Random walks on graphs: ideas, techniques and results

2005 J. Phys. A: Math. Gen. 38 R45

(http://iopscience.iop.org/0305-4470/38/8/R01)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) R45–R78 doi:10.1088/0305-4470/38/8/R01

TOPICAL REVIEW

Random walks on graphs: ideas, techniques and results

R Burioni and D Cassi

Dipartimento di Fisica, INFM and INFN, Università di Parma, Parco Area delle Scienze 7/A, 43100 Parma, Italy

Received 5 October 2004, in final form 30 November 2004
Published 9 February 2005
Online at stacks.iop.org/JPhysA/38/R45

Abstract

Random walks on graphs are widely used in all sciences to describe a great variety of phenomena where dynamical random processes are affected by topology. In recent years, relevant mathematical results have been obtained in this field, and new ideas have been introduced, which can be fruitfully extended to different areas and disciplines. Here we aim at giving a brief but comprehensive perspective of these progresses, with a particular emphasis on physical aspects.

PACS numbers: 02.10.Ab, 02.40.Sf, 05.40.Fb, 05.50.+q

Contents

1. Introduction

A graph is the most general mathematical description of a set of elements connected pairwise by some kind of relation. Therefore, it is not surprising that graph theory has been successfully applied to a wide range of very different disciplines, from biology to social science, computing, psychology, economy, chemistry and physics.

In recent times, physicists have been mainly interested in graphs as models of complex systems, in condensed matter and in network theory. Indeed, these structures have proven to be very useful to describe inhomogeneous structures such as disordered materials, glasses, polymers, biomolecules as well as electric circuits, communication networks, statistical models of algorithms, and applications of statistical mechanics to different (non-physical) systems.

The function of graphs in physics, however, is not purely descriptive. Geometry and topology have a deep influence on the physical properties of complex systems, where the presence of a large number of interacting degrees of freedom typically matters more than the interaction details. In fact, the most specific interest of a physicist concerns the properties of a graph which most affect the dynamical and thermodynamical behaviour of the system it describes. On the other hand, the study of complex systems requires the introduction of statistical methods, to give an effective description of a number of quantities otherwise too difficult to control.

Random walks are probably the simplest stochastic process affected by topology and, at the same time, the basic model of diffusion phenomena and non-deterministic motion. They have been extensively studied for decades on regular structures such as lattices, and most of the common wisdom concerning them relies on the results obtained in this particular geometry. The richer topology of a generic graph can have a dramatic effect on the properties of random walks, especially when considering infinite graphs, which are introduced to describe macroscopic systems in the thermodynamic limit. There, the asymptotic behaviour at long time typically exhibits universal features, only depending on large scale topology. On lattices, such features are known to be related to the Euclidean dimension only. On general graphs, universality allows us to generalize the concept of dimension to inhomogeneous structures, providing a very powerful tool to investigate a large class of different physical models, apparently not connected to diffusion processes. On the other hand, a new and unexpected phenomenon arises in the presence of strong inhomogeneity, namely the splitting between local and average properties. This provides a fundamental conceptual framework to investigate complex systems even from an experimental point of view.

Most results concerning random walks on graphs in physics have been obtained in the last two decades and are scattered over a large number of technical papers. This review is intended to provide the reader with a rigorous, self-contained and up-to-date account of the present knowledge about this subject. Particular attention has been paid to give a simple and general framework effectively resuming rather different results. As for specific calculations, we refer to bibliography, unless otherwise required for clarity. The emphasis is always put on the physical meaning. The reader more interested in formal aspects can find a presentation focused on mathematics in another recent review [1].

The paper is organized as follows: In the first sections we give a brief mathematical description of graphs and random walks, introducing the language and the formalism we will use through the whole paper. Then we present a simple treatment of the finite graphs case, before dealing with infinite graphs. The latter require the introduction of specific concepts, which are fully discussed in an introductory section. Then, the asymptotic behaviour of random walks on infinite graphs is studied and used to define the type problem and the spectral dimension. The difference between local and average properties is evidenced in the following sections. The concluding sections are devoted to the analysis of a large class of specific graphs and to the relations of random walks with different physical problems.

2. Mathematical description of graphs

Let us begin by introducing the basic mathematical definitions and results concerning graphs [2].

A graph $\mathcal{G}$ is a countable set V of vertices (or sites) (i) connected pairwise by a set E of unoriented links (or bonds) $(i, j) = (j, i)$. If the set V is finite, $\mathcal{G}$ is called a finite graph and we will denote by N the number of vertices of $\mathcal{G}$. Otherwise, when V is infinite, $\mathcal{G}$ is called an infinite graph. A subgraph $\mathcal{S}$ of $\mathcal{G}$ is a graph whose set of vertices $S \subseteq V$ and whose set of links $E' \subseteq E$.

A path $C_{i\to j}$ in $\mathcal{G}$ connecting points i and j is a sequence of consecutive links $\{(i, k)(k, h)\cdots(n, m)(m, j)\}$ and a graph is said to be connected, if for any two points $i, j \in V$ there is always a path joining them. In the following we will consider only connected graphs.

Every connected graph $\mathcal{G}$ is endowed with an intrinsic metric generated by the chemical distance r_{ij} which is defined as the number of links in the shortest path connecting vertices i and j.

A particular class of graphs, often occurring in physical applications, is characterized by the absence of closed paths containing an odd number of links. These graphs are called *bipartite*, since we can divide their sites into two sets V_1 and V_2 such that the points of V_1 are connected by a link only to points V_2 and vice versa. Square and hypercubic lattices are the most typical examples of bipartite graphs, as well as all trees (graphs without closed self-avoiding paths). The graph topology can be algebraically represented introducing its adjacency matrix A_{ij} given by

$$A_{ij} = \begin{cases} 1 & \text{if} \quad (i, j) \in E \\ 0 & \text{if} \quad (i, j) \notin E. \end{cases} \tag{1}$$

The Laplacian matrix Δ_{ij} is defined by

$$\Delta_{ij} = z_i\delta_{ij} - A_{ij}, \tag{2}$$

where $z_i = \sum_j A_{ij}$, the number of nearest neighbours of i, is called the coordination number of site i.

In order to describe disordered structures we introduce a generalization of the adjacency matrix given by the ferromagnetic coupling matrix J_{ij}, with $J_{ij} \neq 0 \iff A_{ij} = 1$ and $\sup_{(i,j)} J_{ij} < \infty$, $\inf_{(i,j)} J_{ij} > 0$. One can then define the generalized Laplacian

$$L_{ij} = I_i\delta_{ij} - J_{ij}, \tag{3}$$

where $I_i = \sum_j J_{ij}$.

3. The random walk problem

Let us now introduce the so-called *simple random walk* on a graph $\mathcal{G}$. Assuming the time (t) to be discrete, we define at each time step t the jumping probability p_{ij} between nearest neighbour sites i and j:

$$p_{ij} = \frac{A_{ij}}{z_i} = (Z^{-1}A)_{ij}, \tag{4}$$

where $Z_{ij} = z_i\delta_{ij}$.

This is the simplest case we can consider: the jumping probabilities are isotropic at each point and they do not depend on time; in addition the walker is forced to jump at every time step. As we will see later, the last condition, i.e. the impossibility of staying on the site, although crucial for the short time behaviour, has no significant influence on the long time regime.

Usually, the random walk problem is considered to be completely solvable if, for any $i, j \in \mathcal{G}$ and $t \in N$, we are able to calculate the functions $P_{ij}(t)$, each representing the probability of being at site j at time t for a walker starting from site i at time 0. These probabilities are the elements of a matrix $P = \|P_{ij}(t)\|$ which is equal to the tth power of the jumping probabilities matrix $p = \|p_{ij}\|$:

$$P_{ij}(t) = (p^t)_{ij}. \tag{5}$$

Relation (5) can be easily proven by induction on t. It also has an interesting physical interpretation as a sum over paths; developing the matrix products term by term we can write the whole expression as

$$P_{ij}(t) = (p^t)_{ij} = \sum_{C_{i\to j}(t)} w(C_{i\to j}(t)) \tag{6}$$

where the sum is over all t-step paths between i and j. The weight $w(C_{i\to j})$ is the probability for the walker of going from i to j following exactly the path $w(C_{i\to j})$:

$$w(C_{i\to j}(t)) = \prod_{(k,l)\in C_{i\to j}(t)} p_{kl} \tag{7}$$

the product being over all the t links belonging to the path.

The calculation of all $P_{ij}(t)$, which is straightforward as far as relatively small graphs are concerned, for large or infinite graphs becomes practically impossible and, above all, of little significance. In fact, for large systems we are mainly interested in global and collective properties as typically happen in statistical physics. Therefore, a small subset of all these quantities is usually chosen, together with some other related to them, which give an effective physical description of the random walker behaviour. The most relevant of them is from many points of view the probability $P_{ii}(t)$ of returning to the starting point after t steps, also called the *random walk autocorrelation function*. As we will see, its asymptotic behaviour gives the most direct characterization of the large scale topology for infinite graphs. A related quantity is the average number P_{ii} of returns to the starting point i, which can be generalized to the average number P_{ij} of passages through j starting from i:

$$P_{ij} \equiv \lim_{t\to\infty} \sum_{k=0}^{t} P_{ij}(k), \tag{8}$$

where the limit can be infinite.

The mean displacement $r_i(t)$ from the starting site i after t steps is deeply related to the diffusion properties and is defined as

$$r_i(t) \equiv \sum_j r_{ij} P_{ij}(t). \tag{9}$$

Note that, unlike the case of random walks in continuous Euclidean space, here we consider r instead of r^2, the latter having no particular significance in the absence of a Euclidean metric.

The quantities introduced up to now are not 'sensible to the history'. Indeed, we can in principle determine all of them simply by considering the situation of the walker at time t regardless of his previous behaviour. In order to keep track of what happened before the instant t, a different class of functions is introduced, starting with the *first passage probability* $F_{ij}(t)$. The latter denotes the conditional probability for a walker starting from i of reaching for the first time the site $j \neq i$ in t steps. For $i = j$ the previous definition would not be interesting, the walker being at i at $t = 0$ by definition. Therefore, one defines $F_{ii}(t)$ to be the probability of returning to the starting point i for the first time after t steps and one sets $F_{ii}(0) = 0$. In spite of the deeply different nature of P and F, a fundamental relation can be established between them if all time steps from 0 to t are taken into account (in other words, we have to give up the time locality):

$$P_{ij}(t) = \sum_{k=0}^{t} F_{ij}(k) P_{jj}(t-k) + \delta_{ij}\delta_{t0}. \tag{10}$$

This can be easily obtained by considering that each walker which is at j at time t only has two possibilities: either it gets there for the first time, or it has reached j for the first time at a previous time k and then it has returned there after $t - k$ steps. The first passage probability is in turn connected to other meaningful history dependent quantities. The probability F_{ij} of ever reaching the site j starting from i (or of ever returning to i, if $i = j$) is given by

$$F_{ij} = \sum_{t=0}^{\infty} F_{ij}(t). \tag{11}$$

By $S_i(t)$ we denote the average number of different sites visited after t steps by a walker starting from i. Its relation to $F_{ij}(t)$ is

$$S_i(t) = 1 + \sum_{k=1}^{t} \sum_j F_{ij}(k). \tag{12}$$

Finally, the *first passage time* t_{ij}, i.e. the average time at which a walker starting from i, and passing at least once through j, reaches j for the first time (or returns for the first time to i, if $i = j$) is

$$t_{ij} = \lim_{t\to\infty} \frac{\sum_{k=0}^{t} k F_{ij}(k)}{F_{ij}}. \tag{13}$$

The simple random walk can be modified to give a richer behaviour and to describe more general physical problems. Indeed, one can introduce anisotropic jumping probabilities by substituting in (4) the adjacency matrix with a ferromagnetic coupling matrix:

$$p_{ij} = \frac{J_{ij}}{I_i} = (I^{-1}J)_{ij}, \tag{14}$$

where $I_{ij} = I_i\delta_{ij}$ and $I_i = \sum_k J_{ik}$. Depending on the specific properties of J_{ij}, this can produce only local effects or introduce a global bias which destroys the leading diffusive behaviour giving rise to transport phenomena.

Moreover, one can relax the constraint of jumping at each time step by introducing waiting and traps on the sites. The jumping probabilities are then modified to

$$p_{i,j} = \frac{J_{i,j} + w_i \delta_{i,j}}{I_i + w_i + d_i}, \tag{15}$$

where both w_i and d_i are real positive numbers. From (15), $w_i/(I_i + w_i + d_i)$ is the probability for the walker to stay on site i instead of jumping away and $d_i/(I_i + w_i + d_i)$ is the probability of disappearing (or dying, or being trapped forever) at site i. As we will see later, waiting only affects the short time behaviour, while traps can also dramatically modify the long time asymptotic properties.

