Long range hops and the pair annihilation reaction $A+A\rightarrow 0$: Renormalization group and simulation

Daniel C. Vernon*
Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6
(Received 17 April 2003; published 10 October 2003)

A simple example of a nonequilibrium system for which fluctuations are important is a system of particles which diffuse and may annihilate in pairs on contact. The renormalization group can be used to calculate the time dependence of the density of particles, and provides both an exact value for the exponent governing the decay of particles and an ϵ expansion for the amplitude of this power law. When the diffusion is anomalous, as when the particles perform Lévy flights, the critical dimension depends continuously on the control parameter for the Lévy distribution. The ϵ expansion can then become an expansion in a small parameter. We present the renormalization group calculation and compare these results with those of a simulation.

DOI: 10.1103/PhysRevE.68.041103 PACS number(s): 05.40.Fb, 64.60.Ak, 64.60.Ht

Many different approaches have been used to study the dynamics of systems far from equilibrium [1–3]. These include exact solutions derived by mapping the problem to a quantum spin system [4] or by studying various particle distribution functions [5,1], renormalization group methods [6], and simulations. Many of these systems can be assigned to a small number of universality classes, based on the time dependence of a few measurable quantities. Renormalization group methods are particularly useful in characterizing this universal behavior, as they make it possible to examine the action describing the behavior of the system and determine which scaling variables are relevant. Systems of particles which can diffuse and undergo reactions are straightforward examples, which can be studied far from equilibrium. One of the simplest examples of a reaction-diffusion system is the pair-annihilation reaction, in which members of a single species of particle, denoted by A, react at some rate λ to form an inert product. This reaction is written $A+A\rightarrow 0$. This reaction and some related ones have been studied for some time. For some examples, see the work of Smoluchowski [7], who studied the coagulation of colloidal particles using a mean-field approach, and Ovchinnikov and Zeldovich [8], who examined the effects of fluctuations on the reaction $A+B\rightarrow 0$. The solution to the (mean-field) rate equation

$$\frac{\partial n}{\partial t}=D\nabla^2 n-\lambda n^2 \tag{1}$$

for the density of particles is the correct result for spatial dimension $d>2$, but for lower dimensions fluctuations become important. If the number density of particles scales as $n\sim At^{-\alpha}$ for large t, then $\alpha=1$ for $d>2$. A renormalization group study by Lee [9] produced the exact result $\alpha=d/2$ for $d<2$, and also yielded the amplitude A as an expansion in $\epsilon=2-d$. The agreement between this amplitude and the exact result [10] for a specific model in $d=1$ was poor, as might be expected, as the expansion parameter $\epsilon=1$ is large here. However, the ϵ expansion does provide a systematic picture of the scaling behavior of this process.

This paper extends the renormalization group calculation of Ref. [9] to the case of anomalous diffusion, which is modeled by a long range hopping process in which the distance a particle travels in each time step is chosen from a Lévy distribution. These distributions form a family that share with the Gaussian the property that they are ''stable,'' in the sense that the probability distribution of the sum of two numbers chosen from a Lévy distribution is the same distribution, up to a trivial rescaling. The probability distribution for each of these distributions has a Fourier transform

$$P(k)=e^{-D_A k^\sigma} \quad (0<\sigma\leqslant 2), \tag{2}$$

where σ is a parameter that controls the shape of the distribution and D_A scales the distribution. For $\sigma<2$, the real-space distributions have power-law tails, $P(r)\sim r^{-(d+\sigma)}$ for large r. These distributions appear in a number of physical contexts [11], including diffusion in disordered media [12] and motion of particles in turbulent flow, in both experiments [13,14] and theoretical calculations [15]. Hinrichsen and Howard [16] previously simulated the process studied here and determined the exponent α, but did not perform a renormalization group calculation and did not measure the amplitude.

The calculation of the density of particles uses reasonably standard renormalization group techniques, and will only be summarized here. The density of particles can be found by solving the Langevin equation

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t}=(D_N\nabla^2+D_A\boldsymbol{\nabla}^\sigma)\phi(\mathbf{x},t)-\lambda\phi^2(\mathbf{x},t)+\phi(\mathbf{x},t)\zeta(\mathbf{x},t) \tag{3}$$

with an initial condition set by the initial density of particles n_0. The anomalous diffusion term $D_A\nabla^\sigma$ is defined by its action in Fourier space,

$$D_A\boldsymbol{\nabla}^\sigma e^{i\mathbf{k}\cdot\mathbf{x}}=-D_A|\mathbf{k}|^\sigma e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{4}$$

and the noise term ζ has correlations of the form

*Email address: dvernon@sfu.ca

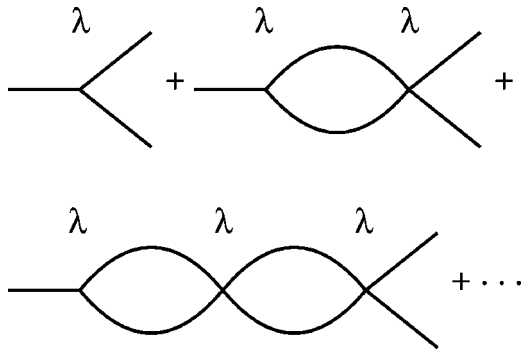

FIG. 1. The diagrams contributing to the renormalized annihilation rate. Time flows from right to left.

