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A simple soluble model of discrete sequential fragmentation

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Abstract. A simple model of discrete sequential fragmentation consists in first breaking a unit segment into $q(\geqslant 2)$ pieces of equal length. A fragment is then selected at random among all fragments and broken in turn into q pieces of equal length and so on *ad infinitum*. Fragments of size $L = q^{-s} (s = 0, \ldots, f)$ are thus produced after f fragmentation events. The distribution of the ensemble averaged number of fragments of 'size' s is calculated exactly in terms of signless Stirling numbers of the first kind and shown to tend asymptotically to a Poisson distribution with parameter $(q/(q-1)) \log(f)$. An asymptotic lognormal distribution is thus found for the distribution of L.

1. Introduction

Fragmentation phenomena are encountered in numerous scientific fields from nuclear to astronomic scale, in real or in abstract spaces (see for instance Grady and Kipp 1985, Derrida and Flyvbjerg 1985, Brown 1989, Redner 1990, Mekjian 1990, Mekjian and Lee 1991, Englman 1991, Botet and Ploszajczak 1994, Elattari *et al* 1995 and references therein). Numerous thorough experimental and theoretical efforts are devoted, among other things, to the characterization of their ubiquitous properties, such as their scale-independent properties. Various semi-empirical distributions have been proposed to describe the distributions of the fragment sizes: Mott, Weibull, exponential, ..., lognormal. Baker *et al* (1992) have recently argued that the lognormal distribution (Aitchison and Brown 1957) is particularly suitable in that context. It seems interesting, thus, to investigate the distributions of fragment sizes in simple and exactly soluble models, with a small number of free parameters. One such model of discrete sequential fragmentation is described in the present paper. It is inspired by a model of 2-dimensional cellular structures generated by a sequential fragmentation procedure: at a given time, one cell is selected at random among all cells and broken into two cells and the process is iterated (Delannay and Le Caër 1994). Strongly disordered structures, which have remarkable topological properties, are thus constructed. A first simplified approach to the characterization of their metric properties consists in breaking the selected cell into two cells of equal areas. For further simplification, the starting structure is a hexagonal 2-dimensional structure with cells of identical areas. A straightforward generalization of the latter fragmentation process yields the model investigated in the following.

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2. A soluble model of discrete sequential fragmentation

The present model is more precisely a particular case of the usual rate equation approach which is used to describe fragmentation. The system is supposed to break up sequentially and no recombination is allowed. The discrete set of all possible fragment sizes can be arranged in order of decreasing sizes and indexed by an integer s, the size indexed by $s = 0$ being the initial maximum size. The function $n_s(f)$ yields the average number of s-fragments after f fragmentations. The evolution of the distribution of fragment sizes is then given by (Peterson *et al* 1985):

$$n_s(f+1) - n_s(f) = -a(s)n_s(f) + \sum_{s'=0}^{s-1} a(s')b(s|s')n_{s'}(f) \tag{1}$$

where the number f of fragmentations plays the role of time, so that the left-hand side term of (1) is just analogous to $\partial n_s/\partial t$. In (1), the function $a(s)$ is the rate at which s-fragments disappear by breakup while $b(s|s')$ is the rate at which s-fragments are produced by the breakup of s'-fragments. Both are assumed to be independent of f. In the present work, we focus on the case where all fragments have the same probability to be selected for breakup. In other words, the rate function $a(s)$ is independent of s and equals then $1/m(f)$, where $m(f)$ is the total number of fragments after exactly f breakups. Summing (1) over all possible sizes yields:

$$m(f+1) = m(f) + \frac{\sum_{s'} n_{s'}(f)(\sum_{s=s'+1}^{\infty} b(s|s'))}{\sum_{s'} n_{s'}(f)} - 1. \tag{2}$$

The sum $\sum_{s=s'+1}^{\infty} b(s|s')$ is just the average number of fragments produced during breakup of a s'-fragment. Let us suppose that this quantity, called here q, independent of f is also independent of s': q is a constant all along the cascade of fragmentations. The average number of fragments is thus:

$$m(f) = 1 + (q-1)f. \tag{3}$$

Only the binary case ($q = 2$) is treated, usually because of its simplicity. In some experiments, however, the proper value of q, if any, is still in debate. For example, in nuclear experiments of heavy-ion fragmentation the fact is that a controversy holds between proponents of the sequential binary fragmentation ($q = 2$) and those of multifragmentation ($q = \infty$) (Gross *et al* 1982, Borderie *et al* 1992).

