\infty$.

II. MODEL

Let particles A with concentration a_0 be initially uniformly distributed in the island $x \in (-L, L)$ surrounded by the unlimited sea of particles B with concentration b_0 on the left-hand side $x \in (-\infty, -L)$ and on the right-hand side $x \in (L, \infty)$ of the island. Particles A and B diffuse with diffusion constants $D_{A,B}$ and reversibly react $A+B\leftrightarrow C$ with the production of particles C, which diffuse with diffusion constant D_C and are originally absent in the system, $c_0=0$. We will assume that the system's dimension is $d>d_c$, therefore, the local production rate of C particles can be represented in the mean-field form

$$R = k(ab - gc), \tag{7}$$

where $a(x,t)$, $b(x,t)$, and $c(x,t)$ are the local concentrations of A, B, and C, respectively, k is the forward reaction constant, and $g=G/k$ is the reduced backward reaction constant (equilibrium constant).

By symmetry our effectively one-dimensional problem is reduced to the solution of the system

$$\partial a/\partial t = D_A \nabla^2 a - R,$$

$$\partial b/\partial t = D_B \nabla^2 b - R,$$

$$\partial c/\partial t = D_C \nabla^2 c + R \tag{8}$$

in the interval $x \in [0, \infty)$ at the initial conditions

$$a(x,0) = a_0\theta(L-x), \quad b(x,0) = b_0\theta(x-L),$$

$$c(x,0) = 0, \tag{9}$$

with the boundary conditions

$$\nabla(a,b,c)|_{x=0} = 0, \quad b(\infty,t) = b_0, \tag{10}$$

where $\theta(x)$ is the Heaviside step function.

To simplify the problem essentially we will assume, as usually, $D_A=D_B=D_C=D$. Then, by measuring the length, time, and concentration in units of L, L^2/D, and b_0, respectively, i.e., assuming $L=D=b_0=1$, and defining the ratio of initial concentrations $a_0/b_0=r$, we come from (8)–(10) to the simple diffusion equations for $a+c$, $b+c$, and $a-b$ with the solutions

$$a + c = r\mathcal{F}, \quad b + c = 1 - \mathcal{F}, \tag{11}$$

and

$$s = a - b = (r+1)\mathcal{F} - 1, \tag{12}$$

where

$$\mathcal{F}(x,t) = \frac{1}{2}\left[\operatorname{erf}\left(\frac{1+x}{2\sqrt{t}}\right) + \operatorname{erf}\left(\frac{1-x}{2\sqrt{t}}\right)\right]. \tag{13}$$

The conservation laws (11) and (12) are valid at any values of dimensionless control parameters r, k, and g. Of primary interest for us here is the behavior of the system (7)–(10) in the region of the parameters $r,k \gg 1$ and $g \ll 1$. We will show that in agreement with [24] at large $r,k \gg 1$ there forms and quasistatically propagates a sharp reaction front which at small $g \ll 1$ is sustained to be quasistatic during the crossover from the irreversible to reversible propagation regime. In the first part of the work we give a general analysis of the crossover irreversible regime–reversible regime in the framework of the quasistatic approximation and find the key condition for the quasistatic front propagation in the reversible regime. In the second part of the work we develop a systematic perturbation theory which allows one to obtain the asymptotically exact analytic solution for $a(x,t)$, $b(x,t)$, $c(x,t)$, and $R(x,t)$.

III. QUASISTATIC FRONT PROPAGATION: CROSSOVER FROM THE IRREVERSIBLE TO REVERSIBLE REGIME

A. Irreversible regime

According to [24] in the irreversible limit $g=0$ with large k at times $t \propto k^{-1} \ll 1$ there forms and quasistatically propagates a sharp reaction front $w/x_f \ll 1$, which separates the domains $s>0$ ($a=s$, $b=0$) and $s<0$ ($a=0$, $b=|s|$) 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. (12) gives

$$\mathcal{F}(x_f,t) = 1/(r+1). \tag{14}$$

From Eq. (14) it follows [24] that at large $r \gg 1$ the reaction front $x_f(t)$ (and with it the whole of the island domain $s>0$) first moves towards the sea (expansion stage), reaching a maximal amplitude

$$x_f^M = (r+1)\sqrt{2/\pi e} \tag{15}$$

at the time moment (turning point of the front)

$$t_M = (r+1)^2/\pi e, \tag{16}$$

and then it comes back to the island center (contraction stage), reaching it at the time moment

$$t_c = (r+1)^2/\pi, \tag{17}$$

wherein the domain of A-particle excess $s>0$ disappears. According to (17) at large $r \gg 1$ the lifetime of the island $t_c \propto r^2 \gg 1$, so the majority of the A particles die at times $t \gg 1$, when the diffusive length exceeds appreciably the initial island size. The same as in the work [24], the evolution of the island in such a large-t regime is of principal interest to us here, and its analysis is the main goal of the present paper.

In the limit $r,t \gg 1$, Eq. (13) acquires the form

$$\mathcal{F}(x,t) = \frac{(1-\chi)}{\sqrt{\pi t}} e^{-x^2/4t}, \tag{18}$$

where $\chi = (1 - x^2/2t)/12t + \cdots$, and, hence, according to (14), the law of the front motion is

$$x_f = 2\sqrt{t}(1+\epsilon)\ln^{1/2}\left[\left(\frac{r+1}{\sqrt{\pi t}}\right)(1-\epsilon)\right], \tag{19}$$

where $\epsilon = 1/12t + \cdots$. Introducing according to [24] the reduced coordinate $\zeta = x/x_f^M$ and time $\tau = t/t_c$, and neglecting the terms χ, ϵ, from Eqs. (12), (18), and (19) we immediately obtain the scaling law for the distribution of particles

$$s(\zeta,\tau) = e^{-\zeta^2/2e\tau}/\sqrt{\tau} - 1, \tag{20}$$

and the scaling law of the front motion (4),

$$\zeta_f(\tau) = \sqrt{e\tau|\ln \tau|}. \tag{21}$$

The front width being neglected, Eqs. (20) and (21) define the scaling law of the island particle number $N(\tau) = x_f^M \int_0^{\zeta_f} s(\zeta,\tau)d\zeta$ evolution

$$\mathcal{G}(\tau) = \gamma \frac{N(\tau)}{N_0} = \operatorname{erf}(\sqrt{|\ln \tau|/2}) - \sqrt{2\tau|\ln \tau|/\pi} \tag{22}$$

[here $N_0=r$ is the reduced initial particle number and $\gamma = r/(r+1) \approx 1$] and give the law of decay of the boundary current $J = -dN/dt = -\partial s/\partial x|_{x=x_f}$,

$$J(\tau)/J_M = \sqrt{\frac{|\ln \tau|}{e\tau}}, \quad J_M = 1/x_f^M, \tag{23}$$

which according to (2) defines the evolution of the reaction front width and amplitude.

Equations (20)–(23) were obtained in [24] for the annihilation reaction $A+B \to 0$, so, the behavior of particles C was not considered there. Here we will complement this analysis for the more general irreversible process $A+B \to C$. Let us show that in the limit of a sharp quasistatic front the distribution of particles C on the left-hand side c_- (island) and right-hand side c_+ (sea) of the front automatically follows from the two conservation laws (11). Indeed, assuming $b(x<x_f) \approx 0$ and $a(x>x_f) \approx 0$ we find from (11)

$$c_- = 1 - \mathcal{F}, \quad c_+ = r\mathcal{F}. \tag{24}$$

By matching these solutions in the vicinity of the front center [i.e., by assuming $(a_f, b_f)/c_f \to 0$] we obtain

$$c_f = r\mathcal{F}_f = \gamma \approx 1. \tag{25}$$

The calculation of diffusive currents of C particles in the vicinity of the front $J_- = -\partial c_-/\partial x|_{x=x_f}$ and $J_+ = -\partial c_+/\partial x|_{x=x_f}$ according to (24) gives

$$J_- = -J/(r+1), \quad J_+ = rJ/(r+1) \tag{26}$$

whence it follows that

$$J_+/|J_-| = r, \quad |J_-| + J_+ = J. \tag{27}$$

From Eqs. (26) and (27) we conclude that at $r, t \gg 1$ in the process of expansion and subsequent contraction of the island practically all the forming C particles diffuse from the front towards the sea

$$J_A = |J_B| = J \approx J_+$$

as according to Eqs. (18) and (24) in the island center $c_-(0,t) \sim 1 - 1/\sqrt{\pi t} \approx 1$ and, therefore, at the quasistatic motion of the sharp front $(w/x_f \ll 1)$ the concentration of C particles within the island is sustained nearly constant, $c_- \approx 1$. It is interesting to note that the ratio of the currents $J_+/|J_-|$ does not depend on the time and direction of the front motion.

B. Crossover from the irreversible to reversible regime

According to [27,28] at finite g in the GR sea-sea (SS) problem there exists some crossover time $t_*(g)$ between the intermediate irreversible regime of the front propagation $t \ll t_*$ where the influence of the backward reaction is not yet manifested, and the asymptotic reversible regime $t \gg t_*$ where a quasiequilibrium $ab \approx gc$ is established. A remarkable property of this crossover is that in the limit of small $g \to 0$ the front is sustained sharp enough $w/L_D \propto \sqrt{g} \to 0$ and propagates quasistatically up to $t/t_* \to \infty$. Thus, the crossover irreversible regime–reversible regime radically changes only the local dynamics in the vicinity of the front leaving unchanged the distribution of particles outside of it $|x - x_f| \gg w$ and, as a consequence, leaving unchanged the law of the front center motion $x_f(t)$. It will be shown below that for the island-sea problem in the limit of large k and small g this remarkable property of the crossover irreversible regime–reversible regime holds up to the narrow vicinity of the critical point $t \approx t_c$. Importantly that in the island-sea problem a relative front width $\eta = w/x_f$ grows rapidly with the time, therefore, as qualitatively different from the sea-sea problem, in this case the sharp front propagation in the reversible regime is possible only at the condition $t_* \ll t_c$ which imposes a strict limitation on the parameters g and k.

We will assume the backward reaction constant g to be sufficiently small so that while crossing over from the irreversible to reversible regime the front is sustained sharp enough $(\eta = w/x_f \ll 1)$ and, as a consequence, propagates quasistatically (the conditions which are imposed by this requirement will be self-consistently revealed below). Then from the conservation laws (11) and (12) it automatically follows that irrespective of the regime the distribution of particles beyond the front $(|x - x_f| \gg w)$ is determined by Eqs. (20) and (24). This implies that irrespective of the regime the center of the front moves by the law (21), the "incoming" diffusive current of A and B particles, J, decays by the law (23), and the "outcoming" diffusive currents of C particles are connected with J by the relations (26). Our goal here is to generalize the QSA for the reversible reaction $A + B \leftrightarrow C$, and, based on it, to obtain the dependences of the width $w(J)$ and the amplitude $R_f(J)$ of the front on the incoming current J as on the parameter and to find the characteristic crossover current J_* between the irreversible and reversible regimes.

