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New solutions to the fragmentation equation

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Abstract. A new general class of exact, explicit scaling solutions to the fragmentation equation is given This class is described by a breakage rate $a(x)=x^{\lambda}$ and the daughter distribution function $y\bar{b}(x|y)=a\gamma(x/y)^{\gamma-2}+(1-a)\delta(x/y)^{\delta-2}$, and includes as special cases all previously-known scaling solutions to the fragmentation equation. For a subset of this class, with $\gamma=\lambda$ and $a=\delta/(\delta-\lambda)$, the complete time-dependent solution for a monodisperse initial condition is also given

1. Introduction

The process of fragmentation occurs in a large variety of situations, including rock crushing and grinding ('comminution'), polymer degradation (mechanical, thermal, and radiation-induced), droplet breakage, and aggregate breakage. The fragmentation process results in the evolution of the size distribution $c(x, t)$, where x is the size of the particles and t is the time. Much effort has been expended in finding solutions $c(x, t)$ to the discrete and continuous fragmentation equations, both to study specific practical problems and to provide a general understanding of the behaviour of these systems (see, for example, [1-27]). While the basic equations are linear and in principle soluble, the number of explicit solutions that have been found has been rather limited. Additional solutions would be very useful for both theoretical and practical applications

Of special interest are the scaling or self-similar solutions. These are essentially the solutions in the long-time, small-size limit where the distribution evolves to a simpler form, and universal in the sense that it becomes independent of the initial conditions. Most experimental systems evolve to the point where this behaviour is reached.

Recently, Peterson [20] has given the scaling solution where the breakage rate $a(x)$ and the daughter-size distribution $\bar{b}(x|y)$ are both power laws, $a(x)=x^{\lambda}$ and $y\bar{b}(x|y)=\gamma(x/y)^{\gamma-2}$. (In fact, for this class of models, the complete time-dependent solution is also known [9, 21].) This is a very general and useful class, and most physical systems will have $a(x)$ given by a simple power-law. However, the simple power-law form puts a strong restriction on the daughter distribution, and implies for example the average number of daughters is fixed by γ and is given by $\gamma/(\gamma-1)$.

A few other specific solutions have been found, such as those by Goren [12] and by Ziff and McGrady [19]. While these models go beyond the general power-law form of $y\bar{b}(x|y)$ in the above class, they represent specific breakage functions and daughter distributions and have no adjustable parameters.

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In this paper, we give a scaling solution for a new general class of models, characterized by $a(x)=x^\lambda$ and $y\bar{b}(x|y)=a\gamma(x/y)^{\gamma-2}+(1-a)\delta(x/y)^{\delta-2}$. This class of multiple fragmentation models as special cases includes all of the models that have been solved previously. It has the three adjustable parameters a, γ and δ in $\bar{b}(x|y)$, as well as the adjustable λ, to allow a quite breakup behaviour to be fit. One can fit the parameters, for example, to a specific value for the average number of daughter particles per breakup event, which is given by $\bar{N}=[\gamma\delta-a\gamma-(1-a)\delta]/[(\gamma-1)(\delta-1)]$.

These solutions are examined for the case $\lambda>0$ only. For $\lambda<0$ it is known that mass conservation breaks down as a cascading of fragmentation of smaller particles leads to loss of mass at $x=0$. This process is termed 'disintegration' [9] or 'shattering' [21]. Then normal scaling arguments will not apply—and indeed, the system will also show very large fluctuations in the distribution about the mean [9]. We will not discuss these cases further.

Besides giving the new solution, we also summarize some of the formal relations concerning the fragmentation equation, in section 2. We utilize the method of moments as developed by Ramkrishna [15] and by Cheng and Redner [23, 24]. In section 3, the solution to the new class is presented, and in section 4, a subset of this class is solved for the complete time dependence for a monodisperse (and therefore arbitrary) initial condition.

