Transition from random to ordered fractals in fragmentation of particles in an open system

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We consider the fragmentation process with mass loss and discuss self-similar properties of the arising structure both in time and space, focusing on dimensional analysis. This exhibits a spectrum of mass exponents θ, whose exact numerical values are given for which $x^{-\theta}$ or $t^{\theta z}$ has the dimension of particle size distribution function $\psi(x,t)$, where z is the kinetic exponent. We obtained conditions for which the scaling and fragmentation process altogether breaks down, and we give an explicit scaling solution for a special case. Finally, we identify a new class of fractals ranging from random to nonrandom and show that the fractal dimension increases with increasing order and a transition to a strictly self-similar pattern occurs when randomness completely ceases.

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The kinetics of the irreversible and sequential breakup of particles occurs in a variety of physical processes and has important applications in science and technology. These include erosion [1], grinding and crushing of solids [2], polymer degradation and fiber length reduction [3], breakup of liquid droplets [4], etc., to name just a few. In recent years, there has been increasing interest in studying fragmentation, resulting in variations that increase the flexibility of the theory in matching such conditions of real phenomena as an extension to higher dimensions [5], agglomerate erosion [1], mass loss [6], volume change [7], and fragmentation annihilation [8]. The kinetic equation approach of fragmentation is described by a linear integrodifferential equation where mass or size is the only dynamical quantity. This theoretical approach is mean field in character since fluctuations are ignored altogether.

In this paper, we study the kinetics of fragmentation with continuous mass loss, an interesting variant of the classical fragmentation equation introduced by Edwards *et al.* [6]. This is relevant in all fragmentation processes mentioned earlier where mass loss might occur due to evaporation, oxidation, sublimation, dissolution, melting, etc., or in the Yule-Furry process of cosmic shower theory where energy loss occurs due to collision [9]. Although there exist a series of paper devoted to this problem, the explicit scaling solution with exact numerical exponents, the geometric properties of the arising pattern, and the interplay between fragmentation and mass loss remain unexplored. In addition to obtaining these, we give an alternative interpretation of the existing scaling theory by considering dimensional analysis, and we give an explicit bound to the exponent of the breakup rate for which the kinetic equation fails. A strong motivation for the present investigation came from the desire to know how fractal geometry of the resulting object changes with the degree of order, which is quantified by the global exponent and is typically known as the fractal dimension.

The evolution of the particle size distribution function $\psi(x,t)$ for fragmentation with mass loss in one dimension is

$$\frac{\partial\psi(x,t)}{\partial t} = -\psi(x,t)\int_0^x F(y,x-y)\,dy + 2\int_x^\infty dy\;\psi(y,t)F(x,y-x) + \frac{\partial}{\partial x}(m(x)\psi(x,t)), \tag{1}$$

where $F(x,y)$ is the breakup kernel describing the rules and the rate at which a particle of size $(x+y)$ breaks into sizes x and y. Equation (1) describes a process whereby cuts are equivalent to seeds being sown on the fragmenting objects, thus producing two new segments. This immediately creates two more new ends belonging to the two different, newly created fragments; in doing so, fragments start losing their masses immediately from either end until they encounter another seed or become dustlike, thereby stopping the loss of their masses. Equation (1) also describes the sequential deposition of point-size particles that grow once deposited successfully and stop growing upon collision with another point or growing particle. In other words, the present model describes nucleation and growth when $\psi(x,t)$ describes the gap size distribution of size x at time t or how space is covered by growing objects. This occurs in a number of natural phenomena, including phase separation, wetting, droplet growth, and growth of breath figures. Recently, a variant of the present model was considered in [10] in which the deposition of growing rods instead of growing seeds was addressed.

