Constant flux relation for aggregation models with desorption and fragmentation

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We study mass fluxes in aggregation models where mass transfer to large scales by aggregation occurs alongside desorption or fragmentation. Two models are considered. (1) A system of diffusing, aggregating particles with influx and outflux of particles (in-out model) (2) A system of diffusing aggregating particles with fragmentation (chipping model). Both these models can exist in phases where probability distributions are power laws. In these power law phases, we argue that the two point correlation function should have a certain homogeneity exponent. These arguments are based on the exact constant flux scaling valid for simple aggregation with input. Predictions are compared with Monte Carlo simulations.

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I. INTRODUCTION

A variety of aggregation–diffusion models have been constructed over the years by defining simple stochastic rules governing the evolution of a set of particles on a discrete lattice. Some of the interest in models of this type comes from the fact that they can be considered as minimal models of physical aggregation diffusion systems which provide a theoretical framework in which to study such phenomena as flocculation and gelation in aerosols and emulsions [1]. In addition, certain aggregation models have been shown to be related to models describing seemingly unrelated things such as the geometry of river networks [2], the distribution of forces in granular media [3] or the directed abelian sandpile model [4]. In analysing such models, most of the theoretical effort has focussed on determining the average mass density, \( \langle m, t \rangle \). In situations where a mean-field description is appropriate, this can be calculated by solving a Smoluchowski–like kinetic equation [2]. However, many of the applications are in low spatial dimensions where mean-field theory is typically inapplicable [6, 7, 8]. In such situations, diffusive fluctuations dominate, rendering the determination of \( \langle m, t \rangle \) quite non-trivial. Nevertheless, much progress has been made for specific models.

Despite the fact that fluctuations lead to non-trivial statistics for the mass distribution, very little is known, even numerically, about higher order correlation functions [9, 10]. This is the issue which we would like to address here. We consider a subclass of aggregation–diffusion models, specifically those which include deposition of monomers. Such models reach a statistically stationary state where the input of small masses is balanced by the depletion of small masses to generate larger ones by aggregation. In recent work [11, 12] we argued that it is useful to think of this stationary state as analogous to the stationary state of a turbulent system with the mass flux playing the role of the energy flux. One of the most important fruits of this analogy is the realisation that aggregation models having a stationary state with constant mass flux must satisfy an analogue of Kolmogorov’s 4/5 Law [13, 14]. This constraint, which we call the Constant Flux Relation (CFR), fixes exactly the scaling of a special correlation function of the mass distribution, namely the one which carries the mass flux. The power of this result is that it does not require any mean-field assumptions and holds equally well in the fluctuation dominated regime. In fact, it determines exactly the scaling of the flux-carrying correlation function for a broad class of homogeneous aggregation kernels even if the scaling of \( \langle m, t \rangle \) itself is not known. While the determination of a single correlation function is a modest step when faced with the problem of determining the full statistics, it can nevertheless be a powerful marker. For example, knowledge of the CFR exponent allowed us to give a relatively simple proof of the multifractality of the mass distribution for constant kernel aggregation in one dimension [15].

In our earlier paper [12], we derived CFR for a simple aggregation–diffusion model which we referred to as the Mass Model (MM). It was a model of diffusing particles undergoing mass conserving aggregation along with input of particles of small mass. The cascade was in the mass space with driving at small mass scales, dissipation at infinity, conserved quantity being mass and aggregation the process transferring mass to larger mass scales. We also derived analogous results for a collection of other models, aiming to stress the ubiquity of the approach and the central role played by conservation laws. In this paper we restrict ourselves to the implications of CFR for aggregation models. For clarity we will restate the argument for the MM. In addition, we ask whether the argument leading to CFR for the MM can tell us anything when the conservation law is less obvious, or when the one.
driving and dissipation scales are not widely separated as in the MM. We address this question in the context of two models studied earlier in relation to nonequilibrium phase transitions \[16\]. These models, which we call the in-out model and the chipping model, are generalisations of the MM. In both, the simple transfer of mass in the MM is disrupted all mass scales by evaporation in the former model and by fragmentation in the latter. In addition, the source of small mass scales is generated from within for the chipping model and not controlled from outside. The analysis for the MM was exact. Here we proceed by analogy in cases where an exact approach is yet to be developed, backing up our heuristic arguments with numerical simulations.

The rest of the paper is organised as follows. In Sec. [II] the two models are defined and known results are briefly reviewed. Sec. [III] describes the CFR for these models, and predicts the scaling behaviour of the two point joint probability distribution function. Sec. [IV] contains the results of Monte Carlo simulations. Sec. [V] contains a summary and conclusions.

## II. MODELS AND REVIEW

In this section, the two models- in-out model and chipping model - are defined and relevant earlier results are reviewed. The in-out model describes a system of diffusing, aggregating particles with influx and outflux of particles. The chipping model describes a closed system of diffusing, aggregating particles with fragmentation.