2. The fragmentation equation

The general form of the multiple fragmentation equation can be written

$$\frac{\partial c(x,t)}{\partial t}=-a(x)c(x,t)+\int_x^\infty a(y)\bar{b}(x|y)c(y,t)\,\mathrm{d}y \tag{1}$$

where $a(x)$ gives the rate of fragmentation of particles of size x, and $\bar{b}(x|y)$ is the average number of particles of size x produced when a particle of size y breaks up. Conservation of mass requires

$$\int_0^y x\bar{b}(x|y)\,\mathrm{d}x=y. \tag{2}$$

Furthermore, the average number of particles produced in a fragmentation event is given by

$$\int_0^y \bar{b}(x|y)\,\mathrm{d}x=\bar{N}(y) \tag{3}$$

which may be infinite. Physical restrictions require that $\bar{N}\geqslant 2$, and also put additional constraints on $\bar{b}(x|y)$ as discussed below.

Often, the fragmentation is a binary process in which only two fragments are produced in each event. Then, the kinetic equation can be written [2, 3, 7]

$$\frac{\partial c(x,t)}{\partial x}=-c(x,t)\int_0^x F(z,x-z)\,\mathrm{d}z+2\int_x^\infty c(y,t)F(x,y-x)\,\mathrm{d}y \tag{4}$$

where $F(x,y)=F(y,x)$ is the rate that particles of length $x+y$ break up into particles of length x and y. The corresponding expressions for $a(x)$ and $\bar{b}(x|y)$ are found from

$$a(x)=\int_0^x F(y,x-y)\,\mathrm{d}y \tag{5}$$

and

$$\bar{b}(x|y) = 2F(x, y-x)/a(y). \tag{6}$$

Note that these imply $\bar{N}=2$. A slightly different form of a binary fragmentation equation has been given by Melzak [6].

The scaling transformation is found by substituting

$$c(x, t) = s(t)^{-2}\phi(x/s(t)) \tag{7}$$

into (1). Assuming that $a(x)=x^{\lambda}$ and $y\bar{b}(x|y)=b(x/y)$, one finds $s(t)=t^{-1/\lambda}$, and that $\phi(\xi)$ satisfies [9, 11–13, 20, 24]

$$2\phi(\xi)+\xi\phi'(\xi) = -\lambda\xi^{\lambda}\phi(\xi)+\lambda\int_{\xi}^{\infty}\phi(\eta)\eta^{\lambda-1}b(\xi/\eta)\,\mathrm{d}\eta \tag{8}$$

where we have set the (arbitrary) separation constant equal to $1/\lambda$, so that $s(t)$ has a coefficient of unity. We define the moments of the scaling function $\phi(\xi)$ and of the daughter-size distribution $\bar{b}(r)$ by

$$\phi_n \equiv \int_0^{\infty}\xi^n\phi(\xi)\,\mathrm{d}\xi \tag{9}$$

$$b_n \equiv \int_0^1 r^n b(r)\,\mathrm{d}r \tag{10}$$

with $b_0=\bar{N}$ and $b_1=1$. Normalization of the mass implies $\phi_1=1$. Equation (8) implies that these moments are related to each other by [24]

$$\frac{\phi_{n+\lambda}}{\phi_n} = \frac{n-1}{\lambda(1-b_n)}. \tag{11}$$

Thus, a scaling solution of (1) can be verified simply by showing that its moments satisfy (11).

A somewhat different approach to fragmentation is through the introduction of the cumulative size distribution [9, 13, 15]. This approach leads to a scaling assumption of the form

$$c(x, t) = \lambda x^{-2}\Phi(tx^{\lambda}). \tag{12}$$

Thus Φ is related to ϕ by $\phi(\xi)=\lambda\xi^{-2}\Phi(\xi^{\lambda})$. It follows that the scaling function $\Phi(z)$ satisfies [15]

$$\Phi(z) = \int_z^{\infty}\Phi(w)B[(z/w)^{1/\lambda}]\,\mathrm{d}w \tag{13}$$

where

$$B(u) \equiv \int_0^u rb(r)\,\mathrm{d}r \tag{14}$$

is the cumulative mass distribution of the products, with $B(1)=1$. In terms of ϕ, (13) is equivalent to

$$\phi(\xi) = \lambda\xi^{-2}\int_{\xi}^{\infty}\phi(\eta)\,\eta^{\lambda+1}B(\xi/\eta)\,\mathrm{d}\eta \tag{15}$$

which also follows directly from (8) by integration Again, we introduce the moments of $\Phi(z)$ and $B(u)$

$$\Phi_n \equiv \int_0^\infty z^n \Phi(z)\,\mathrm{d}z = \phi_{\lambda(n+1)+1} \tag{16}$$

$$B_n \equiv \int_0^1 u^n B(u)\,\mathrm{d}u = (1-b_{n+2})/(n+1) \tag{17}$$

and find from (13) that [15]

$$\frac{\Phi_{n-1}}{\Phi_n} = \lambda B_{\lambda n-1} \tag{18}$$

which is equivalent to, but of a somewhat more convenient form than, (11). Note that $\bar{N} = 1 + B_{-2}$, and $\Phi_{-1} = 1$.

