Crossover in nonequilibrium multicritical phenomena of reaction-diffusion systems

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A field-theoretic renormalization-group method is used to investigate crossover behavior in nonequilibrium multicritical phenomena of one-component reaction-diffusion systems. A system composed of $2n-1$ reactions, $lX \rightarrow l'X$ $(l>l')$, $lX \rightarrow l''X$ $(l<l'')$ (with $l=1,2,\ldots,n-1$), and $nX \rightarrow n'X$ $(n>n')$, is discussed. An expression for crossover exponents is derived and mean-field values of them are obtained as a function of n. For the process of $n=3$, the crossover exponent is determined to first order in $\epsilon=d_c-d$ $(d_c=3)$ and logarithmic corrections to scaling at $d=d_c$ are calculated.

I. INTRODUCTION

In a recent paper[1] (hereafter referred to as I), we investigated nonequilibrium critical phenomena of one-component reaction-diffusion systems on the basis of a field-theoretic renormalization-group method and clarified the breakdown of the fluctuation-dissipation theorem and the existence of two different susceptibility exponents. There, a superposition of three reactions of type

$$mX \rightarrow m'X \quad (m>m') , \tag{1.1}$$

$$mX \rightarrow m''X \quad (m<m'') , \tag{1.2}$$

$$nX \rightarrow n'X \quad (n>n') \tag{1.3}$$

was discussed. The lowest-order system, $m=1$ and $n=2$, corresponds to Schlögl's first model[2,3] and is equivalent to the Reggeon field theory[4] and directed percolation.[5] Using the Fock-space formalism,[6] we found that the action describing higher-order processes shows higher-order critical behavior belonging to different universality classes from that of Schlögl's first model. In the comment on the paper by Elderfield and Wilby,[7] where the same subject was treated erroneously, Janssen[8] pointed out that microscopically higher-order reaction systems do not necessarily exhibit higher-order critical phenomena.[9] Multicritical behavior appears when not microscopic but global lower-order reactions on a macroscopic scale vanish. For example, we can expect the existence of multicritical (tricritical) phenomena in a system with both first- and second-order reactions,[10]

$$X \xrightarrow{k_1^-} 0 , \tag{1.4}$$

$$X \xrightarrow{k_1^+} 2X , \tag{1.5}$$

$$2X \xrightarrow{k_2^-} X , \tag{1.6}$$

$$2X \xrightarrow{k_2^+} 3X , \tag{1.7}$$

$$3X \xrightarrow{k_3^-} 2X , \tag{1.8}$$

where k is a rate constant, but generally the multicritical point is not located at $k_2^-=k_2^+=0$. Then microscopically higher-order systems, e.g., $X\rightarrow 0$, $X \rightarrow 3X$, and $3X \rightarrow X$, may belong to the same universality class as Schlögl's first model. In order to observe multicritical behavior, we have to consider combinations of both lower- and higher-order reactions, where crossover behavior plays a significant role. As is seen in I and thermal critical phenonmena, field-theoretic renormalization-group techniques based upon different regularization schemes give different critical points and provide no information on nonuniversal quantities in terms of microscopic variables. However, they are powerful tools to study universal properties like crossover behavior. The purpose of this paper is to investigate crossover behavior around multicritical points and to complete our work on nonequilibrium critical phenomena in one-component reaction-diffusion systems.

In Sec. II we construct a general field-theoretic formalism. An expression for crossover exponents is derived and their mean-field values are given. Section III is devoted to explicit calculations by an ϵ-expansion scheme for the process (1.4)–(1.8). We compute the crossover exponent to first order in $\epsilon=d_c-d$ and logarithmic corrections to scaling at $d=d_c$.