According to (7) at the front center we have

$$a_f b_f = R_f/k + gc_f. \tag{28}$$

Using the approach [6,14], i.e., defining the width of the front w as the region for which the concentrations of both species A and B are non-negligible [for example, using the symmetry $R(\xi) = R(-\xi)$ one can take

$$w = \text{const} \frac{\int_0^\infty \xi R(\xi) d\xi}{\int_0^\infty R(\xi) d\xi},$$

where $\xi = x - x_f$] we can write

$$a_f = b_f \sim Jw.$$

Substituting this result into Eq. (28), using the condition of conservation of the number of particles

$$J \sim R_f w,$$

and taking into account the requirement $c_f = \gamma$ (25), we find from Eq. (28),

$$(Jw)^2 \sim J/wk + \gamma g \tag{29}$$

or, equivalently,

$$(J^2/R_f)^2 \sim R_f/k + \gamma g. \tag{30}$$

From Eqs. (29) and (30) it immediately follows that the parameter of the crossover from the irreversible to reversible regime is

$$\phi = J^2/(\gamma g)^{3/2} k. \tag{31}$$

In the limit of large $\phi \gg 1$ in the right-hand part of (29) and (30) the first term is dominant and we find

$$w = w_i(1 + \text{const}/\phi^{2/3} + \cdots),$$

$$R_f = R_f^i(1 - \text{const}/\phi^{2/3} + \cdots), \tag{32}$$

where in accordance with (2) in the irreversible limit the front width and amplitude are independent of g,

$$w_i = \text{const}/(kJ)^{1/3},$$

$$R_f^i = \text{const}(kJ^4)^{1/3}. \quad (33)$$

In the opposite limit of small $\phi \ll 1$ in the right-hand part of (29) and (30) the second term is dominant, and we find

$$w = w_a(1 + \text{const}\ \phi + \cdots),$$

$$R_f = R_f^a(1 - \text{const}\ \phi + \cdots), \quad (34)$$

where in the reversible limit the front width and amplitude are independent of k,

$$w_a = \text{const}(\sqrt{\gamma g}/J),$$

$$R_f^a = \text{const}(J^2/\sqrt{\gamma g}). \quad (35)$$

Representing the parameter ϕ in the form

$$\phi = (J/J_*)^2,$$

for the crossover current J_* we find from (31),

$$J_* = \sqrt{(\gamma g)^{3/2} k}. \quad (36)$$

C. Scaling of the reaction front in the reversible regime

We show now that, based on the QSA, in the reversible limit $\phi \ll 1$ one can obtain a closed scaling description of the front propagation. Let us introduce the scaling variable $z = 2(x - x_f)/w$. According to the QSA within the domain $|x - x_f|/x_f \ll 1$ (respectively, $|z| \ll x_f/w \to \infty$ at $w/x_f \to 0$) there takes place the condition $\partial^2 s/\partial x^2 = 0$ whence it follows that

$$b - a = Jwz/2. \quad (37)$$

According to (26) a maximal departure of c from c_f at large $|z| \gg 1$ is

$$c_f - c \sim Jw|z|/2 \sim a_f|z|.$$

In the reversible regime $a_f \sim \sqrt{g}$. Therefore, in the limit $g \to 0$ in the wide range $|z| \ll 1/\sqrt{g} \to \infty$ we can take $c = c_f = \gamma \approx 1$. Thus, in the range $|z| \ll 1/\sqrt{g}$ we can write

$$ab = \gamma g + R/k. \quad (38)$$

In the reversible limit $\phi \ll 1$ in the main approximation the term R/k in Eq. (38) can be neglected. Therefore, asymptotically we have

$$a_a b_a = \gamma g. \quad (39)$$

From Eqs. (37) and (39) there immediately follow the asymptotic scaling laws of distribution of A and B species

$$a_a = a_f^a \mathcal{A}(z), \quad b_a = b_f^a \mathcal{B}(z), \quad (40)$$

where the amplitudes

$$a_f^a = b_f^a = \sqrt{\gamma g},$$

the width of the reaction front

$$w_a = 4\sqrt{\gamma g}/J, \quad (41)$$

and the scaling functions

$$\mathcal{A}(z) = \mathcal{B}(-z) = \sqrt{z^2 + 1} - z. \quad (42)$$

Substituting Eqs. (40) into the central QSA condition [15,27]

$$R = \partial^2 a/\partial x^2 = \partial^2 b/\partial x^2 \quad (43)$$

we find the asymptotic scaling law for the reaction profile

$$R_a = R_f^a \mathcal{R}(z), \quad (44)$$

where the amplitude

$$R_f^a = J^2/4\sqrt{\gamma g} \quad (45)$$

and the scaling function

$$\mathcal{R}(z) = 1/(z^2 + 1)^{3/2}. \quad (46)$$

By comparing Eqs. (33) and (35), and the scaling functions $\mathcal{Q}(z)$ [14,15] and $\mathcal{R}(z)$ we conclude that the crossover irreversible regime–reversible regime leads to a radical change of both the front broadening dynamics and shape of the front.

(i) The law of increase of the front width upon the decay of the incoming current $J(t)$ changes from $w_i \propto J^{-1/3}$ in the irreversible regime to $w_a \propto J^{-1}$ in the reversible regime.

(ii) The law of decay of the front "tails" at large $|z| \gg 1$ changes from a rapid exponential

$$\mathcal{Q}(z) \propto |z|^{3/4} e^{-\text{const}|z|^{3/2}}, \quad |z| \gg 1$$

in the irreversible regime to a comparatively slow power one,

$$\mathcal{R}(z) \propto 1/|z|^3, \quad |z| \gg 1,$$

in the reversible regime.

Substituting Eq. (44) into Eq. (38) from Eqs. (37) and (38) one can calculate a and b in the next approximation, and then from Eq. (43) derive in the next approximation the front profile R. Clearly, the sequential iterative application of this procedure enables one to obtain exact expansions of a, b, and R in powers of ϕ and in this way to obtain the exhaustive picture of the crossover to the asymptotics of the reversible regime (40) and (44). After the first iteration we find

$$a = a_f^a \mathcal{A}(z)[1 + \phi \mathcal{A}_1(z) + \cdots],$$

$$b = b_f^a \mathcal{B}(z)[1 + \phi \mathcal{B}_1(z) + \cdots],$$

$$R = R_f^a \mathcal{R}(z)[1 + \phi \mathcal{R}_1(z) + \cdots], \quad (47)$$

where the scaling functions

$$\mathcal{A}_1(z) = \mathcal{B}_1(-z) = \frac{1}{8(1+z^2)^2(\sqrt{1+z^2} - z)},$$

$$\mathcal{R}_1(z) = \frac{5(z^2 - 1/5)}{2(1+z^2)^{5/2}}. \quad (48)$$

From Eqs. (47) and (48) in accordance with (34) we find exactly

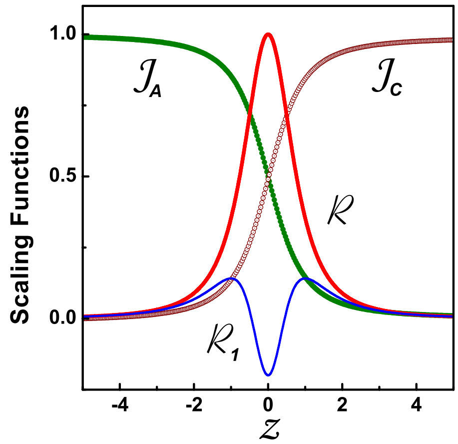

FIG. 1. (Color online) Scaling functions $\mathcal{R}(z)$ (thick line) and $\mathcal{R}_1(z)$ (thin line) calculated according to Eqs. (46) and (48). Also are shown normalized current distributions of A particles $\mathcal{J}_A(z)$ (filled circles) and C particles $\mathcal{J}_C(z)$ (open circles) calculated according to Eq. (42) for $r=10^2$.

$$a_f = a_f^a(1 + \phi/8 + \cdots), \quad R_f = R_f^a(1 - \phi/2 + \cdots).$$

It can easily be seen that $\mathcal{A}_1(z)$ reaches the maximum in the vicinity of the front center, $z_M=1/\sqrt{15}$, asymmetrically decaying at large $|z| \gg 1$ by the laws

$$\mathcal{A}_1(z<0) \propto 1/|z|^5, \quad \mathcal{A}_1(z>0) \propto 1/z^3.$$

More nontrivial is the behavior of $\mathcal{R}_1(z)$. In the interval $-1/\sqrt{5}<z<1/\sqrt{5}$ the function $\mathcal{R}_1(z)$ is negative, reaching in modulus the absolute maximum in the front center, $z_M=0$. As $|z|$ grows, $\mathcal{R}_1(z)$ reverses its sign in the points $z_0=\pm 1/\sqrt{5}$, then it passes through the maximum in the points $z_m=\pm 1$, and at large $|z| \gg 1$ it symmetrically decays by the law

$$\mathcal{R}_1(z) \propto 1/|z|^3.$$

It is easy to check that, as it must be, the global reaction rate $R_G=\int_{-\infty}^{\infty} R d\xi = J$ so that the "crossover" ϕ-containing terms do not contribute into the integral. In Fig. 1 are shown the scaling functions $\mathcal{R}(z)$ and $\mathcal{R}_1(z)$ and, also, the normalized distributions of currents of A-particles $\mathcal{J}_A(z)=J_A^a(z)/J$ and C-particles $\mathcal{J}_C(z)=J_C^a(z)/J=-\mathcal{J}_A(z)+\gamma$ [29].

Though the presented analysis is given as applied to the island-sea problem, it is clear that Eqs. (47) define the key features of the crossover to the reversible regime of the sharp front propagation ($g \ll 1$) at c_f=const for arbitrary laws of behavior of $x_f(t)$ and $J(t)$ which satisfy the quasistaticity conditions. For example, in the trivial particular case of the sea-sea problem ($J \propto t^{-1/2}$) from Eqs. (47) we immediately come to the expansions of a, b, and R in powers of t_*/t [28] with z=const $\xi/\sqrt{t}$ and $t_* \propto g^{-3/2}$. It is important to stress that in the general case Eqs. (47) have the sense of expansions in powers of $1/k$ so that the asymptotic distributions $a_a(z)$, $b_a(z)$, and $R_a(z)$ depend only on the equilibrium constant g, i.e., they are quasiequilibrium diffusion-controlled distributions independent of the forward reaction constant k.

