Universality of a class of annihilation-coagulation models

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A class of d-dimensional reaction-diffusion models interpolating continuously between the diffusion-coagulation and the diffusion-annihilation models is introduced. Exact relations among the observables of different models are established. For the one-dimensional case, it is shown how correlations in the initial state can lead to nonuniversal amplitudes for time-dependent particle density.

PACS number(s): 05.20.Dd, 05.40.+j, 82.20.Mj

I. INTRODUCTION

In the recent years, reaction-diffusion problems have stimulated a large body of work in many different directions [1,2]. The simplest example is provided by the annihilation process $A + A \rightarrow 0$, in which the A particles diffuse and react by pairs on contact.

Usually such kinetic processes are described in terms of macroscopic rate equations giving the time evolution of the local averaged concentrations. One assumes that the reaction is completely described in terms of the local average densities, and that the reaction introduces no correlations between the reacting species. This is reminiscent of a mean-field-like approximation in statistical physics. However, an important aspect of the problem is neglected, namely, the microscopic fluctuations, and it is well known that these fluctuations play an important role in low-dimensional systems [3–5].

Indeed, for the annihilation process $A + A \rightarrow 0$, the rate equation predicts that, in the long-time regime, the concentration of A will decrease in time as $a \simeq \mathcal{A}t^{-1}$ while a calculation taking into account the local microscopic fluctuations in the particle density gives [6] $a \simeq \mathcal{A}t^{\alpha}$, with $\alpha = \min(1, \frac{d}{2})$, where d is the dimensionality of the system. Moreover, for a Poissonian initial state, the amplitude $\mathcal{A}$ is a universal quantity, which is in particular independent of the initial density of the particles. This nonclassical power-law behavior is called anomalous kinetics.

Thus to give a correct description, it is crucial to work within a formalism that is able to keep track of the fluctuations. This is a difficult task, which is the reason that, except for one-dimensional systems, exact analytical results are scarce. Complex reaction-diffusion systems are present in nature [7]. However, the study of simple models, like the diffusion-coagulation process (DC) $A + A \rightarrow A$, or the diffusion-annihilation one (DA) $A + A \rightarrow 0$ provide a very useful testing ground for new theoretical approaches.

Different methods have been explicitly developed for the one-dimensional systems (see, for example, [1,8–15]). In most of them, one maps the initial reaction-diffusion problem onto a different model (quantum chain [1], kinetic Ising model [8], invasion process [10], etc.), which is

exactly solvable. A different approach consists in finding the "good observables" for which an exact equation of motion can be derived and solved. For the DC model, Doering and ben-Avraham [14] have shown that the system was best analyzed in terms of the time-dependent probability $\mathcal{E}(x, y, t)$ that the interval between y and x is empty at time t. The particle density $a(x, t)$ is simply given by $a(x, t) = -\frac{\partial}{\partial x}\mathcal{E}(x, y, t)|_{x=y}$. In the continuous limit, $\mathcal{E}(x, y, t)$ obeys a simple diffusion equation that can be solved analytically. However, Doering and ben-Avraham were not able to find a similar quantity for the DA model.

In arbitrary dimensions, it was soon recognized, based on dynamical renormalization-group arguments [16,17], that the DA and DC models belong to the same universality class. The power-law exponents describing the decay of the particle densities are the same. However, for the amplitude $\mathcal{A}$, the situation turns out to be more subtle. Whereas for the DC model this amplitude seems to be strictly independent of the initial state, this is not the case for the one-dimensional DA model. Indeed, as noticed by Family and Amar [18], short-ranged initial correlations can change the asymptotic amplitude in a continuous way. In their analysis, the DA model is mapped onto a kinetic Ising model at zero temperature [8]. Explicit asymptotic results for the average domain size, average magnetization squared, and pair-correlation function are derived for arbitrary initial conditions. When the initial magnetization is $m_0 = 0$, the results for the DA model with Poissonian initial conditions are reproduced. However, for $m_0 \neq 0$, the particle density has a nontrivial dependence on the initial magnetization. A nonzero value of m_0 means for the DA model that there are some correlations among the particles in the initial state. What is the mechanism responsible for this dependence and could a similar situation also occur in the DC process for which there is no mapping onto a kinetic Ising model?

