Kinetic properties of ballistic aggregation

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We study a recently introduced model of ballistic aggregation by using the scaling theory of Smoluchovski's equations and numerical simulations. The predictions of this mean-field theory for the exponent characterizing typical cluster size are in ageement with the earlier results for all dimensions. Nevertheless, the predicted monomer decay and particle size distribution are totally at variance with the numerical observations in one dimension. The reason for this discrepancy is found to be the fact that high velocity particles coalesce rapidly independent of their mass, which introduces correlations not taken into account by the mean-field treatment. This discrepancy is likely to persist in all dimensions, so that the model has no upper critical dimension. We also generalized our study to the case where the initial velocity distribution function of the particles has a power-law tail. It is found that, at least in one dimension, the typical cluster size behaves in a way that depends on the specific velocity distribution function, whereas the monomer decays regardless of the initial velocity distribution. We study also the case in which the mean velocity is infinite. In this case it is found that the predictions of the Smoluchovski equation theory are completely inconsistent with the numerical results in one dimension.

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I. INTRODUCTION

Irreversible aggregation phenomena have been studied extensively by using scaling theories [1] and rate equations [2]. Numerical studies of explicit models [3-5] and exact solutions [6] have been developed to investigate the kinetic behavior of irreversible aggregation models. Recently, the ballistic agglomeration model was proposed to stimulate the aggregation phenomena with ballistic transport [7]. In this model, particles of a given radius move with random (bounded) initial velocities in a Ddimensional space. Upon two particles colliding, they join to form one larger particle of mass equal to the sum of the two particle masses with a correspondingly larger radius. The resulting velocity of the new larger particle is determined by requiring the conservation of momentum. This problem provides a simple test case for scaling arguments which are being used in fluid mechanics to analyze statistics of the merger of coherent structures such as vortices [4] and thermal plumes. It is also an elementary analog of astrophysical models of the accumulation of cosmic dusts into planetesimals and thence into planets [9]. This model is an idealization for those applications because the particles only interact by collision. Nevertheless, it still captures some of the physics involved in these more complicated problems.

In Ref. [7] a simple scaling analysis has been given for this model, which shows that in D dimensions the average mass of a particle increases like $t^{2D/(D+2)}$. We studied this model from a mean-field viewpoint by using the Smoluchovski equation. Some of the results have been reported briefly [8]. Our purpose is to understand the small- and large-mass behaviors of c(m,t) and the con-

centrations of particles of mass m by studying the corresponding exponents. In order to verify our theory, we performed numerical simulations of the model in one dimension. It is found that the predictions of this meanfield theory for the exponent characterizing typical cluster size are in agreement with earlier results for all dimensions. Nevertheless, the predicted monomer decay and particle size distribution are totally at variance with the numerical observations in one dimension. The reason for this discrepancy is found to be the fact that high velocity particles coalesce rapidly independent of their masses, which introduces correlations not taken into account by the mean-field treatment. We also discussed an interesting generalization in which the initial velocity distribution function has power-law decay for large values of velocity. It is argued that this model may be relevant if the aggregating particles are carried by turbulent fluid.

The paper is organized as follows: In Sec. II we will investigate the asymptotic behavior of the ballistic aggregation from the scaling theory of Smoluchovski equation and give the theoretical results for the case of the initial velocity distribution with a power-law decay. Numerical results will be described and discussed in Sec. III. In Sec. IV we summarize our conclusions.

II. THE GENERAL THEORY

From the point of view of mean-field theory, the ballistic aggregation model can be described by Smoluchovski's equations [10] for the concentrations c(m, u; t) of particles with mass m and velocity u:

$$\dot{c}(m,u;t) = \frac{1}{2} \sum_{m_1 + m_2 = m} \sum_{m_1 u_1 + m_2 u_2 = m\mu} K(m_1, m_2; u_1, u_2) c(m_1, u_1; t) c(m_2, u_2; t)$$

$$-\sum_{m'=1}^{\infty}\sum_{n'=-\infty}^{\infty}K(m,m';u,u')c(m',u';t)c(m,u;t),$$
 (1)

