Renormalization Group Approach to Reaction-Diffusion Systems with Input Particles

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(Received 5 November 1998)

We consider reaction-diffusion systems of a single species \((A + A \rightarrow \phi)\) in the absence and the presence of a particle input. Applying renormalization group theory to a field theoretic description and matching theory to the renormalization group trajectory integrals of the systems, we find that for \(d < 2\) in the absence of an input, the density decays as \(c(t) \sim t^{-\nu}\) with the dynamic exponent \(\nu = d/2\) and in the presence of input the density grows as \(c(t) \sim t^{\mu}\) with the static exponent \(\mu = d/(d + 2)\), while for \(d > 2\) the behaviors are mean-field like and for \(d = 2\) there are logarithmic corrections to the mean-field results. The results for the absence of input are consistent with the previous results obtained using different methods. In addition, we propose a rigorous proof of Racz's conjecture about the relation between the static and the dynamic exponents, \(\mu = \nu/(1 + \nu)\).

Recently, there has been much interest in the kinetics of one-species reaction-diffusion systems, \(A + A \rightarrow \phi\). It is well established that depending on the dimensionality \(d\) of the system in which the reaction and the diffusion take place, fluctuations either can lead to renormalization of the reaction constants or to a dramatic change in the time dependence [1-4]. Mean-field-like kinetic descriptions in terms of the conventional rate equation for the evolution of the average density and their predictions hold only above some upper critical dimension \(d_c\). Below \(d_c\), fluctuations are relevant and lead to the non-mean-field critical exponents, and the associated critical exponents have some universal properties [5-9]. The field theoretic renormalization group approach developed in the framework of equilibrium statistical physics can provide a suitable tool for studying this kind of dynamics [10]. The dynamics of a reaction-diffusion system is described by a master equation governing the time evolution of the probability \(P\{n\}; t\) that the system be in a given microstate \(\{n\}\). The master equation can be mapped to a coarse-grained description by using a Fock space formalism [11-15]. We end up with a model whose dynamics is defined by the action of continuous field theory. From an analysis of the field theory, we find an upper critical dimension \(d_c = 2\), which is associated with the stochastic processes of reaction and diffusion. Hence, for \(d > 2\), one can use a mean-field-like kinetic equation description while for \(d \leq 2\), one must perform a renormalization group calculation.

In this letter, we analyze a field theoretic formulation of the reaction-diffusion process \(A + A \rightarrow \phi\) in the absence and the presence of a particle input. The concentration of \(A\) is initially Poissonian with an average density \(n_0\). We search for the asymptotic decay or growth of the concentration at long times by using renormalization group theory. For the case of the absence of input particles, Peliti [14] and Lee [15] calculated the concentration of particles by solving the Callan-Symanzik equation. We present a different, easier method which uses matching theory to calculate the concentration and show the results are consistent with those in Refs. 14 and 15.

We consider a one-species reaction-diffusion process \((A + A \rightarrow \phi)\) in \(d\) spatial dimensions. For convenience, we define the diffusion so that it proceeds on a cubic lattice. We use a continuous-time master equation to define the way in which the probability of any given configuration of particles changes with time. The master equation for this process [15,16] is

\[
\frac{\partial P\{n\}; t\}}{\partial t} = - \frac{D}{\hbar^2} \sum_{i} [(n_{i+1})P(n_{i-1}, n_{i+1}; t) - n_{i}P(n_{i}, n_{i}; t)] \\
+ \lambda \sum_{i} [(n_{i+2})(n_{i}+1)P(n_{i}+2; t) - n_{i}(n_{i}-1)P(n_{i}t)]
\]
\begin{equation}
\frac{1}{h^d} \sum_i [P(n_i - 1; t) - P(n_i; t)],
\end{equation}

where \( h \) is the lattice spacing, \( I \) is the rate of particle input, \( D \) is the diffusivity of particles, \( n_i \) is the number of particles on lattice site \( i \), and \( \lambda \) is the reaction rate. The summation over \( i \) is over all sites on the lattice, and the summation over \( j \) is over all nearest neighbors of site \( i \). For simplicity, particles with an average number density \( n_0 \) are initially placed at random on the lattice.