To answer this question we shall, in this paper, revisit the problem of universality in the DC and DA models. The strategy is to study the field theory that can be associated to a reaction-diffusion process, following the method introduced by Doi [19] and revisited by Grassberger and Scheunert [20] and Peliti [21]. We shall con-

sider a class of diffusion-coagulation-annihilation models (called α models), allowing us to go continuously from the DC process to the DA one.

The paper is organized as follows. In Sec. II, the way to associate a field theory to a reaction-diffusion process is briefly reviewed and the α models are introduced. Within a functional integral formalism, different d-dimensional α models are related one to the others. In Sec. III, the one-dimensional DC model is revisited. It is shown how the equation for the time-dependent probability $\mathcal{E}(x, y, t)$ that an interval between y and x is empty at time t can be obtained within the field theoretical framework. In Sec. IV, we introduce the quantity $\mathcal{T}^{(\alpha)}(x, y, t)$, which is the natural generalization for the α model of $\mathcal{E}(x, y, t)$. Its equation of motion is derived and exactly solved, leading to an exact expression for the asymptotic behavior of the particle density. It is shown explicitly how and when the amplitude universality can be violated. In particular, it is proved that for an initial state in which particles are pairwise correlated, the violation of the amplitude universality is only possible for the DA model. Finally, possible extensions of this work are discussed.

II. FIELD-THEORETICAL APPROACH

For the sake of completeness and to set up the notations, we briefly sketch the main steps necessary to derive

$$\partial_t P_n(x_1, \ldots, x_n; t) = D \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} P_n(x_1, \ldots, x_n; t)$$

$$-\frac{1}{2} \sum_{i \neq j} V(|x_i - x_j|) P_n(x_1, \ldots, x_n; t) + \frac{1}{2} \int dy dz \; V(|y - z|) P_{n+2}(y, z, x_1, \ldots, x_n; t), \qquad (2)$$

where D is the diffusion constant.

We introduce a Fock space representation for the states of the system. Space-valued annihilation $\psi(x)$ and creation $\pi(x) = \psi^\dagger(x)$ operators are introduced. The vacuum state $|0\rangle$ is defined by

$$\psi(x)|0\rangle = 0$$

and the annihilation and creation operators obey bosonic commutation relations:

$$[\psi(x), \pi(y)] = \delta(x - y).$$

The state specified by the set $\Phi = \{P_n\}_{n=0,\ldots,\infty}$ reads

$$|\Phi\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \cdots dx_n$$

$$\times P_n(x_1, \ldots, x_n) \pi(x_1) \cdots \pi(x_n)|0\rangle \qquad (3)$$

and the statistical average $\langle A \rangle$ over the state Φ of an observable $\{A_n(x_1, \ldots, x_n)\}_{n=0,\ldots,\infty}$ defined by

$$\langle A \rangle = \sum_n \frac{1}{n!} \int dx_1 \cdots dx_n \; A_n(x_1, \ldots, x_n) P_n(x_1, \ldots, x_n)$$

the field theory associated to a d-dimensional reaction-diffusion process. We follow the method introduced by Doi [19] and revisited by Grassberger and Scheunert [20] and Peliti [21].

We start with a description of the system in terms of the probabilities $P_n(x_1, \ldots, x_n; t)$ that a configuration with n particles at points $x_1, \ldots, x_n$ is realized at time t. As we are not interested in specifying which particle is where, we choose $P_n(x_1, \ldots, x_n; t)$ to be a symmetric function in the variables $x_1, \ldots, x_n$. Note that, as the particle number is not conserved, a state of the system must be specified by the entire set $\Phi(t) = \{P_n(t)\}_{n=0,\ldots,\infty}$ with the normalization

$$\sum_n \frac{1}{n!} \int dx_1 \cdots dx_n \; P_n(x_1, \ldots, x_n; t) = 1.$$

The dynamics is defined by the master equation

$$\partial_t P_n(x_1, \ldots, x_n; t) = [\mathcal{H}P]_n(x_1, \ldots, x_n; t), \qquad (1)$$

where $\mathcal{H}$ is an operator acting on the set of the probabilities [19,20].