where the dot indicates a time differential and K(m',m;u',u) are phenomenological constants describing the rate at which a particle of mass m' and velocity u' reacts with another particle with mass m and velocity u. Here we take the reaction kernel to be a homogeneous function of its arguments, i.e.,

$$K(am,am';bu,bu') = a^{\lambda_m} b^{\lambda_u} K(m,m';u,u') . \tag{2}$$

Once K(m,m';u,u') is known, an extensive scaling theory [2] exists that allows one to find the long-time, small- and large-mass behaviors of c(m,u;t). One has, in particular, for marginal distribution $c_m(t) = \int du \ c(m,u;t)$

$$c_{m}(t) \sim m^{-2} \Phi(m/s(t)) ,$$

$$s(t) \sim t^{z} \quad (t \to \infty) ,$$

$$\Phi(x) \sim x^{w/z} \quad (x \to 0) ,$$

$$c_{m(t)} \sim m^{-\tau} \quad [1 \ll m \ll s(t)] ,$$

$$(3)$$

where s(t) is the typical cluster size, $\Phi(x)$ a scaling function, and w, τ , and z exponents related by the scaling law $(2-\tau)z=w$.

Since our main interest focuses on the nongelling regimes of our model, we have a conservation law for the total mass, i.e.,

$$M(t) = \int_{0}^{\infty} \int_{-\infty}^{\infty} m \ dm \ du \ c(m, u; t) = 1$$
 (4)

In order to satisfy this condition, we propose the following scaling ansatz:

$$c(m,u;t) = \overline{m}^{-2}\overline{u}^{-1}\phi(m/\overline{m},u/\overline{u}), \qquad (5)$$

where \overline{m} is the typical mass and \overline{u} the rms value of the velocity. Before we proceed in calculating the scaling exponents, let us first check on the possible relations between the velocity of the aggregate and its mass, resulting from aggregation. Suppose the aggregate consists of sufficiently numerous "monomers" whose velocities are initially randomly distributed. Then according to the momentum conservation and the central limit theorem, one finds $\overline{m}(t) \sim \overline{u}(t)^{-1/2}$. Generally, we assume that

$$\dot{\bar{u}}/\bar{u} = \beta \dot{\bar{m}}/\bar{m} . \tag{6}$$

Substituting (2), (5), and (6) into (1) one obtains

$$\dot{\overline{m}} = w' \overline{m}^{\lambda_m} \overline{u}^{\lambda_u} \ . \tag{7}$$

It then follows that

$$\overline{m} \sim t^z$$
, (8) $\overline{u} \sim t^{\beta z}$,

with z being given by

$$z = 1/(1 - \lambda_m - \beta \lambda_u) . (9)$$

From Eq. (9) it is noted that the dynamic exponent z is characterized by the homogeneity exponents λ_m and λ_u of reaction kernels as well as the mass-velocity relation of the aggregating clusters described by the coefficient β . The homogeneity exponents are determined by the specific physical or chemical process. For instance, if we assume that the collision probability of two aggregates is proportional to the product of the mutual cross section of the two particles with their relative velocity, then the reaction kernel for this process is given by

$$K(m_1, m_2; u_1, u_2) = K_0(m_1, m_2)|u_1 - u_2|,$$
 (10)

with

$$K_0 = (m_1^{1/D} + m_2^{1/D})^{(D-1)}. (11)$$

From Eq. (9) one immediately finds that

$$z = 2D/(D+2)$$
 (12)

This result has been obtained in Ref. [7] by using a simple scaling reasoning, but here it comes as a specific assumption of a reaction kernel.

