Phase transition in annihilation-limited processes

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Abstract
A system of particles is studied in which the stochastic processes are one-particle type-change (or one-particle diffusion) and multi-particle annihilation. It is shown that, if the annihilation rate tends to zero but the initial values of the average number of the particles tend to infinity, so that the annihilation rate times a certain power of the initial values of the average number of the particles remain constant (the double scaling) then if the initial state of the system is a multi-Poisson distribution, the system always remains in a state of multi-Poisson distribution, but with evolving parameters. The large time behavior of the system is also investigated. The system exhibits a dynamical phase transition. It is seen that for a $k$-particle annihilation, if $k$ is larger than a critical value $k_c$, which is determined by the type-change rates, then annihilation does not enter the relaxation exponent of the system; while for $k < k_c$, it is the annihilation (in fact $k$ itself) which determines the relaxation exponent.

PACS numbers: 05.40.-a, 02.50.Ga
Keywords: reaction-diffusion, annihilation, diffusion-limited, phase transition

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1 Introduction

People have studied reaction-diffusion systems, using analytical techniques, approximation methods, and simulations. A large fraction of exact results belong to low-dimensional (specially one-dimensional) systems, as solving low-dimensional systems should in principle be easier [1–13]. Despite their simplicity, these systems exhibit rather rich and non-trivial dynamical and stationary behavior. Studies on the models far from equilibrium have shown that there is a remarkably rich variety of critical phenomena [1]. Among the important aspects of reaction-diffusion systems, are the stationary state of the system (or one of the quantities describing the system) and the relaxation behavior of the system towards this configuration.

Field theoretic methods have been used to study diffusion, recombination, and other dynamic manifestations of non-quantum-mechanical objects (for a review see [14]). The techniques of field theory on a lattice are used to examine the diffusion and reaction processes of particles [14]. The field theoretic methods and the dynamic renormalization group (RG) have been applied to study the universal scaling properties of reaction-diffusion models [15,16]. They have also been used to study fluctuations in reaction-diffusion problems, for example to study the single-species annihilation of $k$ particles to $l$ particles ($l < k$) [15]. In [17] a model is investigated where organisms die and give birth with equal rates, and also diffuse. It is shown there that at dimensions smaller than or equal to 2, there is aggregation, while at larger dimensions there is no clustering. In [18, 19], a model is investigated where particles are created, annihilated, and diffused on a lattice. For the case of one- or two-particle annihilation and creation, exact results are obtained. In all these cases, bosonic formulations have been used, meaning that each site can be occupied by more than one particle.

In this paper, a stochastic model is considered in which the (stochastic) variables of the system are the numbers of various types of particles. The term type can refer to species as well as position of the particle. There are single-particle type-changes, as well as $k$-particle annihilations. Specially, a case is studied where the annihilation rate tends to zero while this rate times the $(k - 1)'$th power of the initial values of the average particle-numbers remain constant. It is shown that in this double-scaling limit, the evolution equations for the annihilation operators contain only annihilation operators. Specifically, if the initial state of the system is a multi-Poisson distribution, then the system always remains in a state of multi-Poisson distribution, but with evolving parameters. The parameters evolve in a set of equations which in fact are the mean field equations.

It is further shown that the system exhibits a dynamical phase transition. The large time behavior of the system is controlled by the spectrum of the evolution operator corresponding to single-particle type-changes, and $k$. It is shown that if $k$ exceeds a critical value $k_c$, which is determined by type-change rates, annihilation does not enter the relaxation exponent of the system; while for $k < k_c$, it is the annihilation which determines the relaxation exponent.
The scheme of the paper is the following. In section 2, some general techniques are introduced, mainly to fix notation. In section 3, the double-scaling is discussed. In section 4, the large-time behavior of the system and the dynamical phase transition are investigated. Section 5 is devoted to the concluding remarks.