II. GENERAL FORMALISM

Most generally, one-component reaction-diffusion systems are expressed as the superposition of reactions of type

$$mX \xrightarrow{k_{mn}} nX , \tag{2.1}$$

where m particles are transformed into n particles with a rate constant k_{mn}. The Fock-space formalism[6] gives an action describing the process (2.1),

$$L=\int dt \int d\mathbf{r} \left[\tilde{\Phi}(\dot{\Phi}-D\,\Delta\Phi)-\sum_m \sum_l K_{ml}\tilde{\Phi}^{\,l}\Phi^m\right] , \tag{2.2}$$

$$K_{ml}=\sum_n ({}_nC_l-{}_mC_l)k_{mn}/n! , \tag{2.3}$$

where $\tilde{\Phi}$ and Φ are fields representing creation and annihilation of particles and D is a diffusion coefficient. Since engineering dimensions of fields $\tilde{\Phi}$ and Φ are positive, higher-order reaction terms with large l or m are less relevant than lower-order terms. Near $d=4$, for instance, only linear and third-order terms ($l+m=2,3$) are relevant and the process belongs to the universality class of Schlögl's first model. When some of the coefficients of relevant terms become zero, as in the Φ^6 theory of thermal tricritical phenomena, the action shows multicritical behavior where most relevant terms with nonzero coefficients control the process. Note that some coefficients have a definite sign. When $m<l$, for example, K_{ml} is always positive and cannot be zero except at $k_{mn}=0$ for all n.

In the present work we limit ourselves to reaction-diffusion systems composed of $2n-1$ reactions,

$$lX \xrightarrow{k_l^-} l'X \quad (l>l')\ , \tag{2.4}$$

$$lX \xrightarrow{k_l^+} l''X \quad (l<l'') \text{ (with } l=1,2,\ldots,n-1) \tag{2.5}$$

$$nX \xrightarrow{k_n^-} n'X \quad (n>n')\ . \tag{2.6}$$

Equations (2.4) and (2.5) represent lth-order annihilation and creation and Eq. (2.6) stands for nth-order annihilation. The system (2.4)–(2.6) corresponds to the process of $m=1$ in I. As mentioned before, $K_{12}\geq 0$. As far as first-order reactions exist, therefore, the process with $m>1$ in I cannot be realized. The relevant action is given by

$$L=\int dt \int d\mathbf{r} \left[\tilde{\Psi}(\dot{\Psi}-D\Delta\Psi)+\sum_{l=1}^{n-1} Ds_l(\tilde{\Psi}\Psi^l) + Du(\tilde{\Psi}\Psi^n-\tilde{\Psi}^2\Psi) \right]\ , \tag{2.7}$$

where $\tilde{\Psi}=\tilde{\Phi}/a$, $\Psi=\Phi a$, $Ds_l=-K_{l1}a^{1-l}$, $Du=-K_{n1}a^{1-n}=K_{12}a$, and $a=(-K_{n1}/K_{12})^{1/n}$. We study the multicritical behavior around

$$s_1=s_2=\cdots=s_{n-1}=0\ . \tag{2.8}$$

The physical meaning of $s_l=0$ is the vanishment of global lth-order reactions due to balance between creation and annihilation. As discussed in the Introduction, this does not necessarily mean the absence of microscopic lth-order reactions.

We now follow the usual field-theoretic renormalization-group scheme.[11] Some of the following overlap the corresponding parts of I. Engineering dimensions in terms of time t and an inverse length scale Λ are written as

$$[\tilde{\Psi}]=\Lambda^{d_{\tilde{\Psi}}},\quad d_{\tilde{\Psi}}=\frac{n-1}{n}d\ , \tag{2.9}$$