Now we turn to the scaling function $\phi(\xi, \eta)$ since it contains the information of the small- and large-mass behaviors of the concentration. For simplicity, we restrict ourselves to the one-dimensional case. In order to get an equation for scaling function ϕ , we consider the mass flow from $m \le m_0$ to $m \ge m_0$, which is defined as

$$-\dot{M}^{(m_0)} = -\int_0^{m_0} \int_{-\infty}^{\infty} \dot{c}(m, u; t) m \, dm \, du$$

$$= \frac{\dot{m}}{m} \int_0^x \xi \, d\xi \int_{-\infty}^{\infty} d\eta [2\phi + \beta\phi + \xi\phi_{\xi} + \eta\phi(\eta)] ,$$
(13)

where $x = m_0/\overline{m}$, $\xi = m/\overline{m}$, and $\eta = u/\overline{u}$. In view of the following identity

$$\sum_{m=1}^{m_0} \sum_{u=-\infty}^{\infty} \sum_{m_1+m_2=m} \sum_{m_1u_1+m_2u_2=mu} mK(m_1,m_2;u_1,u_2)c(m_1,u_1;t)c(m_2,u_2;t)$$

$$=2\sum_{u=-\infty}^{\infty}\sum_{u'=-\infty}^{\infty}\sum_{m=1}^{\infty}\sum_{m'=1}^{m_0-m}mK(m,m';u-'u)c(m,u;t)c(m',u';t),$$

one obtains an integral equation for the scaling function ϕ

$$-w'\int_{x}^{\infty}\xi\,d\xi\int_{-\infty}^{\infty}d\eta[(2+\beta)\phi+\xi\phi_{\xi}+\beta\eta\phi_{\eta}]$$

$$=\int_{0}^{x}\xi\,d\xi\int_{-x-\xi}^{\infty}d\xi'\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}d\eta\,d\eta'K(\xi,\xi';\eta-\eta')\phi(\xi,\eta)\phi(\xi',\eta'). \quad (14)$$

This is the desired integral equation for the scaling function $\phi(x,y)$, in which the parameter β is determined by the initial distribution of velocity and $K(\xi,\xi';\eta-\eta')$ by the reaction mechanisms. In the case of $\beta=-\frac{1}{2}$, this equation can be further simplified into

$$w'x^{2}\int_{-\infty}^{+\infty}\phi(x,\eta)d\eta = \int_{0}^{x}\xi\,d\xi\int_{x-\xi}^{+\infty}d\xi'\int_{-\infty}^{\infty}\int_{-\infty}^{+\infty}d\eta\,d\eta'K(\xi,\xi';\eta-\eta')\phi(\xi,\eta)\phi(\xi',\eta'). \tag{15}$$

In principle Eq. (15) can be solved to give the features of the scaling function $\phi(\xi,\eta)$ for various kinds of kernels. But very often one has to use some approximation schemes. Since our interest centers on the large-mass behavior, we use the following Fourier transform

$$\phi(\xi,\eta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \ \hat{\phi}_k(\xi) \exp(ik\eta) \ . \tag{16}$$

In the one-dimensional case we consider a kernel of the form

$$K(\xi, \xi'; \eta - \eta') = K_0(\xi, \xi') |\eta - \eta'| \exp(-|\eta - \eta'|/N)$$

$$(N \to \infty) . \qquad (17)$$

The Fourier transform of the kernel is given by

$$\hat{K}(\xi,\xi';k) = K_0(\xi,\xi')\sqrt{2/\pi} \frac{N^2(1-K^2N^2)}{(1+k^2N^2)} \quad (N \to \infty) .$$

(18)

After Fourier transform, Eq. (15) turns into

$$w'x^2\widehat{\phi}_0(x)$$

$$= \int_0^x \xi \, d\xi \int_{x-\xi}^\infty d\xi' \int_{-\infty}^\infty dk \, \widehat{K}(\xi, \xi'; k) \widehat{\phi}_k(\xi) \widehat{\phi}_{-k}(\xi') . \tag{19}$$

Expanding $\hat{\phi}_x(x)$ near k=0, we get

$$\hat{\phi}_k(x) = \sum_{n=0}^{\infty} \frac{k^n}{n!} \phi_0^{(n)}(x) , \qquad (20)$$

where

$$\phi_0^{(n)}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \eta^n \widehat{\phi}(x, \eta) d\eta .$$

In the case of normal distribution of velocity, i.e., $\beta = -\frac{1}{2}$, one has $u(m) \sim 1/\sqrt{m}$. It then follows that

$$\phi_0^{(2)}(\xi) \sim \phi_0^{(0)}(\xi)/\xi$$
.