$$\langle \zeta(\mathbf{x},t)\zeta(\mathbf{x}',t')\rangle = -2\lambda\,\delta^d(\mathbf{x}-\mathbf{x}')\,\delta(t-t'). \tag{5}$$

The average density is then given by an average of solutions to Eq. (3) over noise histories, $n=\langle\phi\rangle$. The normal diffusion term $D_N\nabla^2$ appears if the distribution of hops has any component proportional to k^2 in its Fourier transform. This term will be dropped, as it is less relevant than the anomalous term and flows to zero under renormalization.

The form of the noise term and the noise-noise correlation function given by Eq. (5) are not determined by equilibrium physics, but can be derived from the master equation describing the microscopic behavior of the system, using the procedure developed by Doi [17,18] and Peliti [19]. Their procedure produces an effective field theory describing the behavior of the system, with an action given by

$$S=\int d^dx\Bigg[\int_0^t dt\{\hat\phi(\partial_t - D_A\nabla^\sigma)\phi + 2\lambda\hat\phi\phi^2+\lambda\hat\phi^2\phi^2\} - n_0\hat\phi(0)\Bigg]. \tag{6}$$

The field $\hat\phi$ is a response field, which plays the same rôle as that in the Martin-Siggia-Rose approach [20]. This field theory can then be used to derive a Langevin equation by integrating out the response field, applying the Martin-Siggia-Rose approach [20] in reverse. For examples of this derivation applied to similar problems, see Refs. [6,21]. Either the field theory or the Langevin equation can be used to develop a renormalized perturbation expansion for the density of particles.

The sum of tree diagrams is equivalent to the solution of Eq. (3) without the noise term. Divergences appear when diagrams with loops are included, and these can be handled by renormalizing the annihilation rate λ. Power counting shows that the critical dimension is $d_c=\sigma$, so that the expansion will be in $\epsilon=\sigma-d$. The diagrams in Fig. 1 give the full renormalization of the annihilation rate and represent the sum

$$\lambda_R(\mathbf{k},t)=\lambda-2\lambda^2\int\frac{dk_1}{(2\pi)^d}\frac{dk_2}{(2\pi)^d}(2\pi)^d\delta(k-k_1-k_2)\times e^{-k_1^\sigma t}e^{-k_2^\sigma t}+\cdots. \tag{7}$$

This sum can be done to all orders after a Laplace transformation $\lambda_R(\mathbf{k},s)=\int_0^\infty dt e^{-st}\lambda_R(\mathbf{k},t)$ to give

$$\lambda_R(\mathbf{k}=\mathbf{0},s)=\frac{\lambda}{1+\lambda C s^{-\epsilon/\sigma}\Gamma\left(\frac{\epsilon}{\sigma}\right)}, \tag{8}$$

with

$$C=\frac{1}{\sigma}\frac{2^{2-d/\sigma}}{(4\pi)^{d/2}}\frac{\Gamma\left(\frac{d}{\sigma}\right)}{\Gamma\left(\frac{d}{2}\right)}, \tag{9}$$

and so, after a renormalization point $s=\kappa^\sigma$ is chosen, the exact flow function for the renormalized annihilation rate $g_R=\kappa^{-\epsilon}\lambda_R(\mathbf{0},\kappa)$ is

$$\beta=\kappa\frac{\partial g_R}{\partial\kappa}=-\epsilon g_R+\epsilon C\Gamma\left(\frac{\epsilon}{\sigma}\right)g_R^2. \tag{10}$$

This has a nontrivial fixed point, which is stable for $d<\sigma$, at $g_R^*=[C\Gamma(\epsilon/\sigma)]^{-1}$.