$$[\Psi]=\Lambda^{d_\Psi},\quad d_\Psi=\frac{1}{n}d\ , \tag{2.10}$$

$$[s_l]=\Lambda^{d_{sl}},\quad d_{sl}=2-\frac{l-1}{n}d\ , \tag{2.11}$$

$$[D]=t^{-1}\Lambda^{-2}\ , \tag{2.12}$$

$$[u]=\Lambda^{d_u},\quad d_u=2-\frac{n-1}{n}d\ . \tag{2.13}$$

The condition $d_u(d_c)=0$ determines the upper critical dimension,

$$d_c=2n/(n-1)\ . \tag{2.14}$$

Power counting tells us that $n+3$ primitive divergences appear in vertex functions Γ_{1l} ($l=1,2,\ldots,n$) and Γ_{21}, where $\Gamma_{\tilde{N},N}$ is a vertex function with $\tilde{N}$ truncated $\tilde{\Psi}$ legs and N truncated Ψ legs. Hence, we need $n+3$ renormalizations,

$$\tilde{\Psi}_0=Z_{\tilde{\Psi}}^{1/2}\tilde{\Psi}\ , \tag{2.15}$$

$$\Psi_0=Z_{\Psi}^{1/2}\Psi\ , \tag{2.16}$$

$$s_{l0}=Z_{sl}s_l\ , \tag{2.17}$$

$$D_0=Z_D D\ , \tag{2.18}$$

$$u_0=Z_u u\Lambda^{d_u}\ , \tag{2.19}$$

where Z is a renormalization constant and a subscript zero denotes a bare quantity. The renormalization-group equation is derived from the requirement that bare vertex functions are independent of Λ and reads

$$\left[\Lambda\frac{\partial}{\partial\Lambda}+\beta_u\frac{\partial}{\partial u}+\sum_{l=1}^{n-1}\kappa_l x_l\frac{\partial}{\partial x_l}+\zeta D\frac{\partial}{\partial D} -\frac{\tilde{N}\tilde{\mu}}{2}-\frac{N\mu}{2}\right]\Gamma_{\tilde{N},N}=0\ , \tag{2.20}$$

$$\beta_u=\Lambda\frac{\partial u}{\partial\Lambda}\bigg|_0\ , \tag{2.21}$$

$$\kappa_l x_l=\Lambda\frac{\partial x_l}{\partial\Lambda}\bigg|_0\ , \tag{2.22}$$

$$\zeta D=\Lambda\frac{\partial D}{\partial\Lambda}\bigg|_0\ , \tag{2.23}$$

$$\tilde{\mu}=\Lambda\frac{\partial}{\partial\Lambda}(\ln Z_{\tilde{\Psi}})\bigg|_0\ , \tag{2.24}$$

$$\mu=\Lambda\frac{\partial}{\partial\Lambda}(\ln Z_{\Psi})\bigg|_0\ , \tag{2.25}$$

where a subscript zero means differentiation under constant bare parameters. Scaling fields x_l are generally expressed as

$$x_l=s_l+f_l(s_{l+1},s_{l+2},\ldots,s_{n-1};u)\ . \tag{2.26}$$

A zero point of the β function gives a fixed point u^* of a coupling constant

$$\beta_u(u^*)=0\ . \tag{2.27}$$

At $u=u^*$, the renormalization-group equation (2.20) leads to

$$\Gamma_{\tilde N,N}(\Lambda,x_1,x_2,\ldots,x_{n-1},D;\{\mathbf{k},\omega\})=\Lambda^{(\tilde N\tilde\mu^*+N\mu^*)/2}\Gamma^*_{\tilde N,N}(x_1\Lambda^{-\kappa_1^*},x_2\Lambda^{-\kappa_2^*},\ldots,x_{n-1}\Lambda^{-\kappa_{n-1}^*},D\Lambda^{-\zeta^*};\{\mathbf{k},\omega\}) , \quad (2.28)$$

where $\kappa_l^*=\kappa_l(u^*)$, $\zeta^*=\zeta(u^*)$, $\tilde\mu^*=\tilde\mu(u^*)$, and $\mu^*=\mu(u^*)$. In the Fourier space, a Green function $G_{\tilde N,N}$, that is, a correlation function of particles, is related to $\Gamma_{\tilde N,N}$ as

$$G_{\tilde N,N}\sim(\Gamma_{1,1})^{-(\tilde N+N)}\Gamma_{N,\tilde N} . \quad (2.29)$$