One of the new results presented below shows that observable quantities can be found in some cases which allow experimental determination of the parameter q. For now, let us replace $a(s)$ by $1/(1 + (q-1)f)$ in equation (1) to write the rate equation as:

$$n_s(f+1) = \frac{1}{f + (1/(q-1))}\left[f n_s(f) + \sum_{s'=0}^{s-1} \frac{b(s|s')}{q-1} n_{s'}(f)\right]. \tag{4}$$

Equation (4) can be considered as a matrix recurrence equation acting on the vector $\boldsymbol{n}(f)$ whose components are $n_s(f)$. The dimension of $\boldsymbol{n}$ after any number of fragmentations can be extended beyond its minimum value to any desired value by adding as many zeros as necessary. If A denotes the lower triangular matrix with $b(s|s')$ as its (s, s') element $(s \geqslant s' + 1)$, (4) may thus be rewritten as:

$$\boldsymbol{n}(f+1) = \frac{1}{f + (1/(q-1))}\left[f\mathsf{I} + \frac{\mathsf{A}}{(q-1)}\right]\boldsymbol{n}(f). \tag{5}$$

The solution of (5) then writes:

$$\boldsymbol{n}(f) = C_f(q)\left\{\prod_{k=0}^{f-1}\left[k\mathbf{I} + \frac{\mathbf{A}}{q-1}\right]\right\}\boldsymbol{n}(0) \tag{6}$$

where the coefficient $C_f(q)$ is:

$$C_f(q) = \prod_{k=0}^{f-1}\left[k + \frac{1}{q-1}\right]^{-1} = \frac{\Gamma(1/(q-1))}{\Gamma(f+(1/(q-1)))}. \tag{7}$$

The product $\prod_{k=0}^{f-1}[k+x] = \frac{\Gamma(f+x)}{\Gamma(x)}$ can be expanded as a finite sum of powers of x with signless Stirling numbers of the first kind, noted here $|S_f^{(j)}|$, as coefficients (Abramowitz and Stegun 1965, Johnson *et al* 1992):

$$\prod_{k=0}^{f-1}[k+x] = \sum_{j=0}^{f}|S_f^{(j)}|x^j. \tag{8}$$

We recall that the $|S_f^{(j)}|$ satisfy the following recurrence relation:

$$|S_f^{(j)}| = (f-1)|S_{f-1}^{(j)}| + |S_{f-1}^{(j-1)}| \tag{9}$$

with $|S_0^{(0)}| = 1$ and $|S_f^{(0)}| = 0$ for $f > 0$ among others (Abramowitz and Stegun 1965, Johnson *et al* 1992). As $\mathbf{I}$ and $\mathbf{A}$ commute, the product of matrices which appears in (6) can be expanded in the same way as the product (8), simply replacing x by $\mathbf{A}/(q-1)$:

$$\prod_{k=0}^{f-1}\left[k\mathbf{I} + \frac{\mathbf{A}}{(q-1)}\right] = \sum_{j=0}^{f}|S_f^{(j)}|\frac{\mathbf{A}^j}{(q-1)^j}. \tag{10}$$

Under the assumption that the overall rate of breakup is independent of the size during this sequential q-nary fragmentation process, the average size distribution of the fragments is thus seen to be written down naturally as a finite combination of Stirling numbers:

$$\boldsymbol{n}(f) = C_f(q)\sum_{j=0}^{f}|S_f^{(j)}|\frac{\mathbf{A}^j\boldsymbol{n}(0)}{(q-1)^j}. \tag{11}$$

The remaining technical problem is to be able to calculate the vectors $\mathbf{A}^j\boldsymbol{n}(0)$, given the initial state of the system $\boldsymbol{n}(0)$.

