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# ON A TRANSFORMATION PROPERTY OF THE SMOLUCHOWSKI AGGREGATION EQUATION

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Using a specific time-reversal transformation, the Smoluchowski equation for aggregation processes is proved to be formally equivalent to the equation obeyed by the partition function of random cascading models of multiparticle production processes with intermittent fluctuations. This result gives an unexpected connection between intermittent patterns of fluctuations, spin-glass systems and the dynamics of aggregation and gelling, first described for brownian motion by Smoluchowski already 75 years ago.

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## 1. Introduction: from random cascading and spin-glasses to aggregates

Random cascading models were proposed as a prototype of models exhibiting intermittent-like fluctuations of multiplicity in multi-particle production [1]. However, their connection with other fields of Physics was soon recognized. Inspired at the beginning by a mathematical description of fully-developed turbulence in fluids [2], they can be related [3] to popular models of spin-glass systems [4]. It is thus natural to ask the question whether this nontrivial connection can be extended further to other dynamical processes. In the present paper, one will demonstrate that this is indeed the case for coagulation, aggregation and gelling as described by the well-known Smoluchowski equation. The hope is that establishing such a link will allow a

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more basic understanding of intermittent phenomena in Particle Physics. In fact, one will show that it provides a quite general approach to solutions of the Smoluchowski equation.

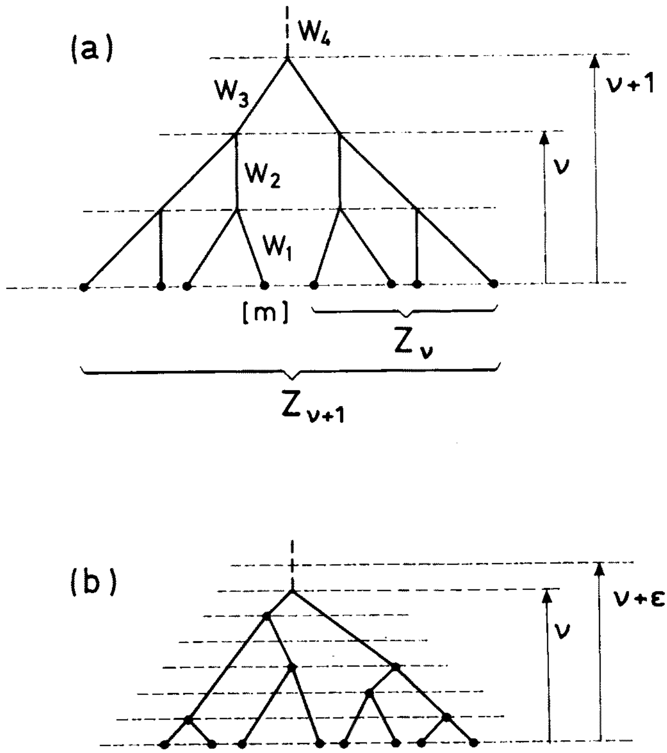


Fig. 1. Tree diagrams of random cascading models. (a) Fixed branching. Each path $[m]$ in the tree is in a one-to-one correspondence with a bin in phase space. The fluctuations density in the bin is described by the product of random weights $W_1\, W_2\, W_3\, W_4$ along the path $[m]$. The tree can be separated into 2 branches. Each of these branches defines a random value $Z_\nu$ of the partition function, the tree itself corresponding to $Z_{\nu+1}$. (By convenience, one here chooses to count the generation number "$\nu$" starting from the smallest bins considered). (b) Random branching. Same structure as in (a), but with small increase $\varepsilon$ of the total number of steps $\nu$ and random branching with probability also equal to $\varepsilon$.

Random cascading models of simplest type are described in Fig. 1. A set of fluctuating densities $\{\rho_m\}$, — where $m$ denotes the phase-space element where the density is observed — is generated by a product of random weights $W_S$.

