

Scaling of the propagation velocity in the contact propagation regime of stirred percolation

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For regimes of flame propagation and diffusion-limited aggregation in which cluster contact is rate limiting, we find that the propagation velocity exhibits a new form of scaling related to percolation. We compute a "propagation exponent" ψ and derive it in terms of static exponents. We also derive bounds on a "transport exponent" ψ' governing the critical diffusivity of fast tracers in lattice gases and the critical conductivity of stirred binary mixtures.

Scaling properties of contact processes have been investigated in recent studies of diffusion-reaction systems modeled as directed percolation problems.¹ Here, we consider a different type of contact process associated with "stirred percolation,"^{2,3} which is a dynamical generalization of ordinary (undirected) percolation.

In stirred percolation, the random process which generates the "allowed" region incorporates time evolution, introducing the processes of cluster merging (contact) and separation. If we postulate a propagation process in the allowed region, dynamical evolution proceeds on two levels, namely, propagation within a cluster and the time evolution of clusters. Intracuster transport in the absence of cluster evolution has been studied intensively,⁴ and it has been shown that many aspects of transport near the percolation threshold are governed by purely geometrical considerations.

For the case of stirred percolation, we postulate an intracuster propagation process for which the dynamics again reduce to a purely geometrical problem. Specifically, we assume that intracuster propagation is so rapid that the cluster equilibrates completely in a time short compared to the time scale for cluster evolution. At first glance, this seems no different from the frozen-cluster assumption. Here, however, we consider the dynamics on the slow time scale, so that the intracuster propagation process becomes trivial, while the influence of cluster evolution introduces a rich, new structure. In particular, novel scaling behavior is obtained far from as well as close to the percolation threshold, though only the latter is considered in detail here.

We introduce the contact process associated with cluster evolution in the context of a flame propagation problem.⁵ If the fuel vapor and air are not fully mixed, the flammable zone at each instant may consist of isolated regions, and yet the flame propagates because advection ("stirring") brings ignited regions into contact with flammable unignited regions. We consider the regime in which this contact process is rate limiting (a regime denoted here as "contact propagation"), so that it is valid to assume instantaneous propagation through a flammable region. Thus, details of the process of flame propagation through a flammable region are irrelevant on the time scale of interest. We focus on the dependence of the flame propagation velocity v on the flammable volume fraction p , followed by a brief examination of the relationship between the propagation velocity and transport coefficients.

We model contact propagation on a lattice on which independent random walkers are randomly distributed, allowing multiple walkers per site, with an average of ϕ walkers

per site (except in one computation involving mutually avoiding walkers). Sites which are occupied at a given epoch are denoted flammable (F), and vacant sites are nonflammable (N). The lattice analog of the flammable volume fraction is the site occupation probability, $p = 1 - \exp(-\phi)$. At each time step, a fraction q of the walkers, randomly chosen, move to nearest-neighbor sites. We consider finite- q processes as well as the continuous-time regime $q \ll 1$.

It is important to note that the random walkers employed here represent the time evolution of the flammable region, while the random walkers employed in the studies cited earlier represent intracuster transport in a frozen geometry. This is the essential manifestation of the distinction between the slow and fast time scales.

We distinguish two types of walkers: ignited and unignited. After the walkers move, clusters of flammable sites are identified, and if a given cluster has at least one ignited walker, all walkers within the cluster are redesignated as ignited. (This is the instantaneous propagation of the flame through the flammable region.) Treating ignition as a site property at a given epoch, F sites are thus either ignited (I) or unignited (U). If all walkers in the half space $x < 0$ ($x > 0$) are initially ignited (unignited), then after a transient, the mean propagation velocity relaxes to a value $v = r/p$, where r is the mean rate of increase of the number of I sites per lattice row in the $+x$ direction.⁶

As p approaches the percolation threshold p_c , we expect that v is dominated by propagation of the ignition through large clusters at each time step. By analogy to the scaling theory of percolation clusters,⁷ we anticipate a scaling regime $v \sim (p_c - p)^{-\psi}$. We have verified scaling and estimated the "propagation exponent"⁸ ψ by means of Monte Carlo simulations on triangular, square, honeycomb, and simple-cubic lattices.