Thus one obtains a closed equation for scaling function $\phi_0(x) \equiv \phi_0^{(0)}(x)$

$$w'x^{2}\phi_{0}(x) = \int_{0}^{x} \xi \, d\xi \int_{x-\xi}^{\infty} d\xi' \overline{K}(\xi,\xi')\phi_{0}(\xi)\phi_{0}(\xi,\xi') ,$$
(21)

with \overline{K} being defined by

$$\overline{K}(\xi, \xi') \sim K_0(\xi, \xi')(\xi^{-1/2} + \xi'^{-1/2})$$
 (22)

For a physical kernel K_0 given by Eq. (11), it is easy to see that Eq. (22) corresponds to the type III kernels in the Smoluchovski theory of the aggregation [2], which gives the result

$$\phi_0(x) \sim \exp(-|x|^{-\mu}), \quad \mu = (2-D)/2D$$
. (23)

In one dimension this yields

$$\phi(x) \sim \exp(-|x|^{-1/2}) \quad (x \to 0) ,$$

$$c_1(t) \sim \exp(-t^{1/3}) \quad (t \to \infty) .$$
(24)

Here the Smoluchovski equation theory predicts that the monomer decays exponentially, as determined by Eq. (24). However, our numerical simulations on the one-dimensional ballistic aggregation reveal that $c_1(t)$ decays approximately as t^{-1} , which is inconsistent with the prediction of the mean-field theory.

In all of the above, we assumed that the initial velocity distribution function (VDF) had finite variance so that the central limit theorem could be invoked to yield $v(m) \sim m^{-1/2}$. An interesting generalization is the case where the initial VDF has a broad distribution of exponent μ

$$p(v) \sim v^{-(1+\mu)}, \quad (v \to \infty) . \tag{25}$$

In this case the particle number conservation states that the sums of independent variables v_i [13]

$$V_N = \sum_{i=1}^N v_i$$

are given by the following.

For $0 < \mu \le 1$, the typical value of V_N is

$$V_N \sim N^{1/\mu} \ (\mu < 1) ,$$

 $\sim N \ln N \ (\mu = 1) ;$ (26)

for $1 < \mu < 2$, the typical value of the difference $V_N - \overline{V}_N$ reads

$$(V_N - \overline{V}_N)^2 \sim N^{2/\mu} \quad (\mu < 2) ,$$

 $\sim N \ln N \quad (\mu = 2) ;$ (27)

for $\mu > 2$, one recovers a purely linear dependence on N.

As we have already known from Eq. (9), the dynamic exponent z depends on β , which is determined by the velocity-mass relation. Combining the results of the particle number conservation and the momentum conservation, one finds that the typical velocity of a cluster is re-

lated to its mass by

$$v_{\rm rms}(m) \sim m^{1/\mu - 1} \ (0 < \mu \le 2)$$
, (28)

with a logarithmic correction for $\mu=1$. Therefore one has

$$\beta = \frac{1}{\mu - 1}$$

for the initial velocity distribution Eq. (25). In the onedimensional case, one finds that the case $0 < \mu \le 1$ corresponds to the type II kernels and $\mu > 1$ to type III kernels [2]. The behavior of the typical mass $\overline{m}(t)$ can be estimated as the following [14]: The rate of increase of the typical mass can be assumed to be the rate at which two aggregates of typical mass react with one another. This is so because the definition of typical size is such that it is not influenced by the presence of a background of small clusters. Thus it follows that the increase of $\overline{m}(t)$ is

$$\frac{d\overline{m}(t)}{dt} \sim \overline{K}(\overline{m}, \overline{m}) \sim \overline{m}^{\overline{\lambda}},$$

where the effective kernel \overline{K} is given by

$$\overline{K}(x,y) = (x^{1/D} + y^{1/D})^{D-1}(x^{1/\mu-1} + y^{1/\mu-1})$$
 (29)

so that

$$\overline{m}(t) \sim t^z$$
, $z = 1/(1-\overline{\lambda})$. (30)