4. The generating functions

Even if we consider only the few fundamental quantities devised at the end of the last section, their direct calculation can be in practice a hard or impossible task on general graphs. However, a powerful indirect mathematical technique exists allowing us to overcome a series of typical difficulties: this is the discrete Laplace transform, which maps a time function onto its *generating function*. The generating function $\tilde{f}(\lambda)$ of $f(t)$ is defined by

$$\tilde{f}(\lambda) = \sum_{t=0}^{\infty} \lambda^t f(t), \tag{16}$$

where λ is a complex number. The inverse equation giving $f(t)$ from $\tilde{f}(\lambda)$ is

$$f(t) = \left. \frac{\partial^t \tilde{f}(\lambda)}{\partial \lambda^t} \right|_{\lambda=0}. \tag{17}$$

This equation is useful as far as we are interested in small t behaviour, but it becomes absolutely ineffectual in the study of asymptotic regimes for $t \to \infty$. In this case a very powerful tool is provided by the Tauberian theorems, relating the singularities of $\tilde{f}(\lambda)$ to the leading large t behaviour of $f(t)$. We give here a rather general Tauberian theorem, which is particularly useful when dealing with random walks. The main assumption we make concerns the analytical form of the leading singularity: we only consider power laws and logarithmic behaviour, since all cases discussed in this paper as well as all physically meaningful cases belong to this class. Suppose that $\tilde{f}(\lambda)$ has its singularity nearest to $\lambda = 0$ in $\lambda = r$ and that $\tilde{f}(r - \epsilon)$, for $\epsilon \to 0^+$, goes as

$$\tilde{f}(r - \epsilon) \sim h(\epsilon) + \text{const} \prod_{i=0}^{\infty} ({}^i \ln(1/\epsilon))^{\alpha(i)}, \tag{18}$$

where ${}^i \ln x \equiv \ln^{i-1} \ln x$, with ${}^0 \ln x \equiv x$ and $h(\epsilon)$ is finite for $\epsilon \to 0^+$.

Then, for $t \to \infty$

$$f(t) \sim \text{const}' r^{-t} \prod_{i=0}^{\infty} {}^i \ln^{\beta(i)}(t), \tag{19}$$

where $\beta(i)$ are related to $\alpha(i)$ by

$$\beta(i) = \begin{cases} \alpha(0) - 1 & \text{for} \quad i = 0 \\ \theta(i - m)(\alpha(i) + 1) - 1 - \delta_{i,m} I(\widetilde{d}/2) & \text{otherwise} \end{cases} \tag{20}$$

where

$$m = \min\{i \geqslant 0 | \beta(i) \neq -1\} \tag{21}$$

and

$$I(\widetilde{d}/2) = \begin{cases} 1 & \text{if } \widetilde{d}/2 \text{ is integer} \\ 0 & \text{otherwise.} \end{cases} \tag{22}$$

The const′ is in general a function of const and of all the exponents appearing in the previous formulae. We do not give here its rather involved explicit expression, since it is not relevant for the purposes of this paper.

The generating functions are usually easier to calculate, since they allow us to exploit some peculiar properties of random walk functions. Moreover, a series of relevant random walk parameters which are non-local in time, can be obtained directly from a generating function, without calculating the corresponding time dependent quantities. A good example is given by P_{ij}, F_{ij} and t_{ij} which are related to $\tilde{P}_{ij}(\lambda)$ and $\tilde{F}_{ij}(\lambda)$ by

$$P_{ij} = \lim_{\lambda \to 1^-} \tilde{P}_{ij}(\lambda) \tag{23}$$

$$F_{ij} = \tilde{F}_{ij}(1) \tag{24}$$

$$t_{ij} = \lim_{\lambda \to 1^-} \frac{\partial \log \tilde{F}_{ij}((\lambda)}{\partial \lambda}. \tag{25}$$

The basic property of random walk generating functions arises from the deconvolution of equation (10), which after some straightforward steps becomes

$$\tilde{P}_{ij}(\lambda)\tilde{F}_{ij}(\lambda)\tilde{P}_{jj}(\lambda) + \delta_{ij}. \tag{26}$$

In other words, the relation which was non-local in time becomes local in λ. As we will see in practical application, many iteration techniques for the analytical calculation of generating functions are based on this property.

5. Random walks on finite graphs

Finite graphs consist of a finite number of sites and links. In principle, every physical structure is composed of a finite number of elements, but it is well known that a series of behaviour occurring in macroscopic systems is better described in the thermodynamic limit. Indeed, the typical singularities and power laws characterizing phase transitions and asymptotic regimes, such as large scale, long times, low temperature and low frequency behaviour, can only be found on infinite graphs.

However, finite graphs are appropriate when dealing with mesoscopic structures and finite size effects. The random walk problem on finite graphs is simplified by the finiteness of the adjacency matrix. In fact, the analytical study is reducible to a spectral problem on a real finite-dimensional vector space, and numerical simulations are easily implemented by Monte Carlo techniques.

Let us first consider the case of a random walk without traps, whose jumping probabilities are given by (15) with $d_i = 0\ \forall i$. The matrix elements p_{ij} satisfy the relations

$$p_{ij} \geqslant 0 \qquad \forall i, j \tag{27}$$

$$\sum_{j=1}^{N} p_{ij} = 1 \qquad \forall i \tag{28}$$

defining a *stochastic matrix*.

The stochastic matrices we are considering exhibit different properties according to some general features of the graph and of the jumping probabilities [3]. We distinguish two cases:

1. If $\mathcal{G}$ is not bipartite, or if it has a staying probability on at least one site, then it has only one eigenvalue $p_{\max}$ with maximal modulus and $p_{\max} = 1$. Moreover, the eigenvector corresponding to $p_{\max}$ has the same entry on each site (usually one chooses $v_{\max} = (1, 1, 1, \ldots, 1)$ for simplicity).
2. If $\mathcal{G}$ is bipartite without staying probabilities, then the spectrum of p is symmetric with respect to the origin of the complex plane. Therefore, in addition to $p_{\max}$ it has a second maximal modulus eigenvalue $p_{\min} = -1$. The eigenvector $v_{\max}$ has the same properties as the previous case, while $v_{\min}$ has all entries on V_1 equal to the same number v and all entries on V_2 equal to $-v$ (usually one chooses $v = 1$).

In case 1, one can easily show that the random walk is *ergodic*, i.e. that it admits limit probabilities for $t \to \infty$:

$$P_{ij}^{\infty} = \lim_{t\to\infty} P_{ij}(t) \qquad \forall i, j \tag{29}$$

and that

$$P_{ij}^{\infty} = \frac{1}{N} \qquad \forall i, j. \tag{30}$$

This means that, independently of the initial conditions, the asymptotic probabilities are the same over all the graph sites. Moreover, this uniform limit value is reached exponentially and the exponential decay of each matrix element is no slower than p_2^t, p_2 being the second greatest eigenvalue of p_{ij}.

In case 2, the random walk is not ergodic. In particular, we have

$$P_{ij}(t) = 0 \tag{31}$$

for all t such that $t - r_{ij}$ is odd. On the other hand, considering for each couple of sites i and j only the values t'_{ij} of t having the same parity as r_{ij}, one can show that

$$P_{ij}^{\infty} = \lim_{t'_{ij}\to\infty} P_{ij}(t'_{ij}) \qquad \forall i, j \tag{32}$$

with

$$P_{ij}^{\infty} = \frac{2}{N} \qquad \forall i, j \tag{33}$$

and the limit is reached exponentially as in case 1.

Similarly, one can easily prove that

$$\lim_{t\to\infty} F_{ij}(t) = 0 \qquad \forall i, j \tag{34}$$

and

$$\lim_{t\to\infty} S_i(t) = N \qquad \forall i \tag{35}$$

the limit values being reached exponentially.

Moreover,

$$P_{ij} = \infty \qquad \forall i, j \tag{36}$$

$$F_{ij} = 1 \qquad \forall i, j \tag{37}$$

and

$$t_{ij} < \infty \qquad \forall i, j. \tag{38}$$

The introduction of at least one trap, setting $d_i > 0$ for at least one site i in (15), dramatically changes the random walk behaviour. The jumping probabilities matrix p is no longer stochastic, since condition (28) is not satisfied. However, condition (27) (i.e. non-negativity) still holds, implying relevant properties. We can still distinguish between cases 1 and 2, but the corresponding properties are modified as follows:

1. If $\mathcal{G}$ is not bipartite, or if it has a staying probability on at least one site, then it has only one eigenvalue $p_{\max}$ with maximal modulus and $p_{\max} < 1$. Moreover, the entries $v_{\max i}$ of the eigenvector $v_{\max}$, corresponding to $p_{\max}$, have the same sign, and $v_{\max}$ is the only eigenvector having such a property.
2. If $\mathcal{G}$ is bipartite without staying probabilities, then the spectrum of p is symmetric with respect to the origin of the complex plane. Therefore, in addition to $p_{\max} < 1$ it has a second maximal modulus eigenvalue $p_{\min} = -p_{\max}$. The eigenvector $v_{\max}$ has the same properties as the previous case, while $v_{\min}$ can be chosen in such a way that all its entries $v_{\min i}$ on V_1 are equal to $v_{\max i}$ and all its entries $v_{\min j}$ on V_2 are equal to $-v_{\max j}$.

In both cases the random walk is ergodic and the limit probabilities vanish:

$$P_{ij}^{\infty} = 0 \qquad \forall i, j. \tag{39}$$

However, in case 2 the time parity still has to be taken into account and (31) holds. Moreover, the asymptotic decay is exponential and no slower than $p_{\max}^t$. Finally, as for the other random walk functions we get

$$\lim_{t\to\infty} F_{ij}(t) = 0 \qquad \forall i, j \tag{40}$$

$$\lim_{t\to\infty} S_i(t) < N \qquad \forall i \tag{41}$$

the limit values being reached exponentially,

$$P_{ij} < \infty \qquad \forall i, j \tag{42}$$

$$F_{ij} < 1 \qquad \forall i, j \tag{43}$$

$$t_{ij} < \infty \qquad \forall i, j. \tag{44}$$

6. Infinite graphs

When dealing with macroscopic systems, composed of a very large number N of sites, one usually takes the thermodynamic limit $N \to \infty$. This means that we have to consider infinite graphs, i.e. graphs composed by an infinite number of sites. This is particularly convenient for two main reasons:

- First of all, a single infinite structure effectively describes a very large (infinite, indeed) number of large structures having different sizes, but similar geometrical features.
- The singularities in thermodynamic potentials typical of critical phenomena as well as a series of universal asymptotic behaviour only occur on infinite structures.

As for random walks on large real structures, the time dependence of physical quantities exhibits different features according to the time scale which is considered. For very long times, the walker can explore every site and its behaviour is described by the finite graph laws introduced in the previous section. However, if the time is long enough to explore large portions of the system, but still too short to experience the finite size effects, many significant quantities are quite insensitive to local details and exhibit power law time dependence with universal exponents. Often, this is the most interesting regime in physical applications. On infinite graphs, this is the true asymptotic regime even for very large times; therefore, we can reproduce the universal behaviour of a huge variety of finite large structures simply by considering infinite graphs with similar topological features.

To deal with infinite graphs, some further mathematics has to be introduced. In particular, we need tools to 'explore' large scale topology. For this purpose, we define the generalized Van Hove spheres (GVHS): a GVHS $\mathcal{S}_{o,r}$ of centre o and radius r is the subgraph of $\mathcal{G}$, given by the set of vertices $V_{o,r} = \{i \in V | r_{i,o} \leqslant r\}$ and by the set of links $E_{o,r} = \{(i, j) \in E | i \in V_{o,r}, j \in V_{o,r}\}$.

Let us use $|S|$ to denote the number of elements of a set S. Then $|V_{o,r}|$, as a function of the distance r, describes the growth rate of the graph at the large scales [4]. In particular, a graph is said to have *polynomial growth* if $\forall o \in V_X \; \exists c, k$, such that

$$|V_{o,r}| < c\, r^k. \tag{45}$$

For a graph satisfying (45), we define the upper growth exponent d_g^+ and the lower growth exponent d_g^- as

$$d_g^+ = \inf\{k | |V_{o,r}| < c_1\, r^k, \forall o \in V\} \tag{46}$$

and

$$d_g^- = \sup\{k | |V_{o,r}| > c_2\, r^k, \forall o \in V\}. \tag{47}$$

If $d_g^+ = d_g^-$, which usually happens on physically interesting structures, we call them the growth exponent d_g, or the *connectivity dimension*.

The connectivity dimension d_g is known for a large class of graphs: on lattices, it coincides with the usual Euclidean dimension d, and for many fractals it has been exactly evaluated [5]. In general, we can think of it as the analogue of the fractal dimension, when the chemical distance metric is considered instead of the usual Euclidean metric.

Infinite graphs are too general to describe systems of physical interest. Indeed, the discrete structures usually studied in physics are characterized by some important properties, often implicitly assumed in the literature, which can be translated into mathematical requirements:

(a) We consider only connected graphs, since any physical model on disconnected structures can be reduced to the separate study of the models defined on each connected component and hence to the case of connected graphs.

(b) Since physical interactions are always bounded, the coordination numbers z_i, representing the number of neighbours interacting with the site i, have to be bounded; i.e. $\exists z_{\max} \,|\, z_i \leqslant z_{\max} \forall i \in V$.

(c) Real systems are always embedded in finite dimensional spaces. This constraint requires for the graph $\mathcal{G}$ the conditions:

(1) $\mathcal{G}$ has a polynomial growth (definition (45))

(2)

$$\lim_{r\to\infty} \frac{|\partial V_{o,r}|}{|V_{o,r}|} = 0 \tag{48}$$

where $\partial V_{o,r}$ denotes the border of $V_{o,r}$, i.e. the set of points of $V_{o,r}$ not belonging to $V_{o,r-1}$ (the existence itself of the limit is a physical requirement on $\mathcal{G}$). This condition is equivalent to requiring that boundary conditions are negligible in the thermodynamic limit.

Note that some graphs studied in the physical literature, such as the Bethe lattice, do not satisfy (1) and (2), while many random graphs do not fulfil (b).

For a large class of physically interesting graphs we have considered so far, conditions (1) and (2) appear to be equivalent. However for the equivalence of the two conditions a rigorous result is still lacking. A graph satisfying (a), (b) and (c) will be called a *physical graph*. Conditions (a) and (b) represent strong constraints on $\mathcal{G}$ and, as we will see later, they have very important consequences.

7. Random walks on infinite graphs

Considering random walks on infinite structures, some further mathematical constraints are to be introduced to describe physical situations.