In the simulations, periodic boundary conditions are imposed in the transverse direction(s) for moving the walkers and for propagating the ignition through flammable clusters. At regular intervals, the computational domain is shifted in the direction of propagation so that propagation can be simulated over an x interval much larger than the longitudinal span of the computational domain. Details of the algorithm are presented elsewhere.⁹

Care was exercised to assure that finite-size and initial-transient biases were negligible. Transient relaxation took tens of time steps near p_c , but more time steps for lower p . Computational domains as large as $x \times y = 600 \times 400$ were required near p_c . [In three dimensions (3D), an $80 \times 80 \times 80$

box was employed.] Five replicate simulations were used to estimate ν for each p .

Figure 1 exhibits the anticipated scaling. For $q=1$ (a discrete-time process), simulations performed on 2D lattices give the estimates $\psi_{tri}=1.51 \pm 0.03$, $\psi_{squ}=1.48 \pm 0.03$, and $\psi_{hon}=1.44 \pm 0.03$.¹⁰ Taking these results to be indicative of the universality⁷ of ψ , we pool these estimates to obtain $\psi=1.48 \pm 0.02$. Computations on a simple-cubic lattice¹¹ give the estimate $\psi=0.80 \pm 0.06$ for $d=3$.

The continuous-time ($q \ll 1$) regime was simulated on the triangular lattice. For given p , ν was computed for successively smaller q until it approached a constant value. Convergence consistently occurred at $q \leq 0.02$. Scaling is again exhibited, with $\psi=2.44 \pm 0.06$. We also performed computations for $q \ll 1$ employing mutually avoiding rather than independent walkers. In this case, a given site is occupied by at most one walker, so $p=\phi$. We obtain $\psi=2.43 \pm 0.02$, which indicates the insensitivity of ψ to the spatial random process governing the walkers.¹²

For the continuous-time regime we propose that ψ is equal to the cluster size exponent⁷ γ . Near p_c , the singular part of ν is proportional to the mean number of sites ignited per unit time due to I-U contacts in a given lattice row. This quantity is equal to the mean size S of a newly ignited cluster times the number N of I-U contacts per lattice row per unit time. We take S to be the mean cluster size for static percolation, so that $S \sim (p_c - p)^{-\gamma}$ for $p \leq p_c$. N is proportional to the width W of the propagation front times the number density ρ_u of "unscreened"¹³ I sites, i.e., I sites adjacent to unignited clusters. If we assume that individual-cluster properties are applicable, then $W \sim \xi$ [ξ is

the "correlation length,"⁷ which diverges as $(p_c - p)^{-\nu}$], and $\rho_u \sim \xi^{d/d_f + d_f - d - 2}$ (Ref. 13), where d_f is the fractal dimension of a cluster. Since $d_f \leq d$, the exponent of ξ in the product $W\rho_u$ is negative, implying that N vanishes near criticality. Since N must be at least of order unity, we infer that individual-cluster properties are not applicable in this instance and we take N to be nonsingular. Therefore, $\nu \sim S$, which gives $\psi = \gamma$. For $d=2$, $\gamma = \frac{43}{18} = 2.389 \dots$,¹⁴ in fairly good agreement with the computed results.

For finite q , a given cluster can experience multiple I-U contacts simultaneously, so a modification of this scaling argument is needed to avoid multiple counting of newly ignited clusters. Since the largest clusters should experience the most multiple counting, we expect ψ to decrease with increasing q . In particular, we consider the regime $1 \ll q \ll \xi$. ($q > 1$ signifies more than one nearest-neighbor step per walker per time step.) In this regime we assume that all unignited clusters bordering the propagation front at a given time step are contacted so the propagation front advances a distance ξ per time step, giving⁶ $\nu \sim (1/q)(p_c - p)^{-\nu}$. Holding q fixed as p approaches p_c , we obtain $\psi = \nu$.

ν equals $\frac{4}{3}$ for $d=2$ and has an estimated value of 0.88 ± 0.02 for $d=3$.¹⁴ The computed results for ψ for the $q=1$ process are close to these values,¹⁵ indicating the approximate correctness of the above reasoning for q of order unity.