3. An explicit solution for a simple model of sequential q-nary fragmentation process

Hereafter, we have chosen to investigate a simple model of sequential q-nary fragmentation process: consider a segment of length 1 and break it first into $q(q \geqslant 2)$ pieces of length $1/q$. A fragment is selected at random amongst the q latter fragments and is broken in turn into q pieces of length $1/q^2$. The process is then pursued: at every step a fragment is selected at random amongst all fragments and broken into q fragments of equal length $L = q^{-s}$. We will investigate the ensemble averaged distribution $n_s(f)$ of the number of fragments of length $L = 1/q^s$ after f fragmentation events ($s = 0, \ldots, f$), where $s = -\log(L)/\log(q)$ is the size index (section 2). As a fragment of length $1/q^i$ is broken into q fragments of length $1/q^{(i+1)}$, the matrix $\mathbf{A}$ is filled up with elements equal to zero, except for the elements $A_{i+1}, i = q$. The matrices $\mathbf{A}^j$ have all the same sort of structure with elements

$(\mathbf{A}^j)_{i+j,i} = q^j$ as the sole non-zero elements. We deduce from (11) that the average number of s-fragments after f fragmentations is $(s = 0, \ldots, f)$:

$$n_s(f) = C_f(q)\left[\frac{q}{q-1}\right]^s |S_f^{(s)}|. \tag{12}$$

Using (12) and defining $H_{f_m}(x)$ as:

$$H_{f_m}(x) = \sum_{k=0}^{f-1} \frac{1}{(x+k)^m} \tag{13}$$

it is straightforward to deduce that the average $\langle s\rangle_f$ is:

$$\langle s\rangle_f = xH_{f_1}(x) \tag{14}$$

with $x = q/(q-1)$. Similarly:

$$\langle(s - \langle s\rangle)^2\rangle_f = xH_{f_1}(x) - x^2 H_{f_2}(x) \tag{15}$$

and

$$\langle(s - \langle s\rangle)^3\rangle_f = xH_{f_1}(x) - 3x^2 H_{f_2}(x) + 2x^3 H_{f_3}(x). \tag{16}$$

The $H_{f_m}(x)$s are finite constants for $m > 1$ when $f \to \infty$ while $H_{f_1}(x)$ is asymptotically equal to $\log(f)$ (Abramowitz and Stegun 1965). The first three moments about the mean are thus asymptotically equal to:

$$\lambda_g = \frac{q}{q-1}\log(f). \tag{17}$$

This suggests that the asymptotic distribution of $k = s-1$ ($s-1$ because $\mathrm{prob}(s=0) = 0$) is a Poisson distribution. For proving it, we calculate the generating function $G(t) = \langle(1+t)^k\rangle_f$ whose expansion when $t \to 0$ yields the factorial moments $\mu'_{[n]} = \langle\prod_{p=0}^{n-1}[k+p]\rangle_f$. For a Poisson distribution of parameter λ, $G(t)$ is equal to $\mathrm{e}^{\lambda t}$ with $\mu'_{[n]} = \lambda^n$. Let us recall that the classical moments are linearly related to the factorial moments via Stirling numbers of the second kind and that the probabilities can also be calculated from the $\mu'_{[n]}$ for a discrete distribution (Johnson *et al* 1992). Using equations (8) and (12), $G(t)$ is expressed for very large f as:

$$G(t) = \left[\frac{\Gamma(q/(q-1))}{(1+t)\Gamma(q(1+t)/(q-1))}\right]\mathrm{e}^{\lambda_g t}. \tag{18}$$