D. Time dependences: Conditions of propagation of the quasistatic quasiequilibrium front

As qualitatively different from the sea-sea problem [25–28], where due to the relation $w_a/L_D \sim \sqrt{g} \ll 1$ the formed quasiequilibrium quasistatic front is sustained quasistatic for an unlimitedly long time, in the island-sea problem due to the rapid growth of the relative front width $\eta = w/x_f$ according to Eq. (6) the front can hold quasistatic $\eta \ll 1$ only to a certain vicinity $|\mathcal{T}|=|(t-t_c)/t_c| \sim \mathcal{T}_Q$ of the critical point t_c. So, together with the requirement $g \ll 1$ the requirement $t_* \ll t_c$ is a necessary condition for the island death in the regime of quasistatic quasiequilibrium front. According to Eq. (5) this requirement is equivalent to the requirement $t_* \ll t_M$ which, in turn, is reduced to the condition $J_* \gg J_M \sim 1/r$. Substituting here Eq. (36) we come to the key condition

$$g_\star = 1/(r^2 k)^{2/3} \ll g \ll 1. \tag{49}$$

Substituting then Eq. (23) into Eqs. (31), (41), and (45) we derive the time dependences

$$R_f^a = \frac{A_R \gamma^{3/2}}{r^2\sqrt{g}} \frac{|\ln \tau|}{\tau}, \tag{50}$$

$$w_a = \frac{A_w r}{\sqrt{\gamma}} \left(\frac{g\tau}{|\ln \tau|}\right)^{1/2}, \tag{51}$$

$$\phi = A_\phi \sqrt{\gamma} \left(\frac{g_\star}{g}\right)^{3/2} \frac{|\ln \tau|}{\tau}, \tag{52}$$

(here $A_R=\pi/8$, $A_w=4\sqrt{2/\pi}$, and $A_\phi=\pi/2$) and using Eqs. (15) and (21) we finally find

$$\eta_a = w_a/x_f = \frac{4\sqrt{\gamma g}}{|\ln \tau|}. \tag{53}$$

In the vicinity of the critical point $|\mathcal{T}|=|\tau-1|=|(t-t_c)/t_c| \ll 1$ from Eq. (53) we obtain

$$\eta_a \sim \mathcal{T}_Q/|\mathcal{T}|, \quad \mathcal{T}_Q \sim \sqrt{g}, \tag{54}$$

where $\mathcal{T}_Q$ is a characteristic time at which the QSA is violated. By extrapolating to $\mathcal{T}_Q$ the expressions $N/N_0 \sim |\mathcal{T}|^{3/2}$ and $\zeta_f \sim \sqrt{|\mathcal{T}|}$, following from Eqs. (21) and (22) at small $|\mathcal{T}| \ll 1$, we find

$$N_Q/N_0 \sim g^{3/4}, \quad \zeta_f^Q \sim g^{1/4} \tag{55}$$

and conclude that in the limit of small $g_\star/g \ll 1$, $\sqrt{g} \ll 1$, the majority of the island particles die in the regime of quasistatic quasiequilibrium front. Let us estimate the ultimate value of $g_\star$. For a perfect diffusion-controlled three-dimensional (3D) reaction $k \sim D r_R$, where r_R is the reaction radius. Thus, as our k is measured in units of $D/L^2 b_0$ for the dimensionless k we have $k \sim r_R L^2 b_0$ [24,30]. Substituting here $r_R \sim 10^{-8}$ cm, $L \sim 0.1$ cm, and $b_0 \sim 10^{21}$ cm^{-3} we find $k \sim 10^{11}$. Substituting this value into Eq. (49) and taking $r = 10^2$ we find $g_\star \sim 10^{-10}$. We thus conclude that the QSA description of the quasiequilibrium front propagation has a broad applicability range. As an illustration, Figs. 2 and 3

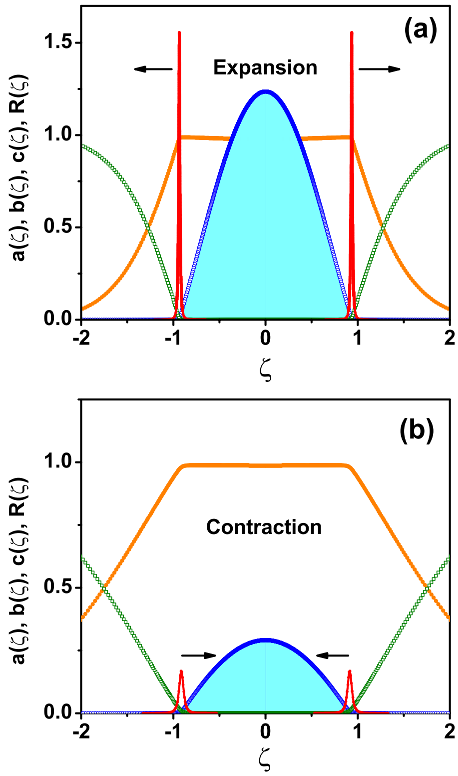

FIG. 2. (Color online) Distributions of particles $a(\zeta)$ (open circles), $b(\zeta)$ (open squares), and $c(\zeta)$ (filled circles), and the reaction front profile $50R(\zeta)$ (lines) at the stages of the island expansion (a) and contraction (b) calculated according to Eqs. (58), (61), (65), and (66) at $g_\star = 10^{-6}$, $g = 10^{-4}$, and $r = 10^2$ for the time moments $\tau = 0.2$ (a) and $\tau = 0.6$ (b). For completeness are shown the both island fronts $\pm\zeta_f(\tau)$ [the left-hand part of the distribution ($\zeta < 0$) is obtained through the mirror reflection of the right-hand one ($\zeta > 0$)]. The island region under the curve $a(\zeta)$ is colored.

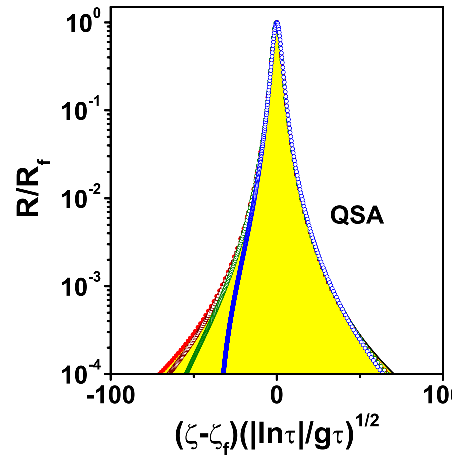

FIG. 3. (Color online) Evolution of the reaction front profile in the scaling coordinates R/R_f vs $(\zeta - \zeta_f)\sqrt{|\ln \tau|/g\tau}$ calculated according to Eqs. (65) and (66) at $g_\star = 10^{-6}$, $g = 10^{-4}$, and $r = 10^2$ for the time moments $\tau = 0.2$ (filled circles), $\tau = 0.4$ (open squares), $\tau = 0.6$ (open hexagons), and $\tau = 0.8$ (open circles). The region under the QSA profile (46) (solid line) is colored.

show the evolution of the distribution of particles and the front profile calculated in accordance with the exact Eqs. (58), (61), (65), and (66) for $g = 10^{-4}$, $g_\star = 10^{-6}$, and $r = 10^2$. It is seen from Fig. 2 that in accordance with Eq. (24) at expansion and subsequent contraction of the island, the distribution of C particles within the island is sustained nearly constant. Figure 3 demonstrates the evolution of the front shape in scaling coordinates R/R_f vs $(\zeta - \zeta_f)\sqrt{|\ln \tau|/g\tau}$. It is seen that up to $\eta_a \sim 0.2$ the departure from the QSA profile (46) manifests itself only at the edges of the profile $R/R_f < 10^{-2}$.

IV. SYSTEMATIC THEORY OF THE ISLAND DEATH IN THE REVERSIBLE REGIME OF FRONT PROPAGATION

The presented QSA analysis of the crossover to the quasiequilibrium front regime imposes a strict requirement of quasistaticity $\eta_a \ll 1$ and describes the propagation of the front only to some vicinity of the critical point $|\mathcal{T}| \gg \mathcal{T}_Q \sim \sqrt{g}$. In this section we develop a free of these limitations systematic theory of perturbations in powers of $1/k$ which gives the asymtotically exact description of evolution of the quasiequilibrium distributions of $a(\zeta,\tau), b(\zeta,\tau), c(\zeta,\tau)$ and of the front profile $R(\zeta,\tau)$ up to $\tau \to \infty$. In the framework of this theory the strict substantiation of the QSA will be given and it will be shown that in the limit of small $g \to 0$ the theory automatically leads to the QSA results (47) and (50)–(52).

A. General solution

Combining Eqs. (7), (11), and (12) we find exactly

$$c = (1/2)(g - s + 2r\mathcal{F}) - \sqrt{\Phi},$$

$$a = \sqrt{\Phi} - (1/2)(g - s),$$

$$b = \sqrt{\Phi} - (1/2)(g + s), \tag{56}$$

where

$$\Phi = (1/4)(s + g)^2 + g(1 - \mathcal{F}) + R/k. \tag{57}$$

By assuming that k is sufficiently large and neglecting in (57) the term R/k for the asymptotic quasiequilibrium distribution,

$$a_a b_a = g c_a,$$

we derive the closed equations

$$c_a = (1/2)(g - s + 2r\mathcal{F}) - \sqrt{\Phi_a},$$

$$a_a = \sqrt{\Phi_a} - (1/2)(g - s),$$

$$b_a = \sqrt{\Phi_a} - (1/2)(g + s), \tag{58}$$

where

$$\Phi_a = (1/4)(s + g)^2 + g(1 - \mathcal{F}). \tag{59}$$

Substituting then a_a, b_a or c_a into Eqs. (8), from any of these equations, for example, from the equation

$$R_a = \nabla^2 a_a - \partial_t a_a,$$

we find the asymptotic quasiequilibrium reaction profile in the compact form,

$$R_a = \frac{gr(r+g+1)}{4\Phi_a^{3/2}}(\nabla\mathcal{F})^2. \tag{60}$$

Substituting R_a into the expression (57), $\Phi=\Phi_a+R/k$, and taking $R_a/k\Phi_a \ll 1$, in the linear $1/k$ approximation for $\delta a_1, \delta b_1$, and δc_1, deviations from the quasiequilibrium distributions, we have from Eqs. (56),

$$\delta a_1 = \delta b_1 = -\delta c_1 = \frac{R_a}{2k\sqrt{\Phi_a}}. \tag{61}$$