Let us consider as an example the following DA process. The A particles diffuse and annihilate each other with a reaction rate $V(|x - y|)$ depending on the distance. The corresponding master equation reads

takes the form of a scalar product:

$$\langle A \rangle = \langle |A|\Phi\rangle,$$

where A is the corresponding operator of the Fock space, such that $\langle 0|\psi(x_1) \cdots \psi(x_n) A|\Phi\rangle = A_n(x_1, \ldots, x_n)$ and $\langle |$ is a projection state given by

$$\langle | = \langle 0|e^{\int dz \; \psi(z)},$$

having the property $\langle |\pi(x) = \langle |$. In particular, the particle density is given by $c(x) = \langle \psi(x) \rangle$ and the n-point correlation functions by $\rho(x_1, \ldots, x_n) = \langle \psi(x_1) \ldots \psi(x_n) \rangle$. The normalization of the state is expressed by the condition $\langle |\Phi\rangle = 1$. A correlated state, characterized by the p-point cumulants,

$$\langle \psi(x_1) \cdots \psi(x_p) \rangle_{\text{cum}} = g_{(p)}(x_1, \ldots, x_p)$$

has the form

$$|\Phi\rangle = \exp\left[\sum_{p=1}^{\infty} \frac{1}{p!} \int dx_1 \cdots dx_p \; g_{(p)}(x_1, \ldots, x_p)\right.$$

$$\left. \times [\pi(x_1) - 1] \cdots [\pi(x_p) - 1]\right]|0\rangle. \qquad (4)$$

It can be shown that the master equation can be written in the Schrödinger-like form:

$$\frac{\partial}{\partial t}|\Phi(t)\rangle = H|\Phi(t)\rangle. \qquad (5)$$

For our annihilation model, the non-Hermitian evolution operator H is given by

$$H = H_0 + H_a,$$

with

$$H_0 = D \int dz \, \pi(z)\nabla^2\psi(z) \qquad (6)$$

and

$$H_a = -\int dzdz' \, V_a(|z-z'|)[\pi(z)\pi(z') - 1]\psi(z)\psi(z'). \qquad (7)$$

A second example is provided by the diffusion-

coagulation process. The interaction part of the evolution operator becomes

$$H_c = -\int dzdz' \, V_c(|z-z'|)[\pi(z)\pi(z') - \pi(z)]\psi(z)\psi(z'). \qquad (8)$$

If now both coagulation and annihilation reactions are simultaneously allowed, one has

$$H_{a+c} = H_a + H_c = -\int dzdz' \, [(V_a + V_c)\pi(z)\pi(z')$$
$$-V_c\pi(z) - V_a]\psi(z)\psi(z'). \qquad (9)$$

Although not Hermitian, these evolution operators have the property to preserve the normalization $\langle|H = 0$. The evolution equation of an observable A is

$$\frac{\partial}{\partial t}\langle A\rangle = \langle AH\rangle = \langle[A,H]\rangle. \qquad (10)$$

It can be shown [21] that the correlation functions may be expressed in terms of functional integrals as

$$\langle\psi(x_1,t_1)\cdots\psi(x_n,t_n)\rangle_{S,F_0} = \int \mathcal{D}\psi\mathcal{D}\bar{\psi} \, \psi(x_1,t_1)\cdots\psi(x_n,t_n)e^{-S}F_0[\bar{\psi}(x,0)]. \qquad (11)$$

The action S appearing in the measure e^{-S} is related to H as follows:

$$S[\bar{\psi},\psi] = \int dtdx \, \bar{\psi}\dot{\psi} - \int dt \, H[\pi = \bar{\psi}+1, \psi].$$

F_0 is a functional of the auxiliary field $\bar{\psi}$ at t=0, and is related to the cumulants of the initial state by

$$F_0[\bar{\psi}] = \exp\left[\sum_{p=1}^{\infty}\frac{1}{p!}\int dx_1\cdots dx_p \, g_{(p)}(x_1,\ldots,x_p;0)\bar{\psi}(x_1)\cdots\bar{\psi}(x_p)\right]. \qquad (12)$$

Let us now assume that V_c is proportional to V_a. This leads us to introduce a class of model (called the α models) depending on a continuous real parameter α and defined by the following action:

$$S_\alpha = \int dtdz \, \bar{\psi}\left(\dot{\psi} - D\nabla^2\psi\right) + \int dtdzdz' \, V(|z-z'|)[\bar{\psi}(z)\bar{\psi}(z') + \alpha\bar{\psi}(z)]\psi(z)\psi(z'). \qquad (13)$$

The simple coagulation and annihilation reactions correspond, respectively, to $\alpha = 1$ and $\alpha = 2$ and will be labeled by the indices c and a in the following. Thus the α models ($\alpha \in [1,2]$) interpolate between the coagulation process and the annihilation one.