The engineering dimension of $G_{\tilde N,N}$ is

$$[G_{\tilde N,N}(\{\mathbf{k},\omega\})]=t^{\tilde N+N-1}\Lambda^{\tilde Nd_{\tilde\Psi}+Nd_\Psi-(\tilde N+N-1)d} . \quad (2.30)$$

From Eqs. (2.28)–(2.30) together with the dimensional analysis, we find that $G_{\tilde N,N}$ has a scaling form

$$G_{\tilde N,N}=x_1^{-\gamma_{\tilde N,N}}F_{\tilde N,N}(x_2x_1^{-\phi_2},x_3x_1^{-\phi_3},\ldots,x_{n-1}x_1^{-\phi_{n-1}}, \{\mathbf{k}x_1^{-\nu},\omega x_1^{-\theta}\}) , \quad (2.31)$$

$$\nu=1/(d_{s1}-\kappa_1^*) , \quad (2.32)$$

$$z=\theta/\nu=2+\zeta^* , \quad (2.33)$$

$$\gamma_{\tilde N,N}/\nu=(\tilde N+N-1)(d+z)-(\tilde Nd_{\tilde\Psi}+Nd_\Psi)-(\tilde N\tilde\mu^*+N\mu^*)/2 , \quad (2.34)$$

$$\phi_l=(d_{sl}-\kappa_l^*)/(d_{s1}-\kappa_1^*) \text{ (with } l=2,3,\ldots,n-1) . \quad (2.35)$$

As discussed in I, there are two different (probably independent at $n>2$) susceptibility exponents: the static exponent γ_s describing spatial fluctuations at steady states and the dynamic exponent γ_d characterizing time evolution of the process. Among $n+3$ renormalization constants, Z_u yields a fixed point u^* and the remaining $n+2$ constants determine critical exponents. In general, therefore, the system has $n+2$ independent critical exponents: ν, z, γ_s, γ_d, and $n-2$ crossover exponents ϕ_l (with $l=2,3,\ldots,n-1$). Constants $Z_{\tilde\Psi}$, Z_Ψ, Z_{s1}, and Z_D give rise to ν, z, γ_s, and γ_d via $\tilde\mu$, μ, κ_1, and ζ. Crossover exponents ϕ_l are obtained from Z_{sl} through κ_l. Calculating engineering dimensions at $d=d_c$, we get mean-field values of critical exponents, because $\kappa_l^*=\zeta^*=\tilde\mu^*=\mu^*=0$ at d_c. The results for ν, z, γ_s, and γ_d were presented in I and that for ϕ_l is

$$\phi_{l0}=(n-l)/(n-1) \text{ (with } l=2,3,\ldots,n-1) , \quad (2.36)$$

where a subscript zero denotes a mean-field value.

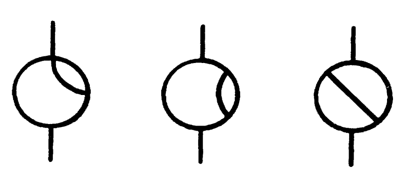

FIG. 1. Relevant diagrams to two-loop order for $\Gamma_{1,1}$.

III. CALCULATIONS FOR $n=3$

In this section we perform explicit calculations for $n=3$ based upon the usual ϵ-expansion technique. The upper critical dimension is 3,

$$d_c=3 , \quad (3.1)$$

and the relevant action becomes

$$L=\int dt\int d\mathbf{r}[\tilde\Psi(\dot\Psi-D\,\Delta\Psi+Ds\,\Psi)+Dv(\tilde\Psi\Psi^2)+Du(\tilde\Psi\Psi^3-\tilde\Psi^2\Psi)] , \quad (3.2)$$

where s and v denote s_1 and s_2. When $v=0$, the action (3.2) reduces to that [Eq. (4.1)] treated in Sec. IV of I. Thus most of the results are the same as those in I. In this paper we present only new results associated with the presence of the term $Dv(\tilde\Psi\Psi^2)$.