The moments of the distribution

$$M_n(t) = \int_0^\infty x^n c(x,t)\,\mathrm{d}x \tag{19}$$

satisfy

$$\frac{\mathrm{d}M_n}{\mathrm{d}t} = (b_n - 1)M_{n+\lambda} = -(n-1)B_{n-2}M_{n+\lambda} \tag{20}$$

which is valid even in the absence of scaling, assuming only homogeneity in $a(x)$ and $y\bar{b}(x|y)$. When scaling holds, the moments are given by

$$M_n(t) = \Phi_{(n-1)/\lambda-1}t^{-(n-1)/\lambda} = \phi_n t^{-(n-1)/\lambda}. \tag{21}$$

As an example of the application of these relations, first we consider the model studied by Filippov [9], Peterson [20], McGrady and Ziff [21], and Williams [27] defined by $a(x) = x^\lambda$ and $b(r) = \gamma r^{\gamma-2}$. It follows that $B(u) = u^\gamma$, $B_n = 1/(n+\gamma+1)$, and $\bar{N} = \gamma/(\gamma-1)$. The known scaling solution $\Phi(z) = z^{\gamma/\lambda}\,\mathrm{e}^{-z}/\Gamma(\gamma/\lambda)$ yields $\Phi_n = \Gamma(n+\gamma/\lambda+1)/\Gamma(\gamma/\lambda)$, which implies that

$$\frac{\Phi_{n-1}}{\Phi_n} = \frac{\lambda}{\lambda n+\gamma} = \lambda B_{\lambda n-1} \tag{22}$$

thus verifying that the scaling equation is satisfied. For the monodisperse initial condition $c(x,0) = \delta(x-l)/l$, the movements of the solution are given by [21] $M_n = l^{n-1}M(m, m+\gamma/\lambda, -tl^\lambda)$, where $m = (n-1)/\lambda$ and $M(a,b,z)$ is the confluent hypergeometric function. It can easily be verified these moments satisfy (20) by making use of the relation [28] $(\mathrm{d}/\mathrm{d}z)M(a,b,z) = (a/b)M(a+1,b+1,z)$.

3. A new class of solutions

We consider the class defined by

$$\begin{aligned} a(x) &= x^\lambda \\ b(r) &= a\gamma r^{\gamma-2} + (1-a)\delta r^{\delta-2} \end{aligned} \tag{23}$$

where $\lambda>0$, $\gamma>0$, $\delta>0$, and a are constants. (Note that this constant a should not be confused with the function $a(x)$). It follows that $B(u)=au^{\gamma}+(1-a)u^{\delta}$,

$$B_n=\frac{n+(1-a)\gamma+a\delta+1}{(n+\gamma+1)(n+\delta+1)} \tag{24}$$

and

$$\bar{N}=\frac{\gamma\delta-a\gamma-(1-a)\delta}{(\gamma-1)(\delta-1)}. \tag{25}$$

Note that this model is symmetrical under the interchange of $a\leftrightarrow 1-a$ and $\gamma\leftrightarrow\delta$. For convenience, we let $g\equiv\gamma/\lambda$, $d\equiv\delta/\lambda$, $a'=1-a$. Substituting (24) into (18) and solving iteratively for $n=1,2,3,\ldots$, we deduce that Φ_n is given by

$$\Phi_n=C\frac{\Gamma(n+g+1)\Gamma(n+d+1)}{\Gamma(n+a'g+ad+1)} \tag{26}$$

where the constant C is determined by the requirement that $\Phi_{-1}=1$

$$C\equiv\frac{\Gamma(a'g+ad)}{\Gamma(g)\Gamma(d)}. \tag{27}$$

One can readily verify that (24)-(26) satisfies (18)

$$\frac{\Phi_{n-1}}{\Phi_n}=\frac{n+a'g+ad}{(n+g)(n+d)}=\lambda B_{\lambda n-1}. \tag{28}$$