From Eq. (29) it follows that

$$\bar{\lambda} = \frac{1}{\mu} - \frac{1}{D}$$
,

and

$$z = \frac{\mu D}{\mu D - D + \mu} \tag{31}$$

Note that the above argument holds only if $\bar{\lambda} < 1$. In the general theory of the Smoluchovski equation, for $\bar{\lambda} > 1$ one expects the occurrence of gelatin transition. In the nongelling cases with $\bar{\lambda} < 1$ $(\mu > \frac{1}{2})$, one has the scaling ansatz

$$c_m(t) \sim \overline{m}(t)^{-2} \phi(m/\overline{m}) , \qquad (32)$$

where the scaling function $\phi(x)$ is qualitatively different for types of kernels. In one dimension, the scaling theory of Smoluchovski's equation gives the approximate results for the scaling function

$$\phi(x) \sim \exp(-|x|^{-|1/\mu - 1|}) \quad (x \to 0, \mu > 1)$$
, (33)

$$\phi(x) \sim x^{-\tau} \quad (x \to 0, \frac{1}{2} < \mu < 1)$$
, (34)

$$\tau = 2 - P_{(1/\mu) - 1} / w' ,$$

$$P_{\alpha} = \int_{0}^{\infty} dx \ x^{\alpha} \phi(x) .$$
(35)

Only in special nongelling models are there exact results. For
$$K(x,y)=1(\mu=1)$$
, one finds $\phi(x)\sim \exp(-2wx)$,

For $K(x,y)=1(\mu=1)$, one finds $\phi(x)\sim \exp(-2wx)$, and for K(x,y)=x+y ($\mu=1/2$), one finds $\phi(x)\sim x^{-3/2}\exp(-x/2)$.

So far we have developed a Smoluchovski-type meanfield theory for the ballistic aggregation. In order to compare the numerical simulation results, we introduce a real physical reaction mechanism for the reaction kernel in one dimension, i.e., $K(m,m';u,u') \sim |u-u'|$ and approximated our principal theoretical result Eq. (15) by Eq. (21), which has been studied in Ref. [2].

In the next section, we discuss our numerical results which show that the scaling theory predicts the dynamic exponent z correctly up to the so-called Cauchy distribution of VDF, i.e.,

$$p(v) = \frac{1}{1+v^2} ,$$

which corresponds to $\mu = 1$. Beyond the Cauchy distribution, that is, in the case of $0 < \mu < 1$, the whole theory seems to breakdown.

III. NUMERICAL RESULTS AND DISCUSSIONS

We have performed numerical simulations on the onedimensional case of the ballistic aggregation model. Initially there were 10^5 particles with mass m=1 randomly or uniformly distributed in a finite interval. The initial velocities were either uniformly distributed between -1and 1 (the normal case) or distributed according to some broad distributions (the anomalous cases). Freeboundary conditions were used, except in the case of very low reaction rates, where it was necessary to use periodic boundary conditions.

The results of these simulations, shown in Fig. 1, indicate that $c_1(t)$ decays approximately as t^{-1} . In fact, it can be shown that t^{-1} is a lower bound on $c_1(t)$, as the following conjunction of three events is sufficient for a monomer to survive until time t without reacting.

- (1) It has an initial velocity of the order $t^{2/3}$ or less.
- (2) For all m of order $t^{2/3}$ or less, the sum of the initial momenta of the m particles to its right is positive.
- (3) A similar condition on the sum of the momenta of the particles to the left being negative.

All three events are mutually independent and each has probability $t^{-1/3}$, since events (2) and (3) are equivalent to the event that a one-dimensional random

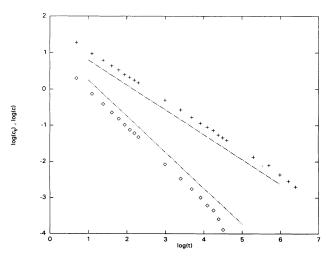


FIG. 1. Double logarithmic plot of particle number c (crosses) and monomer concentration c_1 (diamonds) against time. log stands for the natural logarithm ln.

walk remains positive for a number of steps approximately $t^{2/3}$. Thus

$$c_1(t) \ge \operatorname{const} \times t^{-1} \ . \tag{36}$$

These conditions are also, in essence, necessary, so that $c_1(t) \sim t^{-1}$ as indicated by our simulations.

