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Abstract. We analyse for a class of fragmentation models how the shattering transition is related to the behaviour of the size distribution function, and discuss existence criteria for its moments. For models with homogeneous fragmentation kernels exact expressions are derived for all moments in the shattering and non-shattering regimes.

1. Introduction

Fragmentation occurs in a variety of physical processes such as polymer degradation [1], break-up of liquid droplets [2], and the crushing of rocks [3]. There has been considerable interest during the past few years in describing theoretically the time evolution of this phenomenon [4–7]. Most of the work has been based on a linear rate equation for a distribution of particles of a given size. For certain classes of models exact solutions were discovered [1, 4–6]. A scaling theory based on the linear rate equation was also derived [7] and for quite a large class of models scaling solutions were constructed [6].

The time evolution of the fragmentation process depends qualitatively on the behaviour of the probability of break-up for small particles: for break-up rates increasing sufficiently fast with decreasing mass or size, a cascading break-up occurs in which a finite part of the total mass is transferred to the particles of zero or infinitesimal mass. This so-called *shattering* [5] or *disintegration* [8] phenomenon is accompanied by a violation of the usual dynamical scaling [7].

The shattering behaviour seems to be inconsistent: on the one hand mass is conserved in every single break-up and one can formally prove mass conservation from the dynamic equation, on the other hand the total mass calculated from the exact solution of the rate equation decreases! The naive explanation is that particles of zero mass do not contribute to the standard expression for the total mass, exactly in the same way as particles of zero momentum do not contribute to the naive expression for the total number of particles in the case of the Bose–Einstein condensation. This argument is supported by the analysis of exactly solvable discrete models [1]. There, the total mass is conserved, but a finite fraction of it is contained in the smallest particles—the monomers. In the continuum limit they become points of zero mass and their contribution to the total mass vanishes, while the mass of the remaining particles remains finite and smaller than the initial mass.

A similar phenomenon occurs in the time evolution of atomic collision cascades [9]. Here the relevant quantity is the distribution of particles of a given energy. When a particle with a

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finite energy collides with a zero-energy particle the energy is conserved, but it turns out that for a class of collisional cross-sections the total energy decreases. The physical interpretation of this fact is similar to that given above for the shattering behaviour in fragmentation: the energy is transferred to particles of zero or infinitesimal energy. It is worthwhile noting that the shattering has been known for quite a long time. A rigorous discussion of this phenomenon, contained in the 30 year old paper of Filippov [8], was presented at the seminar of probability theory of the Moscow State University in 1952!

The aim of this paper is three-fold. (i) We present a simple argument that clarifies an apparent inconsistency between a formal proof of the mass conservation law based on the rate equation itself, and the finite mass loss found from the integration of an exact solution of this equation. Our argument leads to a general criterion for shattering in terms of the behaviour of the size distribution function. (ii) We analyse convergence criteria for the moments of the size distribution. This analysis leads to a phase diagram for the shattering transition. (iii) We correct an omission of McGrady and Ziff by calculating for the first time all moments in the shattering regime, as well as giving a concise derivation for the result in the non-shattering regime that was stated in [5] without proof.

2. Shattering scenario

We consider here the time evolution of a distribution of particles of a given mass or size x denoted by $c(x;t)$. A particle of mass y can break up into smaller pieces with probability per unit time $a(y)$. In this fragmentation a particle of mass x is produced with (conditional) probability $b(x|y)$. The time evolution of the mass distribution is thus described by a linear rate equation

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

We consider here the Ziff–McGrady [5] model of fragmentation for which kernels $a(x)$ and $b(x|y)$ are given by homogeneous functions x^α and $(\nu+2)(x/y)^\nu/y$, respectively. A similar class of models was considered by Filippov. However, our qualitative results concerning the shattering scenario are more general.

In every single break-up the mass is conserved. So the distribution of products $b(x|y)$ has to satisfy the condition

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

For integral (2) to exist the exponent ν has to be larger than -2. The average number of fragments resulting from the break-up of a particle of mass y is

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

For homogeneous kernels to achieve the physically admissible $\overline{N} \geqslant 2$ the exponent ν has to be smaller than or equal to 0. Moreover, it follows from (3) that for $-1 < \nu \leqslant 0$ the expected number of fragments $\overline{N}$ is equal to $(\nu+2)/(\nu+1)$ and for $-2 < \nu \leqslant -1$ the average number $\overline{N}$ is infinite.