2 The general technique

To fix notation, let’s briefly introduce the general technique. Consider a system the state of which is characterized by a set of nonnegative integers (say the number of different particles). The vector space corresponding to such a system can be constructed using the raising and lowering operators ($A^{\mu}_\nu$’s and $A^{\mu}$’s, respectively), and the corresponding number operators $N^{\mu}$, through

\[
\begin{align*}
[A^{\mu}, A^{\dagger}_\nu] &= \delta^{\mu}_\nu, \\
[A^{\mu}, A^{\nu}] &= 0, \\
[A^{\dagger}_\mu, A^{\dagger}_\nu] &= 0, \\
A^{\mu} |0\rangle &= 0, \\
N^{\mu} &= \Delta^{\mu}_{\alpha \beta} A^{\dagger}_\alpha A^{\beta}, \\
\Delta^{\mu}_{\alpha \beta} &= \delta^{\mu}_\alpha \delta^{\beta}_\beta, \\
|n\rangle &= \prod_{\mu} (A^{\dagger}_\mu)^{n_\mu} |0\rangle, \\
\langle m|n\rangle &= \delta_{m n},
\end{align*}
\]

where the kets $|n\rangle$ form a basis for the vector space corresponding to the system. Note that by several types of particles, one may mean several species of particles or particles in several places (or both).

Corresponding to any set of probabilities $P_n$ of finding the system in the state $|n\rangle$ (having $n_\mu$ particles of type $\mu$), there is a probability vector in the vector space which is

\[
|P\rangle = \sum_n P_n |n\rangle.
\]

Any physical state of such a system is characterized by a vector like

\[
|P\rangle = f(A^{\dagger}) |0\rangle,
\]

where $f(A^{\dagger})$ is a Taylor series in $A^{\dagger}$ with nonnegative coefficients and with the sum of coefficients equal to one. This last condition can be written as one of the following equivalent forms

\[
\begin{align*}
f(S) &= 1, \\
\langle S| f(A^{\dagger}) &= \langle S|,
\end{align*}
\]
where $S$ is a covector all of its coefficients are equal to one, and
\[
\langle S \rangle = \langle 0 | e^{S_\alpha A^\alpha} .
\] (5)

The observables of such a system are functions of the number operators. The expectation value of the observable $g(N)$ is
\[
\langle g(N) \rangle = \langle S | g(N) | P \rangle,
\]
\[
= \langle 0 | g(N + A) f(A^\dagger + S) | 0 \rangle,
\]
\[
= : \langle 0 | \bar{g}(A) f(A^\dagger + S) | 0 \rangle .
\] (6)

where in the last equality commutation relations between $A$’s and $A^\dagger$’s have been used to rearrange them in $g(N + A)$ so that $A^\dagger$’s are all in the left of $A$’s. Specially, if the system has a multi-Poisson probability distribution with parameters $\Lambda^\mu$:
\[
| P \rangle = e^{\Lambda^\alpha (A^\dagger_\alpha - S_\alpha)} | 0 \rangle ,
\] (7)

then
\[
\langle g(N) \rangle = \bar{g}(\Lambda) .
\] (8)

A general continuous-time stochastic process is described by a linear operator (Hamiltonian) $H$ with nonnegative nondiagonal elements and the property that
\[
\langle S | H = 0 .
\] (9)

Such a Hamiltonian can be written in terms of the annihilation and creation operators. Specifically, a process involving the annihilation of $k$ particles and creation of $l$ particles is described by the Hamiltonian
\[
H = \langle A^\dagger_\alpha_1 \cdots A^\dagger_\alpha_l A^\beta_1 \cdots A^\beta_k \\
- S_\alpha_1 \cdots S_\alpha_l \Delta^\beta_1 \gamma_1 \delta_1 \cdots \Delta^\beta_k \gamma_k \delta_k A^\dagger_1 \cdots A^\dagger_l A^\beta_k \cdots A^\beta_k \rangle C^{\alpha_1 \cdots \alpha_l \beta_1 \cdots \beta_k} (N),
\]
\[
= \langle A^\dagger_1 \cdots A^\dagger_\alpha_l A^\beta_1 \cdots A^\beta_k - S_\alpha_1 \cdots S_\alpha_l N(N^\beta_1 \cdots N^\beta_k) \rangle C^{\alpha_1 \cdots \alpha_l \beta_1 \cdots \beta_k} (N),
\] (10)

where $C$’s are nonnegative rates, and $N$ means normal-ordering, that is putting $A^\dagger$’s at the left of $A$’s.