One writes

$$\rho_m = \prod_{[m]} W_s\,, \tag{1}$$

where the $W_s$ are independent realizations of a random function $W$ obeying to a probability distribution $r(W)$, and distributed along the links of a tree structure, see Fig. 1(a). A given phase-space bin $m$ corresponds to a well-defined path $[m]$ on the tree, with $s = [1, \ldots, \nu]$ denoting the $\nu$ successive links of the path, or "number of generations". From definition (1) and the mutual independence of the $W_s$, one finds by averaging the following property:

$$\frac{\langle \rho_m^q \rangle}{\langle \rho_m \rangle^q} = [\lambda^\nu]^{\ln(\{W^q\}/\{W\}^q)/\ln\lambda}\,, \tag{2}$$

where $\lambda$ is the branching number ($\lambda = 2$ for the simplest example of Fig. 1) and where

$$\{W^q\} = \int_0^\infty r(W)\, W^q\, dW\,, \tag{3}$$

is the $q^{\text{th}}$ moment of the *local* probability distribution $r(W)$.

Formula (2) can be interpreted as an intermittency property, since the moments of fluctuations have a power-law dependence on the total number of bins $\lambda^\nu$, *i.e.* on the resolution with which one looks for these fluctuations.

The random cascading models, as schematized in Fig. 1(a), can easily be generalized [5] to random cascading — random branching models as described in Fig. 1 (b). In this case, one goes to the case of a large number of cascading steps. At each step, one considers a small probability to get a branching described as previously by a random density factor $W_s$ and unchanged at this step. By choosing a constant probability per cascading step, one obtains [5] an interesting class of continuous differential equations. This limit will be discussed in the next sections in comparison with the Smoluchowski equation. The properties of the random cascading — random branching models appear to be very similar to those with fixed branching, as was shown in details in [5] in connection with models of spin-glass systems.

The connection of random cascading with spin-glasses is best exhibited by studying the "Partition function" $Z(q)$, which is a function defined on the set of fluctuations. As an example with the fixed branching case, one defines:

$$Z(q) = \sum_m \rho_m^q \equiv \sum_{\text{all}\,[m]} \prod_s W_s^q\,, \tag{4}$$

where $Z(q)$, depending on the number of generations (see Fig. 1 (a)), has its own random distribution $\mathcal{P}_\nu(z)$. In the case of spin-glass systems [4,5],

$Z$ can actually be identified as a genuine partition function and $q$ as the inverse temperature. Using techniques developed for spin-glasses, it is possible to compute exactly $\mathcal{P}_\nu(Z)$ or, on a more compact form, the generating functional of moments of $Z$, namely $H_\nu(u) = \langle \exp(-uZ) \rangle_\nu$, where the average is defined over different realizations of $Z$, that is over the distribution $\mathcal{P}_\nu(Z)$. One finds [3] the following recurrence formula, for fixed branching:

$$H_{\nu+1}(u) = \left\{ H_\nu\left(\frac{uW}{\lambda}\right) \right\}_r^\lambda , \tag{5}$$

where the averaging $\{\ \}_r$ refers to the *local* densities $W_S$, as in formula (3). Indeed, formula (5) can easily be generalized to the case of random branching processes [5], where is introduced a constant branching probability $\varepsilon$. One gets, in the case of random cascading-random branching models

$$H_{\nu+\epsilon}(u) = \varepsilon \left( \int r(W)\, dW\, H_\nu\left(\frac{uW}{\lambda}\right) \right)^\lambda + (1-\varepsilon) H_\nu(u)$$

or by going to the $\varepsilon \to 0$ limit:

$$\frac{dH_\nu(u)}{d\nu} = \left( \int r(W)\, dW\, H_\nu\left(\frac{uW}{\lambda}\right) \right)^\lambda - H_\nu(u) . \tag{6}$$

