Topology, hidden spectra and Bose-Einstein condensation on low-dimensional complex networks

2002 J. Phys. A: Math. Gen. 35 1245

(http://iopscience.iop.org/0305-4470/35/5/308)

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

J. Phys. A: Math. Gen. **35** (2002) 1245–1252 PII: S0305-4470(02)28828-9

Topology, hidden spectra and Bose–Einstein condensation on low-dimensional complex networks

R Burioni, D Cassi and A Vezzani

Istituto Nazionale Fisica della Materia (INFM), Dipartimento di Fisica, Università di Parma, parco Area delle Scienze, 7A 43100 Parma, Italy

E-mail: burioni@fis.unipr.it, cassi@fis.unipr.it and vezzani@fis.unipr.it

Received 13 September 2001, in final form 26 October 2001
Published 25 January 2002
Online at stacks.iop.org/JPhysA/35/1245

Abstract

Topological inhomogeneity gives rise to spectral anomalies that can induce Bose–Einstein condensation (BEC) in low-dimensional systems. These anomalies consist in energy regions composed of an infinite number of states with vanishing weight in the thermodynamic limit (hidden states). Here we present a rigorous result giving the most general conditions for BEC on complex networks. We prove that the presence of hidden states in the lowest region of the spectrum is the necessary and sufficient condition for condensation in low dimension (spectral dimension $\bar{d} \leqslant 2$), while it is shown that BEC always occurs for $\bar{d} > 2$.

PACS numbers: 03.75.Fi, 02.10.Ab, 02.40.-k

The recent experimental evidence for Bose–Einstein condensation (BEC) in real systems [1] has stimulated an increasing amount of theoretical works to find the most general conditions inducing such phenomenon in new experimental setups. A key problem in this analysis is the influence of geometry on the physical behaviour of bosonic models. In the classical framework of the ideal Bose gas this influence is encoded in the dependence on the space dimension d of the system: indeed BEC occurs if and only if $d \geqslant 3$ [2].

Recently, the interest in quantum devices such as Josephson junctions, together with the possibility of combining them in complex geometrical arrangements, has stimulated the study of bosonic models on general discrete structures [3]. There, the problem of defining an effective dimension describing large-scale topology has been successfully solved by the introduction of spectral dimension $\bar{d}$ [4, 5], which can be experimentally measured [6] and rigorously defined by graph theory [7]. On the other hand, one expects the influence of topology to be richer and more complex on discrete structures, due to the possible relevance of local geometrical details, in addition to the large-scale structure described by dimensionality.

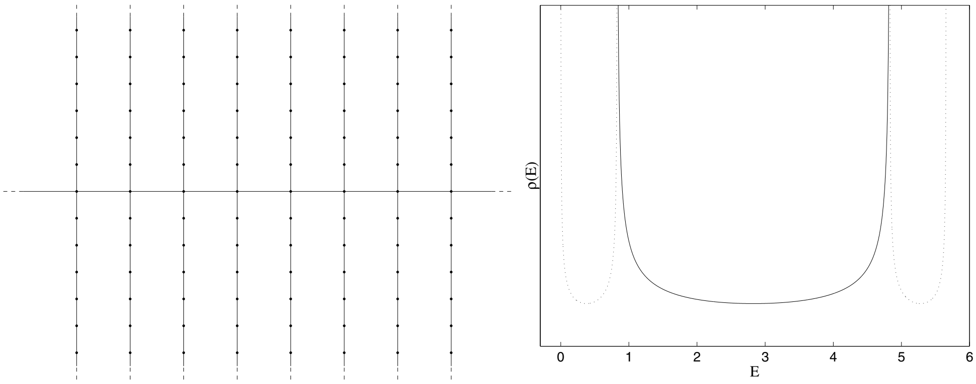

Figure 1. The comb graph and the spectrum of the pure hopping model ($h_{ij} = -tA_{ij}$) defined on this structure. The hidden spectrum is represented with dotted curves. In this case the spectrum is obtained from an exact calculation in the thermodynamic limit. The energy is measured in units of t and the zero has been chosen so that $E_0 = 0$; the density is plotted in arbitrary units (the hidden spectrum and $\rho(E)$ can be normalized to 1 dividing respectively to the number of states belonging to each spectral region).