Substituting, in accordance with Eqs. (8), δa_1 into the equation

$$\delta R_1 = \nabla^2(\delta a_1) - \partial_t(\delta a_1)$$

and using Eq. (60), for the linear $1/k$ deviation δR_1 from the quasiequilibrium profile R_a we find after some transformations

$$\delta R_1 = \frac{gr(r+g+1)}{4k\Phi_a^2}[(\nabla^2\mathcal{F})^2 - 4\omega(\nabla\mathcal{F})^2\nabla^2\mathcal{F} + (3\omega^2 - m/\Phi_a) \times(\nabla\mathcal{F})^4], \tag{62}$$

where $\omega=\frac{d\ln\Phi_a}{d\mathcal{F}}$ and $m=\frac{d^2\Phi_a}{d\mathcal{F}^2}=\frac{(r+1)^2}{2}$. Substituting then $R=R_a+\delta R_1+\cdots$ into (57) and taking $R/k\Phi_a \ll 1$ for the quadratic in $1/k$ additions δa_2, δb_2, and δc_2 we find

$$\delta a_2 = \delta b_2 = -\delta c_2 = -\frac{R_a^2}{8k^2\Phi_a^{3/2}} + \frac{\delta R_1}{2k\sqrt{\Phi_a}}. \tag{63}$$

The iterative repetition of this procedure enables one, in principle, to obtain the systematic expansions

$$\delta R = \sum_{n=1}^{\infty} \delta R_n = \sum_{n=1}^{\infty} \Xi_n(x,t)/k^n,$$

$$\delta a = \delta b = -\delta c = \sum_{n=1}^{\infty} \delta a_n = \sum_{n=1}^{\infty} \Theta_n(x,t)/k^n,$$

which for large k at the condition

$$\sigma = \mathrm{Max}_x(R_a/k\Phi_a) + \mathrm{Max}_x(R_a/kgc_a) \ll 1 \tag{64}$$

rapidly collapse and can be represented by their leading terms.

According to Eq. (18) at $r,t \gg 1$ we have

$$\mathcal{F} = \exp(-x^2/4t)/\sqrt{\pi t}.$$

Substituting this expression into Eqs. (60) and (62), and going to the reduced variables $\zeta=x/x_M$ and $\tau=t/t_c$ we finally find

$$R_a(\zeta,\tau) = \frac{\pi\hat{\gamma}\gamma^3}{8er^2}\frac{g\zeta^2\exp(-\zeta^2/e\tau)}{\Phi_a^{3/2}\tau^3} \tag{65}$$

and

$$\delta R_1(\zeta,\tau) = \frac{\pi^2\hat{\gamma}\gamma^3}{16r^2}\left(\frac{g\mathcal{F}^2}{k\Phi_a^2\tau^2}\right)\{1 + 2(2\omega\mathcal{F}-1)\zeta^2/e\tau + [1-4\omega\mathcal{F} + (3\omega^2 - m/\Phi_a)\mathcal{F}^2]\zeta^4/e^2\tau^2\}, \tag{66}$$

where we have introduced the symbol $\hat{\gamma}=1+g/(r+1)$.

Equations (58)–(66) completely determine the regularities of the crossover to the reversible regime and evolution of the quasiequilibrium reaction profile up to $\tau\to\infty$. In what follows we will concentrate on the key features of the quasiequilibrium front evolution $R_a(\zeta,\tau)$ and then reveal the role of the crossover terms (66), (61), and (63).

B. Trajectories of the front center: Two turning points of the front

From Eqs. (65), (59), and (20) there appear the following key properties of the quasiequilibrium front:

(a) According to Eq. (65) at any g, r, and τ in the vicinity of the island center $R_a(\zeta\to 0)\propto\zeta^2\to 0$. This means that the center of the quasiequilibrium front $\zeta_f(\tau)$, governed by the condition $R_a(\zeta_f)=R_f^a=\mathrm{Max}_\zeta R_a$, never reaches the island center.

(b) According to Eqs. (59), (20), and (12) at large $r\gg 1$, $\Phi_a(g,\zeta,\tau)$ is independent of r and, therefore, irrespective of the initial number of particles in the island, the trajectory of the front center is the universal function $\zeta_f^{(g)}(\tau)$ for any fixed g.

(c) According to Eqs. (59) and (20) at arbitrary g in the long-time limit $\sqrt{\tau}\gg 1$ the function $\Phi_a=(1+g)^2/4+O[(g-1)/\tau^{1/2}]+O(1/\tau)$ becomes practically constant. We thus conclude that in the long-time limit all the trajectories $\zeta_f^{(g)}(\tau)$ converge to the common universal trajectory,

$$\zeta_f^{(u)} = \sqrt{e\tau}. \tag{67}$$

(d) According to Eq. (59) at small $g\ll 1$ and $\tau<1$ at the particular point $s_\star=-g$ the function Φ_a reaches a minimum. In the limit $g\to 0$ in the vicinity of the point $s_\star\to 0$ at finite $\zeta_\star$ we find from Eq. (65),

$$R_a(\zeta_\star) \sim \mathrm{Max}_\zeta R_a \sim \frac{\zeta_\star^2}{r^2\sqrt{g}\tau^2} \to \infty.$$

So, in accordance with the QSA we conclude that in the limit of small $g\to 0$ at $\zeta_\star^2 \gg \sqrt{g}$ the law of the front center motion is governed by the condition $s_\star=s(\zeta_f,\tau)=0$ whence there follows Eq. (21):

$$\zeta_f = \zeta_\star = \sqrt{e\tau|\ln\tau|}.$$

(e) According to Eq. (21), having passed through the turning point $\zeta_f^M=1$ the front center ζ_f moves towards the island center. But in accordance with Eq. (67) asymptotically the front center always moves towards $\zeta\to\infty$. So, we come to the striking conclusion that at small g the front must reverse the direction of its motion twice. Moreover, as at large g the law (67) is realized at $\sqrt{\tau}\gg 1/g$, there should exist some critical value g_c below which *two turning points* appear on the monotonous front trajectory. The numerical calculations of Eq. (65) confirm this conclusion and give $g_c\approx 0.029$.

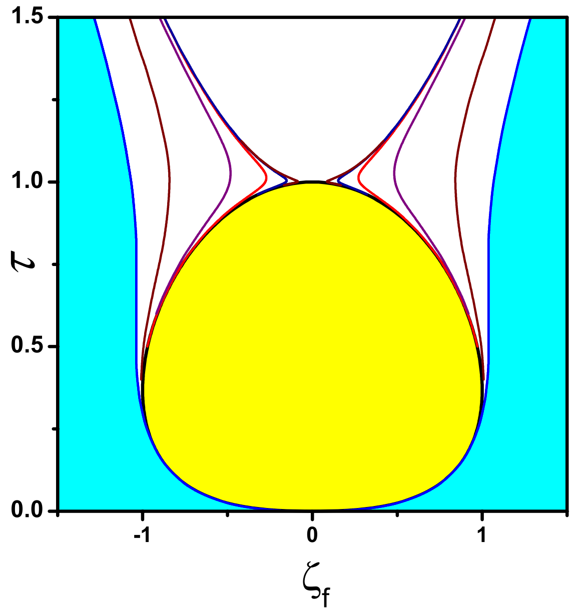

FIG. 4. (Color online) Trajectories of the front center $\zeta_f(\tau)$ calculated from Eq. (65) for the values $g=g_c=0.029$, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, and 10^{-6} (from the periphery towards the center) at $r=10^2$. For completeness is shown the motion of the both island fronts $\pm\zeta_f(\tau)$. The region restricted by the QSA trajectory (21) is colored light (yellow). The region restricted by the trajectory $g=g_c$ is colored dark (cyan).

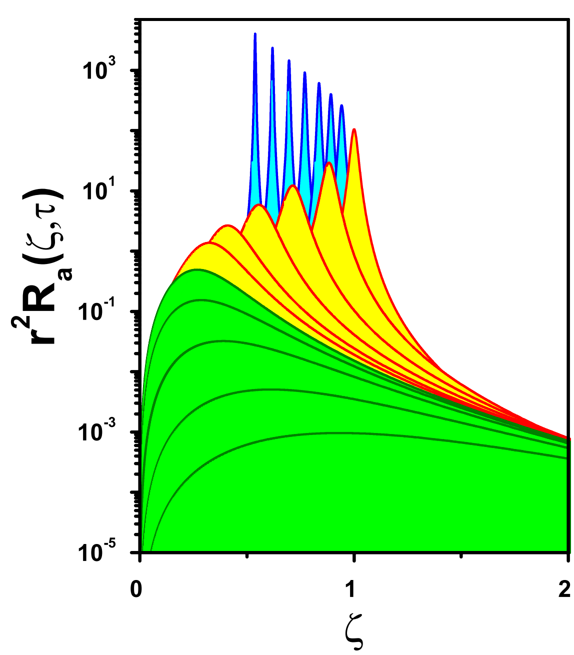

FIG. 5. (Color online) Evolution of the reaction profile $R_a(\zeta,\tau)$ calculated from Eq. (65) at $g=10^{-4}$ and $r=10^2$ for the time moments $\tau=0.03$, 0.045, 0.065, 0.09, 0.12, 0.16, 0.21, $1/e$, 0.629, 0.783, 0.877, 0.941, 0.973, 1.0045, 1.036, 1.098, 1.253, and 1.565 (from top to bottom).

As an illustration, in Fig. 4 are shown the front center trajectories $\zeta_f(\tau)$ calculated according to Eq. (65) for g values in the range from $g=g_c$ to $g=10^{-6}$ at $r=10^2$. It is seen that with the decreasing g the coordinates of the second turning point $\tau_m\to 1$ and $\zeta_f^m\to 0$. Remarkably that in the limit of small $g\to 0$ the front trajectories become universal before and after the turning point (see below). Figure 5 demonstrates the evolution of the reaction profile $R_a(\zeta,\tau)$ calculated from Eq. (65) for $g=10^{-4}$ and $r=10^2$. Our goal will be a detailed analysis of the main stages of this evolution.