Note that, further generalizations of Eqs (5) and (6), can be introduced in different ways. One can consider generation-number dependent probability distributions $r(W,\nu)$ which give interesting phase structures in spin-glass models [4]. It is also possible to consider models [4] where, at each step, one is led to introduce correlations between the $\lambda$ different random factors $W_S$ of the same branching. The different models have essentially the same qualitative properties, the detailed structure being different but studied with the same tools. As an example of simple generation-dependent case, let us introduce a probability $1 - p(\nu)$ of generating a hole ($W = 0$) in the random density distribution for a fixed branching process. One gets the recurrence formula (5), with a modified probability distribution $r(W,\nu) = (1 - p(\nu))\delta(W) + p(\nu) r(W)$.

Formulae (5) and (6) play a central role in the following study of the Smoluchowski equation. Indeed, they nicely exhibit two main features of random cascading models, randomness and the tree geometry, through, respectively, the convolution formula and the non-linear feature of the equations. These two characteristics which are also present in the Smoluchowski equation (see next Section) leads one to the idea that a deep link may exist between both — a priori very different — approaches.

As another remark, it is known from spin-glass models that a phase transition may exist whose features can be studied [4,6] from the moments of the partition function. This phase transition is specific of spin-glass systems and the low temperature phase possesses [4,5] a hierarchical structure in domains, which is very different from the usual order/disorder transition. Properly writing, in random cascading models the temperature itself is not fixed [6] and therefore different phases may coexist [7]. Compared to this situation, the hierarchical structure and the dynamical features of aggregation phenomena are similar and are suggesting a comparison with random cascading. However it is clear that some-time reversal transformation has to be invoked, since aggregation and cascading follow an opposite geometrical evolution. This is the purpose of this paper to explain this time reversal transformation.

In Section 2, one shall present the Smoluchowski equation [8] for aggregation processes and show how a specific time-reversal transform leads to an equivalent formula. In Section 3, one shows, taking the generic example of "multiplicative weights" that the Smoluchowski equation is exactly equivalent to formula (6) for random cascading-random branching processes with $\lambda = 2$. Generalization to other classes are briefly outlined. In the final Section 4, possible applications of the proposed transformation are envisaged, both for aggregation problems and for current questions about random cascading and its application to Particle Physics.

## 2. The Smoluchowski equation and its time-reversal transformation

The Smoluchowski equation [8] describes in a simple way the time evolution of an aggregation process. At a given time $t$, the variation of the number $N(n,t)$ of aggregates of "mass" $n$ is the algebraic sum of two contributions: one positive, is the aggregation of two clusters whose total mass is $n$ and one, negative, is the aggregation of $n$-clusters to other ones (see Fig. 2). In the case of a continuous process in time, one writes

$$\frac{dN(n,t)}{dt} = \tfrac{1}{2} \sum_{i+j=n} N(i,t)N(j,t)K_{ij} - N(n,t) \sum_{i\geq j} N(i,t)K_{in}, \qquad (7)$$

where the aggregation coefficients $K_{ij}$ define the dynamics of the process. In some popular cases [9,10], they can be chosen *multiplicative* ($K_{ij} = K_i K_j$) or *additive* ($K_{ij} = K_i + K_j$), but can be more complicated in specific problems [9]. One could also consider a discrete time equation. The system of equation (7) can be conveniently expressed in terms of a compact equation for a formal Laplace transform [10]

$$G(u,t) = \sum_{n\geq 1} N(n,t)u^n , \tag{8}$$

from which the weights can be obtained by differentiation at $u = 0$.

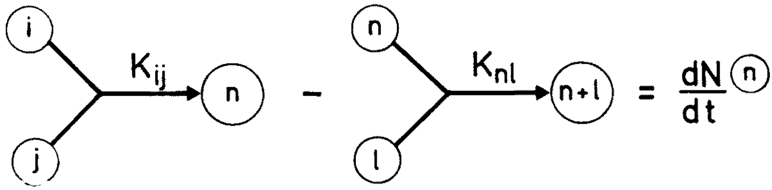


Fig. 2. Aggregation diagram of Smoluchowski equation. The clusters of mass $n$ is sketched by a symbolic equation. The clusters are represented by circles. The aggregation coefficients $K_{ij}$ are shown on the figure (where summation over $i, j$ $(i + j = n)$, and $\ell$ is left implicit) by links.

