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Liên hệ dịch tài liệu :

thanhlam1910_2006@yahoo.com hoặc frbwrthes@gmail.com hoặc số 0168 8557 403 (gặp Lâm)

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Exact solution of Random Graph fragmentation and physical, chemical and biological applications	Nghiệm chính xác của quá trình phân mảnh đồ thị ngẫu nhiên và ứng dụng trong vật lý, hóa học và sinh học.
Abstract. Random graphs (RG), also called mean field percolation in the frame of mesoscopic physics, are a	Tóm tắt. Các đồ thị ngẫu nhiên (RG) hay còn gọi là thẩm thấu trường trung bình trong khuôn khổ

basic model composed solely of connected entities called nodes. The connections, called bonds, can be active of broken. When the number of broken bonds is too large, the system of entities separates into a set of fragments called a partition. The exact solution for the micro-canonical partition probabilities of finite size systems was yet unresolved, thus a series of fundamental questions about the model could not be answered. We have established the exact equations of RG partition probabilities as a function of the number of nodes and of the number of broken bonds. From these probabilities, it is also possible to deduce intrinsic properties of RG. Many actual networks, while composed of complex interactions, behave like RG. We show examples where information was deduced, using RG, from systems consisting of sets of nucleons, atoms or termite nest chambers.

hệ vật lý trung mô, là mô hình cơ bản chỉ bao gồm các thực thể kết nối nhau còn được gọi là các nút. Các kết nối, được gọi là các liên kết có thể bị bẽ gãy. Khi số liên kết bị bẽ gãy quá lớn, hệ thực thể tách thành một tập hợp các mảnh được gọi là một phân vùng. Chúng ta vẫn chưa tìm được nghiệm chính xác của xác suất phân vùng vi chính tắc của những hệ kích thước hữu hạn, vì thế hàng loạt các câu hỏi về mô hình vẫn chưa được giải quyết. Chúng tôi đã xây dựng các phương trình chính xác của xác suất phân vùng RG theo số nút và số liên kết bị bẽ gãy. Từ những xác suất này, chúng ta cũng có thể suy ra được những tính chất nội tại của RG. Nhiều mạng thực, trong khi bao gồm các tương tác phức tạp, lại có đặc tính giống như RG. Chúng tôi trình bày các ví dụ trong đó nhờ vào RG, chúng ta có thể rút ra được thông tin từ những hệ cấu thành từ tập hợp các nucleon, các nguyên tử hoặc termite nest chamber (khoang tổ mối)

1. Introduction

Random Graphs (RG) [1] are the most general and the most studied model of sets of connected entities. Its importance is due to its simplicity, to the richness of its properties and to the fact that it has shown its usefulness to describe and analyze real-world systems. When the size of the system tends to infinity, it shows a phase transition and its evolution near the critical point has been described precisely via a set of universal parameters [2, 3]. New interest has been triggered by the study of mesoscopic objects, such as

nano-objects or atomic clusters, that cannot be considered as infinite and that are not necessarily close the critical points. Hence, we have calculated the exact equations of microcanonical RG for finite systems [4], using the tools of statistical physics. Indeed, the nodes of RG can be seen as particles or molecules and the bonds as binding energies. The resulting equations give the probabilities of fragment partitions.

Many real-life networks, while composed of complex interactions, show a behavior close RG This model can therefore be used as a tool to evidence properties or correlations in physical systems submitted to fragmentation or to nucleation. Different examples are shown where physical information was deduced, using RG, from systems consisting of sets of nucleons [5] (nuclear spinodal decomposition [6, 7]) of atoms (cluster fragmentation [8, 9]), of molecules [10] and from the topology of insect nests [11].

2. Implementation of the model equation

In the following the number of nodes will be noted S (size of the system) and the number of broken bonds E* as we consider that the breaking of a bond requires a unit excitation energy.

A fragment is a set of connected nodes such that it is possible to go

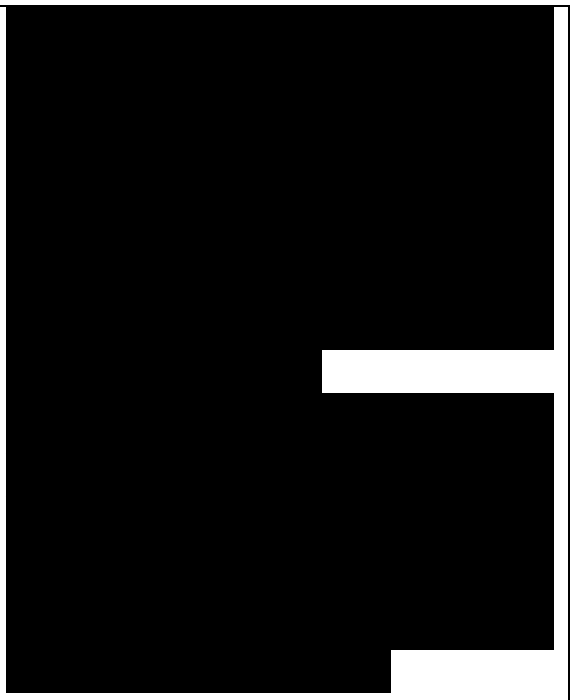
from any node to any other node, directly or indirectly, following active bonds. A fragment partition [12] will be noted as a vector n, whose component ns indicates the number of fragments with size s. The maximum number of bonds is S (S — 1)/2. When enough bonds are broken, the system can separate into fragments.