First of all, the problem of uniform boundedness comes into play. Indeed, in (14) the conditions

$$\exists J_{\min}, J_{\max} > 0 \,|\, J_{\min} \leqslant J_{i,j} \leqslant J_{\max} \quad \forall i, j \tag{49}$$

together with (b) are usually required to exclude the presence of a global bias, which would generate a non-diffusive behaviour.

Moreover, in (15), in the presence of waiting and traps, analogous considerations lead to the following conditions:

$$\exists w_{\min}, w_{\max} > 0| \quad \text{either} \quad w_i = 0, \quad \text{or} \quad w_{\min} \leqslant w_i \leqslant w_{\max} \quad \forall i \tag{50}$$

$$\exists d_{\min}, d_{\max} > 0| \quad \text{either} \quad d_i = 0, \quad \text{or} \quad d_{\min} \leqslant d_i \leqslant d_{\max} \quad \forall i. \tag{51}$$

In the case of finite graphs, the possibility of associating with any matrix an operator acting on a finite-dimensional vector space allowed us to obtain very general and rigorous results. In the infinite case, it is in general impossible to associate a linear operator acting on a Hilbert space with any matrix. However, when (b) holds, the jumping probabilities matrix is quite particular: indeed, it only has a limited number of non-vanishing entries in each row and column. Due to this property, the elements of a matrix product are given by finite sums, as in the finite graphs case, instead of being sums of series. Therefore, the typical convergence problems of infinite-dimensional space do not arise, allowing for a simple and effective study of random walk properties.

Despite the increased mathematical complexity, many general results about infinite graphs have been rigorously proven. Some have correspondents in the finite graphs case, but most of them concern quantities and properties which cannot even be defined on finite structures. The rest of this section is devoted to the former: following the same format used in section 5 we summarize the main differences with respect to the finite case. The new properties arising in the thermodynamic limit will be discussed in the following sections.

First of all, let us consider random walks without traps on infinite graphs satisfying (a), (b), (49) and (50). It can be shown that

$$P_{ij}^{\infty} = \lim_{t\to\infty} P_{ij}(t) = 0 \qquad \forall i, j \tag{52}$$

even for bipartite graphs. However, for bipartite graphs without staying probabilities, we still have

$$P_{ij}(t) = 0 \tag{53}$$

for all t such that $t - r_{ij}$ is odd. Therefore, to study the large times asymptotic behaviour, as in the finite case we usually consider, for any given couple of sites i and j, only the values t'_{ij} of t having the same parity as r_{ij}. Unlike the finite case, the limit in (52) in general is not reached exponentially. Indeed, if (c) also holds, i.e. for physical graphs, the asymptotic behaviour is typically a power law, whose exponent only depends on topology, as we will discuss in details in the next sections. Note that the widely studied case of Bethe lattices, not satisfying (c), is still characterized by an exponential decay.

Similarly, one can easily prove that

$$\lim_{t\to\infty} F_{ij}(t) = 0 \qquad \forall i, j \tag{54}$$

and

$$\lim_{t\to\infty} S_i(t) = \infty \qquad \forall i, \tag{55}$$

the asymptotic behaviour being always bounded from above by t.

As for the quantities concerning the number of visits and the first visit probabilities, the situation is far more complex. Indeed, dramatically different behaviour can occur, according to the graph topology. In particular

$$P_{ij} = \infty \qquad \forall i, j \qquad \text{or} \qquad <\infty \quad \forall i, j \tag{56}$$

$$F_{ij} = 1 \qquad \forall i, j \qquad \text{or} \qquad <1 \quad \forall i, j \tag{57}$$

and

$$t_{ij} < \infty \qquad \forall i, j \qquad \text{or} \qquad =\infty \quad \forall i, j. \tag{58}$$

The classification of infinite graphs according to this possible behaviour is the subject of the next section.

8. Recurrence and transience: the type problem

On finite graphs, in the absence of traps, the probability of ever reaching (or returning to) a site, F_{ij}, is always 1. This means that the walker surely visits each site. This probability can be lowered only by adding traps (where the walker can be destroyed), but in this case the total probability is not conserved, i.e. the walker asymptotically disappears. On infinite graphs, a third possibility arises, which is expressed in (56) and (57): the walker can escape forever from its starting point, or never reach a given site, even in the absence of traps.

This phenomenon was first noticed by Polya in 1921 on lattices: he showed that, while in one and two dimensions $F_{ij} = 1$, for $d \geqslant 3$ $F_{ij} < 1$ [6]. Ever since, the former case has been called *recurrent* and the latter *transient*. Transience is an exclusive property of infinite graphs and it is fundamentally due to large scale topology. In other words, in the transient case, it happens that the number of paths leading the walker away from its starting point is large enough, with respect to the number of returning paths, to act as an asymptotic trap (still conserving the total probability).

As we will see in a while, transience and recurrence of random walks, when (49) and (50) are satisfied, depend only on the graph topology. Therefore they are intrinsic properties of a discrete structure and the classification of infinite graphs according to them is also known as the *type problem*.

Let us define the problem mathematically. First of all, a very general theorem on Markov chains states the following:

$$\exists i, j \in \mathcal{G} \mid F_{ij} = 1 \quad \Rightarrow \quad F_{hk} = 1 \qquad \forall h, k \in \mathcal{G} \tag{59}$$

(where the sites can coincide). This means that recurrence is point independent, or, in other words, that if a walker surely reaches a point j starting from a given point i, then it surely reaches any point k starting from any point h. It is straightforward to see that an analogous result follows for the case $F_{ij} < 1$. Therefore, recurrence and transience are global properties of a random walk.

Another important result relates F_{ij} and P_{ij}. Indeed, from (23), (24) and (26), it follows that

$$F_{ij} = 1 \quad \Leftrightarrow \quad P_{ij} = \infty \tag{60}$$

and

$$F_{ij} < 1 \quad \Leftrightarrow \quad P_{ij} < \infty \tag{61}$$

i.e., a walk is recurrent (transient) if and only if any site is visited an infinite (finite) number of times. The latter can be taken as an alternative definition of recurrence and transience. However, as we will see, the situation is more complex when considering averages over all the sites. A consequent property concerns the way the walker explores the sites of $\mathcal{G}$. Indeed, it can be shown that

$$F_{ij} = 1 \quad \Leftrightarrow \quad \lim_{t\to\infty} \frac{S_i(t)}{t} = 0 \tag{62}$$

while

$$F_{ij} < 1 \quad \Leftrightarrow \quad 0 < \lim_{t\to\infty} \frac{S_i(t)}{t} < 1. \tag{63}$$

In the first situation, where the number of distinct visited sites increases slower than the number of steps, is sometimes called *compact exploration*, since the subgraphs of the visited sites present a negligible number of 'holes'.

Recurrent graphs exhibit a further relevant property: one can show that

$$\lim_{\lambda\to 1^-} \frac{\tilde{P}_{ij}(\lambda)}{\tilde{P}_{hk}(\lambda)} = \lim_{t\to\infty} \frac{P_{ij}(t)}{P_{hk}(t)} = \frac{z_j}{z_k} \qquad \forall i, j, h, k. \tag{64}$$

The most important properties in the type problem concern its invariance with respect to a wide class of dynamical and topological transformations, establishing its independence on the graph details.

First of all, consider two different random walks (without traps) on the same graph $\mathcal{G}$, one (W) defined by the ferromagnetic coupling matrix J_{ij} and by the waiting probabilities w_i, and the other (W') by J'_{ij} and w'_i . It can be shown [7] that, if both satisfy (49) and (50), then W is recurrent if and only if W' is. In other words, any local bounded rescaling of ferromagnetic couplings and waiting probabilities leave the random walk type unchanged. Therefore, provided the previously mentioned boundedness conditions are satisfied, the walk type only depends on the graph topology.

Moreover, even the local topological details are irrelevant to determining the type of a graph. Indeed, it is possible to show that recurrence and transience are left invariant by adding and cutting of links satisfying the *quasi-isometry* conditions. More precisely, two graphs $\mathcal{G}$ and $\mathcal{G}'$ are called *quasi-isometric* if there are a mapping $\varphi : \mathcal{G} \to \mathcal{G}'$ and constants $A > 0$, $B \geqslant 0$ such that

$$A^{-1} r_{ij} - B \leqslant r'_{\varphi i,\varphi j} \leqslant A r_{ij} + B$$

for all $i, j \in \mathcal{G}$, and

$$r'_{i',\varphi\mathcal{G}} \leqslant B$$

for every $i' \in \mathcal{G}'$.

If $B = 0$ then we say that $\mathcal{G}$ and $\mathcal{G}'$ are *metrically equivalent*. Quasi-isometries can be defined between arbitrary metric spaces and represent the most general local topology deformations. Typical examples of them are given by the decimation transformations used on fractals and in real-space renormalization. In some sense, we can consider quasi-isometries as their extension to general networks.

All results presented so far refer to random walks without traps, i.e. to jumping probabilities given by (15) with $d_i = 0$. The introduction of at least one trap, setting $d_i > 0$ for at least one site i, has a very general and simple influence on the random walk behaviour: indeed transience is left unchanged, while recurrent random walks always become transient.

9. The local spectral dimension

As well as happening for recurrence and transience properties, large-scale topology affects the long time dependence of random walk quantities on infinite graphs. Indeed, it has been known for many years that, on regular (translation invariant) lattices, the exponents of the asymptotic power laws of random walks only depend on the lattice (Euclidean) dimension d. For example,

$$P_{ii}(t) \sim t^{-d/2} \qquad \text{for} \quad t \to \infty, \quad \forall i \tag{65}$$

and

$$S_i(t) \sim t^{\min(1,d/2)} \qquad \text{for} \quad t \to \infty, \quad \forall i, \qquad \text{for} \quad d \neq 2 \tag{66}$$

(while, for $d = 2$, $S_i(t) \sim t/\ln t$). As we mentioned before, these laws typically present power behaviour even on general physical graphs, and the exponents of such powers can be used to define a generalized dimension.

Let us consider a random walk without waitings and traps satisfying (49), and suppose that, for a given $i \in \mathcal{G}$

$$P_{ii}(t) \sim t^{-\widetilde{d}/2} \qquad \text{for} \quad t \to \infty \tag{67}$$

then it can be shown that

$$P_{hk}(t) \sim t^{-\widetilde{d}/2} \qquad \text{for} \quad t \to \infty, \quad \forall h, k \tag{68}$$

(for bipartite graphs, the usual assumptions on the parity t are understood). This means that the exponent of the power law is site independent and, therefore, it is a parameter characterizing the whole random walk. Since $\widetilde{d} = d$ on a regular lattice, we can consider it as a dimension associated with the random walk on $\mathcal{G}$. More precisely, we shall call *local spectral dimension* the limit

$$\widetilde{d} = -2 \lim_{t\to\infty} \frac{\ln P_{ii}(t)}{\ln t} \tag{69}$$

when it exists.

Note that the existence of this limit for a given i implies it exists and has the same value for any $j \in \mathcal{G}$. Moreover, the definition given in (69) is more general than (67), since it includes the case of possible multiplicative corrections to the asymptotic behaviour, provided they are slower than any power law (e.g. logarithmic corrections).

From a historical point of view, the term 'spectral dimension' was first introduced by Alexander and Orbach in 1982 [8], studying the anomalous vibrational dynamics on fractals. In the same work, they suggested that even the random walks should be ruled by the same parameter and wrote equation (67). Then the definition was generalized to general networks by Hattori, Hattori and Watanabe [9]. Later, it was shown that the anomalous dimension involved in vibrational dynamics is the *average spectral dimension* [10] we shall discuss in further sections, which coincides with $\widetilde{d}$ only for particular graphs, such as exactly decimable fractals.

As for the existence of the limit (69), a general theorem is still lacking, but it can be easily proven that the asymptotic decay of $P_{ii}(t)$ is always bounded from above and from below by power laws. In any case, on all known cases of random walks on physical graphs, the local spectral dimension has been shown to exist. Note that for the Bethe lattice, which does not fulfil the polynomial growth condition, the limit (69) is infinite. From now on, we shall consider random walks on graphs where $\widetilde{d}$ is defined. Then, one can easily derive the following results:

- Random walks are recurrent if $\widetilde{d} < 2$ and transient if $\widetilde{d} > 2$. For $\widetilde{d} = 2$, if (67) holds, random walks are recurrent. However, subleading corrections to the power law can change the type to transient.
- When (67) holds,

$$S_i(t) \sim t^{\min(1,\widetilde{d}/2)} \qquad \text{for} \quad t \to \infty, \quad \forall i, \quad \text{for} \quad \widetilde{d} \neq 2 \tag{70}$$

otherwise, in general,

$$\lim_{t\to\infty} \frac{\ln S_i(t)}{\ln t} = \min(1, \widetilde{d}/2) \qquad \forall i, \quad \text{for} \quad \widetilde{d} \neq 2. \tag{71}$$

- When (67) holds,

$$F_{ij}(t) \sim t^{\min(\widetilde{d}/2-2,-\widetilde{d}/2)} \qquad \text{for} \quad t \to \infty, \quad \forall i, j \quad \text{for} \quad \widetilde{d} \neq 2 \tag{72}$$

otherwise, in general,

$$\lim_{t\to\infty} \frac{\ln F_{ij}(t)}{\ln t} = \min(\widetilde{d}/2 - 2, -\widetilde{d}/2) \qquad \forall i, j \quad \text{for} \quad \widetilde{d} \neq 2. \tag{73}$$

The case $\widetilde{d} = 2$ is rather particular. Indeed $\widetilde{d} = 2$ is a critical dimension for random walks, discriminating recurrence from transience. The asymptotic behaviour of $S_i(t)$ and $F_{ij}(t)$ have a different dependence on $\widetilde{d}$ for $\widetilde{d} < 2$ and $\widetilde{d} > 2$. In particular, the probability of the first visit has the same time decay of P_{ij} for $\widetilde{d} > 2$ while it decays faster for $\widetilde{d} < 2$. When $\widetilde{d} = 2$, the behaviour of $S_i(t)$ and $F_{ij}(t)$ is strongly affected by subleading corrections.