As only the exponential term in (18) depends on f, the bracketed term gives negligible contributions to the successive terms of the expansion of $G(t)$ when $t \to 0$ and can be simply replaced by 1. The factorial moments tend thus to those of a Poisson distribution of parameter λ_g when $f \to \infty$. We have further observed numerically that the Poisson distribution is already a very good approximation of the distribution of $(s-1)$ for moderate values of f (figure 1), at least of the order of some tens, with a parameter

$$\lambda_f = \langle s\rangle_f - 1 = \lambda_g - \frac{q}{q-1}\Psi\left(\frac{q}{q-1}\right) - 1$$

where $\Psi(x)$ is the digamma function (Abramowitz and Stegun 1965). As the parameter of the Poisson distribution $\lambda_g \to \infty$ with f, the cumulative distribution of $(k-\lambda_g)/\lambda_g^{1/2}$ tends to the cumulative distribution of a standard Gauss distribution $N(0,1)$. Consequently the cumulative distribution of the fragment size L is asymptotically equal to that of a lognormal distribution. Such distributions of fragment sizes are often found experimentally (see for instance Baker *et al* 1992, Ishii and Matsushita 1992, Sotolongo-Costa *et al* 1996). The

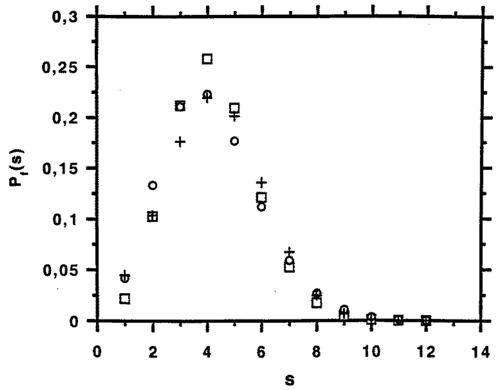

Figure 1. A comparison of the distribution of fragment sizes $P_f(s) = n_s(f)/m(f)$ (open squares) for $q = 4$ and $f = 20$ with a Poisson distribution of parameter $\lambda_f = 3.22$ shifted by $+1$ ($s = k + 1$, open circles) and with a binned normal distribution (mean = 4.22, standard deviation = 2.88, crosses).

convergence to a normal distribution of $\log(L)$ is observed from our numerical simulations to be much faster when q is selected at random at every breakup according to some given distribution.

4. Consequences of the simple model and conclusion

The exact distribution (12) is simple enough to allow computation of various average quantities. For example, using relations (8) and (12), the moments $\langle L^n \rangle_f$ write:

$$\langle L^n \rangle_f = \frac{\Gamma(q/(q-1))}{\Gamma(q^{1-n}/(q-1))} \frac{\Gamma(f + (q^{1-n}/(q-1)))}{\Gamma(f + (q/(q-1)))} \tag{19}$$

from which we calculate for instance $\langle L \rangle_f = 1/m(f)$ (relation (3)) as expected. For large values of f, the moments $\langle L^n \rangle_f$ show a power-law behaviour ($\langle L^n \rangle_f \propto f^{-\beta_n}$ with $\beta_n = q/(q-1)[1-(1/q^n)]$) and therefore:

$$\frac{\langle L^n \rangle_f}{\langle L^{n-1} \rangle_f} \propto f^{-q^{(1-n)}}. \tag{20}$$

The latter result shows in particular that there is no characteristic length since all these quantities scale differently with f. Let us mention that asymptotic multiscaling behaviour has also been reported for the fragment length in a simple model of oriented 2-dimensional fragmentation, where the fragments are always rectangular (Krapivsky and Ben-Naim 1994). By contrast, the area distribution function derived for the latter model is characterized by a single length scale. Relation (20) moreover shows that the study of the dependence of $\langle L^2 \rangle_f / \langle L \rangle_f$ on $\langle L \rangle_f$ provides a direct measure of the value of q since:

$$\frac{\langle L^2 \rangle}{\langle L \rangle} \propto \langle L \rangle^{\frac{1}{q}}. \tag{21}$$

Relation (21) remains valid when q is no longer fixed but is selected at random before each breakup according to a distribution with a finite mean $\bar{q}$ and a finite variance (figure 2). However, a simple calculation shows that the exponent $1/q$ has to be replaced in that case by $(1-\overline{(\frac{1}{q})})/(\bar{q}-1)$. That expression, which is derived by replacing a sum of f independent