From the above and the scaling relation of Eq. (3), it follows that $\tau = \frac{1}{2}$. We check that this is indeed correct (Fig. 2). It is noted that this is at variance with the mean-field prediction, that the particle size distribution should be bell shaped, that is, peaked around the typical size and decaying sharply for both large and small particle sizes (so-called type III behavior [2]).

Such a complete failure of the mean-field theory is rather surprising: indeed it is natural to think of D = 1 as the upper critical dimension for processes involving ballistic transport, as is the case for D=2 in the case of diffusive aggregation [3,12]. To find the explanation, we look at the mass dependence of v(m). In the above treatment, we had assumed that v(m) goes as $m^{-1/2}$. While this is true for the typical velocity of a cluster of typical mass, we see that at fixed time the velocity is essentially independent of mass. In one dimension this can be explained by noting that any particle with an exceptionally high velocity would quickly disappear by reacting with one of its neighbors. Such is not the case, however, if the reaction rate $k \ll 1$. In this case, one expects that for intermediate times a regime of mean-field behavior would be found. We have performed simulations to verify this hypothesis. In these simulations, whenever two particles collide, they react with probability k to form a larger particle and pass through one another without any change in velocity with probability 1-k. (This latter case may not appear very realistic, but it is a way to eliminate correlations and thus check whether our mean-field treatment is indeed the appropriate one.) The results are shown in Fig. 3 for the case of the reaction rate k=0.05. The monomer concentration is found to decay approximately as $\exp(-Ct^{1/3})$ over a time range extending from 10 to

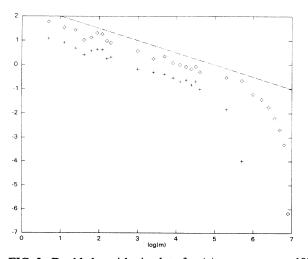


FIG. 2. Double logarithmic plot of $c_m(t)$ versus m at t = 1000 (diamonds) and t = 5000 (crosses). The slope of the best fit line is approximately $-\frac{1}{2}$, as predicted by the theory. log stands for the natural logarithm ln.

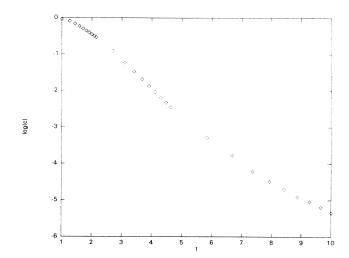


FIG. 3. Plot of $\log c_1(t)$ against $t^{1/3}$ for the reaction rate k equal to 0.05. An approximate straight line regime corresponding to times less than 100 is seen. The later decay (not shown in this figure) can be found as t^{-1} . log stands for the natural logarithm ln.

100, which then crosses over to the expected t^{-1} decay in large time. A plot of v(m) against m also reveals the expected behavior of $m^{-1/2}$. It should be pointed out that the usual t^{-1} behavior is always recovered in the long-time limit. This allows one to reject the suggestion that the discrepancy with mean-field theory is due to the pathological feature that particles cannot avoid each other in one dimension.

We have also performed simulations for the anomalous distribution of the initial velocity, which is described by a particle number conservation distribution of exponent μ as defined by Eq. (25). The mean-field theory, combined with the particle number conservation theory, yields $z=\mu/(2\mu-1)$ in one dimension. These results have been confirmed by the numerical simulations both for $\mu=1$ and $\mu=\frac{3}{2}$ (see Figs. 4 and 5). As for the decay of mono-

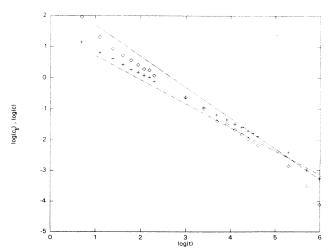


FIG. 4. Double logarithmic plot of particle number (crosses) and monomer (diamonds) concentration against time for an initial VDF with a power-law tail $P(v) \sim v^{-(1+\mu)}$ with $\mu = \frac{3}{2}$. log stands for the natural logarithm ln.