The evolution of the state vector of the system ($| P(t) \rangle$) is through
\[
| P(t) \rangle = U(t, 0) | P(0) \rangle ,
\] (11)

where
\[
\frac{\partial}{\partial t} U(t, 0) = H U(t, 0),
\]
\[
U(0,0) = 1 .
\] (12)

So the expectation value of an observable $Q$ at the time $t$ can be written like
\[
\langle Q(t) \rangle = \langle S | Q | P(t) \rangle ,
\]
\[
= \langle S | Q^H(t) | P(0) \rangle ,
\] (13)
where

\[ Q^H(t) := U^{-1}(t, 0) Q U(t, 0), \]
\[ \frac{d}{dt} Q^H(t) = [Q^H(t), H^H(t)], \]  \hspace{1cm} (14)

One notes that the Heisenberg operators \( Q^H \) are in fact the ordinary operators in them \( A \)'s and \( A^\dagger \)'s are substituted by \( A(t) \)'s and \( A^\dagger(t) \)'s.

One also has

\[ \langle Q(t) \rangle = \langle 0 | \hat{Q} | \hat{P}(t) \rangle, \]
\[ = \langle 0 | \hat{Q}^H(t) | \hat{P}(0) \rangle, \]  \hspace{1cm} (15)

where

\[ |\hat{P}\rangle := e^{S_{\alpha} \mu^\alpha} |P\rangle, \]
\[ \hat{Q} := e^{S_{\alpha} \mu^\alpha} Q e^{-S_{\alpha} \mu^\alpha}, \]
\[ \hat{Q}^H(t) := \hat{U}^{-1}(t, 0) \hat{Q} \hat{U}(t, 0), \]  \hspace{1cm} (16)

and \( \hat{U} \) is defined similar to (12), but with \( \hat{H} \) in place of \( H \). It is seen that the effect of tilde on the operators is just to change \( A^\dagger_\alpha \) to \( (A^\dagger_\alpha + S_\alpha) \).

3 Double scaling in annihilation processes of low rates

Consider a reaction-annihilation process with the Hamiltonian

\[ H = H_0 + H_1, \]  \hspace{1cm} (17)

where

\[ H_0 := M^\alpha_\beta A^\dagger_\alpha A^\beta, \]  \hspace{1cm} (18)
\[ H_1 := \sum_k C_{\beta_1 \ldots \beta_k} [A^{\beta_1} \ldots A^{\beta_k} - N(N_{\beta_1} \ldots N_{\beta_k})], \]  \hspace{1cm} (19)

where

\[ S_\alpha M^\alpha_\beta = 0. \]  \hspace{1cm} (20)

Since only the symmetric part of \( C \) enters the Hamiltonian, from now on it is assumed that \( C \) is symmetric. \( H_0 \) describes a reaction, change of a particle of type \( \beta \) to a particle of type \( \alpha \) with the rate \( M^\alpha_\beta \), while \( H_1 \) describes annihilations.

For the observable \( g(N) \), one has then

\[ \langle g[N(t)] \rangle = \langle 0 | \hat{U}^{-1}(t, 0) \check{g}(A) \hat{U}(t, 0) | \hat{P}(0) \rangle, \]  \hspace{1cm} (21)
where the evolution of $\tilde{U}$ is governed by by $\tilde{H}$:

$\tilde{H} = M_{\alpha \beta} A_{\alpha}^\dagger A_{\beta} + \sum_k C_{\beta_1 \ldots \beta_k} \{ A_{\beta_1} \ldots A_{\beta_k} - N \sum_k \{ A_{\beta_1} \ldots A_{\beta_k} \} \}$,

and

$|\tilde{P}(0)\rangle = \tilde{f}(A^\dagger) |0\rangle$.  

(22)

Suppose that the initial state vector describes a large number of particles, and the annihilation rates are small, specifically so that $\tilde{f}(A^\dagger/\lambda)$ and $(\lambda^{k-1} C_{\beta_1 \ldots \beta_k})$ (for all $k$’s) both exist as $\lambda \to \infty$. One can then define another pair of annihilation and creation operators through the transformation

$A_{\beta} =: \lambda a_{\beta}$,

$A_{\alpha}^\dagger =: \lambda^{-1} a_{\alpha}^\dagger$.  