C. Scaling regime of the sharp front

Using Eq. (20) we can represent Eq. (65) in the form

$$R_a(\zeta,\tau) = \frac{\text{const}\ \zeta^2(s+1)^2}{\tau^2\Phi_a^{3/2}}. \tag{68}$$

Assuming $|\zeta-\zeta_f|/\zeta_f \ll 1$, $|s|\ll 1$ and $g\to 0$ we find

$$R_a(\zeta,\tau) = \frac{\text{const}\ \zeta_f^2}{\tau^2(s^2/4+\gamma g)^{3/2}},$$

whence it immediately follows that $s_f=0$ and

$$R_a = \frac{R_f^a}{(1+z^2)^{3/2}}, \tag{69}$$

where the front amplitude R_f^a is governed by Eq. (50) and $z=-s/2\sqrt{\gamma g}$. Using the condition $|\zeta-\zeta_f|/\zeta_f\ll 1$, we find from Eq. (20),

$$s = e^{-(\zeta-\zeta_f)\zeta_f/e\tau} - 1,$$

whence, with the complementary requirement $|\zeta-\zeta_f|/\zeta_f \ll e\tau/\zeta_f^2 = 1/|\ln \tau|$ it follows that

$$s = -(\zeta-\zeta_f)\zeta_f/e\tau + \cdots . \tag{70}$$

Defining now the reduced reaction front width $\bar{w}_a$ by the condition $z=-s/2\sqrt{\gamma g}=2(\zeta-\zeta_f)/\bar{w}_a$ and using Eqs. (21) and (70), in exact agreement with the QSA result (51) we obtain

$$\bar{w}_a = w_a/x_f^M = 4\sqrt{e\gamma}\left(\frac{g\tau}{|\ln \tau|}\right)^{1/2}.$$

The presented analysis clearly demonstrates that the sharp QSA-front forms in the vicinity of the Φ_a minimum on the scale $|\zeta-\zeta_f|/\zeta_f\ll 1$ where the function $(\nabla\mathcal{F})^2 \sim \zeta^2(s+1)^2 \approx \text{const}$. As it has been mentioned, in the long-time limit $\sqrt{\tau}\gg 1$, where Φ_a becomes $\approx$const, precisely the function $(\nabla\mathcal{F})^2$ defines the shape of the reaction profile at the final relaxation stage.

D. Long-time asymptotics

In the long-time limit $\sqrt{\tau}\gg 1$ at arbitrary g we come from Eq. (65) to the scaling relaxation law

$$R_a = R_f^a\mathcal{S}\left(\frac{\zeta}{\zeta_f}\right), \quad \zeta_f = \sqrt{e\tau}, \tag{71}$$

where scaling function $\mathcal{S}(y)=y^2e^{(1-y^2)}$ and amplitude

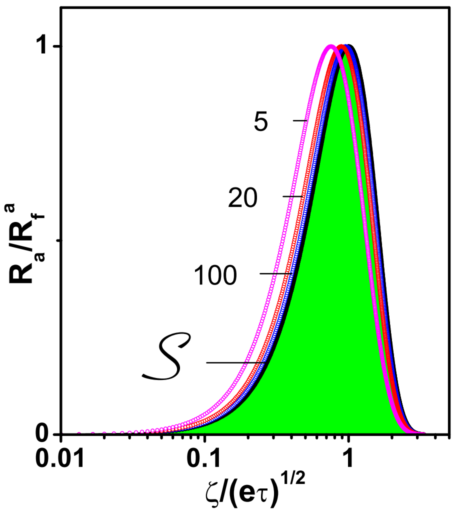

FIG. 6. (Color online) Dependences R_a/R_f^a vs $\zeta/\sqrt{e\tau}$ calculated from Eq. (65) at $g=10^{-4}$ and $r=10^2$ for $\tau=5$, 20, and 100. The region under the $\mathcal{S}$ profile (71) (solid line) is colored.

$$R_f^a = \Gamma(r,g)/\tau^2 \tag{72}$$

with

$$\Gamma(r,g) = \frac{\pi\hat{\gamma}\gamma^3}{er^2}\frac{g}{(1+g)^3}.$$

We conclude that at the final universal stage the reaction profile expands self-similarly by the trivial law $w_u \sim \zeta_f^{(u)} \propto \sqrt{\tau}$ with the rapidly decaying $\propto 1/\tau^2$ amplitude. Figure 6 demonstrates the dependences R_a/R_f^a vs $\zeta/\sqrt{e\tau}$ calculated according to Eq. (65) at $g=10^{-4}$ and $r=10^2$ for $\tau=5,20,100$. It is seen that already at $\tau>5$ the calculated dependences rapidly collapse to the scaling function $\mathcal{S}$.

E. Scaling laws of passage through the critical point

Let us now turn to the central and most interesting problem of the front evolution in the vicinity of the critical point t_c in the limit of small g. As at $g \ll 1$ and $r \gg 1$ the coefficients $\hat{\gamma}$ and γ are close to unity, in what follows we will assume for simplicity $\hat{\gamma}=\gamma=1$.

1. Trajectory of the reaction front center

Deriving the front center position ζ_f from the condition $dR_a/d\zeta=0$, from Eq. (65) we find

$$\frac{(s_f+g)(s_f+1)}{(s_f^2/4+g)} = \frac{\lambda\tau}{\zeta_f^2}(\zeta_f^2/e\tau - 1), \tag{73}$$

where $\lambda=8e/3$. Equation (73), combined with the following from (20), equation

$$s_f = \frac{e^{-\zeta_f^2/2e\tau}}{\sqrt{\tau}} - 1 \tag{74}$$

completely determines the dynamics of the front center motion $\zeta_f(\tau)$. At the stage of the quasistatic regime, taking $|\ln \tau| \gg \sqrt{g}$, we find from (73) and (74),

$$\zeta_f = \sqrt{e\tau|\ln \tau|}(1+\epsilon_f), \tag{75}$$

where

$$\epsilon_f = -\frac{s_f}{|\ln \tau|} = \frac{g}{|\ln \tau|}\left(1 + \frac{8}{3}\frac{(1-|\ln \tau|)}{|\ln \tau|} + O(g)\right).$$

Equation (75) determines the exact correction to the law of the quasistatic front motion (21) dictated by the finiteness of g. It is seen that in the vicinity of the critical point $|\mathcal{T}|=|\tau-1| \ll 1$ in agreement with the quasistaticity condition $\eta_a \ll 1$ the requirement $\epsilon_f \ll 1$ is reduced to the requirement $|\mathcal{T}| \gg \sqrt{g}$. Assuming that at either side of the critical point $|\mathcal{T}|$, $|s_f|$, $\zeta_f \ll 1$, we come from Eqs. (73) and (74) to the compact equation for the trajectory of passage through the critical point

$$s_f = -(2/\lambda)(\zeta_f^2 \mp \sqrt{\zeta_f^4 - g\lambda^2}), \tag{76}$$

whence for the coordinate $\zeta_f^m = \min \zeta_f$ of the front turning point we immediately find

$$\zeta_f^m = \sqrt{\lambda} g^{1/4}, \quad s_f^m = -2\sqrt{g}. \tag{77}$$

According to Eq. (74) at small $|\mathcal{T}| \ll 1$ and $\zeta_f^2 \ll 1$ we have

$$s_f = -\mathcal{T}/2 - \zeta_f^2/2e + \cdots. \tag{78}$$

Substituting (77) into Eq. (78) we obtain

$$\mathcal{T}_m = (4/3)\sqrt{g}. \tag{79}$$

Substituting then Eq. (78) into Eq. (76) we finally derive

$$\zeta_f = \sqrt{(e/4)[(3^2\mathcal{T}^2 + 2^7 g)^{1/2} - \mathcal{T}]}. \tag{80}$$

Equation (80) suggests that in the vicinity of the critical point the trajectory of the front center demonstrates the remarkable property of *self-similarity*,

$$\zeta_f = g^{1/4}\Lambda(\mathcal{T}/g^{1/2}).$$

Introducing the reduced coordinate $\mathsf{z}=\zeta/g^{1/4}$ and time $\mathsf{T} = \mathcal{T}/g^{1/2}$ we have

$$\mathsf{z}_f = \Lambda(\mathsf{T}), \tag{81}$$

where $\mathsf{z}_f^m = \sqrt{\lambda}$ and $\mathsf{T}_m = 4/3$. According to Eq. (80) at large $|\mathsf{T}| \gg 1$ the scaling function $\Lambda(\mathsf{T})$ has the asymptotics

$$\Lambda = \sqrt{e|\mathsf{T}|}(1 + 8/3\mathsf{T}^2 + \cdots), \quad -\mathsf{T} \gg 1 \tag{82}$$

and

$$\Lambda = \sqrt{e\mathsf{T}/2}(1 + 16/3\mathsf{T}^2 + \cdots), \quad \mathsf{T} \gg 1. \tag{83}$$

We thus conclude that beyond the vicinity $|\delta\mathcal{T}| \propto g^{1/2} \to 0$ the trajectories of the front center go to the universal (g-independent) asymptotics

$$\zeta_f^{(-)}(\mathcal{T}<0) = \sqrt{e|\mathcal{T}|} + \cdots$$

and

$$\zeta_f^{(+)}(\mathcal{T}>0) = \sqrt{e\mathcal{T}/2} + \cdots.$$

Figure 7 shows the calculated, according to Eq. (80), trajectory of the front center in scaling variables z_f vs T. Also are

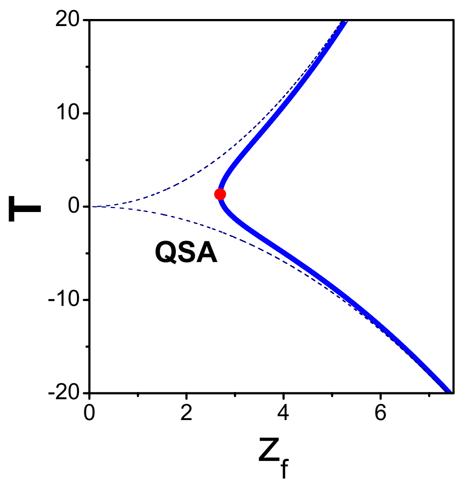

FIG. 7. (Color online) Trajectory of the front center passage through the critical point in the scaling variables $\mathsf{z}_f=\zeta_f/g^{1/4}$ vs $\mathsf{T}=\mathcal{T}/g^{1/2}$ calculated according to Eq. (80). The universal asymptotics $\zeta_f^{(-)}$ (QSA) and $\zeta_f^{(+)}$ are shown in the dashed lines. The red circle marks the position of the second turning point of the front.

shown the universal asymptotics $\zeta_f^{(-)}$ (QSA) and $\zeta_f^{(+)}$. Figure 8 demonstrates the data of Fig. 4 replotted in the rescaled variables $\zeta_f/g^{1/4}$ vs $(\tau-1)/g^{1/2}$ for the values of g in the range from 10^{-2} to 10^{-6}. It is seen that as g is decreased the rescaled trajectories rapidly collapse to the scaling function $\Lambda(\mathsf{T})$.