The first case corresponds to non-shattering break-up, whereas the second and third ones correspond to shattering fragmentation. Note that only (10) agrees with the formal result (4). In the second case we obtain finite, non-zero mass current to the particles of zero or infinitesimal mass. The third case corresponds to the instantaneous, non-physical shattering. We want to stress here that this shattering scenario is not restricted to models with homogeneous kernels—only the power-law behaviour of a, b and c for $x \to 0$ is required. For the rate equation with homogeneous kernels the exact solution was given by Ziff and McGrady [5]. Since the rate equation is linear it is sufficient to consider the solution for a monodisperse initial condition $c(x;0) = \delta(x-l)$:

$$c(x;t) = \exp(-tl^{\alpha})\left\{\delta(x-l) + (\nu+2)tl^{\alpha-\nu-1}x^{\nu}\,{}_1F_1(1+(\nu+2)/\alpha, 2; (l^{\alpha}-x^{\alpha})t)\right\} \tag{13}$$

where ${}_1F_1(a,b;z)$ denotes the confluent hypergeometric function [10]. The analysis of the exact solution (13) shows that for non-diverging break-up rates, i.e. for $\alpha \geqslant 0$, exponent θ is equal to $-\nu$. From the existence of integral (2) it follows that in this case

$$\theta = -\nu < 2 < \alpha + 2 \tag{14}$$

the mass is conserved and there is no shattering. To investigate the behaviour of $c(x;t)$ as $x \to 0$ for diverging break-up rates we need the asymptotic behaviour [10] of the confluent hypergeometric function ${}_1F_1(a,b;z)$ for $z \to -\infty$:

$${}_1F_1(a,b;z) \sim \frac{\Gamma(b)}{\Gamma(b-a)}(-z)^{-a} \tag{15}$$

where $\Gamma(x)$ is the gamma function. It follows from (13) and (15) that for $\alpha \leqslant 0$

$$\theta = \alpha + 2 \tag{16}$$

there is a finite, non-zero mass current to particles of zero or infinitesimal mass, and a shattering fragmentation occurs. Instantaneous shattering does not exist within this model.

3. Moments

We consider here the moments of the distribution of particles of a given size for the fragmentation model with homogeneous kernels $a(x) = x^{\alpha}$ and $b(x|y) = (\nu+2)(x/y)^{\nu}/y$:

$$M_n(t) = \int_0^{\infty} \mathrm{d}x\, x^n\, c(x;t)\,. \tag{17}$$

Since the evolution equation for $c(x;t)$ is linear, it is sufficient to consider moments for the monodisperse initial condition $c(x;0) = \delta(x-l)$. From the exact solution (13) we obtain

$$M_n(t) = l^n \exp(-tl^{\alpha}) + \exp(-tl^{\alpha})(\nu+2)tl^{\alpha-\nu-1} \times \int_0^{l} \mathrm{d}x\, x^{\nu+n}\,{}_1F_1(1+(\nu+2)/\alpha, 2; (l^{\alpha}-x^{\alpha})t)\,. \tag{18}$$

First we consider moments in the non-shattering regime $\alpha > 0$. In this case the integrand behaves as $x^{\nu+n}$ for $x \to 0$, and the nth moment exists, i.e. the integral is convergent, for

According to (2) the mass is conserved in every single break-up and a straightforward integration of (1) gives formally the mass conservation law

$$\dot{M} = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty \mathrm{d}x\, xc(x;t) = 0\,. \tag{4}$$

However, it turns out that for fragmentation rates $a(x)$ increasing sufficiently fast as $x \to 0$, a more subtle analysis is required and (4) is not always valid. Let us consider first a cut-off mass M_ϵ and then take the limit $\epsilon \to 0^+$:

$$M_\epsilon = \int_\epsilon^\infty \mathrm{d}x\, xc(x;t)\,. \tag{5}$$

The cut-off mass loss is

$$\dot{M}_\epsilon = -\int_\epsilon^\infty \mathrm{d}x\, xa(x)c(x;t) + \int_\epsilon^\infty \mathrm{d}x \int_x^\infty \mathrm{d}y\, xb(x|y)a(y)c(y;t)\,. \tag{6}$$

By interchanging the integration over x and y and slighty rewriting the resulting formula we arrive at

$$\dot{M}_\epsilon = -\int_\epsilon^\infty \mathrm{d}x\, xa(x)c(x;t) + \int_\epsilon^\infty \mathrm{d}y \int_0^\infty \mathrm{d}x\, xb(x|y)a(y)c(y;t) - \int_\epsilon^\infty \mathrm{d}y \int_0^\epsilon \mathrm{d}x\, xb(x|y)a(y)c(y;t)\,. \tag{7}$$

The first two terms cancel due to condition (2) and we obtain

$$\dot{M}_\epsilon = -\int_\epsilon^\infty \mathrm{d}y \int_0^\epsilon \mathrm{d}x\, xb(x|y)a(y)c(y;t)\,. \tag{8}$$