We are now in the position to relate the dynamics of different α models in a very simple way. Taking the coagulation case as reference, Eq. (13) gives

$$S_\alpha[\bar{\psi},\psi] = S_c\left[\frac{\bar{\psi}}{\alpha}, \alpha\psi\right]$$

and, by simply rescaling the functions in the functional integral, we get the following relations between correlation functions:

$$\langle\psi(x_1,t_1)\cdots\psi(x_n,t_n)\rangle_{\alpha,F_0}$$
$$= \alpha^{-n}\langle\psi(x_1,t_1)\cdots\psi(x_n,t_n)\rangle_{c,F_0^{(1/\alpha)}}, \qquad (14)$$

where

$$F_0^{(1/\alpha)}[\bar{\psi}] = F_0[\alpha\bar{\psi}].$$

In particular this means that, if at $t = 0$ we consider two states $|\Phi_\alpha(0)\rangle$ and $|\Phi_c(0)\rangle$ such that

$$\langle|\psi(x_1)\cdots\psi(x_n)|\Phi_\alpha(0)\rangle = \alpha^{-n}\langle|\psi(x_1)\cdots\psi(x_n)|\Phi_c(0)\rangle,$$

for all n, then this relation is conserved for all times, if $|\Phi_\alpha\rangle$ evolves according to the dynamic of the α model and $|\Phi_c\rangle$ according to the dynamic of the coagulation one. Moreover, if a set of equations among correlation func-

tions, or more generally among operators, is satisfied for the coagulation case, then a similar set of relations exists for the α model, providing that one rescales the fields according to $\psi \rightarrow \alpha\psi$. Note that similar relations have been recently derived in a different context by Simon [15] and Henkel, Orlandini, and Schütz [22].

For the particular case $\alpha = 2$ and for homogeneous Poissonian initial conditions for both $|\Phi_c\rangle$ and $|\Phi_a\rangle$, we have the following relation between the concentrations:

$$c_c(t) = 2c_a(t) \qquad \forall t > 0, \tag{15}$$

providing that initially $c_c(0) = 2c_a(0)$. This result has been already derived by several authors (see, for example, [11,12,15,22]). Moreover, the relation among the actions $\mathcal{S}_c$ and $\mathcal{S}_a$ has been already used in previous works [16,17] for Poissonian initial conditions. However, our results are valid for all the α models and take care explicitly of arbitrary initial conditions. In addition, from Eq. (14), we clearly see that quantities involving correlation functions of the same order are simply related. But more complicated quantities such as, for example, the interparticle distribution function (which involves many correlation functions of different order), are no longer simply related. This may explain why the asymptotic interparticle distribution function between DC and DA models are qualitatively different [23]. This problem will be investigated in details in a further publication [24].

III. THE ONE-DIMENSIONAL COAGULATION MODEL REVISITED

Let us define $\mathcal{E}(x, y, t)$, the time-dependent probability that the interval (y, x) is empty at time t. Our goal is to rederive in the framework of the field theory the equation of motion for $\mathcal{E}(x, y, t)$ obtained by Doering and ben-Avraham [14]. This equation reads

$$\frac{\partial \mathcal{E}(x, y, t)}{\partial t} = D\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\mathcal{E}(x, y, t). \tag{16}$$