The function $\Phi(z)$ whose moments are given by (26) can be written in two forms: the first form, where $h\equiv g-d$, is given by

$$\begin{aligned}\Phi(z)&=\frac{Cz^{g}}{\Gamma(a'h)}\int_1^{\infty}(u-1)^{a'h-1}u^{ah}\,\mathrm{e}^{-uz}\,\mathrm{d}u\\&=Cz^{g}\,\mathrm{e}^{-z}U(a'h,h+1,z)\end{aligned} \tag{29}$$

and the second form, where $h'\equiv d-g=-h$, is given by

$$\begin{aligned}\Phi(z)&=\frac{Cz^{d}}{\Gamma(ah')}\int_1^{\infty}(u-1)^{ah'-1}u^{a'h'}\,\mathrm{e}^{-uz}\,\mathrm{d}u\\&=Cz^{d}\,\mathrm{e}^{-z}U(ah',h'+1,z)\end{aligned} \tag{30}$$

where $U(a,b,z)$ is the confluent hypergeometric function. The second form above follows from the first by means of Kummer's transformation [28], or by the symmetry transformation $a\leftrightarrow a'$, $d\leftrightarrow g$ and $h\leftrightarrow h'$. One can verify directly that the moments of (29) or (30) are given by (26), this verifying that these are scaling solutions to this model.

By taking special values of the parameters λ, a, γ and δ, one can find all the previously-known scaling solutions to (1), as shown in table 1. These solutions can also be written as incomplete Γ-functions or exponential-integral functions. In fact, (29)-(30) reduce to a variety of simpler functions under many other choices of the parameters, corresponding to the special cases of the function $U(a,b,z)$ [28]. Of course, in some cases only one of the integrals (29) or (30) will converge. The small-z behaviour of $\Phi(z)$ follows directly from (29) and (30):

$$\Phi(z)\sim\begin{cases}z^{g} & h<0,\ a'<0\\ z^{d} & h>0,\ a<0\end{cases} \tag{31}$$

Table 1. Special cases of (29)–(30), which yield previously-known scaling solutions to the fragmentation equation

Model	λ	$b(r)$	a	γ	δ	$\bar{N}$	$\Phi(z)$
Filippov[a]	λ	$\gamma r^{\gamma-2}$	1	γ	—	$\gamma/(\gamma-1)$	$z^{\gamma/\lambda}\,\mathrm{e}^{-z}/\Gamma(\gamma/\lambda)$
Goren[b]	1	$12r(1-r)$	4	3	4	2	$10z^4\int_1^\infty (1-1/u)^3\,\mathrm{e}^{-uz}\,\mathrm{d}u$
$F=6xy$[c]	3	$12r(1-r)$	4	3	4	2	$4z/3\int_1^\infty u^{-4/3}\,\mathrm{e}^{-uz}\,\mathrm{d}u$
Ternary[c]	2	$6(1-r)$	3	2	3	3	$3z/2\int_1^\infty u^{-3/2}\,\mathrm{e}^{-uz}\,\mathrm{d}u$

[a] [9, 20, 21]
[b] [12]
[c] [19]

which implies that

$$\phi(\xi) \sim \begin{cases} \xi^{\gamma-2} & h<0, a'<0 \\ \xi^{\delta-2} & h>0, a<0 \end{cases} \tag{32}$$

for $\xi \to 0$

An interesting special case of this model involving a logarithmic term in $b(r)$ is obtained by taking $a=\delta/(\delta-\gamma)$ and letting $\delta\to\gamma$. Then $b(r)=-\gamma^2 r^{\gamma-2}\ln r$, $\bar{N}=[\gamma/(\gamma-1)]^2$, and $\Phi(z)=[\Gamma(2g)/\Gamma(g)^2]z^g\,\mathrm{e}^{-z}U(g,1,z)$.