We consider the breakup kernel to be $F(x,y)=(xy)^{\beta}(x+y)^{\sigma-1}$, for which the breakup rate $a(x)=\int_0^x F(y,x-y)dy = px^{\lambda(\beta,\sigma)}$, where $p=[\Gamma(\beta+1)]^2/\Gamma(2\beta+2)$, the homogeneity index $\lambda(\beta,\sigma)=2\beta+\sigma$, and $\mathrm{Re}(\beta)>-1$. To comply with the present choice of breakup rate $a(x)$, it is essential to consider a similar power-law form for $m(x)$, hence we choose $m(x)\sim mx^{\gamma}$, with m a positive real constant. However, $a(x)$ being the quantity describing the rate at which particles are fragmenting, $x^{-\lambda(\beta,\sigma)}\equiv\tau(x)$ must bear the dimension of time, and this puts a strong constraint on the exponent γ. That is, the dimensional consistency requires

$\gamma=\lambda(\beta,\sigma)+1$. This dimensional consistency has been ignored in all previous studies [6]; instead, $\gamma<\lambda(\beta,\sigma)+1$ was identified as the recession regime and $\gamma>\lambda(\beta,\sigma)+1$ as the fragmentation regime. A closer look at the rate equation reveals that x and t are inextricably intertwined via the dimensional consistency, and hence the system becomes stochastic in nature. So, it is obvious that either of the two can be taken to be an independent parameter when the other one is expressible in terms of this. For example, if x is chosen to be the independent parameter, then using the fact that the dimension of a physical quantity is always expressed as a power monomial, we can define the dimensionless quantity $\xi=t/x^{\alpha}$. It is obvious that the dimension of the governed quantity $\psi(x,t)$ can also be expressed in terms of x alone, and hence we can define another dimensionless quantity $\Pi=\psi(x,t)/x^{-\theta}\sim x^{\theta}\psi(x,x^{\alpha}\xi)\equiv F(x,\xi)$. Since ξ and Π are dimensionless quantities upon transition from one system of units of measurement to another inside a given class, their numerical values must remain unchanged, meaning $\partial F/\partial x=0$. This implies that Π is independent of x and can be completely expressed in terms of ξ alone. Thus we can define $\Pi=\Phi(\xi)$ to enable us to write the spatial scaling ansatz $\psi(x,t)\sim x^{-\theta}\Phi(\xi)$. Had we chosen time t to be the independent quantity, a similar argument would lead us to write the temporal scaling ansatz $\psi(x,t)\sim t^{\theta z}\phi(\eta)$ with $\eta=x/t^{-z}$. We know that $x^{-\lambda(\beta,\sigma)}$ has the dimension of time, therefore $t^{-1/\lambda(\beta,\sigma)}\equiv\delta(t)$ must have the dimension of x. This gives us $z=1/\lambda(\beta,\sigma)$, which is known as the kinetic exponent since $\delta(t)$ describes the mean or typical cluster size and $\alpha=-\lambda(\beta,\sigma)$. Inserting the temporal scaling ansatz into Eq. (1) and requiring scaling to exist would give the same result for the kinetic exponent z. However, dimensional consideration proved to be very instructive and time-saving, yet rich in physics.