First, we have to identify the Fock space operator corresponding to the probability $\mathcal{E}(x, y, t)$. This means that we are looking for a time-independent operator $E(x, y)$ such that, given a state $|\Phi(t)\rangle$, the probability that the interval between y and x is empty at time t is

$$\mathcal{E}(x, y, t) = \langle |E(x, y)|\Phi(t)\rangle. \tag{17}$$

This operator is

$$E(x, y) = e^{-\int_y^x dz\,\psi(z)}. \tag{18}$$

The easiest way to show this consists in using the explicit form of the projection state $\langle | = \langle 0|e^{\int_{-\infty}^{+\infty} dz\,\psi(z)}$ in Eq. (17). Indeed, for a general state $|\Phi\rangle$, we find

$$\mathcal{E}(x, y) = \langle 0|e^{(\int_x^\infty + \int_{-\infty}^y)dz\,\psi(z)}|\Phi\rangle.$$

If we consider the state $|\Phi'\rangle = \pi(z_1)\cdots\pi(z_n)|\Phi\rangle$ obtained

by adding particles in $z_1, z_2, \ldots, z_n$ to the state $|\Phi\rangle$ we obtain

$$\langle E(x, y)\rangle_{\Phi'} = \begin{cases} \langle E(x, y)\rangle_\Phi & \text{if } z_n \notin (y, x) \ \forall n, \\ 0 & \text{otherwise.} \end{cases} \tag{19}$$

This defines the probability $\mathcal{E}(x, y)$ introduced above. Moreover, we have

$$\psi(x) = -\left[\frac{\partial}{\partial x}E(x, y)\right]_{x=y}, \tag{20}$$

in agreement with Doering and ben-Avraham [14].

The basic commutation relation is

$$[E(x, y), \pi(z)] = -f(z, x, y)E(x, y), \tag{21}$$

where the function f is given by

$$f(z, x, y) = \begin{cases} 1 & \text{if } y < z < x, \\ 0 & \text{otherwise.} \end{cases} \tag{22}$$

This commutation relation can be used to prove Eq. (19) without any reference to the explicit form of the projection state.

We can now derive the equation of motion for $\mathcal{E}(x, y, t)$. From Eqs. (8) and (10) and the property (19), we have

$$\begin{aligned}\frac{\partial}{\partial t}\langle E(x, y)\rangle &= \langle E(x, y)(H_0 + H_c)\rangle \\ &= -D\langle E(x, y)[\psi'(x) - \psi'(y)]\rangle \\ &\quad + \int_\Sigma dz\,dz'\,V(|z - z'|)\langle E(x, y)\psi(z)\psi(z')\rangle,\end{aligned} \tag{23}$$

where the domain of integration is

$$\Sigma = \{(z, z') \mid z \notin (y, x),\ z' \in (y, x)\}.$$

To proceed, we have to specify the interaction $V(\xi)$. We choose the following form:

$$V(\xi) = \begin{cases} v & \text{if } 0 < \xi < \sigma, \\ 0 & \text{if } \xi > \sigma \end{cases} \tag{24}$$

and we shall eventually take the $\sigma \rightarrow 0$ limit. For this purpose let us define

$$v\sigma = \lambda \quad \text{and} \quad v\sigma^2 = \chi.$$

Taking into account the form of the domain of integration Σ, the expansion in σ of Eq. (23) gives:

$$\begin{aligned}\frac{\partial}{\partial t}\langle E(x, y)\rangle &= \langle E(x, y)(H_0 + H_c)\rangle \\ &= -D\langle E(x, y)[\psi'(x) - \psi'(y)]\rangle \\ &\quad + \frac{1}{2}\chi\langle E(x)[\psi^2(x) + \psi^2(y)]\rangle + O(\sigma^3).\end{aligned} \tag{25}$$

From the definition of $E(x, y)$ [Eq. (18)], we obtain

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \langle E(x,y) \rangle = -\langle E(x,y)[\psi'(x) - \psi'(y)] \rangle$$
$$+ \langle E(x,y)[\psi^2(x) + \psi^2(y)] \rangle. \quad (26)$$

Thus in the limit

$$\sigma \to 0, \quad v \to \infty \quad \text{such that} \quad v\sigma^2 = \chi \to 2D, \quad (27)$$

we recover the desired equation:

$$\frac{\partial}{\partial t} \langle E(x,y) \rangle = D \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \langle E(x,y) \rangle + O(\sigma^3). \quad (28)$$

The particular choice $\chi \to 2D$ has its physical motivation in the relation between a model on a discrete lattice and its continuous version [24]. Moreover, our closed equation is valid only in the limit (27), which corresponds to an infinite pointlike coupling:

$$V(|z - z'|) \to 2\lambda\delta(z - z'), \quad \text{with} \quad \lambda = v\sigma \to \infty. \quad (29)$$

This fact is not surprising, considering that such a coupling corresponds to an instantaneous coagulation on contact: this is exactly the condition that was used in all the exact solutions [8–15].