We define the models on a one dimensional lattice with periodic boundary conditions; generalisations to \(d\)-dimensional hyper-cubic lattice is straightforward.

### A. In-out model

Each site \(i\) of the lattice has a non-negative integer mass variable \(m_i \geq 0\). Given a certain configuration of masses at time \(t\), the system evolves in an infinitesimal time \(dt\) as follows. A site \(i\) is chosen at random (with probability \(dt\)), and then the following events can occur. (i) Adsorption: with probability \(q/(p+q+1)\), unit mass is adsorbed at site \(i\); thus \(m_i \rightarrow m_i + 1\). (ii) Desorption: if the mass \(m_i\) is greater than zero, then with probability \(p/(p+q+1)\), unit mass is desorbed from site \(i\); thus \(m_i \rightarrow m_i - 1\) provided \(m_i \geq 0\). (iii) Diffusion and aggregation: with probability \(1/(p+q+1)\) the mass \(m_i\) moves to a randomly chosen nearest neighbour; thus \(m_i \rightarrow 0\) and \(m_{i+1} \rightarrow m_{i+1} + m_i\). The initial condition is chosen to be to be one in which density is uniform. The model has two parameters, \(p, q\). We shall refer to this model as the in-out model.

Let \(P(m,t)\) denote probability that a site has mass \(m\) at time \(t\). The large time limit will be denoted by \(P(m)\), i.e., \(P(m) = \lim_{t \rightarrow \infty} P(m,t)\). When the adsorption rate \(q\) is increased keeping the desorption rate \(p\) fixed, the system undergoes a nonequilibrium phase transition across a critical line \(q_c(p)\) from a phase in which \(P(m)\) has an exponential tail to one in which it has an algebraic tail for large mass; i.e.,

\[
P(m) \sim \begin{cases} e^{-m/m^*} & \text{when } q < q_c(p), \\ m^{-\tau} & \text{when } q = q_c(p), \\ m^{-\tau} & \text{when } q > q_c(p), \end{cases}
\]

where \(m^*\) is a \(q\) dependent cut-off, and \(\tau\) and \(\tau_c\) are exponents characterising the power law decay \[16\]. The three phases will be called as the exponential phase \((q < q_c)\), the critical phase \((q = q_c)\) and the growing phase \((q > q_c)\). In addition, it was argued that as a function of the small deviation \(\tilde{q} = q - q_c\), and large time \(t\), \(P(m,\tilde{q},t)\) displays the scaling form

\[
P(m,\tilde{q},t) \sim \frac{1}{m^{\phi/\alpha}} Y \left( \frac{m^{\phi/\alpha}}{m^{\phi/\alpha}} \right),
\]

in terms of three unknown exponents \(\phi, \alpha, \tau, \tau_c\), and the two variable scaling function \(Y\). The three exponents were determined in all dimensions \[18\]. Of interest in this paper is the behaviour in one dimension wherein \[18\]

\[
P(m, t) \sim \begin{cases} \frac{1}{m^{1/6} f_c} \left( \frac{m}{l^{3/5}} \right), & q = q_c(p), \\ \frac{1}{m^{2/3} f_g} \left( \frac{m}{l^{3/5}} \right), & q > q_c(p), \end{cases}
\]

where the scaling functions \(f_c(x), f_g(x) \rightarrow x^0\) when \(x \rightarrow 0\) and \(f_c(x), f_g(x) \rightarrow 0\) when \(x \rightarrow \infty\).

### B. Chipping model

Each site \(i\) of the lattice has a non-negative integer mass variable \(m_i \geq 0\). Given a certain configuration of masses at time \(t\), the system evolves in infinitesimal time \(dt\) as follows. A site \(i\) is chosen at random (with probability \(dt\)), and then the following events can occur. (i) Chipping: with probability \(w/(w + 1)\), unit mass is chipped out from site \(i\) and added to a neighbour; thus \(m_i \rightarrow m_i - 1\) and \(m_{i+1} \rightarrow m_{i+1} + 1\). (ii) Diffusion and aggregation: with probability \(1/(1+w)\), the mass \(m_i\) moves to a randomly chosen nearest neighbour; thus \(m_i \rightarrow 0\) and \(m_{i+1} \rightarrow m_{i+1} + m_i\). The initial condition is chosen to be to be one in which density is uniform. The model has two parameters, \(w\), the mean density and \(w\), the ratio of the chipping rate to the hopping rate. We shall refer to this model as the chipping model.