Note that the exponent θ takes a value for which $x^{-\theta}$ and $t^{\theta z}$ have a dimension of $\psi(x,t)$, hence it is called the mass exponent. The existence of scaling or a self-similar solution actually means that we can choose self-similar coordinates $\psi/t^{\theta z}$ (or $\psi/x^{-\theta}$) and $x/\delta(t)$ [or $t/\tau(x)$] such that their plots for any initial condition collapse into one single curve. It is very instructive to note that at $\lambda(\beta,\sigma)=0$, the governing parameters x,t and the governed parameter ψ all lose their dimensional characters. As a result, the system loses its stochastic nature. This means that one can no longer define self-similar coordinates at $\lambda(\beta,\sigma)=0$, which is conceptually very important and crucial for scaling to exist, hence scaling at $\lambda(\beta,\sigma)\leqslant 0$ breaks down. Note the inherent properties of the fragmentation process, which are the typical or mean cluster size $\delta(t)$, must decrease as time proceeds, and the number density must be an increasing function of time. In order to be so, the system must be governed by some conservation laws. However, this is not true as the homogeneity index $\lambda(\beta,\sigma)<0$, in which case $\delta(t)$ becomes an increasing function of time. This simply goes against the principle of kinetics of fragmentation. Combining all this, we argue that the system fails to show scaling not only at $\lambda(\beta,\sigma)<0$, as was reported by Cheng and Redner [11], but also at $\lambda(\beta,\sigma)=0$. Many authors noticed further anomalous behavior in this regime, e.g., lack of conservation of mass [12] and an absence of self-averaging [13]. Due to this anomalous behavior, this regime was termed a transition to shattering [14]. These heuristic arguments actually imply a possible failure to describe a physically meaningful fragmentation process by the breakup kernel, for which the homogeneity index $\lambda(\beta,\sigma)\leqslant 0$ and the shattering is actually an articulate term for this regime. The above discussion is true for Eq. (1) even when the mass loss term is absent. Therefore, we shall restrict the rest of the discussion to the regime $\lambda(\beta,\sigma)>0$ with $\mathrm{Re}(\beta)>-1$.

We now turn to finding the mass exponent θ, which can only be found if the system follows some conservation laws. For example, for pure fragmentation ($m=0$), the mass or size of the system is a conserved quantity and gives $\theta=2$. Defining the nth moment $M_n(t)=\int_0^{\infty}x^n\psi(x,t)dx$ and combining it with the rate equation (1) for the present choice of $F(x,y)$ and $m(x)$ yields

$$\frac{dM_n(t)}{dt}=-\left(\frac{[\Gamma(\beta+1)]^2}{\Gamma(2\beta+2)}-\frac{2\Gamma(\beta+1)\Gamma(n+\beta+1)}{\Gamma(n+2\beta+2)}+mn\right)\times M_{n+2\beta+\sigma}(t). \tag{2}$$

Note that the number density $M_0(t)$ evolves in the same fashion as it would in the absence of the mass loss term. This means that particles keep losing their mass in a continuous manner by some mechanisms that do not alter the number density. The interesting feature of the above equation is that for $m>0$, there are infinitely many $n=D_f(\beta,m)$ values for which $M_{D_f(\beta,m)}(t)$ are conserved quantities. However, for $m=0$, there is only one conserved quantity $M_1(t)$, i.e., size or mass of the system, and this does not depend on β. The dynamics of the system is governed by conservation laws and, as a consequence, the system shows scale invariance. These conserved quantities in fact are the intrinsic agent responsible for tuning the numerical value of the mass exponent θ, and they introduce universality to the process. However, at $\lambda\leqslant 0$ there is no evidence that there exists any conservation law for which the mean cluster size can be a decreasing function of time while the mean number density can behave in the opposite way. We can find the numerical value of $D_f(\beta,m)$ by searching for the positive and real root of the equation obtained by setting the term in the bracket of Eq. (2) equal to zero, which is a polynomial in n of a degree determined by the β value. Substituting the temporal scaling ansatz into the definition of $M_n(t)$ gives $M_n(t)\sim t^{-[n-(\theta-1)]z}\int_0^{\infty}\eta^n\phi(\eta)d\eta$, and demanding that $M_{D_f}(\beta,m)$ be a conserved quantity immediately gives $\theta=[1+D_f(\beta,m)]$, which clearly depends on β and m only if $m>0$. Owing to the random nature of the process and due to the presence of the mass loss term, it is clear that when the process continues *ad infinitum*, it creates a distribution of points (dust) along a line at an extreme late stage that is different from any known set [15,16]. To measure the size of the set created in the long-time limit, we define a line segment $\delta(t)=M_1(t)/M_0(t)\simeq t^{-1/\lambda(\beta,\sigma)}$, which is the typical cluster size. We can count the number of such segments

needed to cover the set, and in the limit $\delta \to 0$ (i.e., $t \to \infty$) the number $N(\delta)$ will simply measure the set and appear to scale as $N(\delta) \sim \delta^{-D_f(\beta,m)}$. The exponent $D_f(\beta,m)$ is known as the Hausdorff-Besicovitch [15] dimension or the fractal dimension of the arising pattern.