As for the type problem, local spectral dimension presents interesting invariance properties. First of all, it can be shown that waitings satisfying (50) do not affect its value [10]. Moreover, for $\widetilde{d} < 2$, on a given $\mathcal{G}$ it is the same for all ferromagnetic couplings satisfying (49) [9]. Unfortunately, an analogous result has not been proven for $\widetilde{d} > 2$. However, we will see in later sections that the *average spectral dimension* also has this universality property.

The introduction of a finite number of traps does not affect $\widetilde{d}$ if $\widetilde{d} > 2$. If $\widetilde{d} < 2$ a finite number of traps (even only one) changes $\widetilde{d}$ to $\widetilde{d} + 1$. If the traps are infinite the behaviour is more complex and depends on their distribution.

10. Averages on infinite graphs

Usually, infinite graphs describing real systems are inhomogeneous, i.e., in mathematical terms, they are not invariant with respect to a transitive symmetry group. In simpler words, this means that the topology is seen in a different way from every site. The main effect of inhomogeneity is that the numerical values of physical quantities are site dependent. Therefore, one is typically interested in taking averages over all sites. This requires the introduction of suitable mathematical tools.

First of all, the average in the thermodynamic limit $\bar{\phi}$ of a function ϕ_i defined on each site i of the infinite graph $\mathcal{G}$ is defined by

$$\bar{\phi} \equiv \lim_{r\to\infty} \frac{\sum_{i\in S_{o,r}} \phi_i}{N_{o,r}}. \tag{74}$$

The measure $|S|$ of a subset S of V is the average value $\overline{\chi(S)}$ of its characteristic function $\chi_i(S)$ defined by $\chi_i(S) = 1$ if $i \in S$ and $\chi_i(S) = 0$ if $i \notin S$. The measure of a subset of links $E' \subseteq E$ is given by

$$|E'| \equiv \lim_{r\to\infty} \frac{E'_r}{N_{o,r}}, \tag{75}$$

where E'_r is the number of links of E' contained in the sphere $S_{o,r}$. The normalized trace $\overline{\mathrm{Tr}}B$ of a matrix B_{ij} is

$$\overline{\mathrm{Tr}}\, B \equiv \overline{b}, \tag{76}$$

where $b_i \equiv B_{ii}$. If condition (c) holds, then we can prove [13] that the averages of a bounded from below function ϕ_i are independent of the centre o of the spheres sequence, using the fact that $\chi_i(S)$ is bounded and that measures of subsets are always well defined.

Now, due to this site independence, we have a good definition of averages which we will use in dealing with properties of random walks on infinite graphs. As we shall see in the next section, on inhomogeneous networks the averages of site dependent functions can have a very different behaviour from their local counterparts, giving rise to rather unexpected phenomena.

11. The type problem on the average

In the last few years it has become clear that bulk properties are affected by the average values of random walk return probabilities over all starting sites: this is the case for spontaneous breaking of continuous symmetries [11], critical exponents of the spherical model [12] and harmonic vibrational spectra [10]. Therefore the classification of discrete structure in terms of *recurrence on the average* and *transience on the average* appears to be the most suitable. Unfortunately, while for regular lattices the two classifications are equivalent, on more general networks they can be different and one has to study a type problem on the average [13].

This is defined using the return probabilities on the average $\bar{P}$ and $\bar{F}$, which are given by

$$\bar{P} = \lim_{\lambda\to 1^-} \overline{\tilde{P}(\lambda)} \equiv \lim_{\lambda\to 1^-} \overline{\mathrm{Tr}}\, \tilde{P}(\lambda) \tag{77}$$

$$\bar{F} = \lim_{\lambda\to 1^-} \overline{\tilde{F}(\lambda)} \equiv \lim_{\lambda\to 1^-} \overline{\mathrm{Tr}}\, \tilde{F}(\lambda). \tag{78}$$

A graph $\mathcal{G}$ is called *recurrent on the average* (ROA) if $\bar{F} = 1$, while it is *transient on the average* (TOA) when $\bar{F} < 1$.

Recurrence and transience on the average are in general independent of the corresponding local properties. The first example of this phenomenon occurring on inhomogeneous structures was found in a class of infinite trees called NTD (see section 13.3) which are locally transient but recurrent on the average [14].

Moreover, while for local probabilities (26) gives

$$\tilde{P}_{ii}(\lambda)\tilde{F}_{ii}(\lambda)\tilde{P}_{ii}(\lambda) + 1 \tag{79}$$

an analogous relation for (78) and (77) does not hold since averaging (79) over all sites i would involve the average of a product, which due to correlations is in general different from the product of the average. Therefore the double implication $\tilde{F}_i(1) = 1 \Leftrightarrow \lim_{\lambda\to 1} \tilde{P}_i(\lambda) = \infty$ is not true. Indeed there are graphs for which $\bar{F} < 1$ but $\bar{P} = \infty$ (an example is shown in figure 1) and the study of the relation between $\bar{P}$ and $\bar{F}$ is a non-trivial problem.

A detailed study of this relation [13] shows that a complete picture of the behaviour of random walks on graphs can be given by dividing the transient on the average graphs into two further classes, which are called *pure* and *mixed* transients on the average (TOA).

First, considering a ROA graph, it can be proven that if $\bar{F} = 1$ then $\bar{P} = \infty$. The proof can be easily generalized to graphs in which there is a positive measure subset S such that: $\lim_{\lambda\to 1} \overline{\chi(S)\tilde{F}(\lambda)} = |S|$. Indeed in an analogous way it can be proven that

$$\bar{P} \geqslant \lim_{\lambda\to 1} \overline{\chi(S')\tilde{P}(\lambda)} = \infty \qquad \forall S' \subseteq S, |S'| > 0. \tag{80}$$

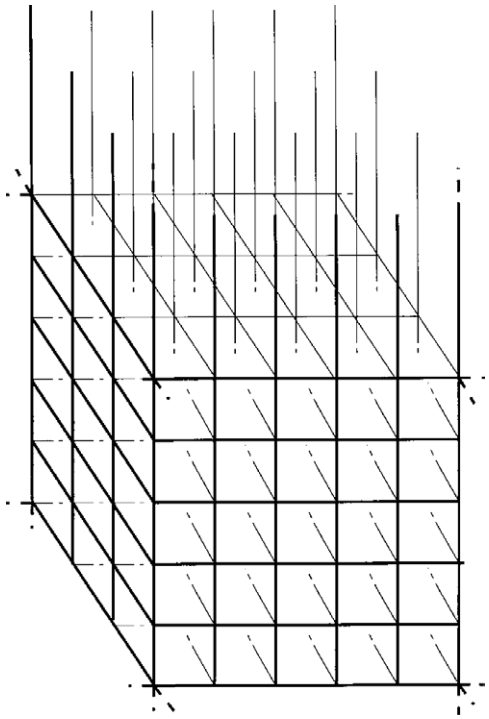

Figure 1. The 'haired cube' graph.

We call *mixed* transient on the average a TOA graph having a positive measure subset S such that

$$\lim_{\lambda\to 1}\overline{\chi(S)\tilde{F}(\lambda)} = |S|, \tag{81}$$

while a graph is called *pure* TOA if

$$\lim_{\lambda\to 1}\overline{\chi(S)\tilde{F}(\lambda)} < |S| \qquad \forall S \subseteq V, |S| > 0. \tag{82}$$

Examples of pure TOA graphs are all the d-dimensional cubic lattices with $d > 2$, while the 'haired cube' of figure 1 is a typical mixed TOA graph. Note that a relevant theorem [13] establishes that for mixed TOA graphs we have $\bar{P} = \infty$, while for pure TOA graphs $\bar{P}$ is finite. A further important property, characterizing mixed TOA graphs, allows us to simplify the study of statistical models on these very inhomogeneous structures. It can be shown [13] that, in this case, the graph $\mathcal{G}$ can always be decomposed into a pure TOA subgraph $\mathcal{S}$ and a ROA subgraph $\bar{\mathcal{S}}$ with independent jumping probabilities by cutting a zero measure set of links $\partial\mathcal{S} \equiv \{(i, j) \in E | i \in \mathcal{S}\, j \in \bar{\mathcal{S}}\}$. The separability property implies that the two subgraphs are statistically independent and that their thermodynamic properties can be studied separately. Indeed, in the thermodynamic limit, the partition functions referring to the two subgraphs factorize [15].

To conclude this section, we note that the same invariance properties of the local type problem under addition of waiting probabilities, coupling rescaling and quasi-isometries still hold for the type problem on the average. This means, as for the local case, that recurrence and transience on the average are intrinsic properties of a graph and not only of a specific random walk defined on it. On the other hand, the introduction of a finite number of traps does

not change the type on the average. Note also that a slightly different definition of the type problem on the average can be found in the mathematical literature [16]; it is more convenient for the formal development of the theory, but it is not directly related to statistical models on graphs.

12. The average spectral dimension

The asymptotic time dependence of the return probability on the average can be used to define a new intrinsic dimension which turns out to be very strictly related to the physical behaviour of statistical models on graphs [11, 10, 17], as we will briefly discuss in the last section.

Indeed, even if the asymptotic time decay of $P_{ii}(t)$ is always the same for all sites i, when the graph topology is strongly inhomogeneous it happens that its average over all the sites decays according to a different law. The average spectral dimension $\bar{d}$ is defined for physical graphs, such as the local one in (67) and (69), by

$$\bar{P}(t) \sim t^{-\bar{d}/2} \qquad \text{for} \quad t \to \infty \tag{83}$$

when the asymptotic behaviour is a power law without subleading corrections, or, more generally, by

$$\bar{d} = -2 \lim_{t\to\infty} \frac{\ln \bar{P}(t)}{\ln t}. \tag{84}$$

Note, however, that, differently from the local case, no physical graphs are known, up to now, where the long time decay is not given by (83). Considerations analogous to those presented for the local case hold here, concerning the existence of the limit (84). Obviously, in all cases where the local type is different from the average type, also the local spectral dimension differs from the average spectral dimension. A typical example, and, historically, the first one, is given again by NTD (see section 13.3 for a detailed account). However, the relations between $\bar{d}$ and the type problem on the average are not the same as in the local case. Indeed, while if $\bar{d} > 2$ the walk is always pure TOA, random walks with $\bar{d} < 2$ can be either pure ROA or mixed TOA.

The most relevant property of $\bar{d}$ is without any doubt its strong invariance with respect to a very large class of dynamical and topological transformations, making it a unique universal parameter associated with a graph $\mathcal{G}$ [10, 18].

These transformations can be divided into three main classes:

1. *Dynamical transformations leaving the graph topology unchanged.* These consist in the addition of waitings and of a finite number of traps, as well as in bounded local rescaling of ferromagnetic couplings.
2. *Topological transformations modifying the number of links but leaving the sites unchanged.* These include 'addition transformations' and 'cutting transformations'. The addition transforms consist in adding links joining sites up to an arbitrary but finite chemical distance from any site, while the cutting transforms are defined to be their inverse. The most general transformations consist in a combination of addition and cutting. Note that even an infinite number of links can be modified with respect to the original graph.
3. *Topological rescaling, i.e. topological transformations modifying both links and sites.* The most general topological rescaling can be realized through two independent steps. The first one is *partition* and consists in dividing the graph $\mathcal{G}$ into an infinite family of connected subgraphs $\mathcal{G}_\alpha$, with uniformly bounded number of points. The second one is *substitution* and consists in generating a new graph $\mathcal{G}'$ by replacing some or all $\mathcal{G}_\alpha$ by a

different (connected) graph $\mathcal{S}_\alpha$, whose number of points ranges from 1 to a fixed $N_{\max}$, and by adding links connecting different $\mathcal{S}_\alpha$ in such a way that two generic $\mathcal{S}_\alpha$ and $\mathcal{S}_\beta$ are connected by some links if and only if $\mathcal{G}_\alpha$ and $\mathcal{G}_\beta$ were. The simplest topological rescaling occurs when every $\mathcal{S}_\alpha$ is composed by just one point. In this case the resulting graph $\mathcal{G}_{\Downarrow}$ is called the *minimal structure* of the partition $\{\mathcal{G}_\alpha\}$.

These three very general classes of geometrical transformations (together with even more general ones violating conditions (b) and (c) and therefore not discussed here [18]) can be applied in all possible sequences to a graph, leading to an overall transformation of coupling strength, number of links and degrees of freedom which does not change its spectral dimension $\bar{d}$. We will call such a transformation an *isospectrality*.

Note that isospectralities include quasi-isometries as a particular case. Indeed, isospectralities include most currently used transformations.

As an example, the usual decimation procedure on fractals is a topological rescaling. In particular, for all exactly decimable fractals (such as e.g. Sierpinski gaskets and T-fractals, as discussed in the next sections), the minimal structure of the graph coincides with the graph itself. Again, an isospectrality relates the usual two-dimensional square lattice, the hexagonal lattice and the triangular lattice, which therefore all have dimension 2. In other words, isospectralities are the theoretical formalization of the intuitive idea of invariance with respect to bounded scale perturbations and disorder and the *isospectrality classes*, defined as the classes of graphs related by such transformations, are the practical realization of the apparently abstract concept of non-integer dimension.

Now, since most dynamical and thermodynamical properties of generic discrete structures depend only on $\bar{d}$, isospectralities provide a very powerful tool to reduce a very complicated geometrical structure to the simplest one having the same $\bar{d}$. The latter turns out to be much simpler to study and still presents the same universal properties.