The system undergoes a transition in the \(\rho-w\) plane \[16\]. There is a critical line \(\rho_c(w)\) in the \(\rho-w\) plane that separates two types of asymptotic behaviours of \(P(m)\). For fixed \(w\), as \(\rho\) is varied across the critical value \(\rho_c(w)\), the large \(m\) behaviour of \(P(m)\) was found to be,

\[
P(m) \sim \begin{cases} e^{-m/m^*} \rho < \rho_c(w), \\ m^{-\tau} \rho = \rho_c(w), \\ m^{-\tau} + \text{infinite aggregate} \rho > \rho_c(w). \end{cases}
\]
Thus, the tail of the mass distribution changes from having an exponential decay to an algebraic decay as $\rho$ approaches $\rho_c$ from below. As one increases $\rho$ beyond $\rho_c$, this asymptotic algebraic part of the critical distribution remains unchanged but in addition an infinite aggregate forms. This means that all the additional mass $(\rho - \rho_c)V$ (where $V$ is the volume of the system) condenses onto a single site and does not disturb the background critical distribution. This is analogous, in spirit, to the condensation of a macroscopic number of bosons onto the single $k = 0$ mode in an ideal Bose gas as the temperature goes below a certain critical value.

The critical density $\rho_c(w)$ was found to be

$$\rho_c(w) = \sqrt{w + 1} - 1,$$

in all dimensions. In addition, it was argued that the exponent $\tau$ is super-universal and was equal to $5/2$ in all dimensions. In particular, it was argued that in one dimension

$$P(m, t) \sim \frac{1}{m^{5/2}} f_{ch} \left( \frac{m}{t^{1/3}} \right),$$

where the scaling functions $f_{ch}(x) \to x^0$ when $x \to 0$ and $f_{ch}(x) \to 0$ when $x \to \infty$.

### III. CONSTANT FLUX RELATION

In this section, we summarise the CFR argument specifically for aggregation models. We then apply it to the in-out model and the chipping model in a heuristic way. The heuristic steps to CFR are as follows. First identify the conserved quantity and the space in which it flows. Second, use the equation of motion to write a Boltzmann like continuity equation for the average density of the conserved quantity in this space. This equation identifies a flux-carrying correlation function, $\Pi$, and a nonlinear coupling, $T$, controlling the flow among degrees of freedom. Dimensional analysis may be used to determine the scaling of $\Pi$ corresponding to constant flux. In Ref. [12], we showed how to make this dimensional argument exact. In this paper we will restrict ourselves to aggregation problems where the conserved quantity is mass, or potentially a power of mass, containing ourselves with a dimensional derivation.

Using the methods of Refs. [11, 21], the mass density in the MM is controlled by an equation with the following structure:

$$\partial_t \langle m P(m, t) \rangle = \int T_{m_1, m_2} \Pi_{m_1, m_2} dm_1 dm_2 + \ldots$$

where $T_{m_1, m_2}$ is the aggregation kernel and $\Pi_{m_1, m_2}$ is the flux-carrying correlation function of interest here. In Refs. [11, 12] we showed that $\Pi_{m_1, m_2}$ takes the form $\Pi_{m_1, m_2} = m P(m_1, m_2) \delta(m - m_1 - m_2)$ where the quantity $P(m_1, m_2)$ should be interpreted physically as the probability of finding particles of masses $m_1$ and $m_2$ on adjacent lattice sites. Of course, when written out properly, Eq. (8) is much more complex, with the “…” representing additional integrals of the form shown (but with permuted arguments), a diffusion term, a source term and a noise term. The diffusion term is neglected since it is zero on average for a statistically homogeneous system. Likewise the noise, having mean zero, is neglected on average. The source term is zero for large masses. We can then take Eq. (8) to define the flux of mass, $J(m, t)$, in mass space:

$$\partial_m J(m, t) \equiv \int T_{m_1, m_2} \Pi_{m_1, m_2} dm_1 dm_2.$$  (9)

Given that the aggregation kernel is homogeneous of degree, $\beta$, and assuming that the flux-carrying correlation function is homogeneous of degree $h$, it follows that the flux itself scales as $J \sim m^{\beta + h + 3}$. The essential observation is that a stationary state of Eq. (8) corresponds, from Eq. (4), to a constant flux of mass, i.e. $J(m)$ independent of $m$. This immediately gives the CFR scaling for the flux-carrying correlation function, $\Pi_{m_1, m_2}$:

$$h = -\beta - 3.$$ (10)

Hence, in the stationary state, we expect that, for large masses, $m P(m_1, m_2) \delta(m - m_1 - m_2) \sim m^{-\beta - 3}$ or,

$$P(m_1, m_2) \sim m^{-\beta - 3}.$$ (11)

Suppose, instead of mass, the conserved quantity was a power of the mass, $m^\gamma$. Formally, this argument would lead us to expect that, in the stationary state, $m^\gamma P(m_1, m_2) \delta(m - m_1 - m_2) \sim m^{-\beta - 3}$. This would give

$$P(m_1, m_2) \sim m^{-\gamma - \beta - 2},$$ (12)

which will be relevant to the subsequent discussion.