To get a physical picture of the role played by m, we set $\beta=0$ for the time being, for which the polynomial equation becomes quadratic in n and the real positive root is $D_f(m) = -\frac{1}{2}(1+1/m)+\frac{1}{2}\sqrt{(1+1/m)^2+4/m}$ when the second root is $D=-[D_f(m)+1+1/m]$. Therefore, the exponent θ is also function of m. The expression for $D_f(m)$ reveals that as the value of m increases, the fractal dimension decreases very sharply and in the limit $m \to \infty$, $D_f(m) \to 0$. This means that as m increases, the size of the corresponding arising set decreases sharply due to the fast disappearance of its member, whereas as $m \to 0$, $D_f(m) \to 1$, that is, we recover the full set (pure fragmentation) that describes a line. On the other hand, had we kept m fixed and let p decrease, the effect would have been the same as was observed for increasing m with $p=1$ (i.e., $\beta=0$). Thus, it is the ratio between m and p that matters rather than their individual increases or decreases. To give a further physical picture of what these results mean, we define the mass length relation for the object as $M_0 \sim \delta^{D_f(m)}$ and $M_e \sim \delta^d$ for the space where the object is being embedded, where d describes the Euclidean space. The density of the property of the object ρ then scales as $\rho \sim \delta^{D_f(m)-d}$. It is thus clear that for a given class of set created by a specific rule, when $D_f(m)$ decreases it means that it is increasingly moving away from d and hence more and more members are removed from the full set. This in turn creates increasingly ramified or stringy objects, since $D_f(m)=d$ describes the compact object with uniform density. Therefore, this shows that increasing the m/p ratio means that the mass loss process becomes stronger than the fragmentation process and vice versa.

We now attempt to find the spatial scaling solution for $\Phi(\xi)$. Note that the dimension of the arising pattern is independent of σ and consequently independent of how fast or slow the system performs the process. Therefore, we can set $\sigma=1$ without the risk of missing any physics, but it certainly simplifies our calculation. Substituting the spatial scaling ansatz into the rate equation (1) for $F(x,y)=1$ and $m(x)=mx^2$ and differentiating it with respect to ξ transforms the partial integrodifferential equation into an ordinary differential equation,

$$\xi(1-m\xi)\Phi''(\xi)+\{(1-\theta)-\xi[2m(2-\theta)-1]\}\Phi'(\xi) -[m(2-\theta)(1-\theta)-(3-\theta)]\Phi(\xi)=0. \quad (3)$$

For $m=1$, this is hypergeometric differential equation [17] whose only physically acceptable linearly independent solutions are ${}_2F_1(1,-(1+2D_f);-D_f;\xi)$ and $\xi^{(1+D_f)}\ {}_2F_1(2+D_f,-D_f;2+D_f;\xi)$, where $D_f=0.414\,213$. From these exact solutions for the spatial scaling function, we can obtain the asymptotic temporal scaling function $\phi(\xi) \sim e^{-D_f\xi}$, which satisfies the condition $\phi(\xi) \to 0$ as $\xi \to \infty$.