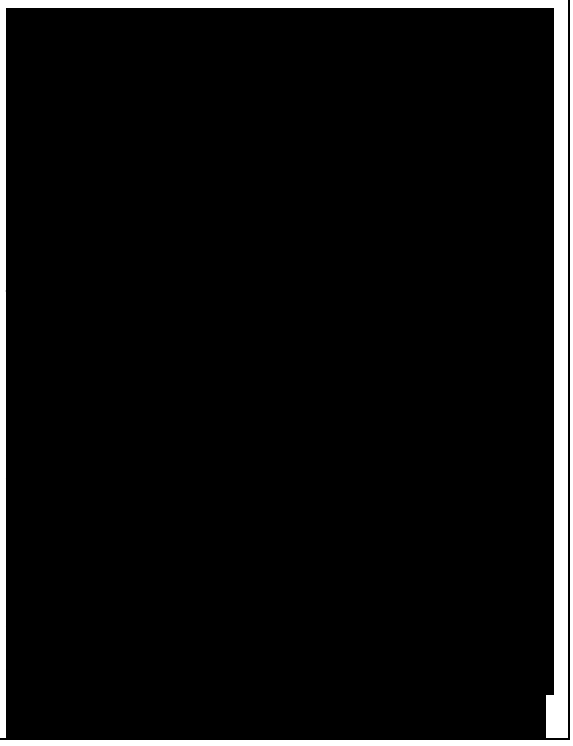
The microcanonical (obtained for a given E*) weight of a fragmentation partition depends both on the number of ways to arrange the nodes among the fragments and on the number of ways to arrange the broken bonds, i.e. the excitation energy, among the fragments.

The first combinatory factor accounts for the number of ways to allocate S nodes to the fragments. There are S! ways to arrange the nodes. However, the permutation of nodes inside a fragment does not change the partition nor does the permutation of equal size fragments. Thus the combinatory factor reads:

(1)

A part of the energy is used to separate the fragments, the remaining energy is distributed among the fragments. For a given fragment i, the density of states p(sj,E*) is equal to the number of ways to choose E* broken bonds among Sj (sj — 1)/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. Moreover, there are different ways to sort the excitation energy among the fragments. The energy sorting is accounted for by a vector E which components are the E* and i E* is the remaining energy.





Thus, the partition weights read:

(2) 10 h 42

All the observables and the thermodynamic features of the model can be deduced from this equation.

The density of states p(S, E*) = w((0,..., 0,1),E*) can easily be computed noticing that the total number of ways to sort E* broken bonds in the system is equal to the sum of all the partition weights. Hence we have:

(3)

Here si and E* are smaller than S and E thus the equation can be used to calculate recursively the densities of states. The results are shown in figure 1. As can be seen, the density of states reaches very high values even for relatively small systems. For fifty nodes, the maximum is of the order of 10367.

Equation (2), gives the microcanonical probabilities. The canonical RG model corresponds to the breaking of bonds according to a breaking probability p playing the role of a temperature. The distribution of the number of broken bonds for a given p is binomial, thus:

(4)

Another way to calculate this quantity was also proposed recently in [13].

Figure 1. Level density (number of stable configurations) as a function of the excitation energy for different system sizes.

Figure 2. Open dots: resilience probability, lines: mean number of cutting bonds as a function of the excitation energy for different system

sizes.

Many real life systems are composed of different types of ”nodes” combinatory factor is given by [4]:
For T types, the
where St the number of type t nodes, nt(s) the number of fragments containing s type t nodes
the number of fragments with s1 type 1 nodes, ..., sT type T nodes.

3. Applications

In [4] we have shown how the preceding equations could be used to evidence an over counting of the fragmentation of the carbon nucleus into three alpha particles, which could sign the Hoyle state [14].

3.1. Networks

From equation (2), different features of the model can be deduced. For example, the resilience probability (probability that the system remains connected if one bond is broken) and the mean number of cutting bonds (bonds such that if they are broken, the system splits into two fragments), which play important roles in the frame of network stability studies, are shown in figure 2. The resilience probability Pr is the ratio of the density of states to the sum of all partition weights and the mean number of cutting bonds is given by the following equation [4]:
(6)

3.2. Distillation process

The simplest two-colour graph is composed of, say, red and blue nodes and of bonds that connect nodes with different colours only. When bonds are broken, two ”phases” appear. The ”gas” gathers the free (unbounded)

nodes and the ”liquid” is composed of the connected nodes. The results (figure 3) illustrate the distillation property that appears when a majority of entities belong to a given species: the relative proportion of the different species in the disordered phase (gas) is systematically more asymmetric than in the ordered phase (liquid). A similar result has been evidenced in atomic nuclei decay [15].