In the MM, and the other cases considered in Ref. [12], the conserved quantity was obvious. In the in-out model and the chipping model, it is not clear what is conserved, and whether there is a cascade in some quantity. In both cases, if we look in the mass space, then there is loss of mass at all mass scales either through desorption or through chipping. In addition, the flux in the chipping model is created from within through the fragmentation process. To apply Eq. (11) or Eq. (12) to the two models being considered, we do the following. Identify $I$ by using the known behaviour of $P(m, t)$. Let $P(m, t)$ have the scaling form

$$P(m, t) = \frac{1}{m^\tau} F \left( \frac{m}{t^{1/3}} \right)$$ (13)

where the scaling function $F(x)$ goes to a constant for small $x$ and to zero for large $x$. We identify $I$ to be $I = m^\gamma$, where $\gamma$ is fixed by the condition that $\langle I \rangle \sim t$. Thus,

$$\gamma = \frac{1}{\delta} + \tau - 1.$$ (14)
For both the models considered $\beta = 0$. In one dimension, for the in-out model $\gamma = 5/2$ at $q = q_c(p)$ and $\gamma = 1$ for $q \gg q_c(p)$. For the chipping model in one dimension $\gamma = 9/2$ at $\rho = \rho_c(w)$. Thus,

$$P(m_1, m_2) \sim (m_1 m_2)^{-9/4}, q = q_c(p), \text{in-out, } d = \mathbf{15}$$
$$P(m_1, m_2) \sim (m_1 m_2)^{3}, q \gg q_c(p), \text{in-out, } d = \mathbf{16}$$
$$P(m_1, m_2) \sim (m_1 m_2)^{-13/4}, \rho = \rho_c, \text{chipping, } d = \mathbf{17}$$

IV. MONTE CARLO SIMULATIONS

In this section, we present simulation results for the in-out and chipping models and compare the results with the predictions in Eqs. (15) and (17). We first present results for the in-out model. CFR predicts that the joint distribution function $P(m_i, m_{i+1}) \sim (m_i m_{i+1})^{-9/4}$. In simulations what we will measure is the quantity

$$\pi(m) = \int_{-\infty}^{\infty} dm' P(m, m'). \quad (18)$$

CFR then predicts that

$$\pi(m) \sim m^{-7/2}, q = q_c(p) \quad \text{in-out model, } d = 1, (19)$$
$$\pi(m) \sim m^{-2}, q \gg q_c(p) \quad \text{in-out model, } d = 1. \quad (20)$$

We did Monte Carlo simulations on a one dimensional lattice of size $L = 4096$. The desorption rate $\rho$ is fixed to be one. For $p = 1$, $q_c \approx 0.3072$. In Fig. 1, we show the variation of $\pi(m)$ with $m$ for $q = 0.3072$. As can be seen, the exponent $-3.5$ is a good fit, thus consistent with CFR. Also shown in Fig. 1 is $\Pi(m)$ for $q = 1.0$. For this value of $q$, the system is in the growing phase, and CFR predicts that $\Pi(m) \sim m^{-2}$. Again, this is borne out by simulations (see top curve of Fig. 1).

For the chipping model, CFR predicts that at $\rho = \rho_c(w)$,

$$\pi(m) \sim m^{-11/2}, \quad \text{chipping model, } d = 1 \quad (21)$$

Monte Carlo simulations were done for lattices of size 4096 and 8192. The chipping rate $w = 24.0$. $\rho$ was chosen to be $\rho = \rho_c = 4.0$. The results are shown in Fig. 2. The data is consistent with the CFR predictions.

V. SUMMARY AND CONCLUSIONS

In this paper, we examined the consequences of a constant flux on two models where there were no obvious conserved quantities and the dissipation and driving scales were not widely separated. The two models considered were examples of systems undergoing nonequilibrium phase transitions. CFR holds in the phases where the probability distributions are power laws. The CFR prediction was borne out by numerical simulations. However, an analytic approach is lacking. For this purpose,

one possibly needs to work with the effective field theories for these models.

For the chipping model, the fact that the two point correlations have a different exponents from the mean field answer clearly shows that the super-universality of $P(m)$ is a coincidence. It is an open problem as to why this exponent does not change with dimension.

![Figure 1](image1.png)  
**FIG. 1:** The variation of $\pi(m)$ with $m$ is shown for different $q$’s in the in-out model. The lower straight line has an exponent $-3.5$ and corresponds to $q = q_c(p)$. The upper straight line has an exponent $-2.0$ and corresponds to the growing phase $q \gg q_c(p)$.

![Figure 2](image2.png)  
**FIG. 2:** The variation of $\pi(m)$ with $m$ is shown for two different lattice sizes in the chipping model. $\rho = \rho_c$. The straight line has an exponent $-5.5$. 

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