(24)

Writing $A$’s and $A^\dagger$’s in terms of $a$’s and $a^\dagger$’s, and sending $\lambda$ to infinity, it is seen that in the Hamiltonian $\tilde{H}$ only those terms survive that are linear in $A^\dagger$.

So in this double-scaling limit, one can use instead of $\tilde{H}$ the Hamiltonian $\tilde{H}_s$:

$\tilde{H}_s := M_{\alpha \beta} A_{\alpha}^\dagger A_{\beta} - \sum_k k C_{\beta_1 \ldots \beta_k} N_{\beta_1} A_{\beta_2} \ldots A_{\beta_k}$,

(25)

where use has been made of the fact that $C$’s are symmetric. It is now easily seen that in this limit,

$\langle g[N(t)] \rangle = \langle 0 | \bar{g}[\tilde{A}_s(t)] | \tilde{P}(0) \rangle$,

(26)

where $\tilde{A}_s(t)$’s satisfy

$\frac{d}{dt} \tilde{A}_s^\beta = \left( M_{\alpha \beta} - \Delta_{\alpha_1 \alpha} \sum_k k C_{\beta_1 \ldots \beta_k} \tilde{A}_{\alpha_1} \ldots \tilde{A}_{\alpha_k} \right) \tilde{A}_s^\beta$.  

(27)

This is a set of differential equations for $\tilde{A}_s^\alpha$’s, which are commuting at $t = 0$ and remain commuting at later times. Specifically, if the initial state of the system is a multi-Poisson distribution (7), then with this evolution the system always remains in a state of multi-Poisson distribution, but with evolving parameters $\Lambda^\alpha(t)$ which satisfy

$\frac{d}{dt} \Lambda^\alpha = \left( M_{\alpha \beta} - \Delta_{\beta_1 \beta} \sum_k k C_{\beta_1 \ldots \beta_k} \Lambda_{\beta_2} \ldots \Lambda_{\beta_k} \right) \Lambda^\beta$.  

(28)

This equation can be solved perturbatively. One defines

$\Lambda^\alpha(t) =: R^\alpha(\beta) Y^\beta(t)$,

(29)

where

$\frac{d}{dt} R = M$,

$R(0) = 1$.  

(30)
To be more specific, let’s consider a system described by a reaction and a $k$-particle annihilation. One has

$$\frac{d}{dt} Y^\alpha = (R^{-1})^\alpha_\sigma D^\sigma_{\beta_1 \ldots \beta_k} (R^\beta_{\alpha_1} Y^{\alpha_1}) \cdots (R^\beta_{\alpha_k} Y^{\alpha_k}), \quad (31)$$

where

$$D^\sigma_{\beta_1 \ldots \beta_k} := -k C_\nu (\beta_2 \ldots \beta_k \Delta^\nu_{\sigma \beta_1}), \quad (32)$$

and the $\beta_2 \ldots \beta_k (\beta_1)$ means that part which is symmetric with respect to the indices. Eq. (31) can be rewritten like

$$Y^\alpha(t) = \Lambda^\alpha(0) + \int_0^t \frac{dt'}{(R^{-1})^\alpha_\sigma (t')} D^\sigma_{\beta_1 \ldots \beta_k} \times [R^\beta_{\alpha_1}(t') Y^{\alpha_1}(t')] \cdots [R^\beta_{\alpha_k}(t') Y^{\alpha_k}(t')], \quad (33)$$

and from that

$$\Lambda^\alpha(t) = R^\alpha_{\beta}(t) \Lambda^\beta(0) + \int_0^t \frac{dt'}{R^\alpha_\sigma (t-t')} D^\sigma_{\beta_1 \ldots \beta_k} \Lambda^\beta_{\alpha_1}(t') \cdots \Lambda^\beta_{\alpha_k}(t'). \quad (34)$$

The above expression can be visualized by a set of graphs. Each graph consists of vertices and directed links. Each vertex has one outgoing link and $k$ incoming links. Each graph is connected, has no loops, and has only one outgoing link. $\Lambda^\alpha(t)$ is the sum of possible such graphs, the values of them are calculated using the following rules.

