Scaling Relationships in Agglomeration and Annihilation Models

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A relation between two exponents characterizing the scaling behavior of random agglomeration models with particle injection is proposed and verified by numerical simulations. This relation, and a link between diffusion-limited agglomeration models with and without injection combined with an exact solution of the latter, leads to a solution of the former in arbitrary dimensionality. [S0031-9007(97)04406-2]

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Agglomeration phenomena are irreversible processes that often lead to scale invariant behavior of various quantities [1–8]. They provide the simplest idealization in a variety of contexts ranging from the coalescence of fluid vortices to the accretion of cosmic dust into planets, and include gelation and aerosols. From a fundamental point of view, studies of agglomeration have shown the important role, in low dimensionalities, of rare fluctuations in modifying the mean field behavior [1]. The principal theme of this Letter is the derivation of a relationship between exponents characterizing the scaling behavior in the steady state of processes in which new particles are being injected at a constant rate during the agglomeration. The scaling arguments employed are general and independent of the microscopic details of the agglomeration process. We have verified this numerically in two different cases; a ballistic agglomeration model in 1D and a diffusive lattice gas in 2D. This relationship is also demonstrated to be useful for obtaining a complete solution of the problem of diffusion-limited agglomeration with injection by relating it to the corresponding problem without injection, for which the exact solution is known [7]. The exact result in 1D [8] is also recovered.

We shall consider two types of dynamics for the agglomerating particles. In both cases, the agglomeration process is assumed to be instantaneous. In the first, we postulate that the particles undergo completely inelastic collisions. When two masses M_1 and M_2 collide and agglomerate, mass and momentum are assumed to be conserved. The agglomerated object has a new mass of $M_1 + M_2$ and the appropriate velocity for momentum conservation to hold. The particles are assumed to move ballistically between collisions. Without injection, this model has been studied previously [2,4–6]. In one dimension, one may start the agglomeration process by considering unit masses with individual velocities chosen randomly from a uniform distribution in, say, the interval between $[-1, 1]$. The masses are assumed to be randomly distributed in space with a mean concentration c_0. Generally, at long times, a scaling regime sets in, during which the average mass grows algebraically with time $\langle M \rangle \sim t^{2/3}$ or, equivalently, the mean concentration decays with time as $c(t) \sim t^{-2/3}$ [2].

A related but more complex problem is one of ballistic agglomeration with injection. Here, one assumes that, during the agglomeration process, unit masses with a velocity distribution as before are being injected randomly into the system at a constant rate. At long times we have observed in computer simulations in $D = 1$ that a steady state is reached in which the concentration of particles is constant and the distribution of masses becomes algebraic,

$$P(M) \sim M^{-\tau}, \tag{1}$$

for masses $M \gg 1$. The upper cutoff for the algebraic behavior increases with time.

We now turn to the second type of dynamics for the agglomerating particles. This involves the diffusion of the particles with the simplifying assumption that the diffusion is independent of the mass of the agglomerated particle. Unlike the case with ballistic dynamics, here it is convenient to put the diffusing particles on a lattice and allow them to move to a randomly chosen nearest neighbor site [1,3,7,8]. Agglomeration occurs if two particles arrive at the same site at the same time. In the absence of injection, this corresponds to the exactly solved random annihilation model or the diffusion-limited reaction $A + A \rightarrow A$ [7], in which the concentration decays as

$$c(t) \sim \begin{cases} t^{-D/2} & D < 2 \\ t^{-1} \ln t & D = 2 \\ t^{-1} & D > 2 \end{cases} . \tag{2}$$

In the presence of injection, the random aggregation model again leads to a steady state characterized by an algebraic distribution of masses of the form given by Eq. (1). This model has been studied in various contexts [8–13] which include Abelian sand piles and the Voter

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model. By a direct study, τ is known to be $4/3$ in $D = 1$ and $3/2$ within mean field theory [8]. Nevertheless, there have been questions raised about the value of the upper critical dimension above which mean field theory is valid, and in which logarithmic corrections to the power law scaling would be expected [8].

Motivated by the algebraic decay of the concentration in the agglomeration process without injection, we introduce a new quantity in the model with injection whose power law scaling will be shown to be related to τ. Consider a snapshot in the steady state of the agglomeration process, ballistic or diffusion limited. All the particles present at that instant are defined to belong to the first generation. During the subsequent agglomeration process, by definition, the number of first generation particles decreases by one when two of them coalesce. A coalescence of a first generation particle and one that is not leads to a merged particle that still carries the first generation label. As in the models without injection, the concentration of first generation particles decays algebraically with time

$$c(t) \sim t^{-\alpha}. \qquad (3)$$

We summarize the key results of our paper as follows:

I. We will show from scaling that τ and α are related to each other by

$$\tau = 1 + \frac{\alpha}{\alpha + 1}. \qquad (4)$$

II. We will present the results of a simulation of the $D = 1$ ballistic agglomeration process with injection from which we find

$$\tau = 1.218 \pm 0.001 \qquad (5)$$

and

$$\alpha = 0.279 \pm 0.05, \qquad (6)$$

in accordance with Eq. (4).