Now suppose that for $x \to 0$ the fragmentation rate and the distribution of products can be approximated by homogeneous kernels $a(x) \sim x^\alpha$ and $b(x|y) \sim (\nu+2)(x/y)^\nu/y$, respectively, and that in the same limit the mass distribution is a power law $c(x;t) \sim A(t)x^{-\theta}$. One can then calculate the contribution to the cut-off mass loss from breakage of the small particles:

$$\dot{M}_\epsilon = -\epsilon^{\nu+2}A(t)\int_\epsilon \mathrm{d}y\, y^{\alpha-\theta-\nu-1}\,. \tag{9}$$

The upper integration limit is not relevant since it does not contribute to the $\epsilon \to 0^+$ limit. It follows from (9) that depending on exponent θ the mass loss $\dot{M} = \lim_{\epsilon\to 0^+} \dot{M}_\epsilon$ is zero, finite but non-zero, or infinite:

$$\dot{M} = \lim_{\epsilon\to 0^+} \dot{M}_\epsilon = 0 \qquad \text{for } \theta < \alpha+2 \tag{10}$$

$$\dot{M} = \lim_{\epsilon\to 0^+} \dot{M}_\epsilon = -\frac{A(t)}{\nu+2} \qquad \text{for } \theta = \alpha+2 \tag{11}$$

$$\dot{M} = \lim_{\epsilon\to 0^+} \dot{M}_\epsilon = \infty \qquad \text{for } \theta > \alpha+2\,. \tag{12}$$

$\nu + n + 1 > 0$. Note that for $-2 < \nu \leqslant -1$ the expected number of fragments in a single break-up $\overline{N}$ is infinite and—as could have been anticipated—the average number of particles, i.e. the zero-moment, is also infinite.

In the *non-shattering region* the exact expression for the nth moment,

$$M_n(t) = l^n \exp(-tl^\alpha)\, {}_1F_1((\nu+2)/\alpha, (\nu+n+1)/\alpha; tl^\alpha) \tag{19}$$

has already been quoted without derivation by Ziff and McGrady [5]. In the appendix we present a concise derivation. Note that for $n = 1$ the confluent hypergeometric function in (19) reduces to a simple exponential and we obtain the mass conservation law $M_1(t) = M_1(0) = l$.

Now let us consider the moments in the shattering regime $\alpha < 0$. It follows from the asymptotic behaviour (15) of the confluent hypergeometric function that the integrand in the expression for the nth moment (18) behaves as $x^{n-\alpha-2}$ for $x \to 0$ and the moment exists, i.e. the integral is convergent, for $n - \alpha - 1 > 0$. Note the surprising fact that for $\alpha < -1$ the 0th moment is always finite, irrespectively of ν. So the average total number of particles could be finite even though the expected number of fragments in every single break-up is infinite! Moreover, a finite fraction of the total mass would be transferred to a finite number of particles with zero or infinitesimal mass! We conclude that a physically acceptable situation corresponds to $\alpha > -1$.

As an important new result, supplementing Ziff and McGrady's result (19), we give here the exact expression for the nth moment in the *shattering region* (the detailed calculation is presented in the appendix):

$$\begin{aligned} M_n(t) = \exp(-tl^\alpha)\Bigg[\!\!\Bigg[l^n\, {}_1F_1\left(\frac{\nu+2}{\alpha}, \frac{\nu+n+1}{\alpha}; tl^\alpha\right) - \frac{\nu+2}{\alpha} t^{1-(\nu+n+1)/\alpha} l^{-\nu+\alpha-1} \\ \times \left\{ \left[\Gamma\left(\frac{\nu+n+1}{\alpha}\right)\Gamma\left(1-\frac{n-1}{\alpha}\right)\right] \Big/ \left[\Gamma\left(2-\frac{\nu+n+1}{\alpha}\right)\Gamma\left(1+\frac{\nu+2}{\alpha}\right)\right]\right\} \\ \times\, {}_1F_1\left(1-\frac{n-1}{\alpha}, 2-\frac{\nu+n+1}{\alpha}; tl^\alpha\right)\Bigg]\!\!\Bigg]. \end{aligned} \tag{20}$$

The above expression is not valid for $(\nu+n+1)/\alpha$ being a negative integer or zero, as both contributions are infinite in this case. To obtain the correct finite result one should take the limit $(\nu+n+1)/\alpha \to$ negative integer or zero of the whole expression (20). From the general formula (20) one can obtain the expression for the average total mass

$$M_1(t) = M(t) = l\left(1 - \frac{\gamma(1-(\nu+2)/\alpha\,; tl^\alpha)}{\Gamma(1-(\nu+2)/\alpha)}\right) \tag{21}$$

where $\gamma(a; z)$ denotes the incomplete gamma function [10]. The total mass monotonically decreases with time.