mers, we found numerically that the value of the exponent w was roughly equal to one independent of μ , in contradiction with the mean-field predictions which claim that the case $\mu = 1$ corresponds to the constant kernel ($\lambda = 0$) while the case $\mu = \frac{3}{2}$ to the type III kernels. To understand this remarkable "superuniversality," consider two typical neighboring clusters at time t. Their constituent particles at t=0 fill two adjacent intervals. If now an additional "test" particle starts between these two intervals and if its initial velocity is sufficiently low to ensure that it would not be likely to collide with either of its two neighbors before time t, this particle will survive as a monomer at time t. If we denote by N(t) the total number of clusters and by $\overline{v}(t)$ the typical velocity at time t, one finds that the probability of a particle being between two such intervals is roughly N(t) and the probability to start with a low enough velocity is about $\overline{v}(t)$. Thus one finds

$$c_1(t) \ge \operatorname{const} \times N(t)\overline{v}(t) \sim t^{-1}$$
 (37)

Again, it appears very likely that this lower bound is in fact exact.

Now let us discuss the case of the super-Cauchy distribution, i.e., the case of $\mu < 1$. In this case, the dynamic exponent z can be obtained from Eq. (31)

$$z = \frac{\mu}{2\mu - 1} \tag{38}$$

in one dimension. For $\mu = \frac{2}{3}$, we have z = 2, which means that the typical cluster size increases with time as $\overline{m}(t) \sim t^2$, or the particle number decreases as $c(t) \sim t^2$. However, the numerical simulations show that both particle number and monomer concentration decay exponentially [see Fig. 6]. In order to understand this discrepancy, we have also checked the behavior of the typical velocity of a cluster. It is found, from Eqs. (28) and (38), that the typical velocity of the cluster will increase with time as $v_{\rm rms} \sim t$, but the numerical results shows that the typical velocity decreases approximately according to some power law [see Fig. 7]. Furthermore, let us look at

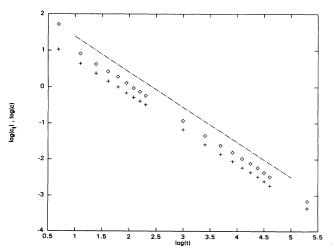


FIG. 5. Double logarithmic plot of particle number (crosses) and monomer (diamonds) concentration versus time, for $\mu=1$, i.e., for the so-called Cauchy distribution. log stands for the natural logarithm ln.

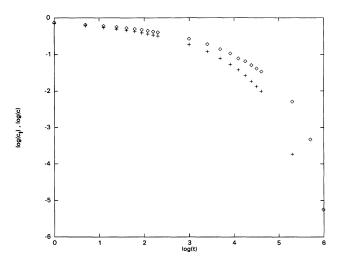


FIG. 6. Double logarithmic plot of particle number (crosses) and monomer (diamonds) concentration against time for the "super-Cauchy" distribution of initial velocity with $\mu = \frac{2}{3}$. log stands for the natural logarithm ln.

the exponent τ . From a general theory of the Smoluchovski equation [2], $\tau=2$ if the particle number decays exponentially. We used the second moment of cluster size distribution $M_2(t)$ to calculate the exponent τ [14]

$$M_2(t) = \sum_{k=0}^{\infty} k^2 c_k(t) . (39)$$

The numerical result is shown in Fig. 8, indicating that $\tau=1$, which is inconsistent with the prediction made from the Smoluchovski-type mean-field theory. This discrepancy might arise from applying the particle number conservation theory [13] to explain the numerical simulation of the finite system. We will study this phenomenon in more detail in a forthcoming publication.

Let us now consider higher dimensions. It is clearly important to know whether the mean-field theory will eventually be correct in some upper critical dimension.

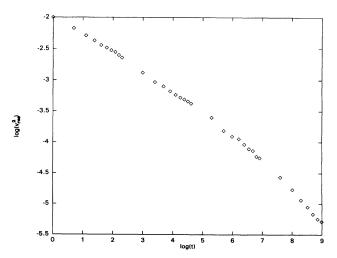


FIG. 7. Double logarithmic plot of typical velocity versus time for $\mu = \frac{2}{1}$, log stands for the natural logarithm ln.

