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Exact Solution of Random Graphs for Cluster Fragmentation

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Abstract. We present the exact solution of a combinatorial fragmentation model and we show how it can be used as a touchstone for the fragmentation of atomic clusters. This model, random graphs (RG), also called mean field percolation, displays a phase transition. In this model, the clusters are solely described as connected entities called nodes. The connections, called bonds, can be active or broken. We have established the algebraic formulas of the probability of all the fragmentation channels. The results depend on the number of nodes and of the number of broken bonds. Using RG, we show an example where information was deduced from fragmentation of systems consisting of finite sets of nodes.

1. Introduction

Random Graphs (RG) were originally introduced in 1959-1960 by Erdős and Rényi [1, 2]. The RG are the most general mathematical models for compound systems of sets of objects in interaction. These models consist only of nodes connected by bonds. At first, this model was used to prove deterministic properties of graphs. Later, interest in random graphs of a different nature arose. Due to the increase of computer power, it has become possible to study real-life networks. Recent applications of RG model are shown in the field of problems of network robustness and of epidemics spreading on contact networks. Typical examples are the termite nest chambers [3], electricity networks or the distribution of diseases [4]. For the physical systems, the nodes represent nucleons, atoms and molecules. The physical information was deduced, using RG, for nuclear spinodal decomposition [5, 6], nuclear fragmentation [7, 8], cluster fragmentation [9, 10] and for the fragmentation of the carbon nucleus into three alpha particles, which could sign the Hoyle state [11].

In this paper, the RG are used as a rigorous formalism allowing to describe and to interpret the fragmentation of clusters. Furthermore, it allows to distinguish the physical correlations, providing information about the system, from the trivial correlations, due to the combinatorial constraints or to conservation laws.

2. Algebraic Formulas of Random Graphs

We consider a homogeneous cluster of S undistinguishable nodes. Each bond between a pair of nodes is associated to the same energy. We consider that the breaking of a bond requires a unit



excitation energy. A cluster is said to be in its ground state when every node pairs is connected by a bond, hence, the ground state energy of S -node clusters is:

$$E_g(S) = -\frac{S(S-1)}{2} \tag{1}$$

A cluster is in an excited state if the number of broken bonds is not enough to break it. In excited states, all nodes are still connected directly or indirectly via the other nodes. When enough bonds are broken, the cluster separates into a set of fragments called a partition. In the example shown in Fig. 1, the parent cluster has 7 nodes (dots) and 21 bonds (lines). After the breaking of 15 bonds (dashed and dotted lines), the parent cluster decays into a partition with 2 fragments (black dots and open dots).

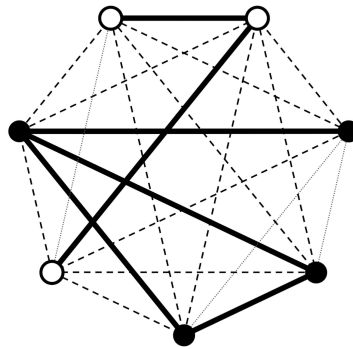


Figure 1. Example of RG fragmentation. The dots represent the nodes and the full lines represent the unbroken bonds. The excitation energy ($E^* = 15$) is shared between the binding energy of the partition ($E_b = 12$, dashed lines) and the individual excitation energies of the fragments ($E_1^* = 2$, for the black dot fragment and $E_1^* = 1$ for the open dot fragment).

A fragment partition [5] will be represented as a vector $\mathbf{n} = (n_1, \dots, n_s, \dots, n_S)$, whose component n_s indicates the number of fragments with size s . The sum of components $M = \sum_s n_s$, is called the multiplicity and the mass (size of the system) conservation reads $\sum_s s n_s = S$. The binding energy $E_b(\mathbf{n})$ of a given partition is the minimal energy to create it. In this model, it is the difference between the number of bonds of the parent cluster and of the sub-clusters in their ground states. Using eq.(1), we can show that it can be also written:

$$E_b(\mathbf{n}) = \frac{1}{2}(S^2 - \sum_{s=1}^S s^2 n_s) \tag{2}$$

When the initial excitation energy E^* (number of broken bonds) injected into the parent cluster is larger than the binding energy of a given partition \mathbf{n} , the remaining energy is distributed among the fragments as individual excitation energy

$$E^* = E_b(\mathbf{n}) + \sum_{i=1}^M E_i^* \tag{3}$$

where E_i^* is the excitation energy of fragment i . For a given initial excitation energy E^* , the microcanonical weight of a fragmentation partition depends on two factors which respectively

represent the number of ways to arrange the nodes among the fragments and on the number of ways to distribute the excitation energy among the fragments.