Inserting (8) into equation (7), one easily gets the following equations:

$$\frac{dG}{dt} = \tfrac{1}{2} G * G - G * G_1 , \tag{9}$$

where, omitting for convenience the arguments of the functions, the convolution operation $*$ is defined by:

$$G * G' = \sum_{i,j\geq 1} N(i,t)N(j,t)(u)^i(u')^j K_{ij} . \tag{10}$$

In formula (9), $G_1$ stands for $G(u = 1, t)$ and is nothing else than the total number of clusters at given time $t$ (see definition (8)). Note that in the multiplicative case, the convolution factorizes and one gets instead of (9)

$$\frac{dG}{dt} = \tfrac{1}{2}\widetilde{G}^2 - \widetilde{G}\widetilde{G}_1 , \tag{11}$$

with

$$\widetilde{G} = \sum_{i\geq 1} N(i,t)K_i u^i , \quad \widetilde{G}_1 = \sum_{i\geq 1} N(i,t)K_i . \tag{12}$$

Our treatment of the Smoluchowski equations begins by deriving the equations for the *normalized* Laplace transform defined as follows

$$\frac{G}{G_1} \equiv \frac{\sum N(n,t)u^n}{\sum N(n,t)} . \tag{13}$$

Using equation (9), once for $G$ and once for $G_1$, one gets

$$\frac{d(G/G_1)}{dt} = \frac{1}{G_1}\frac{dG}{dt} - \frac{G}{G_1^2}\frac{dG_1}{dt} = \frac{1}{2G_1}\{G * G - 2G * G_1 + (G_1 * G_1)(G/G_1)\}\,. \tag{14}$$

Now, we will introduce a time reversal transformation which allows one to simplify expression (14). Let one introduce a variable $\nu$, which plays the role of a continuous "generation number", by the following:

$$\frac{d(G/G_1)}{d\nu} = \frac{dt}{d\nu}\frac{d(G/G_1)}{dt} \equiv \frac{1}{\varepsilon}(G/G_1|_{\nu+\varepsilon} - G/G_1|_{\nu})\,. \tag{15}$$

It becomes clear from equation (14), and also from the consideration of the above mentioned discrete time version of the equations (*e.g.* $\varepsilon = 1$), that the suitable choice of the transformation is given by

$$\frac{d\nu}{dt} \equiv -\frac{G_1 * G_1}{2G_1} = \frac{dG_1}{G_1 dt}\,, \tag{16}$$

where the last equality comes again from Smoluchowski equation for $G_1$.

It is important to note that the same reasoning can be applied to a modified version of the Smoluchowski equation, where one considers the aggregation process by discrete-time steps. In this case, one is led to replace in equations (5), (16), time derivatives by finite differences, and to replace the infinitesimal increment $\varepsilon$ by 1. In this *discrete-time* case, one obtains recurrence relations instead of differential equations. This is the same discussion as the one leading to the different equations (5) and (6) corresponding, respectively, to fixed-branching and random-branching cascading models.