By introducing various asymmetries in the random process governing the walkers, models are obtained which are applicable to diverse physical systems. For example, if the unignited walkers are frozen while the ignited walkers are mobile, we obtain a model of the contact propagation regime for combustion of solids. The onset of mobility represents melting or sublimation due to heat release. The nonflammable zone now represents inert binder material in which the solid propellant is imbedded.

By freezing the ignited walkers rather than the unignited walkers, we obtain a model applicable to diffusion-limited aggregation at high particle concentration. When the concentration of mobile particles is high, the outward advance of the perimeter of the aggregate, rather than the inward diffusive flux of particles, provides the dominant contribution to the growth rate of the aggregate.¹⁶ If the particle concentration in fact approaches the percolation threshold (well defined on a lattice, extended to the continuum by allowing some overlap of the diffusing particles), then the rate of advance of the aggregate perimeter will diverge. To apply our model, we employ mutually avoiding walkers and freeze the motion of the unignited walkers upon contact with ignited walkers, which represent the aggregate. Results computed for the continuous-time regime exhibit the anticipated scaling, but we now obtain $\psi=2.99 \pm 0.07$, higher than previously.

The difference is due to the fact that ignition (aggregation) now occurs only by motion of a walker toward the aggregate. Such a move tends to detach the walker from the unaggregated cluster containing it, thus biasing the mean size of newly aggregated clusters downward from the unconditioned mean cluster size. Therefore, the derivations relating ψ to static exponents are no longer applicable. (This argument further implies that in the previous case, the dominant propagation mechanism near criticality is motion of ignited walkers toward unignited clusters.)

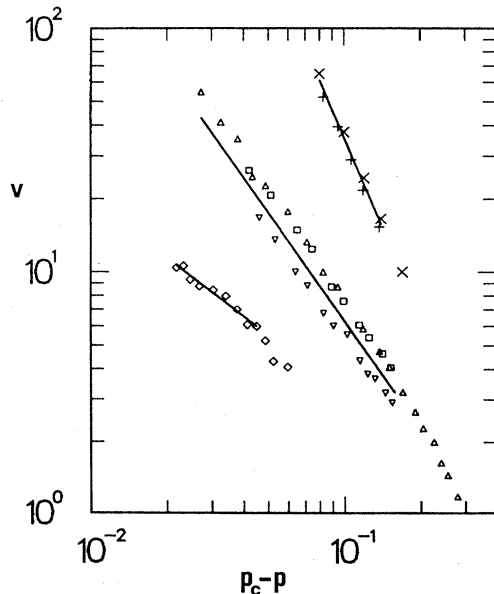


FIG. 1. Log-log plot of propagation velocity ν vs $p_c - p$ for triangular (Δ), square (\square), honeycomb (∇), and simple-cubic (\diamond) lattices. Lines of slopes -1.48 and -0.80 indicate the scaling regime for $d=2$ and $d=3$, respectively. The line segments span the ranges of data used to estimate the propagation exponent ψ for the discrete-time ($q=1$) process. Also shown are results for the continuous-time ($q \ll 1$) regime for a triangular lattice with independent (+) and mutually avoiding (x) walkers. A line segment of slope -2.43 indicates the scaling regime.

Computational procedures and detailed results for these and other asymmetric models are presented elsewhere.⁹

We now consider the relationship between the propagation velocity and transport coefficients for systems in which cluster contact is rate limiting. One application with the latter feature is diffusion of fast tracer particles through the vacancies in a concentrated lattice gas of slow-moving particles,¹⁷ of interest due to the use of muons as fast tracers in studies of hydrogen diffusion in metals.¹⁸ Another application is the conductivity of a stirred binary mixture of conducting and nonconducting components.²