2. Amplitude and shape of the front

We will assume in accordance with Eq. (81) that g is sufficiently small so that $|\mathsf{T}|$ and z may change within broad limits without violating the requirement of smallness of $|\mathcal{T}|\ll 1$, $|s|\ll 1$, and $\zeta \ll 1$. Then from Eqs. (65) and (20) we come to the scaling law of the front profile evolution

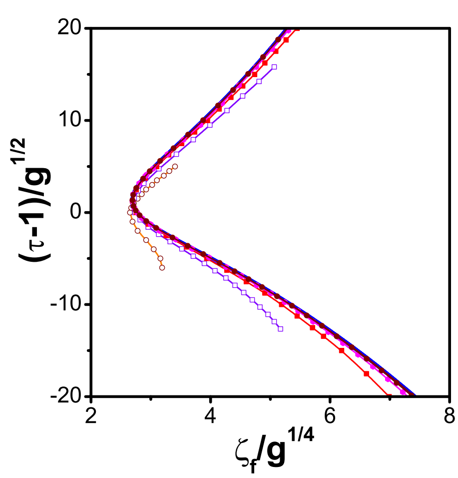

FIG. 8. (Color online) Collapse of the data of Fig. 4 to the scaling function $\Lambda(\mathsf{T})$ (line). The trajectories $\zeta_f(\tau)$ are replotted in the rescaled variables $\zeta_f/g^{1/4}$ vs $(\tau-1)/g^{1/2}$ for the values $g=10^{-2}$ (open circles), 10^{-3} (open squares), 10^{-4} (filled squares), 10^{-5} (filled hexagons), and 10^{-6} (filled circles).

$$R_a=\left(\frac{\pi}{8er^2}\right)\Psi(\mathsf{z},\mathsf{T}), \tag{84}$$

where the scaling function

$$\Psi(\mathsf{z},\mathsf{T})=\mathsf{z}^2/(\mathsf{s}^2/4+1)^{3/2}$$

and

$$\mathsf{s}=s/g^{1/2}=-\mathsf{T}/2-\mathsf{z}^2/2e+\cdots . \tag{85}$$

Substituting into Eq. (84), $\mathsf{z}=\mathsf{z}_f(\mathsf{T})$, for the front amplitude we find

$$R_f^a=\left(\frac{\pi}{8er^2}\right)\Psi_f(\mathsf{T}), \tag{86}$$

where at large $|\mathsf{T}|\gg 1$ the scaling function $\Psi_f(\mathsf{T})$ has the asymptotics

$$\Psi_f=e|\mathsf{T}|(1+8/3\mathsf{T}^2+\cdots), \quad -\mathsf{T}\gg 1$$

and

$$\Psi_f=\left(\frac{256e}{27}\right)\frac{(1-8/3\mathsf{T}^2+\cdots)}{\mathsf{T}^2}, \quad \mathsf{T}\gg 1.$$

From Eq. (86) there follow two remarkable consequences:

(1) In the second turning point the front amplitude does not depend on g. Substituting into Eq. (86), $\mathsf{T}_m=4/3$, we obtain

$$(R_f^a)_m=(\pi/6\sqrt{2})/r^2. \tag{87}$$

Moreover, the ratio of the front amplitudes in the first and second turning points does not depend on the initial number of the island particles

$$(R_f^a)_m/(R_f^a)_M=(4/3e\sqrt{2})\sqrt{g}.$$

(2) In the limit $g\to 0$ the passage through the critical point is accompanied by a sharp drop of the front amplitude ($|\mathsf{T}|\to 1/\mathsf{T}^2$) on the vanishingly small time scale $|\delta\mathcal{T}|\propto g^{1/2}\to 0$ (*amplitude jump*).

In Fig. 9 is shown the calculated from Eq. (86) time dependence of R_f^a in the vicinity of the critical point, $r^2R_f^a$ vs T. Also there are shown the power asymptotics $R_f^{(-)}=\text{const}|\mathsf{T}|$ (QSA) and $R_f^{(+)}=\text{const}/\mathsf{T}^2$.

Let us now focus on the evolution of the scaling function of the front profile, $\Psi(\mathsf{z},\mathsf{T})$, which is convenient to represent in the form

$$\Psi(\mathsf{z},\mathsf{T})=\frac{\mathsf{z}^2}{[\alpha(\mathsf{z}^2+e\mathsf{T})^2+1]^{3/2}} \tag{88}$$

with $\alpha=1/16e^2$. Using Eqs. (82) and (83), and neglecting the term $O(1/\mathsf{z}_f^2)$ in parentheses, we come from Eq. (88) at large $|\mathsf{T}|\gg 1$ to the asymptotics

$$\Psi=\frac{\mathsf{z}^2}{[\alpha(\mathsf{z}^2-\mathsf{z}_f^2)^2+1]^{3/2}}, \quad -\mathsf{T}\gg 1 \tag{89}$$

and

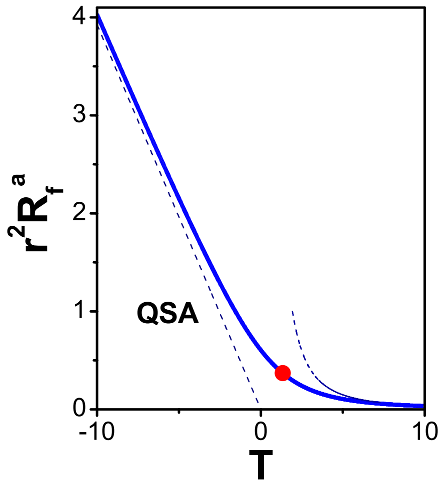

FIG. 9. (Color online) Time dependence of the front amplitude during the passage through the critical point plotted according to Eq. (86) in the scaling variables $r^2R_f^a$ vs $\mathsf{T}=\mathcal{T}/g^{1/2}$. The power asymptotics $R_f^{(-)}$ (QSA) and $R_f^{(+)}$ are shown in the dashed lines. The red circle marks the position of the second turning point of the front.

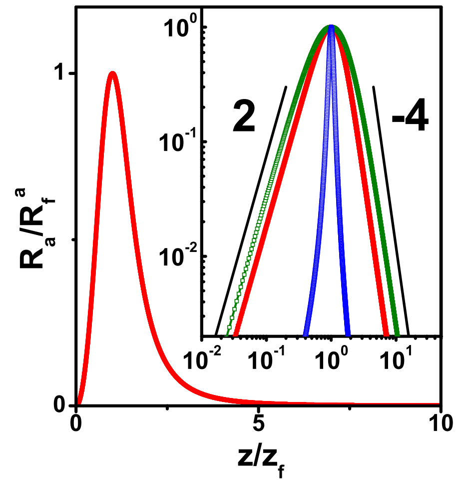

FIG. 10. (Color online) Evolution of the front profile during the passage through the critical point. Inset: Dependences R_a/R_f^a vs z/z_f in double logarithmic coordinates, calculated according to Eq. (88) for $\mathsf{T}=-10$ (open circles), $\mathsf{T}=0$ (line), and $\mathsf{T}=10$ (open squares). Main panel: Front profile R_a/R_f^a vs z/z_f at the critical point $\mathsf{T}=0$.

$$\Psi = \frac{\mathsf{z}^2}{[\alpha(\mathsf{z}^2+2\mathsf{z}_f^2)^2+1]^{3/2}}, \quad \mathsf{T} \gg 1. \tag{90}$$

Equations (88)–(90) give a clear picture of the front profile transformation at the passage through the critical point. The picture is reduced to the following:

(1) Away from the front center z_f the function $\Psi(\mathsf{z})$ at any $|\mathsf{T}|$ decays asymmetrically by the laws $\propto \mathsf{z}^2$ ($\mathsf{z} \ll \mathsf{z}_f$) and $\propto 1/\mathsf{z}^4$ ($\mathsf{z} \gg \mathsf{z}_f$).

(2) In the limit $-\mathsf{T} \gg 1 (\mathsf{z}_f \gg 1)$ in the range $1/\mathsf{z}_f \ll |\mathsf{z}-\mathsf{z}_f| \ll \mathsf{z}_f$ the periphery asymmetric $\mathsf{z}^2 - 1/\mathsf{z}^4$ "tails" are dominated by the sharp symmetric QSA profile $R_a/R_f^a \propto 1/|(\mathsf{z}-\mathsf{z}_f)\mathsf{z}_f|^3$ with the width $w \propto 1/\mathsf{z}_f$.

(3) In the limit $\mathsf{T} \gg 1$ the front profile R_a/R_f^a becomes a universal function of z/z_f that decays by the laws $(\mathsf{z}/\mathsf{z}_f)^2$ and $(\mathsf{z}_f/\mathsf{z})^4$ on the left- and right-hand sides of the front center with the front width $w \propto \mathsf{z}_f$.

We thus arrive at the remarkable conclusion: In the limit $g \to 0$ the passage through the critical point is accompanied by a sharp front broadening $1/\mathsf{z}_f \to \mathsf{z}_f$ and by a radical transformation of its shape on the vanishingly small time scale $|\delta\mathcal{T}| \propto g^{1/2} \to 0$ (abrupt "*delocalization*" of the front). As an illustration, in Fig. 10 are shown the dependences R_a/R_f^a vs z/z_f calculated in accord with Eq. (84) for three time moments $\mathsf{T}=-10$, $\mathsf{T}=0$, and $\mathsf{T}=10$.