Using relations (15) and (16) in the transformation of Eq. (14), one finds the following equation

$$\frac{d}{d\nu}\left(\frac{G_1 - G}{G_1}\right) = \frac{(G_1 - G) * (G_1 - G)}{G_1 * G_1} - \left(\frac{G_1 - G}{G_1}\right)\,. \tag{17}$$

It is to be noticed that the transformation of Eq. (14) into (17) has been only made possible by the change of variable (19), including the change of sign ( $\frac{G_1}{G_1 * G_1}$ is a function of time always positive, *i.e.* $\ln G_1$ is monotonously decreasing). One is thus able to relate an aggregation process (when the variable $t$ increases) to a "time-reversed" cascading (when the number of generations $\nu$ decreases). Equivalently, one could consider the recurrence formula (17) in the normal way for cascading processes ($\nu$ increasing) as a "time-reversed" aggregation mechanism. Note [11] that aggregation is not a reversible mechanism since its "time-reversal" is not identifiable to a physical "desaggregation" mechanism. Note also that the solution of the equations depends on the boundary conditions for some values $(\nu_0, t_0)$ compatible with the change of variable (16). This can be fulfilled by integration of equation (16). One gets the very simple relation

$$\nu - \nu_0 = \ln G_1 - \ln \gamma_1 , \tag{18}$$

where $G_1$ is the total number of clusters, assuming that the condition $\nu = \nu_0$ corresponds to some cluster number $G_1 = \gamma_1$.

The relation (18) shows how the number of generations comes directly from the evolution of the total number of clusters during aggregation. This number often has nice scaling properties [9,10], which will be translated into a function $\nu(t)$ by relation (18).

It is remarkable that the equation (17) can provide a constructive way of solving the general Smoluchowski equation, knowing the coefficients $K_{ij}$. Indeed starting with initial conditions, $G(t, \nu)$ near the initial value $t_0$, one could get the right hand side of equation (17), and the local correspondence between $t$ and $\nu$, through equation (16). By small steps $\nu \to \nu + \varepsilon$ one can numerically integrate the equation (17). However, as will become clear in the next Section, it is possible to get more direct analytic relations. We will show the result explicitly for the multiplicative case (*cf.* (11), (12)), but it can be extended to the other cases.

## 3. From aggregation to random cascading and spin-glasses

Let one consider now the multiplicative case (11) of the equation with the notations defined by (12). The recurrence formula (17) takes the simple form:

$$1 - G/G_1|_{\nu+1} = (1 - \widetilde{G}/\widetilde{G}_1)^2|_\nu . \tag{19}$$

for the discrete-time equation and

$$\begin{aligned} \frac{d}{d\nu}\langle 1 - u^i \rangle_\nu &\equiv \frac{d}{d\nu}\left(\frac{\sum N_i(1-u^i)}{\sum N_i}\right) \\ &= \left(\frac{\sum K_i N_i (1-u^i)}{\sum K_i N_i}\right)^2_\nu - \langle 1 - u^i \rangle_\nu , \end{aligned} \tag{20}$$

for the Smoluchowski equation (17), where we introduced the notation $\langle\ \rangle_\nu$ for the average over the weights $N_i$ at a time corresponding to the generation number $\nu$, see Eq. (18). Let also introduce the inverse Laplace transform of the aggregation coefficients under the following form

$$K_i = C \int_0^\infty r(W)\, dW \left(\frac{W}{2}\right)^i , \tag{21}$$

where $r(W)$ is a normalized, positive, distribution and $C$ is left arbitrary but constant. Formula (20) becomes

$$\frac{d}{d\nu}\left\langle 1-u^i\right\rangle_\nu = \left\{1-p_\nu + p_\nu\langle\widetilde{1-u^i}\rangle_\nu\right\}^2 - \langle 1-u^i\rangle_\nu\,, \tag{22}$$

where the numbers $p_\nu$ are also related to the number of clusters $G_1$ by the following relations

$$p_\nu^{-1} \equiv \frac{\sum K_i N_i}{C\sum N_i} = \frac{\widetilde{G}_1}{CG_1} = \frac{1}{C}\sqrt{\frac{d(2/G_1)}{dt}}\,. \tag{23}$$

One can express $\langle\widetilde{1-u^i}\rangle$ and $\widetilde{G}_1$ by convolution formulae using relation (21). One gets

$$\langle\widetilde{1-u^i}\rangle_\nu = \int_0^\infty r(W)\,dW\langle 1-\left(\frac{uW}{2}\right)^i\rangle\,,$$

$$\widetilde{G}_1 = C\int_0^\infty r(W)\,dW\,G\left(u=\frac{W}{2},t\right)\,. \tag{24}$$

Equation (22), with given initial conditions and evolution of the total member of clusters, gives an equivalent form of the Smoluchowski equation in the multiplicative case. Note that the correspondence has to be completed by the knowledge of the dependence $G_1(t)$ of the total number of clusters, which fixes the law $\nu(t)$ and the normalization of the generating function $G(\nu,t)$.