Moreover, an isospectrality can not only be used to reduce and simplify structures and problems, it can also be applied, with the opposite aim, to build complicated structures with controlled dynamical and thermodynamical properties, starting from simple deterministic geometrical models. This is the point of view of *spectral dimension engineering*, providing a very interesting field of possibilities to polymer physicists and material scientists dealing with non-crystalline materials. In figure 2 we give explicit examples of isospectral structures obtained by applying isospectral transformations (without long range couplings) to the T-fractal and to the square lattice.

On macroscopically inhomogeneous graphs, it can happen that the average value of $P_{ii}(t)$ on infinite subgraphs of $\mathcal{G}$ with positive measure decays with a power law different from (83) [19]. In such cases, it is interesting to look for the maximal (positive-measure) subgraphs having no (positive measure) parts with different power law decay. These are called *spectral classes* and each is characterized by its own spectral dimension. A theorem rather relevant in physical applications establishes that spectral classes can be separated from each other by cutting a zero-measure set of links, implying the same statistical independence property we discussed for mixed TOA graphs [19].

13. A survey of analytical results on specific networks

Apart from the well-known case of regular lattices, where it is completely solved [20], the random walk problem has been studied analytically only on some specific classes of infinite graphs. In these cases, one usually focuses on the asymptotic properties of random walk autocorrelation functions and on the calculation of the local and average spectral dimension.

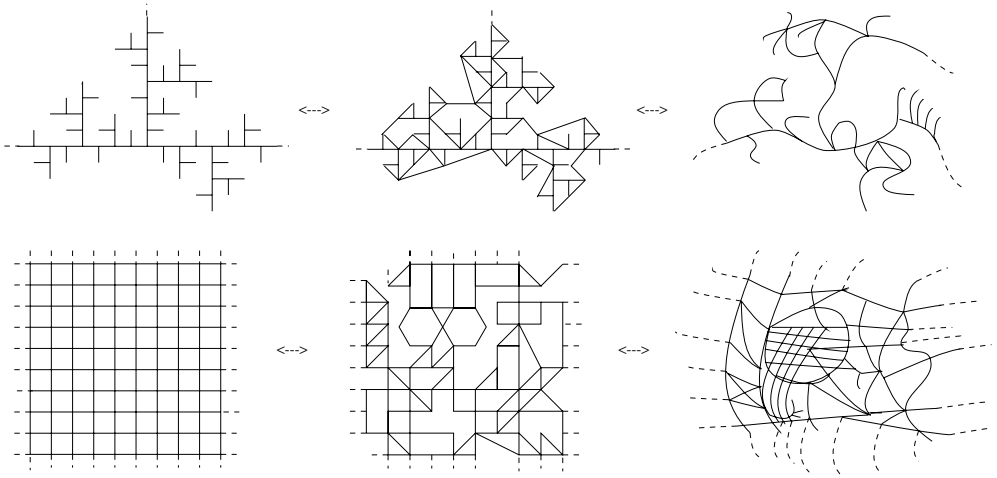

Figure 2. Example of isospectral structures obtained applying isospectral transformations to the *T*-fractal and to the square lattice.

As we discussed in previous sections, these are the most important quantities in statistical physics and thermodynamics. On lattices, the random walk problem is solved by using the translation invariance of the structure, and this allows us to apply powerful mathematical tools, such as the Fourier transform. On general graphs these methods do not apply. Therefore due to the lack of translation invariance, one has to introduce new and alternative techniques, which can be grouped into three main classes: renormalization techniques, combinatorial techniques and mixed techniques. In the next subsections we will review recent and significant results obtained with these techniques.

13.1. Renormalization techniques

Renormalization techniques have been successfully applied to deterministic fractal networks, where one can take advantage of the decimation transformations which connect two consecutive generations. In particular, a well-studied class of fractals is that of *exactly decimable* fractals. On these structures, exact renormalization group calculations based on a real space decimation procedure allow us to obtain all the relevant random walk quantities.

Let us consider a random walk without traps and sources defined by the jumping probabilities (4) and let us write the master equation for the probability P_{0i} of being at site i after t steps for a random walker starting from an origin site 0 at time 0:

$$P_{0i}(t+1) - P_{0i}(t) = \sum_j A_{0j}\left(\frac{P_{0j}(t)}{z_j} - \frac{P_{0j}(t)}{z_i}\right) + \delta_{i0}\delta_{t0}. \tag{85}$$

Equation (85) can be written in terms of the generating function $\widetilde{P}_{ij}(\lambda)$ when $\lambda \to 1^-$ by setting $\lambda = 1 - \epsilon$, writing

$$\widetilde{P}_{ij}(\epsilon) = \sum_{t=0}^{\infty}(1+\epsilon)^{-t} P_{ij}(t) \tag{86}$$

and taking $\epsilon =\!\!\rightarrow 0$:

$$\epsilon\widetilde{P}_{0i}(\epsilon) = \sum_j A_{0j}\left(\frac{\widetilde{P}_{0j}(\epsilon)}{z_j} - \frac{\widetilde{P}_{0j}(\epsilon)}{z_i}\right) + \delta_{0i}. \tag{87}$$

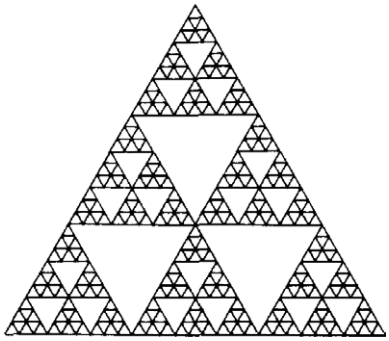

Figure 3. The Sierpinski gasket.

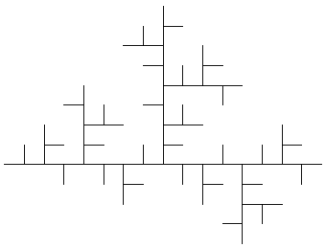

Figure 4. The *T*-fractal.

Note that the system (87) is inhomogeneous and corresponds to a Cauchy problem, which has only one solution. The behaviour of such a solution for $\epsilon \to 0$ is what we need to obtain the local spectral dimension $\widetilde{d}$, as defined in (67), through the Tauberian theorems. On the other hand, to calculate the average spectral dimension $\bar{d}$ we will need to average over all starting points the solution of equation (87), strongly modifying its asymptotic behaviour on inhomogeneous graphs, as we will see in the following.

Exactly decimable fractals are a restricted class of self-similar structures (i.e. not all self-similar structures are exactly decimable) which are geometrically invariant under site decimation. This invariance is explicitly applied in analytical calculations for random walks. A geometrical structure is decimation invariant if it is possible to eliminate a subset of points (and all the bonds connecting these points) obtaining a network with the same geometry as the starting one. From a mathematical point of view this corresponds to the possibility of eliminating by substitution a set of equations from system (85) or (87) obtaining a system which is similar to the initial one after a suitable redefinition of the coupling parameters. Examples of exactly decimable fractals are the Sierpinski gasket (figure 3) [25–28], the *T*-fractal, shown in figure 4 [29, 30], the branched Koch curves, shown in figure 5 [31]. In general, all deterministic finitely-ramified fractals are exactly decimable. Note that the exact decimation is a particular case of isospectrality, as we discussed in previous sections.

Let us consider now the general procedure to decimate the set of equation (85). After eliminating a set of points and substituting the corresponding equation, one finds

$$\epsilon \to \epsilon'(\epsilon) \sim a^2\epsilon. \tag{88}$$

The presence of the term δ_{i0} in (87) requires a redefinition of the quantities $\widetilde{P}_{ij}(\epsilon)$ to assure that, even after the decimation, the initial condition will correspond to the probability of being

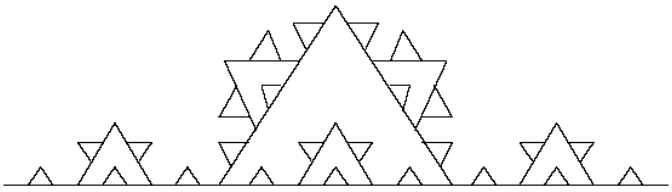

Figure 5. The branched Koch curve.

at a fixed site equal to 1. One introduces a new parameter c and writes the transformation law for $\widetilde{P}_{ij}(\epsilon)$ as

$$\widetilde{P}_{ij}(\epsilon) \to \widetilde{P}'_{ij}(\epsilon') \sim \frac{1}{c}\widetilde{P}_{ij}(\epsilon). \tag{89}$$

From the rescaling of ϵ and $\widetilde{P}_{ij}(\epsilon)$, the local spectral dimension $\widetilde{d}$ is obtained by using a suitable expression for $\widetilde{P}_{00}(\epsilon)$:

$$\widetilde{P}_{00}(\epsilon) \sim \epsilon^{\widetilde{d}/2-1}, \tag{90}$$

which holds only for $\widetilde{d} < 2$. This is always the case for exactly decimable fractals. Using expression (90) one easily finds

$$\widetilde{d} = 2\frac{\log a^2/c}{\log a^2}. \tag{91}$$

As for the average spectral dimension $\bar{d}$, by using the relation between equation (87) and the equation for harmonic oscillations to be discussed later [21], one has that

$$\bar{d} = \frac{\log r}{\log a}, \tag{92}$$

where r is the decimation ratio used in the renormalization procedure. Therefore $\widetilde{d} = \bar{d}$ if

$$r = a^2/c. \tag{93}$$

This can be shown to be the case for all exactly decimable fractals, using results obtained [9] for the Gaussian model.

Equation (92) allows us to calculate the spectral dimension on all exactly decimable fractals, once the decimation procedure is identified, recovering known results.

One of the most studied fractals is without any doubt the Sierpinski gasket [25–28] and its generalizations. For the simplest case one has $r = 3$ and $a = \sqrt{5}$, leading to

$$\widetilde{d} = 2\frac{\log 3}{\log 5}. \tag{94}$$

For d-dimensional generalized Sierpinski gaskets, which are built from a d-dimensional hypertetrahedron of side length b filled with b layers of smaller hypertetrahedra of unit site length, Hilfer and Blumen [26] have shown that for $b = 2$

$$\widetilde{d} = 2\frac{\log d + 1}{\log d + 3} \tag{95}$$

and for $b = 3$

$$\widetilde{d} = 2\frac{\log((d+1)(d+2)/2)}{\log((d+2)(2d^2+9d+19)/(4d+6))}. \tag{96}$$

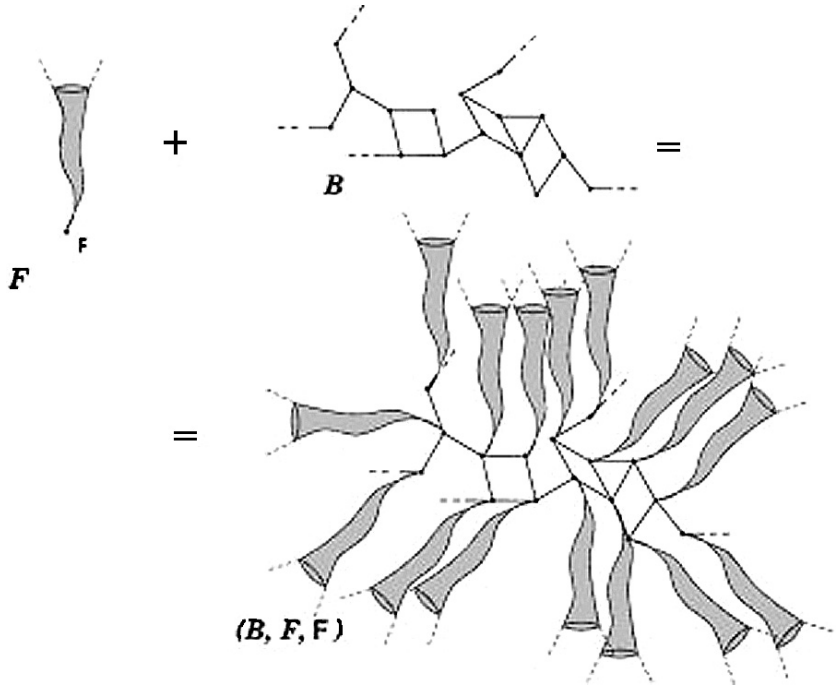

Figure 6. Building process of a bundled graph.

Due to the self-similarity of the structure, the return probabilities on the Sierpinski gasket show a remarkable effect, which has been pointed out in [32]. Indeed, the coefficients have an oscillatory behaviour, which is given by

$$P_{00}(t) = t^{-\widetilde{d}/2} F\left(\frac{\log t}{\log 5}\right), \tag{97}$$

where F is a periodic C^∞-function of period 1 whose Fourier series is given by

$$F(x) = \sum_{k=-\infty}^{\infty} \Gamma\left(1 - \frac{\log 3}{\log 5} + \frac{2\pi k \mathrm{i}}{\log 5}\right)^{-1} \exp(2\pi k \mathrm{i}\, x). \tag{98}$$

Interestingly, it can be shown that the oscillation of the coefficients disappears in the probability of return on the average.

The renormalization techniques can be applied to all exactly decimable fractals. For example, for the T-fractal [29, 30], which is a particular case of hierarchical combs [33], one has $r = 3$ and $a = \sqrt{6}$.