The first factor is the combinatorial factor representing the number of ways to allocate S nodes to the fragments. There are $S!$ number of ordering of all the nodes. However, the permutation of nodes inside a fragment does not change the partition nor does the permutation of equal size fragments. Thus this factor can be written as:

$$w_{\text{comb}}(\mathbf{n}) = \frac{S!}{\prod_{s=1}^S s!^{n_s} n_s!} \quad (4)$$

The second factor is related to the number of the ways to distribute the remaining energy among the fragments of the partition. There are different ways to sort the excitation energy among the fragments. A distribution of the total excitation energy is characterized by a vector \mathbf{E} with M dimensions which components are the E_i^* with the constraints:

$$E_i^* \in [0, (s_i - 1) \times (s_i - 2)/2] \quad \text{and} \quad \sum_i E_i^* = E^* - E_b(\mathbf{n})$$

Moreover, for a given fragment i , the density of states $\rho(s_i, E_i^*)$ is equal to the number of ways to choose E_i^* broken bonds among $s_i \times (s_i - 2)/2$ bonds without breaking the fragment. Hence, the product of the fragments level densities has to be taken into account in the evaluation of the partition weight. Finally, the partition weight corresponding to the given E^* can be expressed as:

$$w(\mathbf{n}, E^*) = w_{\text{comb}}(\mathbf{n}) \sum_{\mathbf{E}} \prod_{i=1}^M \rho(s_i, E_i^*) \quad (5)$$

All the observables and the thermodynamic features of the model can be derived from this equation. Especially, equation (5) allows to determine the partition probabilities as a function of the initial excitation energy. It is calculated by:

$$P(\mathbf{n}|E^*) = \frac{w(\mathbf{n}, E^*)}{\sum_{\mathbf{n}} w(\mathbf{n}, E^*)} \quad (6)$$

where the sum is over all possible partitions. The density of states $\rho(S, E^*) = w((0, \dots, 0, 1), E^*)$ can easily be computed noticing that it is the total number of ways to choose E^* broken bonds among $-E_g(S)$ bonds minus the sum of all the partition weights. Thus we have:

$$\rho(S, E^*) = \binom{-E_g}{E^*} - \sum_{\mathbf{n} \neq (0, \dots, 0, 1)} w_{\text{comb}}(\mathbf{n}) \sum_{\mathbf{E}} \prod_{i=1}^M \rho(s_i, E_i^*) \quad (7)$$

Here s_i and E_i^* are smaller than S and E^* thus the equation can be used to calculate recursively the densities of states.

Real life systems may also be composed of different types of "nodes" (for example protons and neutrons in the nucleus or atomic species in molecules). For T types, the combinatory factor of the heterogeneous RG model is given by [12]:

$$w_{\text{comb}}(\mathbf{N}) = \frac{\prod_{t=1}^T S_t!}{\left[\prod_{s=1}^{\max(S_1, \dots, S_T)} s!^{\sum_t n_{ts}} \right] \left[\prod_{s_1=0}^{S_1} \dots \prod_{s_T=0}^{S_T} N_{s_1 \dots s_T}! \right]} \quad (8)$$

where S_t the number of type t nodes, n_{ts} the number of fragments containing s nodes of type labeled t and $N_{s_1 \dots s_T}$ the number of fragments with s_1 nodes of type 1, ..., s_T nodes of type T .

3. Results

3.1. Diagram for fragmentation channel probabilities

We first present the results obtained from the exact equations of RG partition probabilities as a function of the excitation energy (number of broken bonds). Figures 2 and 3 show the diagram for fragmentation channel probabilities of C_5 ($S = 5$) and C_4H ($S_1 = 4$ and $S_2 = 1$) clusters, respectively. The fragmentation of the same atomic clusters has been studied experimentally by [13] and [14]. The highly excited C_5 and C_4H clusters may decay into seven and twelve fragmentation channels (partitions), respectively. These figures show the thresholds of appearance of the fragmentation channels as well as the dominant partition corresponding to a domain of excitation energy. The C_5 and C_4H clusters do not dissociate up to $E^* = 3$. We note that the partitions having the same number of fragments cover approximately the same range of excitation energy. For example, the two fragment channel: C_3/C_2 and C_4/C of C_5 cluster; C_4/H , C_3H/C , C_3/CH and C_2H/C_2 of C_4H cluster, appear in the range of excitation energy from 4 to 8. In the energy region from 7-9, only the fragmentation channels leading to three fragments play a significant role.