Thus, we have found the scaling solution for a quite general class of models (23). The values of the parameters a, γ and δ are restricted so that (i) $b(r)\geqslant 0$, (ii) $\bar{N}\geqslant 2$, and (iii) the constraint [21]

$$\int_0^u rb(r)\,\mathrm{d}r \geqslant \int_{1-u}^1 (1-r)b(r)\,\mathrm{d}r \tag{33}$$

for $0<u\leqslant 1/2$ are satisfied. These constraints put rather complicated restrictions on the parameters in this model. Note that (33) is a necessary, but most likely not sufficient, physical restriction on $b(r)$.

4. A class of models allowing complete time-dependent solutions

Finally we consider the question of whether general time-dependent solutions, for a monodisperse initial condition, can be found for these models. (Once the solution is known for a monodisperse initial condition, the solution for any initial condition follows simply because of the linearity of the problem.) For the binary model $F(x,y)=6xy$ and the ternary breakup model, it is known that the general solution is very closely related to the scaling integral—essentially, one has to change the limits of integration, and add a δ-function term [19] We have found that a subset of the above class of models can also be generalized in a similar way to find the complete solutions.

We consider the case $\gamma=\lambda$ and $a=\delta/(\delta-\lambda)$. That is, we consider the class of models with

$$\begin{aligned} a(x) &= x^\lambda \\ b(r) &= \frac{\delta\lambda}{\delta-\lambda}(r^{\lambda-2}-r^{\delta-2}). \end{aligned} \tag{34}$$

For this case, $ah' = 1$ and (29) reduces to

$$\Phi(z) = dz \int_1^\infty u^{-d} e^{-uz} \, du = dz^z \, \Gamma(1-d, z) \tag{35}$$

where again $d = \delta/\lambda$, and $\Gamma(a, x)$ is the incomplete Γ-function [28]. This scaling solution implies that $c(x, t)$ is given by

$$c(x, t) = \lambda x^{-2} \Phi(tx^\lambda) = \lambda \delta t x^{\delta - 2} \int_x^\infty y^{\lambda - \delta - 1} e^{-ty^\lambda} \, dy \tag{36}$$

where we have carried out the change of variables $y = xu^{1/\lambda}$ in the integral. Now, following the examples of the $F = 6xy$ and ternary models [19], we hypothesize that the general time-dependent solution for a monodisperse initial condition $c(x, 0) = l^{-1}\delta(x - l)$ (where here $\delta(x)$ represents the Dirac δ-function, while elsewhere δ is a parameter) is given by

$$c(x, t) = l^{-1} e^{-tl^\lambda} \delta(x - l) + \lambda \delta t x^{\delta - 2} \int_x^l y^{\lambda - \delta - 1} e^{-ty^\lambda} \, dy. \tag{37}$$

That is, we have added the time-dependent δ-function term, and changed the upper limit of the integral to l. First, one can verify the $M_1 = 1$ for all time. (With the more general forms of $b(r)$, this normalization generally fails.) Second, one can insert this solution into (1) and verify that it is satisfied, or alternately take the moments and verify that (20) is satisfied. Thus, (37) is indeed the general solution to the class of models specified by (34). Note that for this model, $\bar{N} = \delta\lambda/(\delta - 1)(\lambda - 1)$.

For special cases, $\lambda = 2$, $\delta = 3$ gives the ternary breakup model, with $b(r) = 6(1 - r)$ and $\bar{N} = 3$ [19]:

$$c(x, t) = l^{-1} e^{-tl^2} \delta(x - l) + 6tx \int_x^l y^{-2} e^{-ty^2} \, dy \tag{38}$$

while $\lambda = 3$ and $\delta = 4$ gives the binary $F = 6xy$ model, with $b(r) = 12r(1 - r)$ and $\bar{N} = 2$ [19].

$$c(x, t) = l^{-1} e^{-tl^3} \delta(x - l) + 12tx^2 \int_x^l y^{-2} e^{-ty^3} \, dy. \tag{39}$$

Solutions for the class of models with $\delta = \lambda + 1$ (which includes the two examples above) have also been discussed [26]. Thus, as special cases, the class of solutions (34) includes all models where explicit general solutions were previously known, except for the basic Filippov model, where the time dependent solution involves the confluent hypergeometric function $M(a, b, z)$ [9, 21].

In conclusion, we have presented both new scaling and new general solutions to the fragmentation equation. We note that Williams [27] has recently described a procedure to find general solutions to the fragmentation equation. An interesting problem for future study is to show how the solutions given here follow from Williams' theory.

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