- To each point of the graph (the beginning points, the end point, and the vertices) is assigned a time. The time corresponding to the end of a link should not be smaller than the time corresponding to the beginning of that link. The time corresponding to the beginnings of the incoming links of the graph are 0, and the time corresponding to the end of the outgoing link of the graph is $t$.

- To each directed link is assigned a factor $R$, the argument of which is the time corresponding to the end of the link minus the time corresponding to the beginning of the link.

- To each vertex is assigned a factor $D$.

- To the beginning point of each incoming link of the graph is assigned a factor $\Lambda(0)$.

- The value assigned to a graph is the product of the values assigned to various parts of the graph, integrated over the times corresponding to the vertices.

Using this scheme, one can in principle find $\Lambda(t)$ up to desired order (number of vertices).
4 The large time behavior of the system

The real parts of the eigenvalues of $M$ are nonpositive, and zero is an eigenvalue of $M$. Assuming that the only eigenvalue with nonnegative real part is zero, and that this eigenvalue is nondegenerate, the large time behavior of $R$ is simple. The large time behavior of $R$ depends on the spectrum of $M$ near zero. If there is a gap in the spectrum, that is if the supremum of the real parts of the eigenvalues (apart from zero) is negative, then

$$\lim_{t \to \infty} R^{\alpha \beta}(t) = u^\alpha S_\beta,$$  \hspace{1cm} (35)

where $u$ is the normalized right eigenvector of $M$ corresponding to the eigenvalue 0:

$$Mu = 0, \quad S_\alpha u^\alpha = 1.$$  \hspace{1cm} (36)

If there is no gap in the spectrum of $M$ near the eigenvalue zero, but still the only eigenvalue of $M$ with zero real part is zero, and this eigenvalue is nondegenerate, then

$$R^{\alpha \beta}(t) \sim \left(\frac{t}{\tau}\right)^{-\delta} u^\alpha S_\beta, \quad t \to \infty,$$  \hspace{1cm} (37)

where $\tau$ and $\delta$ are constants depending on the behavior of the spectrum of $M$ near zero.

In the case there is a gap in the spectrum, for $t \to \infty$ one can substitute the right-hand side of (35) for $R$ in the expressions for the graphs, as for most of the times, the argument of $R$ is large. This is equivalent to rewriting (34) as

$$\Lambda^\alpha(t) = u^\alpha \left[ S_\beta \Lambda^\beta(0) + \int_0^t dt' S_\sigma D^\sigma_{\beta_1 \cdots \beta_k} \Lambda^{\beta_1}(t') \cdots \Lambda^{\beta_k}(t') \right],$$  \hspace{1cm} (38)

or

$$\lambda(t) = S_\beta \Lambda^\beta(0) + \int_0^t dt' D[\lambda(t')]^k,$$  \hspace{1cm} (39)

where

$$\Lambda^\alpha(t) =: u^\alpha \lambda(t),$$  \hspace{1cm} (40)

and

$$D := S_\sigma D^\sigma_{\beta_1 \cdots \beta_k} u^{\beta_1} \cdots u^{\beta_k}.$$  \hspace{1cm} (41)

It is easy to solve (39). One has

$$\frac{d\lambda}{dt} = D \lambda^k,$$  \hspace{1cm} (42)

from which one obtains

$$\lambda(t) = \frac{S_\alpha \Lambda^\alpha(0)}{1 - (k - 1) D[S_\beta \Lambda^\beta(0)]^k t} t^{1/(k-1)},$$  \hspace{1cm} (43)
or
\[
\Lambda^\alpha(t) = \frac{u^\alpha S_\gamma \Lambda^\gamma(0)}{\{1 + k (k - 1) C_{\beta_1 \cdots \beta_k} u^{\beta_1} \cdots u^{\beta_k} [S_\beta \Lambda^\beta(0)]^{k-1} t\}^{1/(k-1)}}.
\] (44)