13.2. Combinatorial techniques

Renormalization procedures cannot be applied on non-self-similar graphs. Therefore one has to develop alternative techniques to study the random walk problem. This is the case of bundled structures [22, 23], a large class of very interesting graphs used in condensed matter as realistic models for the geometry and dynamics of polymers and other inhomogeneous systems. Given two graphs $\mathcal{B}$ and $\mathcal{F}$, not necessarily different, and a site F of $\mathcal{F}$, we call a bundled graph with base $\mathcal{B}$ and fibre $\mathcal{F}$ the graph built by joining to each site of $\mathcal{B}$ a copy of $\mathcal{F}$ in such a way that F is the only site $\mathcal{B}$ and $\mathcal{F}$ have in common (figure 6). Examples

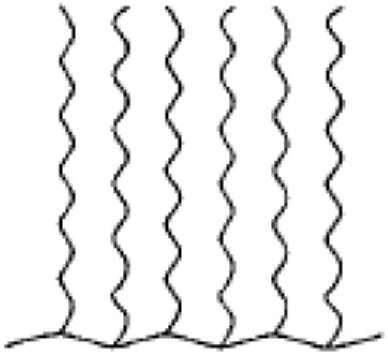

Figure 7. A comb polymer.

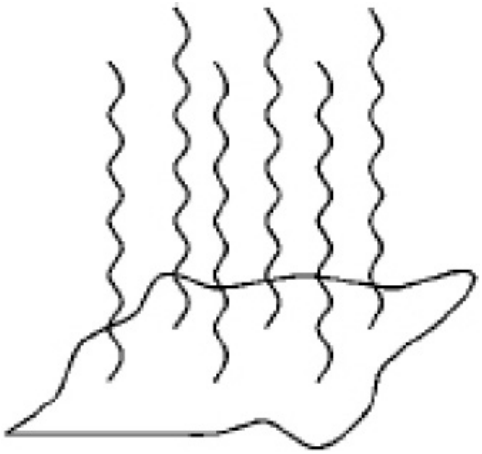

Figure 8. A brush polymer.

of bundled structures are comb polymers [34] (figure 7), brush polymers, shown in figure 8, and many kinds of branched aggregates (figure 9). For these graphs a purely combinatorial technique allows us to calculate the asymptotic properties of the random walk autocorrelation functions.

Let us consider a walker starting from a point belonging to the base and let us restrict ourselves to base graphs with constant coordination number $z_{\mathcal{B}}$. By decomposing the motion of the walker on the fibre and on the base, one can obtain

$$P_0(t) = \sum_{t_{\mathcal{B}}=0}^{\infty} \sum_{t_1=0}^{\infty} \cdots \sum_{t_{\mathcal{B}}+1=0}^{\infty} P_{\mathcal{B}}(t_{\mathcal{B}}) \left(\frac{z_{\mathcal{B}}}{z_{\mathcal{B}} + z_F} \right)^{t_{\mathcal{B}}} P'_{\mathcal{F}}(t_1) \cdots P'_{\mathcal{F}}\big(t_{t_{\mathcal{B}}+1}\big) \delta_{t, t_{\mathcal{B}} + \sum_{i=1}^{t_{\mathcal{B}}+1} t_i}, \tag{99}$$

where $P'_{\mathcal{F}}$ refers to a random walk on $\mathcal{F}$ with a trap at the starting point of $\mathcal{F}$. In terms of the generating functions equation, (99) becomes

$$\widetilde{P}_0(\lambda) = \sum_{t_{\mathcal{B}}=0}^{\infty} P_{\mathcal{B}}(t_{\mathcal{B}}) \left(\frac{\lambda z_{\mathcal{B}}}{z_{\mathcal{B}} + z_F} \right)^{t_{\mathcal{B}}} (\widetilde{P}'_{\mathcal{F}}(\lambda))^{t_{\mathcal{B}}+1} = \widetilde{P}'_{\mathcal{F}}(\lambda) \widetilde{P}_{\mathcal{B}}(\lambda') \tag{100}$$

with

$$\lambda' \equiv \frac{\lambda z_{\mathcal{B}}}{z_{\mathcal{B}} + z_F} \widetilde{P}'_{\mathcal{F}}(\lambda) \tag{101}$$

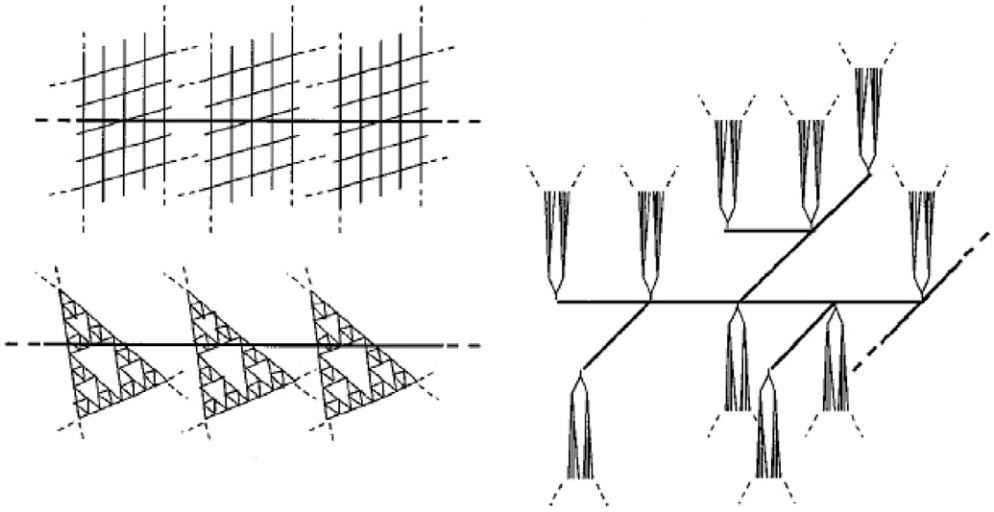

Figure 9. Further examples of bundled graphs.

and

$$\widetilde{P}'_{\mathcal{F}}(\lambda) = \left(1 - \frac{z_F}{z_{\mathcal{B}} + z_F}(1 - (\widetilde{P}_{\mathcal{F}}(\lambda))^{-1})\right)^{-1} \tag{102}$$

with $\widetilde{P}_{\mathcal{F}}(\lambda)$ being the generating function of the probability of returning to the starting point F on $\mathcal{F}$ without the trap. From these relations one obtains the values for the local spectral dimension on general bundled graphs:

$$\widetilde{d} = \begin{cases} \widetilde{d}_{\mathcal{F}} & \text{if} \quad \widetilde{d}_{\mathcal{F}} \geqslant 2 \\ 4 - \widetilde{d}_{\mathcal{F}} & \text{if} \quad \widetilde{d}_{\mathcal{F}} \leqslant 2 \text{ and } \widetilde{d}_{\mathcal{B}} \geqslant 4 \\ \widetilde{d}_{\mathcal{F}} + \widetilde{d}_{\mathcal{B}} - \frac{\widetilde{d}_{\mathcal{F}}\widetilde{d}_{\mathcal{B}}}{2} & \text{if} \quad \widetilde{d}_{\mathcal{F}} \leqslant 2 \text{ and } \widetilde{d}_{\mathcal{B}} \leqslant 4, \end{cases} \tag{103}$$

where $\widetilde{d}_{\mathcal{B}}$ and $\widetilde{d}_{\mathcal{F}}$ are the local spectral dimensions of the base and of the fibre. If the coordination number of the base is not constant, it can be shown that this amounts to introducing waiting probabilities on the points connecting the fibre and the base, which, as shown in the previous section, does not change the value of the spectral dimension.

As for the average spectral dimension, it is easy to show that if the fibre is an infinite graph, the average spectral dimension of the whole graph is the spectral dimension of the fibre. On the other hand, if the fibre is a finite graph, the average spectral dimension coincides with that of the base.

From equations (100), (102) one also obtains the asymptotic laws for the probability of returning to the starting point, which on these structures can contain logarithmic corrections. Indeed, writing

$$P_0(t) \sim \prod_{i=0}^{\infty} {}^{i} \ln^{\beta(i)}(t) \tag{104}$$

and setting

$$m = \min\{i \geqslant 0 | \beta(i) \neq -1\} \tag{105}$$

and

$$I(\widetilde{d}/2) = \begin{cases} 1 & \text{if} \quad \widetilde{d}/2 \text{ is an integer} \\ 0 & \text{otherwise} \end{cases} \tag{106}$$

one has

(a) if $\widetilde{d}_{\mathcal{B}} < 4$ and $\widetilde{d}_{\mathcal{F}} < 2$

$$\beta(i) = \begin{cases} -1 & \text{for} \quad 0 < i < m \\ \left(1 - \frac{\widetilde{d}_{\mathcal{B}}}{2}\right)\left[\beta_{\mathcal{F}}(m_{\mathcal{F}}) + I\left(\frac{\widetilde{d}_{\mathcal{F}}}{2}\right)\right] - I\left(\frac{\widetilde{d}_{\mathcal{F}}}{2}\right) & \text{for} \quad i = mm_{\mathcal{F}} \\ \left(1 - \frac{\widetilde{d}_{\mathcal{B}}}{2}\right)\beta_{\mathcal{F}}(i) + \theta(i - m_{\mathcal{F}} - m_{\mathcal{B}})\beta_{\mathcal{B}}(i - m_{\mathcal{F}}) & \\ \quad + \delta_{i-m_{\mathcal{F}},m_{\mathcal{B}}} I\left(\frac{\widetilde{d}}{2}\right) - \delta_{i,m} I\left(\frac{\widetilde{d}}{2}\right) & \text{otherwise,} \end{cases} \tag{107}$$

where $m_{\mathcal{B}}$ and $m_{\mathcal{B}}$ refer to the base and to the fibre respectively while m refers to the whole graph and is determined by

$$m = m_{\mathcal{F}} + \delta_{\widetilde{d}_{\mathcal{B}},2} m_{\mathcal{B}}. \tag{108}$$

(b) If $\widetilde{d}_{\mathcal{B}} > 4$ and $\widetilde{d}_{\mathcal{F}} < 2$

$$\beta(i) = \begin{cases} -\beta_{\mathcal{F}}(i) - 2\delta_{i,m_{\mathcal{F}}} I(\widetilde{d}_{\mathcal{F}}/2) & \text{for} \quad i \geqslant m_{\mathcal{F}} \\ \beta_{\mathcal{F}}(i) & \text{for} \quad 0 < i < m_{\mathcal{F}}. \end{cases} \tag{109}$$

(c) If $\widetilde{d}_{\mathcal{B}} = 4$ and $\widetilde{d}_{\mathcal{F}} < 2$ and $d_{\mathcal{B}} > -1$,
$\beta(i)$ has to be determined as in (a).

(d) If $\widetilde{d}_{\mathcal{B}} = 4$ and $\widetilde{d}_{\mathcal{F}} < 2$ and $m_{\mathcal{B}} < -1$,
$\beta(i)$ has to be determined as in (b).

(e) If $\widetilde{d}_{\mathcal{F}} > 2$

$$\beta(i) = \beta_{\mathcal{F}}(i) \quad \forall i. \tag{110}$$

The case $\widetilde{d}_{\mathcal{F}} = 2$ has to be treated separately, as the case $\widetilde{d}_{\mathcal{F}} < 2$ if the fibre is a recurrent graph or as the case $\widetilde{d}_{\mathcal{F}} > 2$ if it is transient.

Another interesting way of combining two graphs to obtain a more complex structure is the *Cartesian product*. The Cartesian product of two graphs X, Y has the vertex set $X \times Y$, and two pairs $xy, x'y'$ are adjacent if $x \sim x'$ and $y = y'$, or $x = x'$ and $y \sim y'$. An example of an interesting Cartesian product is that of the Toblerone graph [35], shown in figure 10, which is obtained from the product of a line with a Sierpinski gasket. Using combinatorial techniques analogous to those presented for bundled graphs, it can be shown that the local and the average spectral dimensions on the whole graph are the sums of the corresponding dimensions of the two initial graphs [7].

13.3. Mixed techniques

The random walk problem in some very interesting cases of graphs cannot be studied simply by one of the above cited techniques and it requires instead a 'mixed' use of the two, which gives rise to very interesting phenomena. Indeed, the first example of a difference between the local and the average spectral dimension, the 'dynamical dimension splitting', was observed on the quasi-self-similar graphs NT_D, where the asymptotic properties of the random walk were found by a mixed technique [14].

The fractal trees known as NT_D [36] can be recursively defined as follows: an origin point O (figure 11) is connected to a point 1 by a link, of unitary length; from 1, the tree splits into

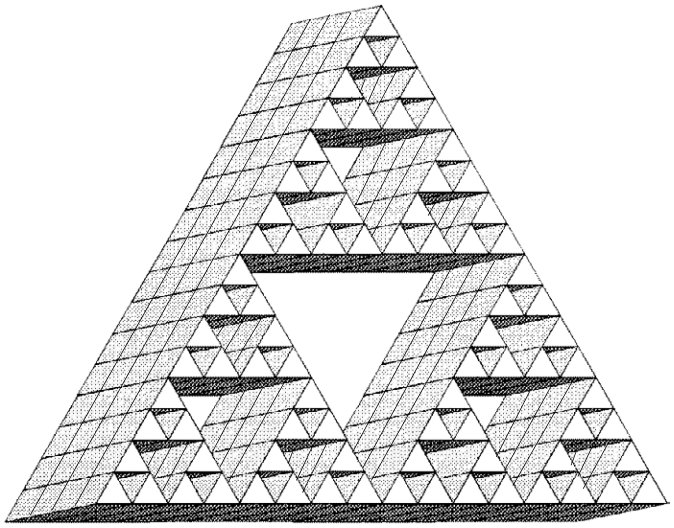

Figure 10. The Toblerone graph.