III. For the simple case of diffusion-controlled agglomeration in which the dynamics of the particles is independent of their mass, the decay exponent of first generation particles may be deduced from the exact solution for the case without injection, Eq. (2), to be

$$\alpha = \begin{cases} \frac{D}{2} & D < 2 \\ 1 & D \geq 2 \end{cases}. \qquad (7)$$

This is because the injected particles do not slow down the coalescence of the first generation particles, unlike in the ballistic case.

IV. The scaling relations then show that

$$\tau = \begin{cases} \frac{2(D+1)}{(D+2)} & D < 2 \\ \frac{3}{2} & D > 2 \end{cases} \qquad (8)$$

with

$$P(M) \sim M^{-3/2}(\ln M)^{1/2} \qquad D = 2, \qquad (9)$$

confirming that the upper critical dimension of the random agglomeration model with injection is $D = 2$.

V. We also show that randomness in the injection in the diffusion-limited case is irrelevant in arbitrary dimensionality. This result was obtained earlier in $D = 1$ [8], using explicitly the exact solution.

We first turn to a proof of the scaling relation (4). To this end, we define a quantity X_i as the *age of the oldest particle* constituting the composite particle with label i. We proceed to make a scaling ansatz for the probability distributions of the masses M and the ages X defined above:

$$P(M,T) = M^{-\tau} f(M/T^{\varphi}), \qquad (10)$$

$$\Pi(X,T) = X^{-\psi} f(X/T), \qquad (11)$$

where T is the total number of time steps. Equation (10) is a generalization of (1) which takes into account finite time effects, while the exponent ψ in Eq. (11) is equal to $(\alpha + 1)$ from Eq. (3). The latter result follows from the observation that Π is simply proportional to the time derivative of c. Note that both X and T have the same dimensions of time. Recognizing that the mean mass (averaged over each of the particles and for all the T time steps) ought to be proportional to T [the proof is given later in Eq. (13) for a more general case] and requiring that $P(M,T)dM = \Pi(X,T)dX$ [14] with $X \sim T \sim M^{1/\varphi}$, one obtains

$$\varphi(2 - \tau) = 1 \quad \text{and} \quad \psi = \varphi, \qquad (12)$$

respectively. Substituting for ψ in terms of α, one obtains the scaling relation (4).

We now consider the proof of result V above. Let $r_i(t)$ and $M_i(t)$ denote independently distributed random variables ≥ 0 that represent the injected mass and the agglomerated mass at site i at time t, respectively. The mean mass, averaged over each of the sites of a hypercubic lattice of linear size L and for all the T time steps, averaged over the randomness is given by

$$\begin{aligned} \langle M(T) \rangle &= \lim_{L\to\infty} \left\langle \frac{1}{L^d T} \sum_{i,t} M_i(t) \right\rangle \\ &= \lim_{L\to\infty} \frac{1}{L^d T} \sum_{i,t} \sum_{j,s<t}' \langle r_j(s) \rangle \\ &= \lim_{L\to\infty} \frac{1}{L^d T} \sum_{j,s} \langle r_j(s) \rangle (T - s) \\ &= \frac{1}{T} \langle r \rangle \sum_s (T - s) = \frac{T-1}{2} \langle r \rangle. \end{aligned} \qquad (13)$$

In the third step $\sum_j'$ is restricted to sites j at time s whose injected masses are agglomerated at site i at time t. Thus if $\langle r \rangle$ is finite, Eq. (13) shows that the arguments used for the uniform injection case are still valid, the scaling laws in Eq. (12) hold, and the exponents remain the same as before. We note that all our results on the diffusion-limited agglomeration model are generalizable to fractal geometries [15] with the spectral dimension playing the role of D.