In this case $\Gamma_{1,1}$, $\Gamma_{1,2}$, $\Gamma_{1,3}$, and $\Gamma_{2,1}$ are primitively divergent. Figures 1 and 2 show relevant diagrams to two-loop order for $\Gamma_{1,1}$ and $\Gamma_{1,2}$. Those for $\Gamma_{2,1}$ and $\Gamma_{1,3}$ are plotted in Figs. 2 and 3 of I. All divergent contributions from these diagrams are described by integrals listed in the Appendix of I. The results for $\Gamma_{1,1}$ and $\Gamma_{1,2}$ are

$$\Gamma^0_{1,1}(\mathbf{k},\omega)=i\omega\left[1+\frac{\sqrt3}{\epsilon}\left[\frac{u_0}{4\pi}\right]^3\right]+D_0k^2\left[1+\frac{7\sqrt3}{9\epsilon}\left[\frac{u_0}{4\pi}\right]^3\right]+D_0\left[s_0-\frac{4\pi-3\sqrt3}{6\pi\epsilon}\left[\frac{u_0}{4\pi}\right]^2v_0^2\right] , \quad (3.3)$$

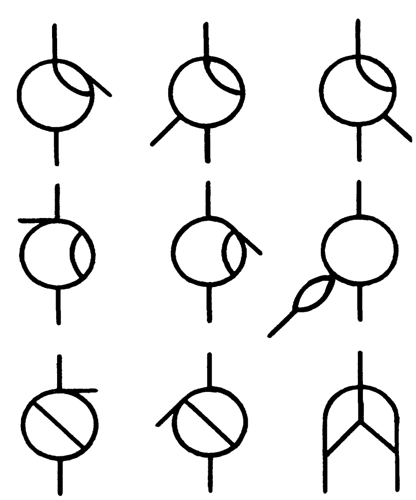

FIG. 2. Relevant diagrams to two-loop order for $\Gamma_{1,2}$.

$$\Gamma^0_{1,2}(\mathbf{0},0)=2D_0v_0\left[1-\frac{20\pi-12\sqrt{3}}{\epsilon}\left[\frac{u_0}{4\pi}\right]^3\right] . \tag{3.4}$$

By using the minimal subtraction method, we have

$$Z_x=1+(7\sqrt{3}/9)u^3\epsilon^{-1} , \tag{3.5}$$

$$Z_v=1+(8\pi-44\sqrt{3}/9)u^3\epsilon^{-1} . \tag{3.6}$$

The scaling field x is written as

$$x=s+[(4\pi-3\sqrt{3})/6\pi\epsilon]u^2v^2\Lambda^{-2\epsilon/3} \times[1-(14\sqrt{3}/9)u^3\epsilon^{-1}] . \tag{3.7}$$

Here a factor 4π is absorbed in u. Renormalization functions are given by

$$\kappa_x=(14\sqrt{3}/9)u^3 , \tag{3.8}$$

$$\kappa_v=(16\pi-88\sqrt{3}/9)u^3 . \tag{3.9}$$

The β function gives

$$u^{*3}=[3/(108\pi-41\sqrt{3})]\epsilon . \tag{3.10}$$

Substituting Eqs. (3.8)–(3.10) into Eq. (2.35), we get

$$\phi=\phi_2=\tfrac{1}{2}-[(6\pi-9\sqrt{3})/(108\pi-41\sqrt{3})]\epsilon+O(\epsilon^2) . \tag{3.11}$$