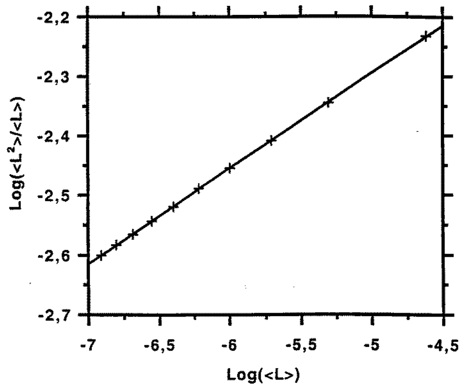

Figure 2. $\log(\frac{\langle L^2\rangle}{\langle L\rangle})$ versus $\log(\langle L\rangle)$: before each fragmentation, q is chosen at random between 2 and 10. The points are plotted for $f = 20n$ ($n = 1, \ldots, 10$). The slope of the least-squares line is 0.160 while $\frac{1-\overline{(1/q)}}{(\bar{q}-1)} = 0.157$.

and identically distributed random variables q_i by f times the common average, holds only for $f \to \infty$ or when q has a fixed value. It constitutes, however, a good approximation of the actual exponent even for moderate values of f (figure 2). In this sort of fragmentation process, the plot (21) can be used to suspect multifragmentation ($q > 2$) when the slope in figure 2 is found different from $\frac{1}{2}$. It would be interesting to know if other analytical models show behaviour like relation (21). We finally mention that 2-dimensional plots of points (x, f) ($1 \leqslant f \leqslant 10\,000$ and $q = 2$), where $x(0 < x < 1)$ is the abscissa of the point at which the initial segment of length 1 is broken at fragmentation number f, produce some sort of statistically self-similar patterns in which points concentrate into bands which are parallel to the f-axis and which are in turn constituted of narrower bands. The formation of bands may be partly explained by the random selection of fragments whatever their length: the breaking of a selected segment increases locally the number of smaller segments that is the probability to select again a breaking point in the same region etc. Such patterns, which remain, however, somewhat intriguing, suggest that the behaviour of the sequential q-nary fragmentation model described in section 3 is worth further investigation.

References

Abramowitz M and Stegun I 1965 *Handbook of Mathematical Functions* (New York: Dover)
Aitchison J and Brown J A C 1957 *The Lognormal Distribution* (Cambridge: Cambridge University Press)
Baker L, Giancola A J and Allahdadi F 1992 *J. Appl. Phys.* **72** 2724–31
Borderie B, Rivet M F and Remaud B 1992 *Phys. Lett.* **302B** 15–17
Botet R and Ploszajczak M 1994 *Int. J. Mod. Phys.* **3** 1033–117
Brown W K 1989 *J. Astrophys. Astron.* **10** 89–112
Delannay R and Le Caër G 1994 *Phys. Rev. Lett.* **73** 1553–6
Derrida B and Flyvbjerg H 1985 *J. Phys. A: Math. Gen.* **20** 5273–88
Elattari B, Richert J, Wagner P and Zheng Y M 1995 *Phys. Lett.* B **356** 181–5
Englman R 1991 *J. Phys.: Condens. Matter* **3** 1019–53
Grady D E and Kipp M E 1985 *J. Appl. Phys.* **58** 1210–22
Gross D H E, Satpathy L, Meng Ta-Chung and Satpathy M 1982 *Z. Phys.* A **309** 41–8
Ishii T and Matsushita M 1992 *J. Phys. Soc. Japan* **61** 3474–7
Johnson N L, Kotz S and Kemp A W 1992 *Univariate Discrete Distributions* 2nd edn (New York: Wiley)
Krapivsky P L and Ben-Naim E 1994 *Phys. Rev.* E **50** 3502–7
Mekjian A Z 1990 *Phys. Rev. Lett.* **64** 2125–8

Mekjian A Z and Lee S J 1991 *Phys. Rev.* A **44** 6294–312
Peterson T W, Scotto M V and Sarofim A F 1985 *Powder Technology* **45** 87
Redner S 1990 *Statistical Models for the Fracture of Disordered Media* ed H J Herrmann and S Roux (Amsterdam: North-Holland) 321–48
Sotolongo-Costa O, Moreno-Vega Y, Lloveras-Gonzalez J J and Antoranz J C 1996 *Phys. Rev. Lett.* **76** 42–5