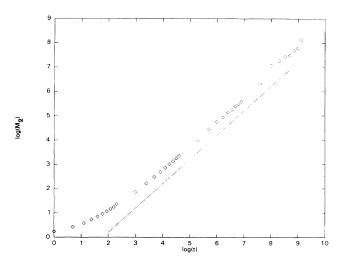


FIG. 8. Double logarithmic plot of the second moment of cluster size distribution $(M_2(t))$ versus time for $\mu = \frac{2}{3}$. log stands for the natural logarithm ln.

We surmise that this will not happen. The ansatz (10), (11) for the kernel K(i,j) gives, in the terminology of Ref. [2], $\mu = -\frac{1}{2}$ and hence

$$\Phi(x) \sim \exp(-|x|^{-1/2}) \quad (x \to 0) ,$$
 $c_1(t) \sim \exp(-t^{d/(d+2)} \quad (t \to \infty) ,$
(40)

which also implies that the particle size distribution is bell shaped. These results have a rather simple physical interpretation: if R(t) is the typical cluster radius, then the total reactive area of the system is roughly $N(t)R(t)^{d-1}$, which decays as $t^{2/(d+2)}$. If one then assumes

$$\dot{c}_1 = -\operatorname{const} \times A(t)c_1 , \qquad (41)$$

one obtains exactly the above formulas.

These results, however, all rely upon the assumption that a VDF of the form $v(m) \sim m^{-1/2}$ is eventually established. In view of the one-dimensional results, this is highly questionable. Indeed, in higher dimensions, the conservation of the total volume fraction ϕ causes the mean free path of a cluster to be of the order of the typical cluster radius. This may well eventually eliminate high-velocity particles regardless of mass and lead to v(m) being mass independent, as in one dimension. In fact, we may repeat the preceding argument: let the constituent particles of distinct clusters at time t be labeled at t=0 by the cluster they belong to at time t. Assume that particles with the same label are initially located in one

regular (more or less spherical) domain of volume approximately s(t), where s(t) is typical cluster size. Then the probability that an additional "test particle" falls in the interstitial region between these domains is of the order of $s(t)^{-1/d}$. If this particle has, in addition, a velocity of order of $\overline{v}(t)$ or less, it will survive as a monomer up to time t. This latter condition has a probability of $\overline{v}(t)^d$, as all components of the velocity must be small so that

$$c(t) \ge \overline{v}(t)^d s(t)^{1/d} \approx t^{-(d^2+2)/(d+2)}$$
, (42)

contradicting (40), which claims stretched exponential behavior for $c_1(t)$. However, it should be remembered that, for many systems of practical interest, one has $\phi \ll 1$, so that the mean free path is infinite in practice. The mean-field theory would then be valid in much the same way as it is valid for low reaction rates in one dimension. Simulations in higher dimensions are clearly desirable, but they are, unfortunately, quite difficult to perform.

IV. CONCLUSIONS

We have studied the ballistic aggregation model by using the scaling theory of the Smoluchovski equation as well as numerical simulations. We find that this model has the exponents $z = \frac{2}{3}$ and w = 1 in one dimension. The latter is incorrectly predicted by the mean-field theory to be a stretched exponential. The reason for this discrepancy lies in the fact that the VDF at large times is independent of mass. The case of initial VDF's obeying a particle number conservation was also studied. Scaling arguments analogous to those used in the previous case were found to agree with numerical work, in the case of finite mean velocity. We found that the value of zchanged continuously with the particle number conservation exponent μ if $\mu \ge 1$, whereas the value of one for the exponent w is unaffected by these variations, thus exhibiting a "universal" behavior. In the case of super-Cauchy distribution of initial velocity, i.e., $\mu < 1$, we found that the mean-field theory of Smoluchovski equation with the particle number conservation theory cannot give the correct predictions of the kinetic behavior of ballistic aggregation, at least, in one dimension. These discrepancies are speculated to persist in higher dimensions, so that there is, strictly speaking, no upper critical dimension for this system. These effects may well be unobservable unless the volume fraction is sufficiently large, however, so that the mean-field theory will presumably be excellent for a large variety of systems with small volume fractions.

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