The field theory is derived by identifying a master equation, writing the master equation in terms of creation and annihilation operators, and using the coherent-state representation. We find that the concentration of particles, averaged over the random initial condition and the random statistics of the reaction-diffusion process, is given by

\begin{equation}
c(x, t) = \langle a(x, t) \rangle
\end{equation}

where the average is taken with respect to \( e^{-S} \). The action \( S = S_0 + S_1 + S_2 \), where

\begin{equation}
S_0 = \int d^d x \int_0^{t_f} dt \bar{a}(x, t) \left[ \partial_t - D \nabla^2 + \delta(t) \right] a(x, t) - n_0 \int d^d x \bar{a}(x, 0),
\end{equation}

\begin{equation}
S_1 = \int d^d x \int_0^{t_f} dt \left[ \bar{a}^2(x, t) a^2(x, t) + 2 \bar{a}(x, t) a^2(x, t) \right],
\end{equation}

\begin{equation}
S_2 = -I \int d^d x \int_0^{t_f} dt \bar{a}(x, t).
\end{equation}

The upper time limit in the action is arbitrary as long as \( t_f \geq t \). The first term in \( S_0 \) represents simple diffusion without an external potential, and the second term comes from the random Poissonian initial condition. The \( \delta \)-function, often left out by convention, forces the initial condition on the free-field propagator. The term \( S_1 \) comes from the reaction terms. The term \( S_2 \) comes from the particle input. In case of no particle input, we will set \( I = 0 \).

A mean-field-like equation can be derived by a saddle-point approximation to the action \( S \) [16,17]. The result is

\begin{equation}
\partial_t c = D \nabla^2 c - \lambda_1 c^2 + I, \quad c(x, 0) = n_0.
\end{equation}

In the absence of a particle input, this equation has the mean-field solution

\begin{equation}
c(t, I = 0) = \frac{1}{n_0^{-1} + \lambda_1 t}
\end{equation}

which behaves as \( c(t) \sim t^{-1} \) in the long-time limit. This result applies only for \( d > d_2 = 2 \). In the presence of a particle input, Eq. (5) has a mean-field steady-state solution which approaches the steady-state density:

\begin{equation}
c(t = \infty, I) \sim I^{1/2}
\end{equation}

which also holds only above the upper critical dimension \( d_c = 2 \).

Below \( d_c \), we apply renormalization group (RG) theory to the action \( S \) to take into account the fluctuation effects. Time ordering prevents a term of the form \( \bar{a}a \) from being generated, and all other relevant terms are already in the action \( S \). We integrate over momenta in the range \( \Lambda/k < k < \Lambda \) and then rescale the fields by \( \bar{a}'(bk, b^{-z}t) = \bar{a}(k, t)/\alpha \) and \( a'(bk, b^{-z}t) = a(k, t)/\alpha \). To achieve fixed points and to keep the time derivative in \( S_0 \) constant, we set \( \alpha = 1 \) and \( \bar{a} = b^d \). We determine the dynamical exponent \( z \) by requiring that the diffusion coefficient remain unchanged. We find the flow equations, to one-loop order, to be

\begin{align}
\frac{d \ln D}{dl} &= z - 2, \\
\frac{d \ln n_0}{dl} &= 2, \\
\frac{d \ln \lambda}{dl} &= z - d - \frac{\lambda}{4\pi D}, \\
\frac{d \ln I}{dl} &= z + d.
\end{align}

The dynamical exponent is given by \( d \ln D/dl = 0 \), i.e., \( z = 2 \). The renormalization group transformation relates the original system at long times and low concentrations to another, renormalized system at short times and high concentrations.

1. Without the Particle Input

In the absence of input particles, we set \( I = 0 \) and seek to understand how the concentration scales with \( t \) in long times. We integrate the flow equations until the renormalized time is short enough so that we can use simple mean-field theory [16]. The matching time, \( t_0 \),

\begin{equation}
t(t') = te^{-\int_0^{t'} \frac{z(t')}{d} dt} \equiv t_0,
\end{equation}

is chosen to be on the order of \( h^2/2D \) so as to be within the range of validity of both RG scaling and mean-field theory. Mean-field theory is a good approximation at this time because \( \lambda \) is small. An expansion in \( \lambda \) generates an expansion in \( t_0 \) that leads to subdominant scaling. For short times, the effective diffusivity is given by the bare value.