3. Distribution of particles

From Eqs. (58) and (59) it follows that in the limit of small g during the passage through the critical point the concentration of particles C in a broad range of z and T is $c_a(\mathsf{z},\mathsf{T})=1$, and distribution of particles A and B is described by the scaling law

$$a_a = g/b_a = g^{1/2}\mathcal{L}(\mathsf{z},\mathsf{T}), \tag{91}$$

where the scaling function

$$\mathcal{L}(\mathsf{z},\mathsf{T}) = \mathcal{L}(\mathsf{s}) = \sqrt{\mathsf{s}^2/4+1} + \mathsf{s}/2 \tag{92}$$

and the function $\mathsf{s}(\mathsf{z},\mathsf{T})$ is defined by Eq. (85). Substituting here $\mathsf{z}=\mathsf{z}_f(\mathsf{T})$ and introducing the reduced concentrations $\mathsf{a}=a_a/g^{1/2}$ and $\mathsf{b}=b_a/g^{1/2}$ for the concentrations of particles in the front center we find

$$\mathsf{a}_f = 1/\mathsf{b}_f = \mathcal{L}_f(\mathsf{T}), \tag{93}$$

where the scaling function $\mathcal{L}_f(\mathsf{T})$ at large $|\mathsf{T}| \gg 1$ has the asymptotics

$$\mathcal{L}_f = 1 - 4/3|\mathsf{T}| + \cdots, \quad -\mathsf{T} \gg 1$$

and

$$\mathcal{L}_f = \left(\frac{4}{3}\right)\frac{(1-16/3\mathsf{T}^2+\cdots)}{\mathsf{T}}, \quad \mathsf{T} \gg 1.$$

Substituting now $\mathsf{s}_f^m=-2$ into Eq. (92) we find that in the second turning point

$$\mathsf{a}_f^m = \sqrt{2}-1, \quad \mathsf{b}_f^m = \sqrt{2}+1. \tag{94}$$

Figure 11 demonstrates the dependences $\mathsf{a}_f(\mathsf{T})$ and $\mathsf{b}_f(\mathsf{T})$ calculated according to Eqs. (92), (85), and (81). It is seen that the passage through the critical point is accompanied by a sharp growth of the B particles concentration so that in the limit $g \to 0$ their concentration growth by a finite number on the time scale $|\delta\mathcal{T}| \propto g^{1/2} \to 0$.

According to Eqs. (85) and (92) during the passage through the critical point:

(1) The tail of $\mathcal{L}$ distribution at $\mathsf{z}/\mathsf{z}_f \gg 1$ independently of T decays as $\mathcal{L}(\mathsf{z}) \propto 1/\mathsf{z}^2$.

(2) At large $-\mathsf{T} \gg 1$ and $|\delta\mathsf{z}|/\mathsf{z}_f = |\mathsf{z}-\mathsf{z}_f|/\mathsf{z}_f \ll 1$ the distribution of particles is reduced to the QSA scaling $\mathcal{L}(\mathsf{s}) = \mathcal{A}(-\mathsf{s}/2) = \mathcal{B}(\mathsf{s}/2)$. Beyond the narrow zone $|\delta\mathsf{z}|/\mathsf{z}_f \gg 1/|\mathsf{T}|$ we find

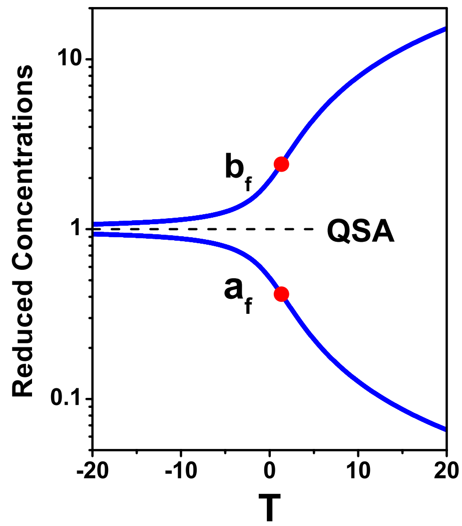

FIG. 11. (Color online) Time dependences of passage through the critical point of the reduced concentrations in the front center $\mathsf{a}_f = a_f^a/g^{1/2}$ and $\mathsf{b}_f = b_f^a/g^{1/2}$ vs $\mathsf{T} = \mathcal{T}/g^{1/2}$, calculated according to Eq. (93). The red circles mark the second turning point of the front.

$$\mathcal{L}/\mathcal{L}_f = \tfrac{1}{2}|\mathsf{T}|[1-(\mathsf{z}/\mathsf{z}_f)^2], \quad -\mathsf{T} \gg 1, \quad \mathsf{z} < \mathsf{z}_f$$

and

$$\mathcal{L}/\mathcal{L}_f = \frac{2}{|\mathsf{T}|[(\mathsf{z}/\mathsf{z}_f)^2-1]}, \quad -\mathsf{T} \gg 1, \quad \mathsf{z} > \mathsf{z}_f.$$

(3) In the limit $\mathsf{T} \gg 1$ the distribution of particles becomes the universal function of z/z_f,

$$\mathcal{L}/\mathcal{L}_f = \frac{3}{[2+(\mathsf{z}/\mathsf{z}_f)^2]}, \quad \mathsf{T} \gg 1.$$

Comparing the concentration gradients at the front center $\nabla \ln \mathcal{L}|_{\mathsf{z}_f} \sim |\mathsf{T}|$ at $-\mathsf{T} \gg 1$ and $\nabla \ln \mathcal{L}|_{\mathsf{z}_f} \sim 1$ at $\mathsf{T} \gg 1$ we conclude that during the passage through the critical point an *abrupt delocalization* of the front is accompanied by an abrupt "*smoothing*" of the distribution of particles.

4. Global reaction rate and number of island particles

To complete the theory of passage through the critical point it remains for us to reveal the laws of decay of the number of island particles, N, and of the global reaction rate R_G. Substituting Eq. (91) into the expression for the number of island particles

$$N = \int_0^\infty a_a dx = x_f^M \int_0^\infty a_a d\zeta,$$

we find

$$N/N_0 = \sqrt{\frac{2}{\pi e}} g^{3/4} \mathcal{L}_N(\mathsf{T}), \tag{95}$$

where the scaling function

$$\mathcal{L}_N(\mathsf{T}) = \int_0^\infty \mathcal{L}(\mathsf{z},\mathsf{T}) d\mathsf{z}$$

at large $|\mathsf{T}| \gg 1$ has the asymptotics

$$\mathcal{L}_N = \tfrac{1}{3}\sqrt{e}|\mathsf{T}|^{3/2} + O(|\mathsf{T}|^{1/2}\ln|\mathsf{T}|), \quad -\mathsf{T} \gg 1$$

and

$$\mathcal{L}_N = \frac{\pi\sqrt{e}}{\mathsf{T}^{1/2}} - O(\mathsf{T}^{-5/2}), \quad \mathsf{T} \gg 1.$$

Substituting Eq. (84) into the expression for global reaction rate

$$R_G = -\dot{N} = \int_0^\infty R_a dx = x_f^M \int_0^\infty R_a d\zeta,$$

we find

$$R_G = \left(\frac{\sqrt{2\pi/e^3}}{8r}\right) g^{1/4} \Psi_G(\mathsf{T}), \tag{96}$$

where in accordance with Eq. (95) the scaling function

$$\Psi_G(\mathsf{T}) = \int_0^\infty \Psi(\mathsf{z},\mathsf{T}) d\mathsf{z}$$

at large $|\mathsf{T}| \gg 1$ has the asymptotics

$$\Psi_G = 4\sqrt{e^3}|\mathsf{T}|^{1/2} + O\left(\frac{\ln|\mathsf{T}|}{|\mathsf{T}|^{1/2}}\right), \quad -\mathsf{T} \gg 1$$

and

$$\Psi_G = \frac{4\pi\sqrt{e^3}}{\mathsf{T}^{3/2}} - O(\mathsf{T}^{-7/2}), \quad \mathsf{T} \gg 1.$$

As it is to be expected the passage through the critical point is accompanied by a sharp drop of the island particles number ($|\mathsf{T}|^{3/2} \to 1/\mathsf{T}^{1/2}$) and of the global reaction rate ($|\mathsf{T}|^{1/2} \to 1/\mathsf{T}^{3/2}$) on the time scale $|\delta\mathcal{T}| \propto g^{1/2} \to 0$.

V. CROSSOVER TERMS

According to the general QSA analysis the key condition of the island death in the quasiequilibrium front regime is reduced to the requirement (49) which in consistence with (52) and (64) may be rewritten in the form

$$k_\star/k = (g_\star/g)^{3/2} \ll 1, \tag{97}$$

where $k_\star = 1/r^2 g^{3/2}$ and $g_\star = 1/(r^2 k)^{2/3}$. This condition is mainly based on the key requirement $|\delta R_1^f|/R_f^a \ll 1$. But in accord with Eqs. (65) and (66) in view of $R_a|_{\zeta=0} = 0$ in the vicinity of the island center $\zeta = 0$ the dominant contribution to R is made precisely by the crossover term δR_1 which forms a satellite maximum of R. In this section we give a complete analysis of the contribution of the crossover terms in the limit of small g and demonstrate that the requirement (97) is the necessary and sufficient condition for the island death in the quasiequilibrium regime. For simplicity we will take $\hat{\gamma} = \gamma = 1$.

A. Sharp front regime

We start with the analysis of the correction $\delta R_1(\zeta,\tau)$ in the sharp front regime $|\ln\tau| \gg \sqrt{g}$. Assuming that $|s| \ll 1$ and neglecting, as compared with $|s|$, the terms $O(g)$ we find from Eq. (59),

$$\omega\mathcal{F} = s/2\Phi_a, \tag{98}$$

whence taking $\sqrt{g} \ll |s| \ll |\ln\tau|$ with allowance for Eq. (70) we derive

$$|\omega|\mathcal{F}\zeta_f^2/e\tau \sim \frac{|\ln\tau|}{|s|} \sim \frac{\zeta_f}{|\zeta-\zeta_f|}. \tag{99}$$

From Eqs. (66) and (99) it immediately follows that in the vicinity of the front center $|\zeta-\zeta_f|/\zeta_f \ll 1$ the dominant contribution to δR_1 is made by the term in the curly brackets in (66) proportional to $\zeta^4/(e\tau)^2$. According to Eq. (98) the leading coefficient for this term may be represented in the form

$$(3\omega^2 - m/\Phi_a)\mathcal{F}^2 = \left(\frac{5}{8}\right)\frac{(s^2-4g/5)}{\Phi_a^2}. \tag{100}$$

Substituting Eq. (100) into Eq. (66) we finally obtain

$$\delta R_1 = \left(\frac{5\pi^2 g g_\star^{3/2}}{128 r^2}\right)\left(\frac{|\ln\tau|}{\tau}\right)^2\frac{(s^2-4g/5)}{\Phi_a^4}. \tag{101}$$

One can easily be convinced that Eq. (101) exactly reproduces the QSA structure of δR_1 with a deep minimum in the front center and two symmetric lateral maxima at $s=\mp 2\sqrt{g}$. Indeed, in the front center from Eq. (101) we find

$$\delta R_1^f = -\frac{\pi^2}{32 r^2 g^{1/2}}\left(\frac{g_\star}{g}\right)^{3/2}\left(\frac{|\ln\tau|}{\tau}\right)^2, \tag{102}$$

whence in accordance with the QSA result (52) there follows

$$\frac{\delta R_1^f}{R_f^a} = -\phi/2 = -\frac{\pi}{4}\left(\frac{g_\star}{g}\right)^{3/2}\frac{|\ln\tau|}{\tau}.$$

At large $|\mathsf{s}| = |s|/\sqrt{g} \gg 1$ in accordance with the QSA equations (47) δR_1 rapidly decays by the law

$$\frac{\delta R_1}{|\delta R_1^f|} = \frac{320}{\mathsf{s}^6}.$$

As an illustration, in Fig. 12 we show the dependences $R_a(\zeta)$ and $\delta R_1(\zeta)$ calculated according to Eqs. (65) and (66) for the time moment of the first turning of the front $\tau=1/e$ ($\zeta_f=1$) at $g_\star=10^{-6}$, $g=10^{-4}$, and $r=10^2$.