The expression (21) has been derived by Filippov [8] and subsequently rederived for the special case of $(\nu+2)/\alpha$ being a negative integer by Ziff and McGrady [5]. The general formula (20) is new.

We conclude with a short overview of the behaviour of the system for different values of α. For $\alpha > 0$ the total mass is conserved whereas the total number of particles can be finite or infinite, depending on the expected number of fragments in a single break-up. For $-1 < \alpha < 0$ the total mass decreases monotonically with time and the total number of particles is always infinite. It is important to note that the shattering transition is connected with the non-conservation of mass and not with the infinite total number of particles.

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Appendix

Let us consider first the moments for non-shattering fragmentation. To calculate the integral in (18) we use the following identity [11]:

$$\int_0^y \mathrm{d}x\,(y-x)^{\mu-1}x^{\lambda-1}\,{}_1F_1(a,b;x) = y^{\mu+\lambda-1}\frac{\Gamma(\mu)\Gamma(\lambda)}{\Gamma(\mu+\lambda)}\,{}_2F_2(\lambda,a;b,\mu+\lambda;y) \tag{A1}$$

where ${}_2F_2(c,d;e,f;y)$ is the generalized hypergeometric function [12]. First we use (A1) with $\mu=(\nu+n+1)/\alpha$ and $\lambda=1$ and express the integral in (18) in terms of ${}_2F_2$

$$\int_0^l \mathrm{d}x\,x^{\nu+n}\,{}_1F_1(1+(\nu+2)/\alpha,2;(l^\alpha-x^\alpha)t)$$
$$=\frac{l^{\nu+n+1}}{\nu+n+1}\,{}_2F_2(1,1+(\nu+2)/\alpha;2,1+(\nu+n+1)/\alpha;tl^\alpha)\,. \tag{A2}$$

Then we use (A1) with $\mu=1$ and $\lambda=1$ and reduce ${}_2F_2$ to the integral of ${}_1F_1$ that can be directly calculated with help of formula (13.4.9) from [10]:

$${}_2F_2(1,1+(\nu+2)/\alpha;2,1+(\nu+n+1)/\alpha;tl^\alpha)$$
$$=(tl^\alpha)^{-1}\int_0^{tl^\alpha}\mathrm{d}z\,{}_1F_1(1+(\nu+2)/\alpha,1+(\nu+n+1)/\alpha;z)$$
$$=\frac{\nu+n+1}{\nu+2}(tl^\alpha)^{-1}\{{}_1F_1((\nu+2)/\alpha,(\nu+n+1)/\alpha;tl^\alpha)-1\}\,. \tag{A3}$$

Using (A2) and (A3) in the general expression for moments (18) we arrive easily at Ziff and McGrady's formula (19).

Now consider the moments for shattering fragmentation. In this case we first rewrite the integral in (18):

$$\int_0^l \mathrm{d}x\,x^{\nu+n}\,{}_1F_1((\alpha+\nu+2)/\alpha,2;(l^\alpha-x^\alpha)t)$$
$$=-\frac{t^{-(\nu+n+1)/\alpha}}{\alpha}\int_0^\infty \mathrm{d}z\,\exp(-z)\,(z+tl^\alpha)^{-1+(\nu+n+1)/\alpha}\,{}_1F_1((\alpha-\nu-2)/\alpha,2;z)\,. \tag{A4}$$

Then using a rather complicated formula (7.627.8) from [12] we express (A4) in terms of the generalized hypergeometric functions

$$-\frac{t^\rho}{\alpha}\int_0^\infty \mathrm{d}z\,\exp(-z)\,(z+tl^\alpha)^{-1-\rho}\,{}_1F_1(1+\eta,2;z)$$
$$=-\frac{t^\rho}{\alpha}\left\{\frac{\Gamma(-\rho)\Gamma(1-\eta+\rho)}{\Gamma(2+\rho)\Gamma(1-\eta)}\,{}_2F_2(1+\rho,1-\eta+\rho;2+\rho,1+\rho;tl^\alpha)\right.$$
$$\left.+\frac{\Gamma(\rho)}{\Gamma(1+\rho)}(tl^\alpha)^{-\rho}\,{}_2F_2(1,1-\eta;2,1-\rho;tl^\alpha)\right\} \tag{A5}$$

where $\rho = -(\nu + n + 1)/\alpha$ and $\eta = -(\nu + 2)/\alpha$. The generalized hypergeometric function in the first term in (A5) can be straightforwardly expressed in terms of the confluent hypergeometric function whereas that in the second term can be reduced to ${}_1F_1$ by using identity (A1) with $\mu = 1$ and $\lambda = 1$ and calculating the resulting integral explicitly. Substituting the result into the general expression for moments (18) we arrive at (20).

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