As is obvious by comparison of equation (22) with the expression (6), they are formally identical. This is explicit for the case $p_\nu\equiv 1$, and by the extension to generation dependent processes (see the end of Sect. 2) the identity is true in all cases. More precisely by choosing a modified random distribution of weights, namely

$$r(W,\nu)\equiv(1-p_\nu)\delta(W)+p_\nu r(W)\,. \tag{25}$$

One proves the equivalence of the form (22) of the Smoluchowski's equation with the one for the partion function of a random cascading random branching model with branching number $\lambda=2$. Note that one could also identify the recurrence equation for a discrete-time Smoluchowski's equation with the equation (5) obtained for random cascading models with fixed branching. As mentioned previously these equivalences can very probably be extended between the general Smoluchowski equation with non-multiplicative weights, *e.g.* random cascading-random branching models with correlated weights at each node.

## 4. Conclusion: an equivalence property

The result of the present study can be briefly summarized as follows.

Equivalence property

*The solutions of the Smoluchowski equation for the kinetics of aggregation are formally identical to those for the partition function distribution of random cascading models.*

The potential consequences of this fact are quite interesting when considering some questions remaining unsolved in both field of research.

*(i)* in models of aggregation, it seems [10] that the investigation of new exact solutions can be helpful. On the other hand, exact solutions have been discussed in the framework of random cascading models [3]. More generally, random cascading models have the same structure as models of spin-glasses [4] and polymers in random potentials [5] whose extensive study is the past years opens the way to applications to aggregation kinetics *via* the equivalence property.

*(ii)* in studies of random energy models, one important question concerns the structure of the "event space" or more precisely the knowledge of the distribution $\mathcal{P}(Z)$. Indeed, a whole hierarchical structure appears in the cases where this distribution is known [4]. This structure is to be related to the one revealed for spin-glass systems where the "event space" is replaced by the "replica-space" [12]. Yet, the interpretation of this structure in random cascading processes is not clear, due to the absence of conditions analogous to a fixed temperature. The random cascading systems appear more similar to complex multifractal systems than to thermodynamical ones [6]. It is thus interesting that a kinetic equation for an irreversible process such as the Smoluchowski equation can be introduced for random cascading models.

*(iii)* in aggregation processes, there exists an interesting phase structure related to the differentphysical regimes:"flocculation" or "gelling",with different scaling behaviour [9]. Flocculation is an aggregation process where the number of aggregates remains large throughout the coagulation process. On the contrary, gelling is characterized first by the formation of an "infinite cluster", that is where a finite fraction of the total mass forms one cluster, and finally ending by a unique cluster of all aggregates. It is intriguing that such involved phase transitions could be in a correspondence with phase transitions which are discussed in Particle Physics, such the confinement transition of quarks and gluons into hadrons, or the mass generating or so-called chiral phase transition.

As a final remainder, one may note again the interesting generalizations which are suggested on both sides — aggregation and random cascading — by the calculation of Sections 2 and 3. Indeed, the convolution formula (10), means that random cascading models, and their main results, can be extended to non-multiplicative cases [4]. On the other hand, the existence of random cascading solutions with an arbitrary branching number $\lambda$, can enlarge the range of aggregation to a modified type of clustering. Finally, time (or generation) dependent aggregation coefficients could be introduced, in much the same way as can be done for random cascading (or spin-glass) models [4].

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