The transport coefficient δ is defined by the relation $j = \delta E$, where E is a driving field which we take to be a concentration gradient. The material flux j is the product of a velocity v , in this instance the contact propagation velocity, and a concentration ρ which is the typical concentration change resulting from a cluster contact event. We consider two clusters of size s_1 and s_2 , respectively, just prior to contact, labeled so that $s_1 \geq s_2$. The concentrations on the two clusters are ρ_1 and $\rho_2 = \rho_1 \pm E\xi$, where the correlation length ξ is an estimate of the mean x separation of the cluster centroids. (This relationship is valid provided that $\rho_1 \gg E\xi$, i.e., in the linear response¹⁹ regime. The sign depends on which cluster centroid is at larger x .) The key premise of contact propagation is that the merged cluster formed upon contact rapidly equilibrates, resulting in a uniform concentration

$$\rho_m = (s_1\rho_1 + s_2\rho_2)/(s_1 + s_2) = \rho_1 \pm E\xi/(1 + R),$$

where R is the size ratio s_1/s_2 . Taking ρ to be the magnitude of the concentration change $\rho_m - \rho_1$ on the larger cluster, we conclude that ρ is of order $E\xi/R$. Combining factors, we obtain

$$\delta = \xi v / R.$$

This result is valid for contact propagation at arbitrary p .

Here, we use it to characterize the divergence of δ near the percolation threshold.

As p approaches p_c , ξ and v diverge with exponents ν and ψ , respectively. R may be nonsingular, or at the other extreme, it may diverge with exponent γ (the cluster size exponent), depending upon the random process governing cluster evolution. (This range of behaviors reflects the previously mentioned possibility of cluster size bias.) Therefore, the transport coefficient diverges as $\delta \sim (p_c - p)^{-\psi'}$, where the "transport exponent" ψ' obeys the inequalities

$$\psi + \nu - \gamma < \psi' < \psi + \nu.$$

Taking $\psi = \gamma$ and using previously quoted values of ν and γ and the estimate $\gamma = 1.73 \pm 0.03$ for $d = 3$,¹⁴ we obtain $\frac{4}{3} < \psi' < \frac{67}{18}$ for $d = 2$ and $0.88 < \psi' < 2.61$ for $d = 3$.

A measurement by Laguës² of the conductivity of a microemulsion in a "stirred" (Brownian motion) regime gives $\psi' = 1.2 \pm 0.1$, within the $d = 3$ bounds. (Our ψ' is his s' . Our notation emphasizes the distinction between contact propagation and static percolation exponents.) He derives the relationship $\psi' = 2\nu - \beta$ (which gives $\psi' \approx 1.3$ for $d = 3$) by generalizing the random-walk model of de Gennes.³ This model omits important features of the contact propagation regime, so we regard the success of his prediction as not fully explained.

We briefly mention some additional results concerning contact propagation. In addition to the scaling regime at $p \leq p_c$, five other scaling regimes have been identified. For $p \ll 1$, we obtain $\nu \sim p^{1/2}$, and for p of order unity but well below p_c , we obtain a regime in which $\nu \sim p$. For $p \geq p_c$, three finite-size scaling regimes are obtained. Details are reported elsewhere.⁹

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⁵The need for a dynamical percolation model of turbulent flame propagation has been noted by N. Peters, Combust. Sci. Technol. 30, 1 (1983).

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⁸The propagation velocity in the model of W. Kinzel (Ref. 1) vanishes rather than diverging at criticality, so his model is of a different universality class than ours.

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¹⁰To estimate ψ we take $p_c = 0.59277$ for the square lattice, based on T. Gebele, J. Phys. A 17, L51 (1984); for the honeycomb lattice, we take $p_c = 0.6962$ based on Z. V. Djordjevic, H. E. Stanley,

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¹¹For the simple-cubic lattice we take $p_c = 0.3117$, based on D. Heermann and D. Stauffer, Z. Phys. B 44, 339 (1981).

¹²To obtain this estimate it was assumed that $p_c = \frac{1}{2}$ as for uncorrelated percolation on the triangular lattice. The computed scaling behavior validates this assumption. The insensitivity of p_c as well as ψ to spatial correlations is analogous to the static percolation results of A. Geiger and H. E. Stanley, Phys. Rev. Lett. 49, 1895 (1982).

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¹⁵For $d = 3$, ψ is less than ν , but the difference between ψ and ν is not statistically significant.

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