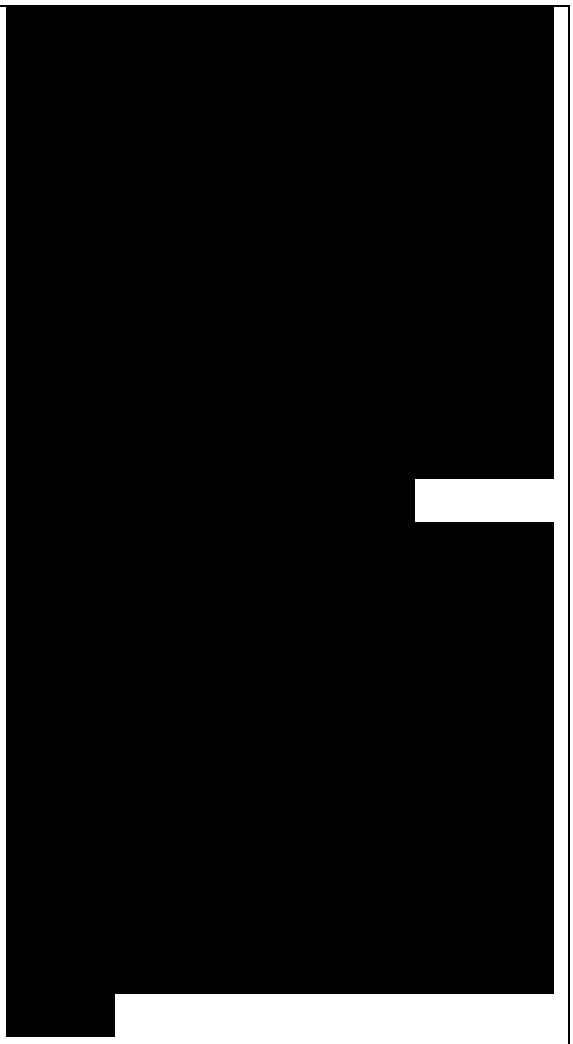


Figure 3. Distillation process in a 2 node- type RG model. The system is composed of 8 blue and 12 red nodes. The curves give the mean proportion of nodes in each phase at a given excitation energy. At low energy, all the nodes are in the ”liquid”. At the evaporation threshold, E* = 8, the ”gas” is composed of red nodes only. Over the threshold, the ”gas” is always more asymmetric than the ”liquid”.

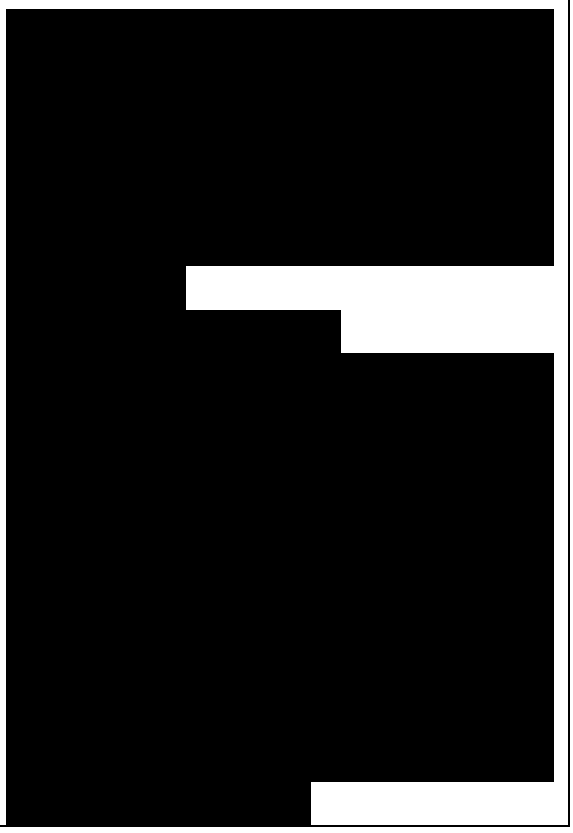


Figure 4. Upper part of a cubitermes nest. The center of the chambers are indicated by dots, cutting corridors by thin lines and non- cutting corridors by bold lines.

3.3. Cubitermes nests

Cubitermes, like ants and termites, build complex nests composed of corridors and chambers (figure 4) [11]. One way to evidence their topological properties is to compare them to RG. As an example, the mean number of cutting corridors is much larger in the nests than in RG which is interpreted in terms of mobility management and of protection against intruders.

4. Conclusions We have established the exact expressions of the RG partition probabilities and shown that a fruitful way to use the result is to apply RG as a null hypothesis to evidence properties of real-life systems.