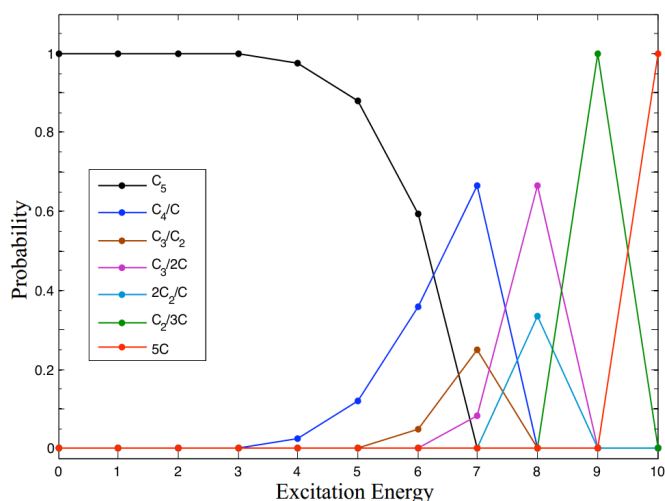


Figure 2. Partition probabilities as a function of the number of broken bonds for the fragmentation of C_5 from RG model.

3.2. Multiplicity probabilities as a function of the excitation energy

The objective of this section is to present the matrix $P(M|E^*)$ representing multiplicity probabilities as a function of the excitation energy E^* to show the correlation between M and E^* . The probability $P(M|E^*)$ is the sum of the equal multiplicity partition probabilities. These probabilities satisfy the following normalization:

$$\forall E^*, \quad \sum_{M=1}^S P(M|E^*) = 1 \quad (9)$$

For a fragmentation partition of the system with size S leading to M fragments, the total minimal number of bonds necessary to connect all the nodes in the fragments is $L_{\min} = S - M$ (each fragment is a linear chain). The maximal excitation energy to produce this fragmentation is thus:

$$E^* = -E_g - (S - M) \quad (10)$$

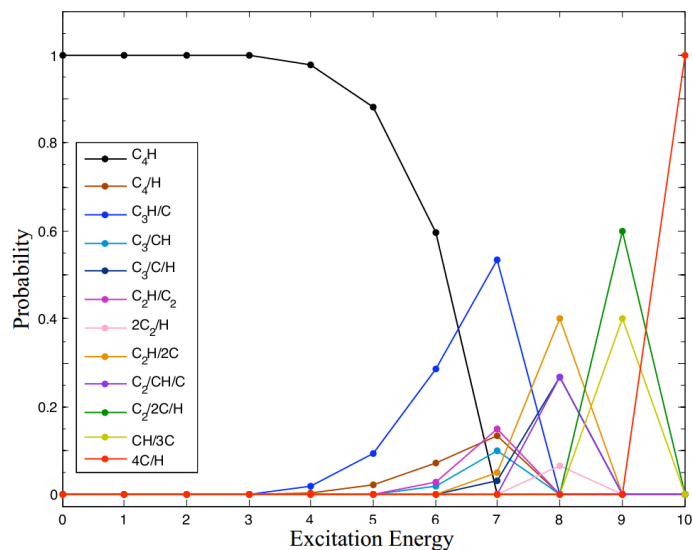


Figure 3. Partition probabilities as a function of the number of broken bonds for the fragmentation of C_4H from RG model.

Using equations (1) and (10), we deduce the relation between M and E^* for the RG model:

$$M = E^* - \frac{S(S-3)}{2} \quad (11)$$

Equation (11) shows that the correlation between M and the maximal excitation energy is linear with a threshold energy $E_{\text{threshold}}^* = S(S-3)/2$.

Figures 4 and 5 represent $P(M|E^*)$ for the system $S = 5$ which interests us and for a larger system $S = 15$ on which the effect is more visible. As can be seen, at high multiplicity, the dispersion according to the excitation energy is very small, the correlation thus becomes linear (see figure 5). The same behavior has been evidenced for atomic clusters by Chabot et al..

3.3. Convergence of a RG Monte Carlo simulation

We have studied the convergence of the Monte Carlo version of the RG model towards the exact algebraic solution. We illustrate here in the case of the system with the size $S = 7$ nodes in the ground state ($E_g = -21$) with the excitation energy $E^* = 15$. The probabilities of the 8 possible partitions are calculated for 3 values of the total number of Monte Carlo events. For each event, the Carlo Monte program breaks randomly 15 bonds among the 21 bonds. The corresponding partition counting rate is indented and the program starts again. The probability of a partition obtained by Monte Carlo simulation, is equal to its counting rate divided by the total number of events. In Fig. 6 are represented the results for 10^2 , 10^3 and 10^4 events. We see that when the total number of events increases, the probabilities obtained by the Monte Carlo simulation converge rapidly towards the probabilities calculated algebraically.

4. Conclusions

We have applied the Random Graphs model to describe the fragmentation of excited homogeneous and heterogeneous systems. We have also established the algebraic equations of the RG model and used that as a tool to evidence properties or correlations in physical systems submitted to fragmentation.