B. Passage through the critical point

From Eqs. (65) and (66) it follows that in the island center $\zeta=0$ where $R_a(0)\equiv 0$ the crossover term $\delta R_1(0)$ forms a local maximum of R which at small $\tau \ll \tau_+ = 1/9$ decays by the law

$$\delta R_1(0) = \frac{\pi^2}{r^2}\left(\frac{g_\star}{g}\right)^{3/2}\frac{g^{5/2}}{\tau}, \quad \tau \ll \tau_+,$$

and then, reaching a minimum in the point τ_+, begins to rapidly grow by the law (Fig. 13)

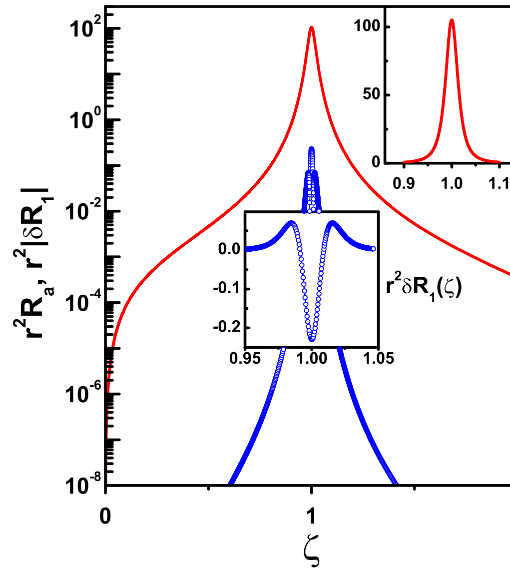

FIG. 12. (Color online) Main panel: Dependences $r^2R_a(\zeta)$ (filled circles) and $r^2|\delta R_1(\zeta)|$ (open circles) plotted in semilogarithmic coordinates according to Eqs. (65) and (66) for the moment of the first turning of the front $\tau=1/e$ ($\zeta_f=1$) at $g_\star=10^{-6}$, $g=10^{-4}$, and $r=10^2$. Insets: Dependences $r^2R_a(\zeta)$ and $r^2\delta R_1(\zeta)$ in the vicinity of the reaction front.

$$\delta R_1(0) = \frac{16\pi^2}{r^2}\left(\frac{g_\star}{g}\right)^{3/2}\frac{\sqrt{g}}{\mathsf{T}^4}, \quad -\mathsf{T} \gg 1,$$

so that according to Eq. (102) the approach to the critical point is accompanied by a sharp growth of the ratio

$$\frac{\delta R_1(0)}{|\delta R_1^f|} \propto \frac{1}{\mathsf{T}^6}, \quad -\mathsf{T} \gg 1. \tag{103}$$

Using Eq. (76) one can easily be convinced that during the passage through the critical point at the front center $|\omega|\mathcal{F}\zeta_f^2 \sim m\mathcal{F}^2\zeta_f^4/s_f^2 \sim O(1)$ and, therefore, $|\delta R_1^f| \approx \delta R_1(0)$ [the same

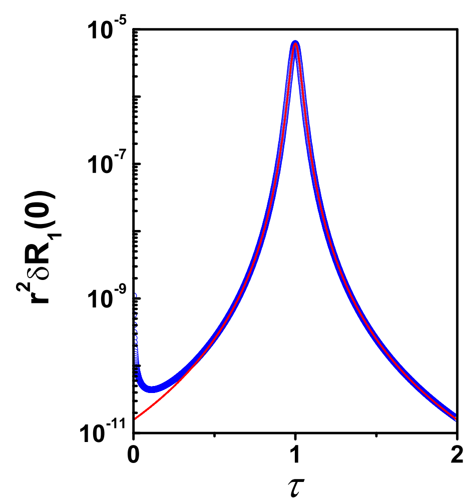

FIG. 13. (Color online) Dependences $r^2\delta R_1(0)$ vs τ calculated according to Eqs. (66) (open circles) and (104) (solid line) at $g_\star=10^{-6}$, $g=10^{-4}$, and $r=10^2$.

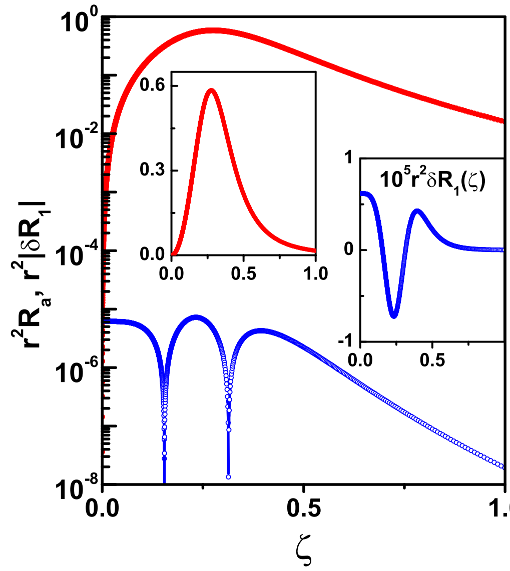

FIG. 14. (Color online) Main panel: Dependences $r^2R_a(\zeta)$ (filled circles) and $r^2|\delta R_1(\zeta)|$ (open circles) plotted in semilogarithmic coordinates according to Eqs. (65) and (66) for the critical point $\tau=1$ at $g_\star=10^{-6}$, $g=10^{-4}$, and $r=10^2$. Insets: Dependences $r^2R_a(\zeta)$ and $10^5r^2\delta R_1(\zeta)$.

result is yielded by the direct extrapolation of Eq. (103) to the critical point domain $|\mathrm{T}|\sim 1$]. Moreover, the numerical calculations show that during the passage through the critical point $\mathrm{Max}_\zeta|\delta R_1|\sim\delta R_1(0)$ (Fig. 14). From Eq. (66) we find that in a wide $|\mathcal{T}|$ range (see Fig. 13)

$$\delta R_1(0)=\frac{\pi^2}{16r^2}\left(\frac{g_\star}{g}\right)^{3/2}\frac{\sqrt{g}}{(1+\mathrm{T}^2/16)^2}, \qquad (104)$$

whence it follows that in the critical point $\mathrm{T}=0\,\delta R_1(0)$ passes through a sharp maximum

$$\mathrm{Max}\ \delta R_1(0)=\frac{\pi^2\sqrt{g}}{16r^2}\left(\frac{g_\star}{g}\right)^{3/2}.$$

By comparing Eqs. (86) and (104) we finally obtain

$$\mathrm{Max}\frac{\delta R_1(0)}{R_f^a}\sim\sqrt{g}\left(\frac{g_\star}{g}\right)^{3/2} \qquad (105)$$

and conclude that at $g_\star \ll g \ll 1$ the influence of the crossover term δR_1 on the evolution of the quasiequilibrium reaction profile R_a may be neglected. The analysis of the corrections δa_1 [Eq. (61)] and $\delta a_2(0)$ [Eq. (63)] suggests the analogous conclusion.

VI. CONCLUSION

In this paper, a systematic theory of propagation of the reaction front $A+B\leftrightarrow C$ in the process of death of an A-particle island in the B-particle sea has been developed and a rich dynamical picture of front evolution has been revealed. The main results may be formulated as follows.

(1) In terms of the QSA a systematic analysis of the crossover from the irreversible to reversible regime of front propagation has been given and the general scaling structure of the sharp quasiequilibrium front has been revealed.

(2) The key condition has been found for the island death in the regime of the quasiequilibrium front.

(3) The systematic perturbation expansion in powers of $1/k$ has been given on the base of which the asymptotically exact description has been derived for the evolution of the quasiequilibrium front profile and distribution of particles up to $\tau\to\infty$.

(4) It has been found that below some critical value of the reduced backward reaction constant $g<g_c$ there appear *two turning points* on the front trajectory. The evolution of the amplitude, width, and configuration of the quasiequilibrium front has been studied in detail in the limit of small g.

(5) It has been shown that (a) the first turning of the front is due to the finite number of island particles and is located on the QSA branch of the trajectory (sharp localized front) so that at the passage through the turning point the structure of the front does not change, (b) the second turning of the front is the result of its radical transformation (*delocalization* of the front) during the passage through the critical point.

(6) A remarkable property of *self-similarity* of the passage through the critical point has been discovered. The scaling laws of passage through the critical point have been derived for the trajectory, amplitude, and configuration of the front and, also, for the distribution of particles, global reaction rate, and the number of island particles. It has been shown that in the singular limit $g\to 0$ these laws lead to a striking consequence, namely, to an *abrupt delocalization* of the front on the time scale $|\delta\mathcal{T}|\propto g^{1/2}\to 0$.

We believe that the presented systematic theory may serve as a basis for the description of propagation and evolution of a quasiequilibrium front in a broad range of finite particle number systems including the systems localized A-particle source–B-particle sea [30] and A-particle island–B-particle island [31,32]. Moreover, we hope that the presented theory provides a solid basis for generalization to important cases of one-dimensional fluctuation front and unequal particle diffusivities. Of particular interest is a formal analogy between the passage through the critical point in the island-sea problem and the passage through the critical point in the problem of annihilation on the catalytic surface of a restricted medium, where for unequal species diffusivities in a recent series of papers [33], the phenomenon of annihilation catastrophe (singular jump of the flux relaxation rate) has been discovered. We are planing to reveal the reasons for such analogy in a future paper.

ACKNOWLEDGMENTS

I wish to thank Misha Sinder who attracted my attention to the generalization of the island-sea problem [24] for the reversible reaction. He informed me that in the asymptotic limit $t\to\infty$ the main terms of the distribution of particles and of the front profile [Eqs. (58)–(60)] may be derived by analogy with the sea-sea problem [27,28]. This communication became a starting stimulus for performing of the present work. This research was financially supported by the RFBR through Grants No. 08-03-00554 and No. 05-03-33143.

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