Imposing the condition that the density be independent of the (arbitrary) normalization point κ, and using dimensional analysis, a renormalization group equation can be written as

$$\left[\sigma D_A t\frac{\partial}{\partial(D_A t)}+\beta(g_R)\frac{\partial}{\partial g_R}-n_0\frac{\partial}{\partial n_0}+d\right]n_R=0. \tag{11}$$

The solution to this, by the method of characteristics, is

$$n_R(D_A t,n_0,g_R,\kappa) = (\kappa^\sigma D_A t)^{-d/\sigma}n_R(\kappa^{-\sigma},(\kappa^\sigma D_A t)^{d/\sigma},\tilde g_R,\kappa), \tag{12}$$

where $\tilde g_R$ is the running coupling, which goes to g_R^* as $t\to\infty$. In a diagrammatic expansion, each loop brings in a higher power of the renormalized coupling, so an expansion in the number of loops is an expansion in g_R^*, which is small near the critical dimension $d_c=\sigma$. The first approximation to the right hand side can be found by summing all tree diagrams generated by expanding either the action [Eq. (6)] or the Langevin equation [Eq. (3)]. The next term, including all diagrams with loops, is calculated by writing an integral equation for the density, as done in Ref. [9]. The leading contribution to the density at long times is then given by

$$n(t)=A(D_A t)^{-d/\sigma}. \tag{13}$$

The exponent is exact and, to the order of ϵ^0, the amplitude is

$$A=\frac{1}{(4\pi)^{d/2}}\frac{\Gamma\left(\frac{d}{\sigma}\right)}{\Gamma\left(\frac{d}{2}\right)}\frac{2^{1-d/\sigma}}{\sigma}\left[\frac{\sigma}{\epsilon}-\frac{5}{2}\right]. \tag{14}$$

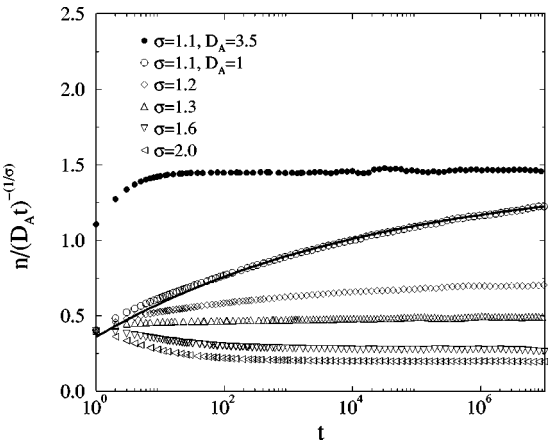

FIG. 2. The density of particles divided by its asymptotic (large time) power law for several values of σ. For σ close to 1 and $D_A=1$ (open symbols), the crossover becomes very slow, but the trend is towards the same value as for simulations done with a larger value of D_A. The filled symbols give the density for $D_A=3.5$. Also shown (solid line) is the crossover function of Eq. (15) for $\sigma=1.1$, with the parameters extrapolated to their $t\to\infty$ values.

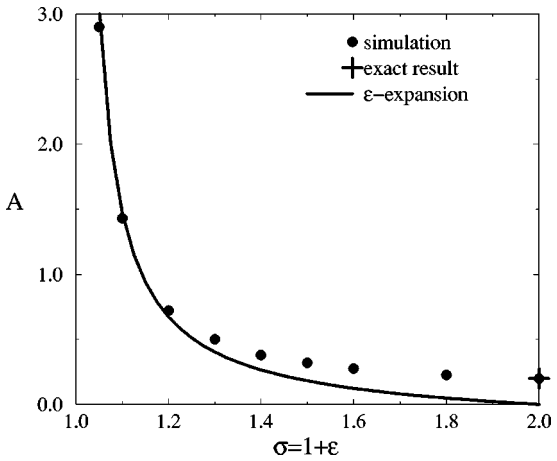

FIG. 3. The amplitude of the power-law decay of the density of particles determined in simulation (circles), compared with the renormalization group prediction of Eq. (14). Also shown is the exact result [10] for the normal diffusion case (cross).

This expression is obtained by expanding factors which are singular as $\epsilon\to 0$ in ϵ and leaving the remainder as an expression in d. The result for the exponent is to be expected, as the decay exponent for annihilation reactions is generally $\alpha=d/d_c$ for annihilation with no single-particle processes (see, for example, Ref. [9]). Here, $d_c=\sigma$, producing the decay given in Eq. (13).

Simulations of a microscopic model in one dimension have been performed and the results compared to the prediction of the renormalization group calculation. The density of particles converged to the predicted power law for all values of σ simulated, as can be seen in Fig. 2.