We now attempt to see the role of β on the system. To judge its role, it is clear from the previous discussion that we ought to give equal weight to all the terms in Eq. (1) so that each of them can compete on an equal footing. This can be done if we set $m=p=[\Gamma(\beta+1)]^2/\Gamma(2\beta+2)$ so that the relative strength between fragmentation and the mass loss process stays the same as the value of β increases. This is a very crucial point to be emphasized. We can obtain the fractal dimension for different values of β, which is simply the real positive root of the polynomial equation in n of degree β. A detailed survey reveals that the fractal dimension increases monotonically with increasing β. To find the fractal dimension in the limit $\beta \to \infty$, we can use Stirling's approximation in the polynomial equation to obtain $\ln[n+1]=(1-n)\ln[2]$ when $n=0.456\,999\,7$ solves this equation. In order to give a physical picture of the role of β in the limit $\beta \to \infty$, we consider the following model: $F(x,y)=(x+y)^\gamma \delta(x-y)$. This model shows that cuts are only allowed to be in the middle in order to produce two fragments of equal size at each time event. This makes $a(x)=\frac{1}{2}x^\gamma$, so we need to choose $m(x)=\frac{1}{2}x^{\gamma+1}$ ($m=\frac{1}{2}$ gives the same weight as for the fragmentation process). Then the rate equation for $M_n(t)$ becomes $M_n'(t)=-[(n+1)/2-2^{-n}]M_{n+\gamma}(t)$. As before, we set the numerical factor on the right-hand side of this equation equal to zero and then take the natural logarithm on both sides to obtain the n value for which $M_n(t)$ is time-independent. In doing so, we arrive at the same functional equation for n as we found for $\beta \to \infty$. This shows that the kernel $F(x,y)=(xy)^\beta(x+y)^{\sigma-1}$ behaves exactly in the same fashion as for $F(x,y)=(x+y)^\gamma\delta(x-y)$. We thus find that in the limit $\beta \to \infty$, the resulting distribution of points is a set with fractal dimension $D_f=0.456\,999\,7$, which is a strictly self-similar fractal as randomness ceases by dividing the fragments into equal pieces. We are now in a position to give a physical picture of the role played by β. First of all, the process with $\beta=0$ that describes the frequency curve of placing cuts about the size of the fragmenting particles is Poissonian in nature. Consequently, the system enjoys the maximum randomness and the corresponding fractal dimension is $D_f=0.414\,213$. For $\beta>0$, the frequency curve of placing cuts about the size of the fragmenting particles is Gaussian in nature, meaning that as the value of β increases, the particles are increasingly more likely to break in the middle than on either end. That is, as β increases, the variance decreases in such a manner that in the limit $\beta \to \infty$, the variance of the frequency curve becomes infinitely narrow, meaning a δ-function distribution for which the fragments are broken into two equal pieces. Therefore, there is a spectrum of fractal dimensions between $\beta \to 0$ when $D_f=0.414\,213$ and $\beta \to \infty$ when $D_f=0.456\,999\,7$. A detailed numerical survey, which we do not present here, confirms that the fractal dimension increases monotonically with β and reaches a constant value when $\beta \to \infty$. The previous density-dimension relation implies that increasing β vis-à-vis increasing order also means that the system loses less and less mass, and this happens despite the fact that now the m/p ratio stays the same. This shows that there exists an interplay between fragmentation and the mass loss process that can be tuned either by changing the ratio of m and p, which is ob-

vious of course, or by changing the degree of order alone, which is indeed a nontrivial result.

In summary, we have identified a new set with a wide range of subsets produced by tuning the degree of randomness only. The process starts with an initiator of unit interval $[0.1]$, and the generator divides the interval into two pieces, deleting some parts from either side of both pieces at each time step. The amount of parts to be deleted is determined by the parameter that controls the intensity of randomness. We quantified the size of the resulting set obtained in this way by fractal dimension and showed that the fractal dimension increases with increasing order and reaches its maximum value when the pattern described by the set is perfectly ordered, which is contrary to some recently found results [18]. We also discussed the scaling theory of the process, emphasizing dimensional analysis, and we showed that the shattering is in fact an articulate term whereby the equation fails to describe a physically meaningful fragmentation process. We have also shown that the interplay between fragmentation and mass loss arises not only from the ratio of their strengths determined by their respective numerical coefficients, but also from the degree of order. We gave an exact numerical value of the mass exponent, which has never been reported, and we obtained the explicit scaling function for a special case of interest. Finally, we argued on the basis of our findings that fractal dimension, degree of order, and the extent of the ramifications of the arising pattern are interconnected.

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