Calculating the renormalized particle concentration at short times with mean-field theory, we find

\begin{equation}
c(t(t'), I') = \frac{1}{n_0^{-1} \lambda(t') + \lambda(t')t(t')}
\end{equation}

as \( t' \to \infty \). The concentration of the original system is related to that of the renormalized system by scaling:

\begin{equation}
c(t, I = 0) = e^{-dt} c(t(t'), I').
\end{equation}
Combining Eqs. (14) and (15) and using Eq. (13) to express the result in terms of \( t \) rather than \( t^* \), we find

\[
c(t) \sim \begin{cases} 
\frac{1}{\ln(\frac{t}{t_0})} & d > 2 \\
\frac{1}{8\pi D t} & d = 2 \\
\frac{1}{\lambda^d \frac{t}{t_0}} & d < 2.
\end{cases}
\]  

(16)

Here, we have used the fact that \( \lambda(t) \) goes to a fixed point value for \( d < 2 \). To first order in \( 2 - d \), we find from Eq. (11) that \( \lambda^* = 4\pi D(2 - d) \). These results are consistent with those of Peliti [14] and Lee [15].

2. With the Particle Input

In the presence of input particles, we consider the limit \( I \to 0 \) and seek to understand how the concentration scales with \( I \) in this limit. We integrate the flow equations until the renormalized input rate is large enough so that we can use simple mean-field theory. The matching input rate, \( I_0 \),

\[
I(I^*) = e^{-(2+d)I} I \equiv I_0.
\]

is chosen to be on the order of \( D/h^{2+d} \) so as to be within the range of validity of both RG scaling and mean-field theory. For this renormalized value of \( I \), the average density is finite, and we can use mean-field theory. In this case, the mean-field theory predicts

\[
c(I(I^*), I^*) \sim \left( \frac{I(I^*)}{\lambda(I^*)} \right)^{1/2}.
\]

(18)

We match the mean-field result to the observed value by using the scaling relation

\[
c(t = \infty, I) = e^{-dI^*} c(I(I^*), I^*).
\]

(19)

We find the following for the concentration in the limit \( I \to 0 \):

\[
c(I) \sim \begin{cases} 
\left( \frac{I}{I_0} \right)^{1/2} & d > 2 \\
\left( \frac{1}{16\pi D} \frac{1}{\ln(I/I_0)} \right)^{1/2} & d = 2 \\
\left( \frac{I}{I_0} \right)^{d/(2+d)} \left( \frac{t}{t_0} \right)^{1/2} & d < 2.
\end{cases}
\]

(20)

Here, we used the fact that \( \lambda(t) \) goes to a fixed point value for \( d < 2 \), just as in the case of no particle input. These predictions are consistent with those of Rey and Droz [18].

In summary, we have shown that the RG and the matching theories are suitable formalisms for calculating the concentration for single-species reaction-diffusion systems with and without a particle input. In particular, we easily calculated the dynamic and the static critical exponents in arbitrary dimension. For \( d = 1 \), it was predicted that the steady-state density of particles depended on the input rate \( I \) with \( \mu = 1/3 \). We confirmed this result rigorously by using the field theoretic approach and matching theory. When \( d = 2 \), we showed that the rate constant \( \lambda \) became marginally irrelevant and that the dynamic and the static exponents were given by mean-field theory, but with logarithmic corrections to the mean-field results. Using scaling arguments, Racz conjectured that the static exponent \( \mu \) and the dynamic exponent \( \nu \) were not independent and that they were related to each other by \( \mu = \nu/(1 + \nu) \) [6]. For all dimensions above the critical dimension \( d_c = 2 \), the mean-field results for the dynamic and the static exponents satisfied this conjecture. For dimensions below the critical dimension, we showed that the dynamic exponent was given by \( \nu = d/z \) and the static exponent by \( \mu = d/(z + d) \) with \( z = 2 \). Consequently, using the field theoretic approach, we propose a rigorous proof of the conjecture by Racz, \( \mu = (d/z)/(1 + d/z) = \nu/(1 + \nu) \).

The authors wish to acknowledge the financial support of the Korea Research Foundation made in the program year of 1997.

REFERENCES