This aspect can also be nicely understood in the renormalization-group framework (see, for example, [2]). The limit $\lambda \to \infty$ corresponds to approaching the nontrivial fixed point of the theory and thus to be in the asymptotic long-time regime. As a consequence, we can interpret the result (28), valid in the limits (27) and (29), as an equation for the asymptotic long-time regime for a diffusion-coagulation problem, with arbitrary reaction rate.

IV. GENERALIZATION TO α REACTIONS

Following the results obtained in Sec. II, about the correspondence between the coagulation model and an α model, we can now find the quantity corresponding to E for the α model and its equation of motion.

Let us define the operator

$$T^{(\alpha)}(x,y) = e^{-\alpha \int_y^x dz\, \psi(z)}. \quad (30)$$

Thus, $\mathcal{T}^{(\alpha)}(x,y) = \langle T^{(\alpha)}(x,y) \rangle$ satisfies the closed equation:

$$\frac{\partial}{\partial t} \mathcal{T}^{(\alpha)}(x,y,t) = D \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \mathcal{T}^{(\alpha)}(x,y,t) + O(\sigma^3). \quad (31)$$

To see the physical meaning of this operator, we consider a state $|\Phi\rangle = \pi(z_1) \cdots \pi(z_n)|0\rangle$. It is then easy to show that

$$\langle T^{(\alpha)}(x,y) \rangle_\Phi = \prod_{i=1}^n a_i,$$
$$a_i = \begin{cases} 1 & \text{if } z_i \notin (y,x), \\ 1 - \alpha & \text{if } z_i \in (y,x). \end{cases} \quad (32)$$

$\mathcal{T}^{(2)}(x,y)$, which is relevant for the annihilation case, is related to the probability of having an even number of particles in the interval between y and x. For a generic vector of the form $|\Phi\rangle = F[\pi]|0\rangle$, we have

$$\mathcal{T}^{(\alpha)}(x,y) = F[1 - f^{(\alpha)}(z)], \quad (33)$$

where the function $f^{(\alpha)}$ is the generalization of (22), i.e.,

$$f^{(\alpha)}(z) = \begin{cases} \alpha & \text{if } y < z < x, \\ 0 & \text{otherwise.} \end{cases}$$

Equation (31) has been solved by Doering, Burschka, and Horsthemke [25], with appropriate boundary conditions at $x = y$ and $x = \infty$ and the initial condition $\mathcal{T}^{(\alpha)}(x,y,0) = \mathcal{T}_0^{(\alpha)}(x,y)$. The solution of this equation is particularly simple if the system is homogeneous. From translational invariance $\mathcal{T}^{(\alpha)}(x,y,t) = \mathcal{T}^{(\alpha)}(x-y,t)$ and Eq. (31) becomes

$$\frac{\partial}{\partial t} \mathcal{T}^{(\alpha)}(x,t) = 2D \frac{\partial^2}{\partial x^2} \mathcal{T}^{(\alpha)}(x,t), \quad (34)$$

with the conditions:

$$\mathcal{T}^{(\alpha)}(0,t) = 1, \quad |\mathcal{T}^{(\alpha)}(\infty,t)| \leq 1,$$

$$\mathcal{T}^{(\alpha)}(x,0) = \mathcal{T}_0^{(\alpha)}(x).$$

The second condition follows from the fact that $T^{(\alpha)}(x,y)$ is a stochastic variable that takes its value in the interval $[-1, +1]$. To take care of the first two boundary conditions, it is judicious to define

$$t^{(\alpha)}(x,t) \equiv \frac{\partial^2}{\partial x^2} \mathcal{T}^{(\alpha)}(x,t), \quad (35)$$

whose equation of motion is

$$\frac{\partial}{\partial t} t^{(\alpha)}(x,t) = 2D \frac{\partial^2}{\partial x^2} t^{(\alpha)}(x,t),$$
$$t^{(\alpha)}(0,t) = t^{(\alpha)}(\infty,t) = 0. \quad (36)$$