Since $d_c=3$, logarithmic corrections to scaling arise under experimental conditions. Here we derive them from the renormalization-group equation (2.20). The general solution of Eq. (2.20) is expressed as

$$\Gamma_{\tilde{N},N}=A_{\tilde{N},N}(\Lambda)\Gamma^*_{\tilde{N},N}(u(\Lambda),x_1(\Lambda),x_2(\Lambda),\ldots,x_{n-1}(\Lambda),D(\Lambda);\{\mathbf{k},\omega\}) , \tag{3.12}$$

where $u(\Lambda)$, $x_l(\Lambda)$, $D(\Lambda)$, and $A_{\tilde{N},N}(\Lambda)$ are solutions of the following equations:

$$\Lambda\frac{\partial u}{\partial\Lambda}=-\beta_u , \tag{3.13}$$

$$\Lambda\frac{\partial x_l}{\partial\Lambda}=-\kappa_l x_l , \tag{3.14}$$

$$\Lambda\frac{\partial D}{\partial\Lambda}=-\zeta D , \tag{3.15}$$

$$\Lambda\frac{\partial A_{\tilde{N},N}}{\partial\Lambda}=\frac{\tilde{N}\tilde{\mu}+N\mu}{2}A_{\tilde{N},N} . \tag{3.16}$$

At $d=d_c$ ($\epsilon=0$), the β function becomes

$$\beta_u=(24\pi-82\sqrt{3}/9)u^4 . \tag{3.17}$$

Then the solution of Eq. (3.13) is

$$u(\Lambda)=u(1)[L(\Lambda)]^{-1/3} , \tag{3.18}$$

$$L(\Lambda)=1+C_u[u(1)]^3\ln\Lambda , \tag{3.19}$$

$$C_u=72\pi-82\sqrt{3}/3 . \tag{3.20}$$

Equations (3.8) and (3.14) lead to

$$x(\Lambda)=x(1)[L(\Lambda)]^{-C_x} , \tag{3.21}$$

$$C_x=7\sqrt{3}/[3(108\pi-41\sqrt{3})] . \tag{3.22}$$

Similar relations are obtained from other renormalization functions. It follows that

$$\Gamma_{\tilde{N},N}=L^{C_{\tilde{N},N}}\Gamma^*_{\tilde{N},N}(uL^{-1/3},xL^{-C_x},vL^{-C_v},DL^{-C_D};\{\mathbf{k},\omega\}) , \tag{3.23}$$

$$C_v=(72\pi-44\sqrt{3})/[3(108\pi-41\sqrt{3})] , \tag{3.24}$$

$$C_D=2\sqrt{3}/[3(108\pi-41\sqrt{3})] , \tag{3.25}$$

$$C_{\tilde{N},N}=(38\pi-16\sqrt{3})\tilde{N}+(-38\pi+19\sqrt{3})N . \tag{3.26}$$

Substitution of Eq. (3.23) into Eq. (2.29) yields

$$G_{\tilde{N},N}=L^{-C_{\tilde{N},N}}G^*_{\tilde{N},N}(uL^{-1/3},xL^{-C_x},vL^{-C_v},DL^{-C_D};\{\mathbf{k},\omega\}) . \tag{3.27}$$

Applying the dimensional analysis, we arrive at the scaling form of $G_{\tilde{N},N}$ with logarithmic corrections:

$$G_{\tilde{N},N}=x^{-\gamma^0_{\tilde{N},N}}L^{-C_{\tilde{N},N}+\gamma^0_{\tilde{N},N}C_x+(\tilde{N}+N-1)C_D}F_{\tilde{N},N}(uL^{-1/3},vx^{-\phi_0}L^{\phi_0C_x-C_v},\{\mathbf{k}x^{-\nu_0}L^{\nu_0C_x},\omega x^{-\theta_0}L^{\theta_0C_x+C_D}\}) , \tag{3.28}$$

$$L=1-(C_u/2)u^3\ln|x| , \tag{3.29}$$

where $\nu_0=\frac{1}{2}$, $\theta_0=1$, $\phi_0=\frac{1}{2}$, and $\gamma^0_{\tilde{N},N}=-(5-3\tilde{N}-4N)/2$ are mean-field critical exponents.

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