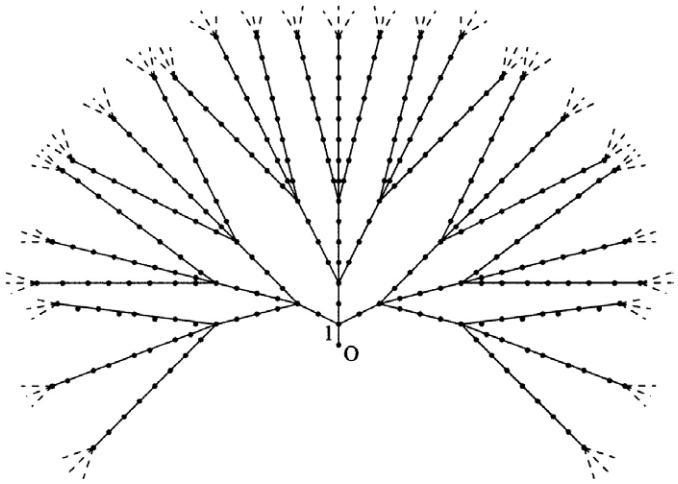

Figure 11. NT_D graph.

k branches of length 2 (i.e. consisting of two consecutive links); the ends of these branches split into k branches of length 4 and so on; each endpoint of a branch of length 2^n splits into k branches of length 2^{n+1}.

As one can easily verify, NT_D are not exactly decimable and therefore the simple decimation techniques cited above cannot be applied. Indeed, after a simple decimation starting from the origin O, one obtains k copies of the original structure joined together at a point instead of the same NT_D. However, NT_D are invariant under a more complex transformation $T = D \cdot C$, consisting of the product of a cutting transform C and a decimation D, which can be described as follows. Let us cut the log of the tree at point 1 and separate the k branches (cutting transform). Now, each branch can be obtained from the initial NT_D by

a dilatation with a factor 2. Eliminating all branches but one and decimating it (decimation transform), one obtains the original NT_D.

The T transform can now be used to solve the random walk problem. Let us sketch the main points of the calculation. The cutting transform gives a relation between random walks on the whole tree and random walks on one of its branches; more precisely one relates $\widetilde{P}_O^{\text{tree}}(\lambda)$, the generating function of the probability of returning to point O after a random walk on the NT_D tree, and $\widetilde{P}_1^{\text{branch}}(\lambda)$, the generating function of the probability of returning to the starting point 1 after a random walk on one of the branches. This relation is given by [14]

$$\widetilde{P}_O^{\text{tree}}(\lambda) = \frac{\widetilde{P}_1^{\text{branch}}(\lambda) + k}{2\lambda \widetilde{P}_1^{\text{branch}}(\lambda) + k}. \tag{111}$$

Now, the decimation transformation is performed using a time-rescaling technique. Indeed, the motion of the random walker on the branch considered only after an even number of steps can be exactly mapped in the motion of a random walker on the tree after the introduction of a staying probability $p_{ii} = 1/2$ at every site i. This equivalence can be translated into terms of generating functions through the substitutions

$$\widetilde{P_O}(\lambda) \to \frac{\lambda}{2-\lambda}\widetilde{P_O}\left(\frac{2}{2-\lambda}\right) \tag{112}$$

$$\lambda \to \lambda^2. \tag{113}$$

Equations (112) and (113) can be used to rewrite (111) as

$$\widetilde{P_O}^{\text{tree}}(\lambda) = \frac{\frac{2}{2-\lambda^2}\widetilde{P_O}^{\text{tree}}\left(\frac{\lambda^2}{2-\lambda^2}\right) + k}{(1-\lambda^2)\frac{2}{2-\lambda^2}\widetilde{P_O}^{\text{tree}}\left(\frac{\lambda^2}{2-\lambda^2}\right) + k}. \tag{114}$$

Choosing a suitable power law expression for the singularity of $P_{OO}^{\text{tree}}(\lambda)$ for $\lambda \to 1^-$ [14] we obtain

$$\widetilde{d} = 1 + \frac{\log k}{\log 2}. \tag{115}$$

To obtain the average spectral dimension, one has to calculate the normalized trace of the return probability $\widetilde{P_O}^{\text{tree}}(\lambda)$. It can be shown that $\overline{d} = 1$ and this can be intuitively understood by noting that the topology of NT_D is dominated by linear chains which become longer and longer in the outer branches [21]. Therefore, while NT_D are locally transient if the ramification k is greater than 2, they are always recurrent on the average. This result has been generalized. Indeed, recently it has been shown that all physical trees, satisfying conditions (a), (b) and (c) are recurrent on the average [37].

The cutting decimation transform can be applied to a large class of non-exactly decimable fractals which correspond to more general cases of the NT_D. These are built with the same recurrence procedure as the NT_D and we shall call them 2^mNT_D, nNT_D and p-polygonNT_D, depending on the growth rules for the branches [24].

The first generalization is that of 2^mNT_D. The 2^mNT_D are infinite fractal trees that can be recursively built using the same recipe as for NT_d but, from point 1, the log splits into k branches of length 2^m (i.e. made of 2^m consecutive links) which, in turn, split into k branches of length 2^{2m} and so on in such a way that each branch of length 2^{nm} splits into k branches of length $2^{(n+1)m}$. The case $m = 1$ corresponds to the usual NT_D previously studied. If $m > 1$ the time rescaling procedure which led to (112) and (113) must be iterated m times obtaining

$$\widetilde{P_O}^{\text{tree}}(\lambda) = \frac{\left(\prod_{i=1}^m \frac{2}{2-\lambda_i^2}\right)\widetilde{P_O}^{\text{tree}}(\lambda_{i+1}) + k}{(1-\lambda^2)\left(\prod_{i=1}^m \frac{2}{2-\lambda_i^2}\right)\widetilde{P_O}^{\text{tree}}(\lambda_{i+1}) + k} \tag{116}$$

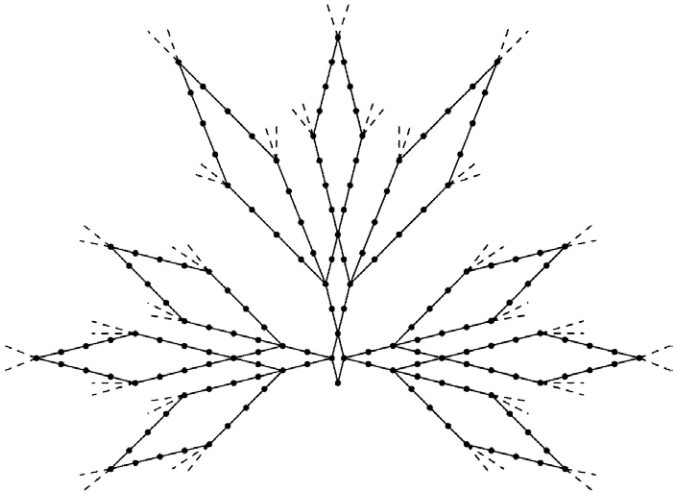

Figure 12. Four-polygon NT_D.

with

$$\lambda_i = \begin{cases} \lambda & i = 1 \\ \frac{\lambda_{i-1}^2}{2-\lambda_{i-1}^2} & i > 1, \end{cases}$$

i being the iteration step. This gives, with the same steps as for $m = 1$:

$$\widetilde{d}_{2^m} = 1 + \frac{\ln k}{\ln 2^m}, \tag{117}$$

which represent the generalization of the result obtained for $m = 1$.

The previous results can be extended to nNT_D, where now n is an integer and not necessarily a power of 2, and to p-polygonNT_D, where the branches of NT_D are replaced by p-vertices regular polygons (figure 12).

Let us consider nNT_D first. While relation (111) for the cutting transform still holds, the exact time-rescaling procedure cannot be applied to the branch of generic length n. However even in this case it is possible to obtain an asymptotic recursion relation applying the renormalization group techniques usually implemented on exactly decimable fractals. Although this procedure cannot give an exact equation for $\widetilde{P_O}^{\text{tree}}(\lambda)$ as in the previous case, nevertheless it can be used to obtain the exact value of $\widetilde{d}$ via an asymptotic estimation.

Indeed, in this case the branch of the nNT_D can be considered as a tree with a dilatation factor equal to n. The log of this tree can be reduced to a unitary length log after the suppression of the $n-2$ sites between the edges and introducing a new link connecting the edges. The same operation can be repeated for branches of every length suppressing the inner $n-2$ consecutive sites in every sequence of n sites and introducing a new link between the surviving points. The final structure is equal to the original tree and the generating function $\widetilde{P}_1^{\text{branch}}(\lambda)$ becomes $\widetilde{P}_1'^{\text{branch}}(\lambda')$ where

$$\lambda' = n^2\lambda \tag{118}$$

$$\widetilde{P}_1'^{\text{branch}}(\lambda') = \frac{1}{n}\widetilde{P}_1^{\text{branch}}(\lambda). \tag{119}$$

Now $\widetilde{P}_1'^{\text{branch}}(\lambda')$ coincides with $\widetilde{P_O}^{\text{tree}}(\lambda')$ since our branch has been transformed into a tree and (111) can be rewritten as

$$\widetilde{P_O}^{\text{tree}}(\lambda) = \frac{n\widetilde{P_O}^{\text{tree}}(n^2\lambda) + k}{2\lambda n\widetilde{P_O}^{\text{tree}}(n^2\lambda) + k}. \tag{120}$$

Using the procedure described in the previous section for $2^m NT_D$, from (120) it follows that for an $n - NT_D$ the spectral dimension is given by

$$\widetilde{d}_n = 1 + \frac{\ln k}{\ln n}. \tag{121}$$

An analogous technique can be used for p-polygonNT_D (figure 12). The log polygon has now p faces of unitary length; from each of $p-1$ of its vertices k polygons depart, whose faces have length n and so on. These structures, though similar to NT_D, are no longer loopless structures nor necessarily bipartite graphs (e.g. the 3-polygon tree). The cutting–decimation transform can be applied to p-polygonNT_D as in the case of NT_D with the same substitutions (118) and (119). Indeed, even if (111) does not hold in this case, a new relation between the generating functions of the tree and that of one of its branches can be obtained using bundled structures theory discussed above [38]. Let us consider a p-polygonNT_D and suppose we attach k branches also in the free vertex of the log (the root of the tree): we obtain a bundled structure having the log polygon as the base and the graph made of k branches as the fibre. Since for a p-polygon

$$\widetilde{P_O}(\lambda) \sim \frac{1}{p(1-\lambda)} \tag{122}$$

as $\lambda \to 1$, we obtain for our bundled structure

$$\widetilde{P_O}^{\text{b.s.}}(\lambda) = \frac{1}{1 - \frac{k}{k+1}\widetilde{F_1}^{\text{branch}}(\lambda)} \frac{1}{p} \left(1 - \frac{\lambda}{k+1} \frac{1}{1 - \frac{k}{k+1}\widetilde{F_1}^{\text{branch}}(\lambda)}\right)^{-1}, \tag{123}$$

where $\widetilde{P_O}^{\text{b.s.}}(\lambda)$ is the generating function of the probability of returning to point O (one of the vertices of the log polygon) after a random walk on the bundled structure and $\widetilde{F_1}^{\text{branch}}(\lambda)$ is the generating function of the probability of returning for the first time to the point of connection with the base after a random walk on the fibre. Now,

$$\widetilde{F_O}^{\text{b.s.}}(\lambda) = \frac{k}{k+1}\widetilde{F_1}^{\text{branch}}(\lambda) + \frac{1}{k+1}\widetilde{F_O}^{\text{tree}}(\lambda), \tag{124}$$

where $F_O{}^{\text{tree}}(\lambda)$ refers to the p-polygonNT_D. From (123) and (124) and using the usual relation between $\widetilde{F_1}^{\text{branch}}(\lambda)$ and $\widetilde{P_1}^{\text{branch}}(\lambda)$, a relation between $\widetilde{P_O}^{\text{tree}}(\lambda)$ and $\widetilde{P_1}^{\text{branch}}(\lambda)$ follows, which represents the cutting transformation. It is now possible to perform the cutting–decimation transform for p-polygonNT_D and get

$$\widetilde{d}_p = 1 + \frac{\ln k(p-1)}{\ln n}. \tag{125}$$

In the same way we can calculate the spectral dimension of an NT_D built with d-dimensional simplexes instead of p-polygons. A d-dimensional simplex is a complete graph of $d+1$ points, i.e. a graph where each point is the nearest neighbour of all other points. The two-dimensional case is the triangle, the three-dimensional one is the tetrahedron and so on. Since for d-simplex $\widetilde{P_O}(\lambda) \sim 1/(d+1)(1-\lambda)$ the spectral dimension is

$$\widetilde{d}_d = 1 + \frac{\ln kd}{\ln n}. \tag{126}$$

14. Relation to other physical problems

As we have shown in previous sections, the random walk problem is strictly related to the graph topology. Indeed, the main physical quantities are simple functions of the adjacency matrix A, which algebraically describes the graph structure. Now, the Hamiltonians of a series of fundamental statistical models are linear in A, therefore even their behaviour is deeply influenced by topology and it can be expressed in terms of random walk functions. For this reason, the main concepts and parameters characterizing random walks, such as recurrence and transience, as well as the spectral dimension, also determine the properties of these models, which have very different physical origins. This provides a very powerful tool to investigate and classify geometrically disordered and inhomogeneous systems, where the usual techniques and ideas developed for lattices do not apply.

14.1. The oscillating network

Probably, the physical model whose connection with random walks has been most extensively explored is the so-called *oscillating network*.

The harmonic oscillations of a generic network of masses m linked by springs of elastic constant K can be studied by writing the equations of motion of the displacements x_i of each mass from its equilibrium position:

$$m\frac{\mathrm{d}^2}{\mathrm{d}t}x_i = -K\sum_j A_{ij}(x_i - x_j) = -K\sum_j \Delta_{ij}x_j, \tag{127}$$

which after Fourier transforming with respect to the time reads

$$\frac{\omega^2}{\omega_0^2}\tilde{x}_i = \sum_j \Delta_{ij}\tilde{x}_j, \tag{128}$$

where $\omega_0^2 \equiv K/m$. In other words, the determination of the normal modes and of the normal frequencies of the oscillating network reduces to the diagonalization of the Laplacian operator δ.