In this direction, recent works on BEC on inhomogeneous networks [8] have put into evidence that strong inhomogeneities can give rise to condensation at finite temperature even in a low-dimensional system such as a comb lattice ($\bar{d} = 1$, see figure 1). This phenomenon arises from a peculiarity of the spectra of inhomogeneous networks we shall refer to as *hidden spectrum*, consisting of an energy region filled by a finite of infinite number of eigenvalues which do not contribute to the normalized spectral density in the thermodynamic limit. Hidden spectra do not usually affect bulk thermodynamic quantities but, as we shall show in the following, can have dramatic effect when bosonic statistics forces the macroscopic occupation of a single quantum state.

Here we give a general mathematical definition of hidden spectra and we prove that the necessary and sufficient condition for condensation when $\bar{d} \leqslant 2$ is the presence of hidden states in the lowest region of the energy spectrum, while BEC at finite temperature always occurs for higher-dimensional systems (i.e. when $\bar{d} > 2$).

A generic discrete network is naturally described by a graph which is a countable set V of vertices (sites) i connected pairwise by a set E of unorientated edges (links) $(i, j) = (j, i)$. We will call nearest neighbours two vertices joined by an edge. The graph topology is algebraically described by its adjacency $A_{ij} = 1$ if (i, j) is a link of the graph and $A_{ij} = 0$ otherwise. The coordination number $z_i = \sum_j A_{ij}$ is the number of nearest neighbours of the site i. A real geometrical structure always has a finite maximum number of nearest neighbours at any site. To take into account this condition in the thermodynamic limit we introduce the uniform boundedness condition: $\max_i z_i < \infty$ on the coordination numbers. A path in G is a sequence of consecutive links $\{(i, k), (k, h), \ldots, (n, m), (m, k)\}$ and a graph is said to be connected if for any two point there is always a path joining them. In the following we will consider only connected graphs; disconnected graphs can be reduced to non-interacting connected components which can be studied separately. Every connected graph is endowed with an intrinsic metric generated by the chemical distance $r_{i,j}$, which is defined as the number of links in the shortest path connecting sites i and j.

The most general Hamiltonian for non-interacting particles on G is

$$H = \sum_{i,j \in V} h_{ij} a_i^\dagger a_j \tag{1}$$

where $a_i^\dagger$ and a_i are the creation and annihilation operators at site i. The bosonic nature of the particles is introduced through the usual commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$. The Hamiltonian matrix h_{ij} is defined by

$$h_{ij} = t_{ij} + \delta_{ij} V_i. \tag{2}$$

The term t_{ij} describes hopping between nearest-neighbour sites and it is directly related to the topology of the graph. Indeed $t_{ij} \neq 0$ if and only if $(i, j) \in E$, i.e. $A_{ij} = 1$. The diagonal term V_i takes into account a potential at site i and both terms must satisfy a a boundedness condition $0 < k < |t_{ij}| < K$ and $0 < c < |V_i| < C$.

To introduce the thermodynamic limit and analyse the conditions for BEC on the graph, we begin by studying models restricted to the Van Hove sphere $S_{r,o}$ of centre o and radius r. This is defined as the set of the vertices whose distance from o is equal or smaller than r. We will call $N_{r,o}$ the number of site in $S_{o,r}$. The Hamiltonian restricted to the sphere is

$$H^{S_{r,o}} = \sum_{i,j \in V} h_{ij}^{S_{r,o}} a_i^\dagger a_j \tag{3}$$

where $h_{ij}^{S_{r,o}} = h_{ij}$ if i and j belong to the sphere and $h_{ij}^{S_{r,o}} = 0$ otherwise. For graphs with polynomial growth, i.e. when $N_{r,o} \sim r^p$ for $r \to \infty$, it is possible to show that the thermodynamic limit is independent from the choice of the centre of the sphere o [9]. In the following we will consider only graphs with polynomial growth, since this is the necessary condition to ensure that the structure can be embedded in a finite-dimensional space. We will then write $H^r = H^{S_{r,o}}$, $h_{ij}^r = h_{ij}^{S_{r,o}}$ and $N_r = N_{r,o}$.

For each finite sphere of radius r the matrix h_{ij}^r defines a normalized density of states $\rho^r(E)$ which is the sum of N_r δ-functions $\delta(E - E_k^r)$, where E_k^r are the eigenvalues of h_{ij}^r. The density $\rho^r(E)$ will be normalized to $1/N_r$.