The solution reads

$$t^{(\alpha)}(x,t) = \int_0^\infty dz\, G(x,z,t) t_0^{(\alpha)}(z), \quad (37)$$

where $G(x,z,t)$ is the Green function:

$$G(x,z,t) = (8\pi Dt)^{-1/2} \left[\exp\left(-\frac{(x-z)^2}{8Dt}\right) \right.$$
$$\left. - \exp\left(-\frac{(x+z)^2}{8Dt}\right)\right]. \quad (38)$$

We can now study the behavior of the particle density. From Eq. (30), it follows that the (homogeneous) density is

$$c_\alpha(t) = \langle \psi(0) \rangle = -\alpha^{-1} \left[\frac{\partial}{\partial x} \mathcal{T}^{(\alpha)}(x,t) \right]_{x=0} \quad (39)$$

and then from (35):

$$c_\alpha(t) = \alpha^{-1} \int_0^\infty dz \, t^{(\alpha)}(z,t). \quad (40)$$

Using Eq. (37) we obtain

$$c_\alpha(t) = \alpha^{-1} \int_0^\infty dz \, \mathrm{erf}\left(\frac{z}{(8Dt)^{1/2}} \right) t_0^{(\alpha)}(z)$$
$$= \alpha^{-1} (2\pi Dt)^{-1/2} \int_0^\infty d\xi \, e^{-\xi^2} \xi \left[1 - \mathcal{T}_0^{(\alpha)}(2\xi t^{1/2}) \right], \quad (41)$$

whose asymptotic behavior for large t is

$$c_\alpha(t) \sim (2\alpha)^{-1} (2\pi Dt)^{-1/2} \left[1 - \mathcal{T}_0^{(\alpha)}(\infty) \right]. \quad (42)$$

This result shows that, besides the trivial dependence on the factor $(2\alpha)^{-1}$, which follows from the rescaling $\psi \to \alpha\psi$, the asymptotic density amplitude depends also on the initial value $\mathcal{T}_0^{(\alpha)}(\infty)$. The study of this quantity for a general initial state is a very hard problem. From (33) and (4) we have

$$\mathcal{T}_0^{(\alpha)}(x) = \exp\left[\sum_{p=1}^\infty \frac{(-\alpha)^p}{p!} \bar{g}_{(p)}(x) \right], \quad (43)$$

where

$$\bar{g}_{(p)}(x) = \int_0^x dx_1 \cdots \int_0^x dx_p \, g_{(p)}(x_1, \ldots, x_p)$$

and it is difficult to predict the value $\mathcal{T}_0^{(\alpha)}(\infty)$, without expliciting the $g_{(p)}$'s.

Let us then consider a translational invariant state having the following properties:

$$g_{(1)}(x) = c, \quad g_{(2)}(x_1, x_2) = g(|x_1 - x_2|),$$
$$\quad (44)$$
$$g_{(p)} = 0, \text{ for } p \geq 3.$$

Such a state can be easily built, as we shall see later. Thus, we have

$$\mathcal{T}_0^{(\alpha)}(x) = \exp\left\{ -\alpha c x + \frac{\alpha^2}{2} \bar{g}_{(2)}(x) \right\}, \quad (45)$$

with

$$\bar{g}_{(2)}(x) = 2x \int_0^x dz \, g(z) - 2 \int_0^x dz \, z \, g(z).$$

If we define

$$A = 2 \int_0^\infty dz \, g(z) \quad \text{and} \quad B = \int_0^\infty dz \, z \, g(z),$$

which are finite for short-range correlations, one sees that in the limit $x \to \infty$ three cases have to be distinguished:

$$
\begin{aligned}
&(1) \quad \alpha c - \frac{\alpha^2}{2} A > 0 : \mathcal{T}_0^{(\alpha)}(\infty) = 0, \\
&(2) \quad \alpha c - \frac{\alpha^2}{2} A < 0 : \mathcal{T}_0^{(\alpha)}(\infty) = \infty, \quad (46) \\
&(3) \quad \alpha c - \frac{\alpha^2}{2} A = 0 : \mathcal{T}_0^{(\alpha)}(\infty) = e^{-\alpha^2 B}.
\end{aligned}
$$

