Exact Solution of Random Graphs for Cluster Fragmentation 2 h 29 15/4 Abstract. We present the exact solution of a combinatorial fragmentation model and we show how it can be used as a touchstone for	Nghiệm chính xác của các đồ thị ngẫu nhiên dùng cho phân mảnh cụm Tóm tắt Chúng tôi trình bày nghiệm chính xác của mô hình phân mảnh tổ hợp và cách sử dụng nó như một chuẩn để phân mảnh

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 of 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 example where information was deduced from fragmentation of systems consisting of finite sets of nodes.

các cụm nguyên tử. Mô hình này có tên gọi là các đồ thị ngẫu nhiên (RG) hay còn gọi là thẩm thấu trường trung bình, cho thấy sự dịch pha. Trong mô hình này, các cụm chỉ được mô tả dưới dạng các thực thể kết nối nhau được gọi là các nút. Những kết nối này được gọi là các liên kết có đặc điểm là có thể bị bẽ gãy. Chúng tôi đã xây dựng các công thức đại số của xác suất của tất cả các kênh phân mảnh. Kết quả phụ thuộc vào số nút và số liên kết bị bẽ gãy. Dùng RG, chúng tôi trình bày ví dụ cho thấy thông tin có thể rút ra từ quá trình phân mảnh hệ thống bao gồm một tập hợp nút hữu hạn.

1. Introduction

Random Graphs (RG) were originally introduced in 1959-1960 by Erdos and Renyi [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, its allow 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:

(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).

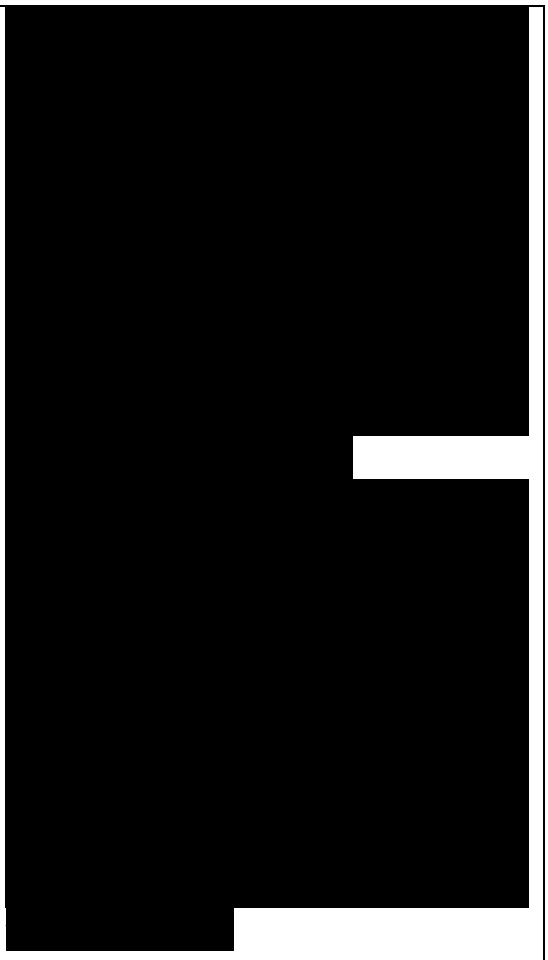


Figure 1. Example of RG fragmentation. The dots represent the nodes and the full lines represent the unbroken bonds. The excitation energy (E* = 15) is shared between the binding energy of the partition (Eb = 12, dashed lines) and the individual excitation energies of the fragments (E* = 2, for the black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

A fragment partition [5] will be represented as a vector n = (ni,..., ns,..., ns), whose component ns indicates the number of fragments with size s. The sum of components M = ^2s ns , is called the multiplicity and the mass (size of the system) conservation reads s sns = S. The binding energy Eb(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:

(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 n, the remaining energy is distributed among the fragments as individual excitation energy

(3)

where E* 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:

(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 E with M dimensions which components are the E* with the constraints:

Moreover, for a given fragment i, the density of states p(si, E*) is equal to the number of ways to choose E* broken bonds among si X (si — 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:

(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:

(6)

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

(7)

Here si and E* 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]:

(8)

where St the number of type t nodes, Uts the number of fragments containing s nodes of type labeled t and NS1...ST the number of fragments with s1 nodes of type 1 , ..., sT 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 C5 (S = 5) and C4H (Si = 4 and S2 = 1) clusters, respectively. The fragmentation of the same atomic clusters has been studied experimentally by [13] and [14]. The highly excited C5 and C4H 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 C5 and C4H 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: C3/C2 and C4/C of C5 cluster; C4/H, C3H/C, C3/CH and C2H/C2 of C4H 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.

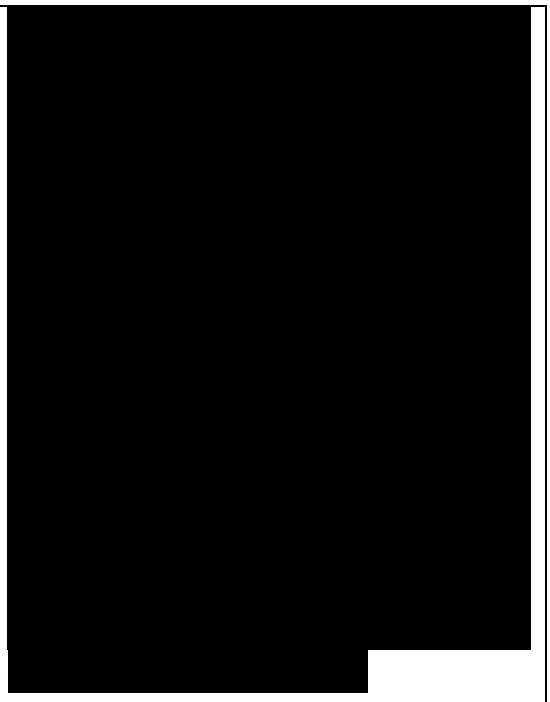


Figure 2. Partition probabilities as a function of the number of broken bonds for the fragmentation of C5 from RG model.