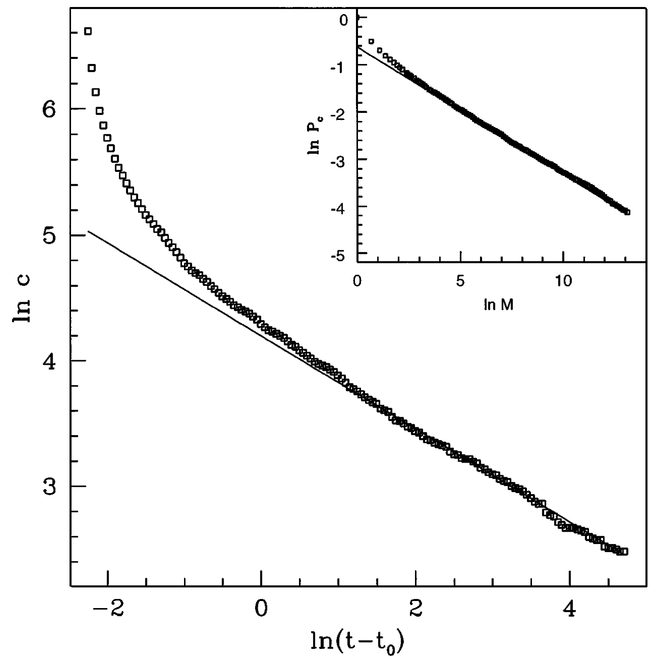

FIG. 1. Plot of the decay of the number of particles present at some initial time t_0 in the steady state for ballistic agglomeration with injection in 1D. The decay is algebraic with an exponent $\alpha = 0.279$. The continuous line is a guide the eye. In the inset, the corresponding integrated mass distribution follows an algebraic distribution giving $\tau = 1.218$.

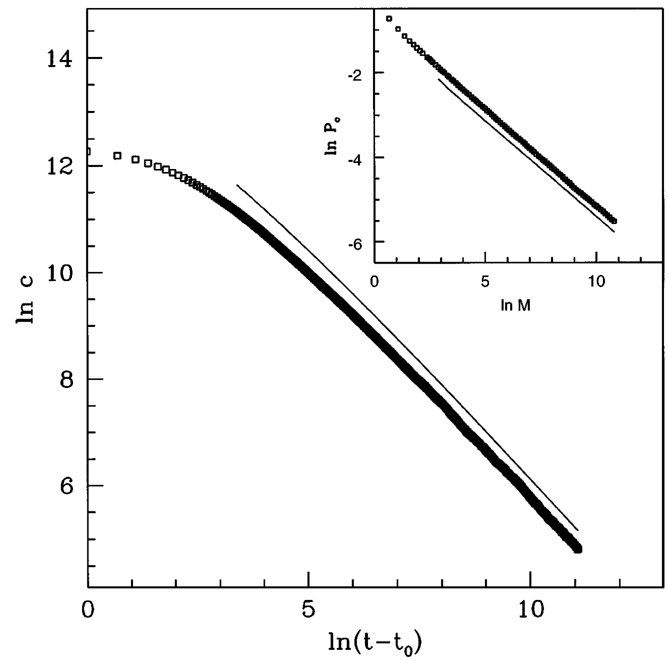

FIG. 2. The decay of the particles present at some time t_0 for diffusive agglomeration with injection in 2D. The line, which has been shifted for clarity, shows the existence of logarithmic corrections as described in the text. The inset shows the corresponding integrated mass distribution which is consistent with Eq. (9).

We have performed numerical simulations in $D = 1$ of the ballistic agglomeration model with injection using an event driven algorithm. In the interval $[0, 1]$ with periodic boundary conditions, we inject particles at a constant rate with a velocity chosen randomly from the interval $[-1, 1]$. When two particles collide they agglomerate to form a single particle with a velocity satisfying momentum conservation. The system reaches a steady state in which the average number of particles is constant. We then monitor the decay of all particles present at some time t_0 (in the steady state) and the mass distribution. Our results are shown in Fig. 1 in the form of a log-log plot of c versus t, where c is the concentration of all labeled particles, and the best fit gives $\alpha = 0.279 \pm 0.05$. The inset shows the integrated probability $P_c = \int_M^\infty P(x)dx$ versus M and our prediction for τ, Eq. (4), using the above estimate of α. The agreement is excellent and supports our scaling analysis.

As a final check of our scaling relation, we have performed numerical simulations of diffusive agglomeration with injection in 2D, where logarithmic corrections are present [16]. Figure 2 shows the decay of labeled particles c and the integrated probability $P_c(M)$. The solid lines are of the form $c \sim t^{-1}\ln(t)$ and $P_c \sim M^{-1/2}\ln(M)^{1/2}[1 + \ln(M)^{-1} - \ln(M)^{-2} + \ldots]$ which confirm the existence of the logarithmic corrections given in Eqs. (2) and (9). These results are in full accord with our scaling hypothesis.

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