Noting that $\Delta = Z(\mathbf{1} - P)$, where $\mathbf{1}$ is the identity matrix and P is given by (4), it is not difficult to establish mathematical correspondences with random walks. In particular, using the universality properties discussed in the previous sections, one can show a fundamental result concerning the density $\rho(\omega)$ of normal modes at low frequencies:

$$\rho(\omega) \sim \omega^{\bar{d}-1} \qquad \text{for} \quad \omega \to 0. \tag{129}$$

This basic connection between random walks and harmonic oscillations was first introduced by Alexander and Orbach in 1982 for the case of fractals. Note that at that time the splitting between local and average spectral dimensions on inhomogeneous structures was not yet known and the exponent describing the scaling of the density of states at low frequencies was simply called spectral dimension, since it was related to the vibrational spectrum. Due to the already mentioned universality properties, the above result holds for the very general case where oscillating masses and elastic constants may have different values on different sites and links, provided they are bounded by positive numbers. More precisely, considering the equations of motion

$$m_i\frac{\mathrm{d}^2}{\mathrm{d}t}x_i = -K\sum_j J_{ij}(x_i - x_j) = -K\sum_j L_{ij}x_j \tag{130}$$

for the same graph of (127), if (49) holds together with

$$\exists m_{\min}, m_{\max} > 0 | m_{\min} \leqslant m_i \leqslant m_{\max} \qquad \forall i \tag{131}$$

then the asymptotic behaviour of the density of vibrational states is still given by (49).

From all the above properties, it follows that the spectrum of the Laplacian operator L also depends on $\bar{d}$: indeed it can be shown [10] that the spectral density $\rho(l)$ of L at low eigenvalues behaves as $\rho(l) \sim l^{\bar{d}/2-1}$.

The average spectral dimension is crucial in determining the behaviour of the oscillating network in equilibrium with a thermal bath at temperature T. Considering the Hamiltonian of the system given by (129)

$$H = \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2} m\omega_0^2 \sum_{ij} J_{ij} x_i x_j \tag{132}$$

and calculating the thermodynamic averages with respect to the Gibbs weight $\exp(-H/kT)$, where k denotes the Boltzmann constant, one can show that, for positive T,

$$\langle \bar{x}^2 \rangle = \infty \qquad \text{for} \quad \bar{d} \leqslant 2 \tag{133}$$

while

$$\langle \bar{x}^2 \rangle < \infty \qquad \text{for} \quad \bar{d} > 2. \tag{134}$$

This is the generalization to graphs of the fundamental Peierls result about the thermodynamic instability of oscillating crystals in low dimensions. In other words, for an infinite oscillating network with $\bar{d} \leqslant 2$ in equilibrium with a thermal bath, the mean square displacement of masses from their equilibrium positions would diverge.

14.2. The Gaussian model

The Gaussian model is the simplest statistical model used to study magnetic systems on lattices. Even if it is not realistic, its properties are fundamental to understand more complex and phenomenologically significant models. In field theory it is also known as the 'free scalar field'. The Gaussian model on $\mathcal{G}$ is defined by the Hamiltonian

$$H = \frac{1}{2} \sum_{ij} \phi_i \big(J L_{ij} + m_i^2 \delta_{ij} \big) \phi_j - h \sum_i \phi_i, \tag{135}$$

where ϕ_i is a real field, $J > 0$ a ferromagnetic coupling, h an external magnetic field and $m_i^2 = \alpha_i m^2$, with $1/K < \alpha_i < K$ for some positive K [10]. Its specific free energy f_G is given by

$$f_G\big(J, m_i^2, h\big) = \lim_{N\to\infty} \frac{1}{N} F = -\lim_{N\to\infty} \frac{1}{N} \log Z, \tag{136}$$

where Z is the partition function calculated according to the Boltzmann weight $\exp(-H)$. The spectral dimension is related to the singular part of f_G for $h = 0$ and $m^2 \to 0$ by

$$\mathrm{Sing}(f) \sim m^{\bar{d}}. \tag{137}$$

The covariance of this Gaussian process reads

$$\langle \phi_i \phi_j \rangle \equiv C_{ij}(m^2) = (\Delta + m^2 \eta)^{-1}_{ij} \tag{138}$$

and hence it satisfies by definition the Schwinger–Dyson (SD) equation

$$(J_i + m^2 \eta_i) C_{ij}(m^2) - \sum_{k\in G} J_{ik} C_{kj}(m^2) = \delta_{ij}. \tag{139}$$

Setting

$$C_{ij} = \frac{(1-W)^{-1}_{ij}}{J_i + m^2 \eta_i}, \qquad W_{ij} = \frac{J_{ij}}{J_j + m^2 \eta_j} \tag{140}$$

Table 1. Critical exponents of the spherical model on a graph of spectral dimension $\bar{d}$.

	$1 \leqslant \bar{d} < 2$	$2 < \bar{d} < 4$	$\bar{d} > 4$
$T = T_c$	$\delta \to \infty$	$\delta = \frac{\bar{d}+2}{\bar{d}-2}$	$\delta = 3$
$T < T_c$	–	γ' does not exist	$\gamma' = 1$
$T > T_c$	$\gamma = -\frac{2}{\bar{d}-2}$	$\gamma = \frac{2}{\bar{d}-2}$	$\gamma = 1$
$T < T_c$	–	$c = \frac{1}{2}K_B$	$c = \frac{1}{2}K_B$
$T > T_c$	$\alpha = \frac{\bar{d}}{\bar{d}-2}$	$\alpha = \frac{\bar{d}-4}{\bar{d}-2}$	$\alpha = 0$
$T < T_c$	–	$\beta = \frac{1}{2}$	$\beta = \frac{1}{2}$

one obtains the standard connection with the random walk (RW) over $\mathcal{G}$ [9]:

$$(1 - W)^{-1}_{ij} = \sum_{t=0}^{\infty} (W^t)_{ij} = \sum_{\gamma: i \leftarrow j} W[\gamma], \tag{141}$$

where the last sum runs over all paths from j to i, each weighted by the product along the path of the one-step probabilities in W:

$$\gamma = (i, k_{t-1}, \ldots, k_2, k_1, j) \quad \Longrightarrow \quad W[\gamma] = W_{ik_{t-1}} W_{k_{t-1}k_{t-2}}, \ldots, W_{k_2k_1} W_{k_1 j}. \tag{142}$$

Note that, as long as $m > 0$, we have $\sum_i (W^t)_{ij} < 1$ for any t, namely the walker has a non-zero death probability. This implies that C_{ij} is a smooth function of m^2 for $m \geqslant \epsilon > 0$. In the limit $m \to 0$ the walker never dies and the sum over paths in equation (141) is dominated by the infinitely long paths which sample the large scale structure of the entire graph ('large scale' refers here to the metric induced by the chemical distance alone). This typically reflects itself into a singularity of C_{ij} at $m = 0$ whose nature does not depend on the detailed form of J_{ij} or η_i, as long these stay uniformly positive and bounded.

Of particular importance is the leading singular infrared behaviour, as $m^2 \to 0$, of the average $[C(m^2)]_G$ of $C_{ii}(m^2)$, which is a positive definite quantity, over all points i of the graph $\mathcal{G}$, which we may write in general as

$$\mathrm{Sing}[C(m^2)]_G \sim c(m^2)^{\bar{d}/2-1}. \tag{143}$$

14.3. Spherical model and O(n) models

The spherical model is again a magnetic model with no direct connection to phenomenology. Nevertheless, it is a little more complex than the Gaussian one and, most important, it exhibits phase transitions at a finite temperature for $\bar{d} > 2$. Moreover, its critical exponents can be exactly determined and they turn out to be simple functions of $\bar{d}$, pointing out the crucial role of the average spectral dimension in phase transitions and critical phenomena. The spherical model can be defined on a generic graph through the Hamiltonian (135) with the *generalized spherical constraint* $\sum_i z_i \phi_i^2 = N$. We assume the coordination numbers to be bound: $1 \leqslant z_i \leqslant z_{\max}$. Its free energy and correlation functions can be expressed in terms of the Gaussian ones. Then the critical behaviour is obtained from the infrared singularities of the latter, i.e. in terms of the long time behaviour of random walks [12]. The results concerning the critical exponents are summarized in table 1, where $T_c = 0$ for $\bar{d} \leqslant 2$.

The so-called $O(n)$ models are defined, for positive integer n, by the Boltzmann weight $\exp(-\beta H_n)$, where

$$H_n[\mathbf{S}] = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} (\mathbf{S}_i - \mathbf{S}_j)^2, \tag{144}$$

the sum extends to all links of a certain graph $\mathcal{G}$, $J_{ij} > 0$ are ferromagnetic interactions, which may vary from link to link, and $\mathbf{S}_i$ is an n-dimensional vector of fixed length normalized by $\mathbf{S}_i \cdot \mathbf{S}_i = n$. They represent more realistic magnetic models, but their exact solution is in general impossible. However, a series of complex but powerful inequalities, relating their correlation functions to the random walk generating functions, allow us to prove some very general results shedding light on the complicated phenomena concerning phase transitions on graphs. In particular it has been proven that:

- they cannot have phase transitions at $T > 0$ if $\mathcal{G}$ is recurrent on the average [11];
- they exhibit phase transitions at $T > 0$ if $\mathcal{G}$ is transient on the average [15];
- for $n \to \infty$ their critical exponents tend to the spherical ones [17].

References

[1] Burioni R, Cassi D and Vezzani A 2004 Random walks and physical models on infinite graphs: an introduction *Random Walks and Geometry* ed V Kaimanovich, K Schmidt and W Woess (Berlin: de Gruyter)
[2] Harary F 1994 *Graph Theory* (Reading, MA: Addison-Wesley)
[3] Gantmacher F 1950 *The Theory of Matrices* (New York: Chelsea)
[4] Mohar B and Woess W 1989 *Bull. Lond. Math. Soc.* **21** 209
[5] Gefen Y, Aharony A and Mandelbrot B B 1980 *Phys. Rev. Lett.* **45** 855
[6] Polya G 1921 *Math. Ann.* **84** 149
[7] Woess W 2000 *Random Walks on Infinite Graphs and Groups* (Cambridge: Cambridge University Press)
[8] Alexander S and Orbach R 1982 *J. Phys. Lett.* **43** L62
[9] Hattori K, Hattori T and Watanabe H 1987 *Prog. Theor. Phys. Suppl.* **92** 108
[10] Burioni R and Cassi D 1996 *Phys. Rev. Lett.* **76** 1091
[11] Cassi D 1996 *Phys. Rev. Lett.* **76** 2941
[12] Cassi D and Fabbian L 1999 *J. Phys. A: Math. Gen.* **32** L93
[13] Burioni R, Cassi D and Vezzani A 2000 *Eur. Phys. J.* B **15** 665
[14] Burioni R and Cassi D 1995 *Phys. Rev.* E **51** 2865
[15] Burioni R, Cassi D and Vezzani A 1999 *J. Phys. A: Math. Gen.* **32** 5539
[16] Bertacchi D and Zucca F 2004 *J. Stat. Phys.* 947
[17] Burioni R, Cassi D and Destri C 2000 *Phys. Rev. Lett.* **85** 1496
[18] Burioni R and Cassi D 1997 *Mod. Phys. Lett.* B **11** 1095
[19] Burioni R, Cassi D and Destri C 2000 *J. Phys. A: Math. Gen.* **33** 3627
[20] Montroll E and Weiss G H 1965 *J. Math. Phys.* **6** 167
[21] Burioni R, Cassi D and Regina S 1996 *Mod. Phys. Lett.* B **10** 1059
[22] Cassi D and Regina S 1993 *Phys. Rev. Lett.* **70** 1647
[23] Cassi D and Regina S 1996 *Phys. Rev. Lett.* **76** 2914
[24] Burioni R, Cassi D, Pirati A and Regina S 1998 *J. Phys. A: Math. Gen.* **31** 5013
[25] Rammal R and Toulouse G 1983 *J. Physique—Lett.* **44** L13
[26] Hilfer R and Blumen A 1984 *J. Phys. A: Math. Gen.* **17** L537
[27] Milosevic S, Stassinopoulos D and Stanley H E 1988 *J. Phys. A: Math. Gen.* **21** 1477
[28] Dhar D 1988 *J. Phys. A: Math. Gen.* **21** 2261
[29] Kahng B and Redner S 1989 *J. Phys. A: Math. Gen.* **22** 887
[30] Maritan A, Sartoni G and Stella A L 1993 *Phys. Rev. Lett.* **71** 1027
[31] Gefen Y, Aharony A and Mandelbrot B B 1980 *Phys. Rev. Lett.* **45** 855
[32] Grabner P J and Woess W 1997 *Stochastic Proc. Appl.* **69** 127
[33] Giacometti A, Maritan A and Stella A L 1991 *Int. J. Mod. Phys.* B **5** 709
[34] de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
[35] Hilfer R and Blumen A 1986 *Fractals in Physics, Proc. VI Trieste Int. Symp. (July 1985)* ed L Pietronero and E Tosatti (Amsterdam: North-Holland)
[36] Doyle P G and Snell J L 1984 *Random Walks and Electric Networks* (Lincoln, NE: The Mathematical Association of America)
[37] Donetti L 2002 *Preprint* condmat 0206149
[38] Cassi D and Regina S 1993 *Phys. Rev. Lett.* **70** 1647