3.2. Multiplicity probabilities as a function of the excitation energy

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

(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 Lmin = S — M (each fragment is a linear chain).

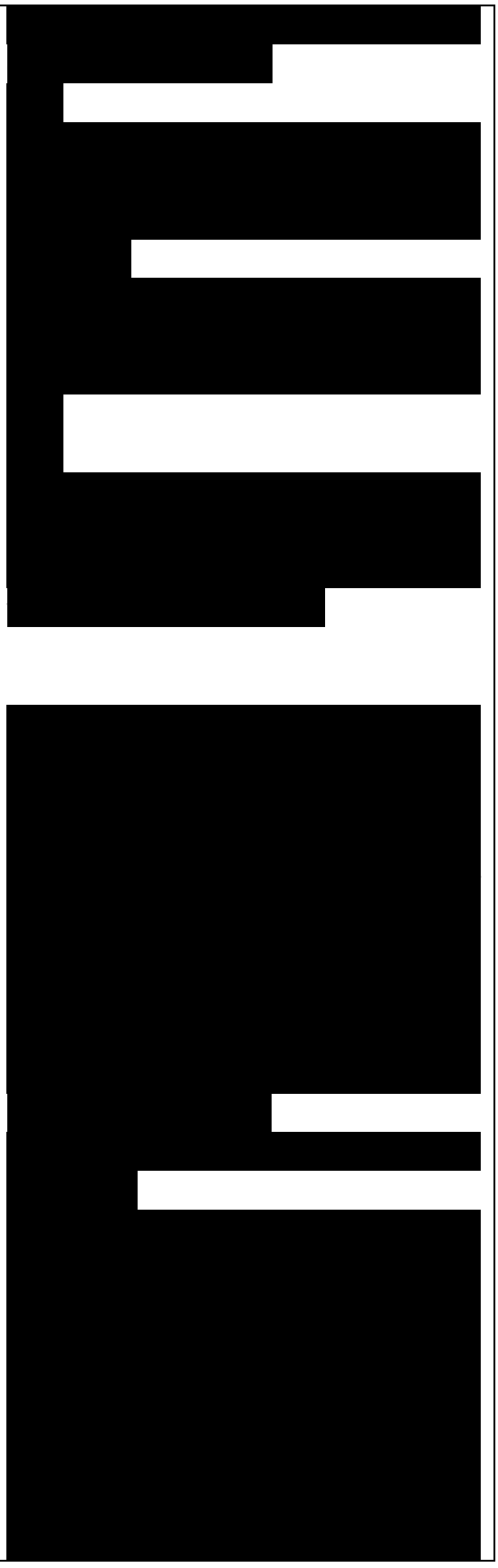
The maximal excitation energy to produce this fragmentation is thus:
(10)
Figure 3. Partition probabilities as a function of the number of broken bonds for the fragmentation of C4H from RG model.
Using equations (1) and (10), we deduce the relation between M and E• for the RG model:
(11)

Equation (11) shows that the correlation between M and the maximal excitation energy is linear with a threshold energy Et*hreshold = 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 (Eg = -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 102, 103 and 10 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.

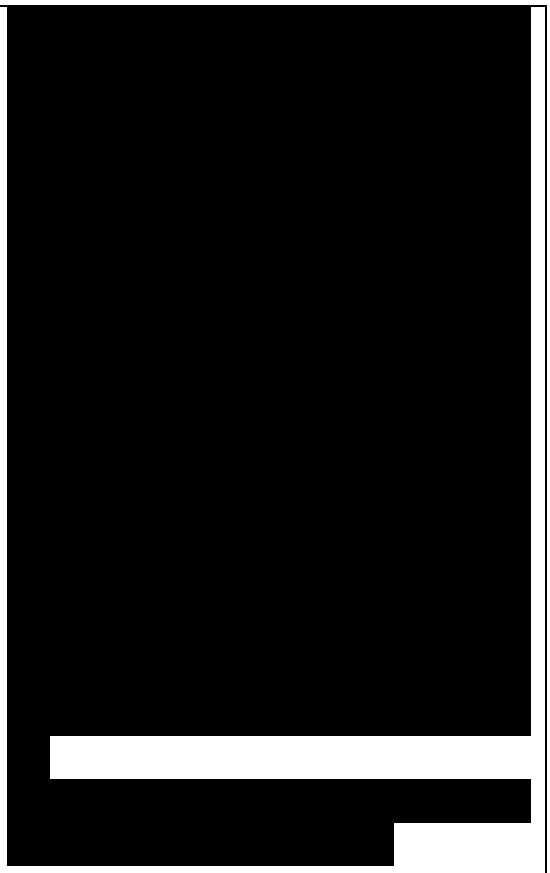


Figure 4. Fragmentation probabilities as a function of the multiplicity M and the

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).