In the thermodynamic limit, we define $\rho(E)$ to be the spectral density of the eigenvalues of h_{ij} if

$$\lim_{r \to \infty} \int |\rho^r(E) - \rho(E)| \, \mathrm{d}E = 0. \tag{4}$$

Let us define $E_m \equiv \mathrm{Inf}\,(\mathrm{Supp}(\rho(E)))$ where $\mathrm{Supp}(\rho(E))$ is the support of the distribution $\rho(E)$. The asymptotic behaviour of the thermodynamic spectral density in this region is described by the spectral dimension $\bar{d}$ [5]:

$$\rho(E) \sim (E - E_m)^{\frac{\bar{d}}{2} - 1} \qquad \text{for} \quad E \to E_m. \tag{5}$$

A *hidden* region of the spectrum is an energy interval $[E_1, E_2]$ such that $[E_1, E_2] \cap \mathrm{Supp}(\rho(E)) = \emptyset$ and $\lim_{r \to \infty} N^r_{[E_1,E_2]} > 0$, where $N^r_{[E_1,E_2]}$ is the number of eigenvalues of h_{ij}^r in the interval $[E_1, E_2]$. Notice that in general $N^r_{[E_1,E_2]}$ can diverge for $r \to \infty$ and the eigenvalues can become dense in $[E_1, E_2]$ in the thermodynamic limit. Therefore this condition not only includes the trivial case of discrete spectrum but is far more general; an interesting example of this new kind of behaviour has been observed in the comb lattice [8] (figure 1), where the hidden region of the spectrum is filled by an infinite number of states.

We now define the lowest energy level for the sequence of densities $\rho_r(E)$, setting $E_0^r = \mathrm{Inf}_k(E_k^r)$ and $E_0 = \lim_{r \to \infty} E_0^r$. In general, $E_0 \leqslant E_m$. If $E_0 < E_m$, then $[E_0, E_m]$ is a hidden region of the spectrum, which will be called the hidden low-energy spectrum.

In the following we will consider models at fixed fillings $f = N/N_r$, where N represents the number of particles in the system. In the macro-canonical ensemble the equation that determines the fugacity z in the thermodynamic limit is

$$f = \lim_{r\to\infty} \int \frac{\rho^r(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1}. \tag{6}$$

Setting $E_0 = 0$ we have that $0 \leqslant z \leqslant 1$.

The integral in equation (6) can be divided into two sums, the first ones considering the energies smaller than an arbitrary constant ϵ and the second the energies larger than ϵ:

$$\int \frac{\rho^r(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1} = \sum_{k=0}^{E_k\leqslant\epsilon} \frac{1}{z^{-1}\mathrm{e}^{\beta E_k^r} - 1} + \int_{E>\epsilon} \frac{\rho^r(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1}. \tag{7}$$

We define

$$n_\epsilon^r \equiv \sum_{k=0}^{E_k\leqslant\epsilon} \frac{1}{z^{-1}\mathrm{e}^{\beta E_k^r} - 1} \tag{8}$$

as the fraction of particles with energy smaller than ϵ. BEC occurs in this systems if there exists a critical temperature $T_c > 0$ such that, for any $T < T_c$, $n_\epsilon \equiv \lim_{r\to\infty} n_\epsilon^r > k > 0$, for all $\epsilon > 0$; i.e. $n_0 \equiv \lim_{\epsilon\to 0} n_\epsilon = k > 0$.

From the definition (8), n_0 can be strictly positive only if $\lim_{r\to\infty} z(r) = 1$. Indeed, if this limit is smaller than 1 it follows that $n_\epsilon \leqslant (1-z)^{-1} \lim_{r\to\infty} N_\epsilon^r/N^r$ where N_ϵ^r is the number of state with energy smaller than ϵ. If the ground state is not infinitely degenerate, $\lim_{\epsilon\to 0} \lim_{r\to\infty}(N_\epsilon^r/N^r) = 0$ and then $n_0 = 0$.

Taking first the limit $r \to \infty$ and then $\epsilon \to 0$ in equation (7) we obtain

$$f = n_0 + \lim_{\epsilon\to 0}\lim_{r\to\infty} \int_{E>\epsilon} \frac{(\rho^r(E) - \rho(E))\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1} + \lim_{\epsilon\to 0}\lim_{r\to\infty} \int_{E>\epsilon} \frac{\rho(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1}. \tag{9}$$

Now, from the boundedness of $(z^{-1}\mathrm{e}^{\beta E} - 1)^{-1}$ for $E > \epsilon$ and from the definition (4), the first of the two limits in the right-hand side of (9) vanishes:

$$f = n_0 + \lim_{\epsilon\to 0} \int_{E>\epsilon} \frac{\rho(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1} = n_0 + \int \frac{\rho(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1} \tag{10}$$

where, again, n_0 can be different from 0 only if $z = 1$.