If there is no gap in the spectrum of \(M\) near zero, one has to substitute (37) in (34). It is then seen that \(\Lambda(t)\) is proportional to \(u\), for large times. Putting the ansatz
\[
\Lambda^\alpha(t) \sim t^{-\mu} u^\alpha, \quad t \to \infty,
\] (45)
along with (37) in (34), one arrives at
\[
t^{-\mu} \sim c t^{-\delta} + I(t),
\] (46)
where
\[
I(t) \sim \int_x^{t-y} dt' (t - t')^{-\delta} t'^{-k\mu}.
\] (47)
x and \(y\) are introduced to ensure that the approximations used for \(R\) and \(\Lambda\) are valid in the integration domain. A dimensional analysis shows that for large \(t\),
\[
I(t) \sim c_1 t^{-\delta} + c_2 t^{-k\mu} + c_3 t^{1-\delta-k\mu}, \quad t \to \infty.
\] (48)
So,
\[
t^{-\mu} \sim c_1' t^{-\delta} + c_2' t^{-k\mu} + c_3' t^{1-\delta-k\mu}, \quad t \to \infty.
\] (49)
The meaning of this, is that the two largest exponents entering this expression should be equal. As \(k > 1\), the exponent \(-k\mu\) is smaller than \(-\mu\). So it cannot be among the largest exponents. There remains three possibilities:
\[
\mu = \begin{cases} 
1 \quad & k \delta < 1 \\
\delta \quad & k \delta > 1 \\
\frac{1-\delta}{k-1} \quad & k \delta > 1
\end{cases}
\] (50)
It can be shown that the third case does not occur. To see this, consider the integration corresponding to the a vertex all of its incoming links are incoming links of a graph. The time dependence of the integral involved is
\[
I'(t) \sim d_1 t^{-\delta} + d_2 t^{-k\delta} + d_3 t^{1-\delta-k\delta},
\] (51)
where \(t\) is the time corresponding to the end of the outgoing link. It is seen that for \(k \delta > 1\), the largest exponent in the right-hand side is \(-\delta\), which shows that the result of the integration is proportional to \(t^{-\delta}\) (for large times). Repeating this for successive vertices, One finds that all graphs are proportional to \(t^{-\delta}\). So the correct value for \(\mu\) is \(\delta\). One can then summarize (50) in
\[
\mu = \max \left( \frac{\delta}{k}, \frac{1}{k} \right).
\] (52)
Defining
\[ k_c := \frac{1}{\delta}, \]  
(53)
it is seen that the system exhibits a dynamical phase transition: for \( k > k_c \), annihilation does not enter the relaxation exponent of the system; while for \( k < k_c \), it is the annihilation which determines the relaxation exponent.

A note is here in order. If instead of (45), one choose an ansatz that the relaxation of \( \Lambda \) is exponential rather than power law, then the integral on the right-hand side of (34) tends to zero faster than \( \Lambda \) itself (as \( k > 1 \)), which means that for large times, only the first term on the right-hand side of (34) determines \( \Lambda \), so it should decay exponentially, which is not the case.

As an example, consider a system consisting of particles of a single species diffusing on a \( d \)-dimensional lattice with symmetric rates. Suppose that there is a \( k \)-particle annihilation (double-scaled) as well. The types of the particles are just the sites of the lattice, denoted by \( x \) (\( d \)-tuples of integers). The matrix \( M \) describing the diffusion is then
\[ M = \sum_{i=1}^{d} r_i (T_i + T_i^{-1} - 2), \]  
(54)
where \( T_i \) is the one-site translation in the \( i \)-th direction. The eigenvalues of \( M \) are
\[ E(\theta) := \sum_{i=1}^{d} 2r_i (\cos \theta_i - 1). \]  
(55)
For a finite lattice, \( \theta \)'s are discrete and there is a gap in spectrum at zero. For an infinite lattice, the spectrum is continuous at zero, and a steepest-descent study shows that
\[ \delta = \frac{d}{2}. \]  
(56)
This shows that in this case, the system never crosses the critical point \( k = k_c \), as \( k_c \leq 2 \) and \( k \geq 2 \).

5 Concluding remarks

A system was investigated consisting of several types of bosonic particles. By bosonic, it is meant there can be more than one particle of each type (at each site). In [17–19], similar systems were investigated and exact results including phase transitions were obtained for the case of at most two particle creation or annihilation. In the case investigated here, there is no creation, but there is \( k \)-particle annihilation, where \( k \) can be larger than 2. The case of small annihilation rate, together with large initial number of particles was investigated in more detail. It was shown that this system exhibits a dynamical phase transition, which is controlled by \( k \) and another parameter related to the rates of one-particle reactions.
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