The simulations are of a one-dimensional lattice, where only one particle may occupy each site. This differs from the renormalization group calculation, in which multiple occupancy is allowed, but the annihilation rate flows to a fixed point and thus the bare annihilation rate does not appear in the final answer, so the results should be similar. At the beginning of the simulation, the lattice contains $L=10^7$ sites, with every site occupied. Whenever the number of particles fell below 1000, the system was doubled by appending an exact copy of the current configuration of particles. While this does make the system momentarily periodic, the two halves subsequently evolve differently. This allowed the simulation to continue to large times without large statistical fluctuations in the density. For $\sigma=1.05$, the final system size was $L=2^9\times 10^7$. The distribution of jumps was chosen to follow a Lévy stable law, using the method given in Ref. [22]. Since this method is for a continuous distribution, which is then made into a discrete distribution by rounding, the values generated were multiplied by a numerically determined factor to produce the correct low-k value of the distribution. Earlier simulations [21,16] used a pure power-law form for the distribution of jumps, which does flow to the desired distribution in the long-time limit. The distribution used here matches the Lévy distribution much more closely after a single step and makes it easier to determine the anomalous diffusion constant D_A.

For some values of σ, the anomalous diffusion constant D_A in the distribution of hop lengths, Eq. (2), was varied. In the field theory or the Langevin equation, this change to the kinetics results in a change in the coefficients of powers of k, which come from an expansion of the hop length distribution. These terms, many of which are irrelevant in the renormalization group sense and are not written in the Langevin equation, can be seen to have a significant impact on the crossover behavior, and it may be useful to vary these parameters in future simulations to examine the crossover.

As can be seen in Fig. 2, the time taken to reach the asymptotic form of the density depends strongly on D_A. For σ close to 1 and $D_A=1$, the crossover is very long, but the amplitude can be extracted from a fit to the form

$$\frac{n(t)}{(D_A t)^{-1/\sigma}}=A(1-Bt^{-\phi}). \tag{15}$$

To obtain the long-time value of the amplitude, the fit was done over many ranges with differing starting times, and extrapolated to $t\to\infty$. For larger values of D_A, this fit is not necessary, as the density reaches its asymptotic value quickly, and several decades of scaling can be seen in the data.

The prediction for the amplitude is compared to simulation results in Fig. 3. The agreement between the ϵ expansion for the amplitude and the simulation result becomes quite good for small ϵ, as expected for this asymptotic power series expansion. As well as being interesting as a model for physical processes with anomalous diffusion, the Lévy flights used here allow this regime, where the expansion parameter is small, to be explored in a simulation.

Thanks to Michael Plischke for several useful suggestions, and to Martin Howard and Tibor Antal for helpful comments on an earlier version of this paper. Financial support was provided by the NSERC of Canada.

[1] *Nonequilibrium Statistical Mechanics in One Dimension*, edited by V. Privman (Cambridge University Press, Cambridge, 1997).
[2] H. Hinrichsen, Adv. Phys. **49**, 815 (2000).
[3] U.C. Tauber, Acta Phys. Slov. **52**, 505 (2002).
[4] G.M. Schütz, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic Press, New York, 2000), Vol. 19.
[5] T.O. Masser and D. ben-Avraham, Phys. Rev. E **63**, 066108 (2001).
[6] J. Cardy, in *The Mathematical Beauty of Physics*, edited by J. M. Drouffe and J.B. Zuber, Advanced Series in Mathematical Physics, Vol. 24 (World Scientific, Singapore, 1996).
[7] M.v. Smoluchowski, Z. Phys. Chem. (Leipzig) **92**, 129 (1917).
[8] A.A. Ovchinnikov and Y.B. Zeldovich, Chem. Phys. **28**, 215 (1978).
[9] B.P. Lee, J. Phys. A **27**, 2633 (1994).
[10] A.A. Lushnikov, Phys. Lett. A **120**, 135 (1987).
[11] J. Klafter, M.F. Shlesinger, and G. Zumofen, Phys. Today **49**(2), 33 (1996).
[12] J.-P. Bouchaud and A. Georges, Phys. Rep. **195**, 127 (1990).
[13] T.H. Solomon, E.R. Weeks, and H.L. Swinney, Phys. Rev. Lett. **71**, 3975 (1993).
[14] E. R. Weeks and H. L. Swinney, Nonlinear Sci. Today (1998).
[15] L. Chen and M.W. Deem, Phys. Rev. E **65**, 011109 (2002).
[16] H. Hinrichsen and M. Howard, Eur. Phys. J. B **7**, 635 (1999).
[17] M. Doi, J. Phys. A **9**, 1465 (1976).
[18] M. Doi, J. Phys. A **9**, 1479 (1976).
[19] L. Peliti, J. Phys. (France) **46**, 1469 (1985).
[20] J. Cardy, *Scaling and Renormalization in Statistical Physics*, Cambridge Lecture Notes in Physics Vol. 5 (Cambridge University Press, Cambridge, UK, 1996).
[21] D. Vernon and M. Howard, Phys. Rev. E **63**, 041116 (2001).
[22] P. Bratley, B.L. Fox, and L.E. Schrage, *A Guide to Simulation*, 2nd ed. (Springer-Verlag, New York, 1987).