The case (2) is unphysical, because the particle density must be positive. Thus the value of A is such that $\alpha A \leq 2c$ for all $\alpha \in [1, 2]$, which implies $A \leq c$. This constraint is a consequence of the assumption $g_{(p)} = 0$ for $p \geq 3$ and $B < \infty$. This also means that the case (3) is only realizable for $\alpha = 2$, $A = c$. From (42) it follows that for an initial state of the type (44), we have the same asymptotic density amplitude for all the α models with $1 \leq \alpha < 2$ and for the pure-annihilation case with $A < c$. But in the pure-annihilation case with $A = c$, the amplitude depends on the value of B.

We now show how to build a state of the form (44) and understand its physical content. Let us take a Poissonian state with density $\hat{c}$

$$|P\rangle = e^{\hat{c} \int dz \, (\pi(z) - 1)} |0\rangle,$$

and the state $|\Phi_\beta\rangle$ obtained by the replacement,

$$\pi(z) \to \pi(z) \left[\beta + \frac{1}{2\hat{c}} \int dy \, \pi(z+y) g(y) \right], \quad 0 \leq \beta \leq 1. \quad (47)$$

The normalization $\langle |\Phi_\beta \rangle = 1$ implies that

$$A = 2 \int_0^\infty dy \, g(y) = 2(1 - \beta)\hat{c}.$$

The modification (47) means that we go from the state $|P\rangle$, where particles are randomly distributed, to the state $|\Phi_\beta\rangle$, where both single particles and pairs are randomly distributed. The probability density that a pair has an extension σ is $\frac{1}{2\hat{c}} g(\sigma)$. If $\beta = 0$ there are only pairs in the state $|\Phi_0\rangle$. A straightforward calculation gives

$$|\Phi_\beta\rangle = \exp\left\{ (2 - \beta)\hat{c} \int dz \, [\pi(z) - 1] \right.$$
$$\left. + \frac{1}{2} \int dz \, dy \, g(z-y)[\pi(z) - 1][\pi(y) - 1] \right\}.$$

Thus we have a state of the type (44) with density $c = (2 - \beta)\hat{c}$. For $\beta = 0$, we have $A = c$. The mean extension of a pair is

$$\bar{\sigma} = \frac{1}{2\hat{c}} \int_0^\infty d\sigma \, \sigma g(\sigma) = \frac{(2 - \beta)B}{2c}.$$

Our α models, with initial correlations can now be parametrized in terms of $(\alpha, \beta, \bar{\sigma}) \in [1,2] \times [0,1] \times [0,\infty)$. The asymptotic density amplitudes are universal for all the values of the parameters, except on the line $(\alpha = 2, \beta = 0, \bar{\sigma})$ where the amplitude is proportional to

$(1 - e^{-4c\bar{\sigma}})$. In this case, the asymptotic density amplitude tends to zero if $\bar{\sigma} \to 0$. The physical reason is that when $\bar{\sigma} = 0$, the two particles of a pair are at the same place and immediately annihilate. This situation cannot occur if coagulation is present, because single isolated particles will remain.

It would be interesting to see how a more general initial state would affect the amplitudes. Note finally that the relations (46), characterizing the initial state, are preserved by the dynamical evolution. Indeed, every evolved state can be considered as a new initial state evolving towards the same asymptotic solution.

V. CONCLUSIONS

We have studied a class of d-dimensional diffusion-reaction models interpolating continuously between the diffusion-coagulation and the diffusion-annihilation models. The field-theoretical approach used leads to exact relations between the observables of these different models. In one dimension, it was shown how correlations in the initial state can lead to a violation of the universality of the amplitude for the DA models.

Several extensions of the present work concerning one-dimensional models with reversible diffusion-reaction systems, or the presence of fronts in inhomogeneous systems, are under investigation. Moreover, one may expect to construct "good observables" in d-dimensional systems for which a closed equation of motion can be derived.

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