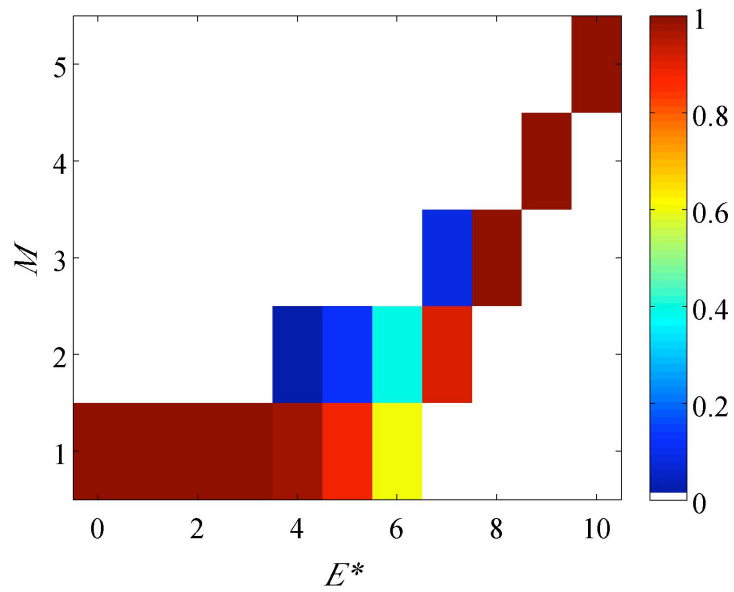


Figure 4. Fragmentation probabilities as a function of the multiplicity M and the excitation energy E^* of the system containing 5 nodes from RG model.

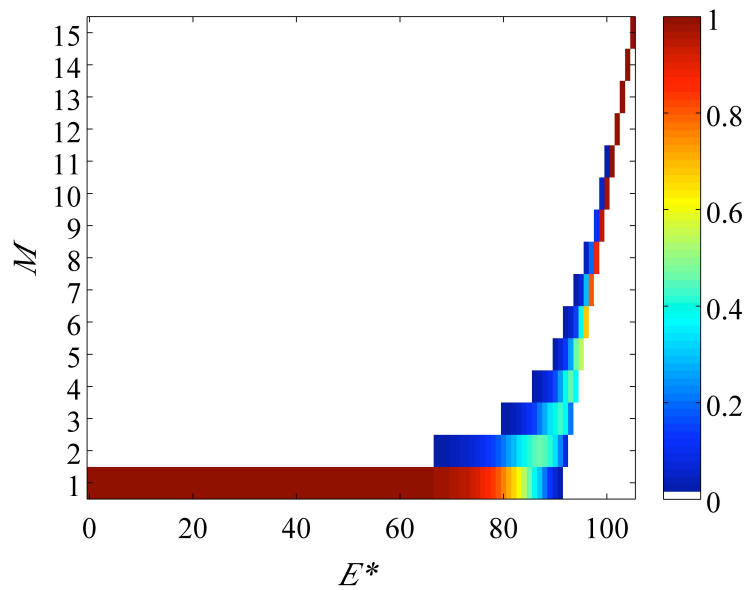


Figure 5. Fragmentation probabilities as a function of the multiplicity M and the excitation energy E^* of the system containing 15 nodes from RG model.

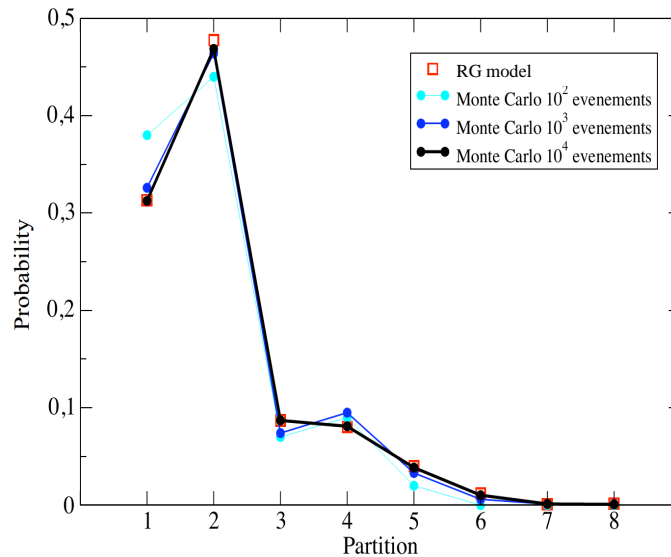


Figure 6. Probabilities of the 8 possible partitions obtained by Monte Carlo simulation and by the algebraic equations of RG model, for the system containing 7 nodes in the ground state with excitation energy $E^* = 15$ (as in Fig. 1).

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