Now the integral in equation (10) is an increasing continuous function of z with $0 \leqslant z < 1$. If the limit

$$f_c(\beta) = \lim_{z\to 1} \int \frac{\rho(E)\,\mathrm{d}E}{z^{-1}\mathrm{e}^{\beta E} - 1} \tag{11}$$

is equal to ∞ we have $z < 1$ and $n_0 = 0$. If the limit is finite, $f_c(\beta)$ is a decreasing function of β with $\lim_{\beta\to\infty} f_c(\beta) = 0$ and $\lim_{\beta\to 0} f_c(\beta) = \infty$. Then, for a suitable β_C, $f_c(\beta_C) = f$. For $\beta > \beta_C$, (i.e. $T < T_C$) $z = 1$ and $n_0 = f - f_c(\beta) > 0$ while for $\beta < \beta_C$, (i.e. $T > T_C$) $z < 1$ and $n_0 = 0$.

From the divergence or finiteness of the limit (11) one obtains the most general conditions for the occurrence of BEC.

First, if $0 = E_0 < E_m$ (i.e. the system presents a low-energy hidden spectrum) the limit (11) is finite and there is BEC at finite temperature:

$$f_c(\beta) \leqslant \frac{1}{\mathrm{e}^{\beta E_m} - 1} \int \rho(E)\,\mathrm{d}E = \frac{1}{\mathrm{e}^{\beta E_m} - 1}. \tag{12}$$

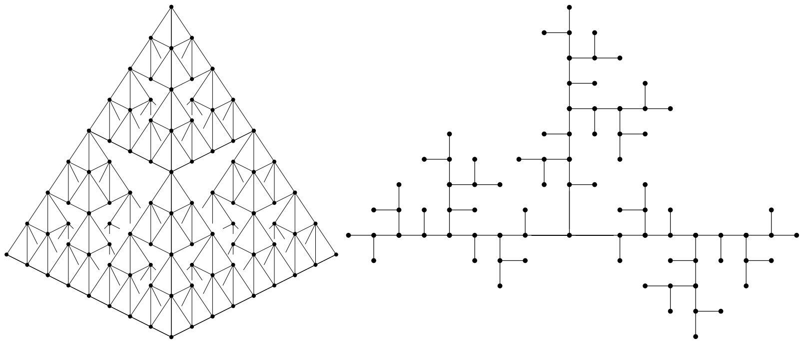

Figure 2. Two classical examples of exactly decimable graph: the three-dimensional Sierpinski gasket ($\bar{d} = 2\ln(4)/\ln(6) < 2$) and the T-fractal ($\bar{d} = 2\ln(3)/\ln(6) < 2$).

On the other hand, when $E_0 = E_m$ the value of the limit (11) is determined by the spectral dimension $\bar{d}$. Indeed if $\bar{d} > 2$

$$f_c(\beta) \leqslant \int_0^\delta \frac{c_1 E^{\frac{\bar{d}}{2}-1}\,\mathrm{d}E}{\beta E} + \int_{E>\delta} \frac{\rho(E)\,\mathrm{d}E}{\mathrm{e}^{\beta E} - 1} < \infty \tag{13}$$

where δ and c_1 are suitable constants. Therefore in this case BEC occurs at finite temperature.

For $d < 2$ we have

$$f_c(\beta) \geqslant \lim_{z\to 1} \int_0^\delta \frac{z c_1 E^{\frac{\bar{d}}{2}-1}\,\mathrm{d}E}{\beta E + 1 - z} = \infty \tag{14}$$

and there is no BEC. When $\bar{d} = 2$ we have to consider the logarithmic correction to (5) and it is possible to show that the limit (11) diverges.

This result applies to many different situations. The simplest example is the discretization of the usual Schrödinger equation for free particles on a graph. In this case the Hamiltonian is given by $h_{ij} = \frac{\hbar^2}{2m} L_{ij}$. L_{ij} is the Laplacian operator on the graph $L_{ij} = z_i \delta_{ij} - A_{ij}$. It can be shown that $E_0 = E_m$ and therefore the occurrence of BEC is determined by the behaviour of the spectrum of L_{ij} at low eigenvalues, described by the spectral dimension as in (5). $\bar{d}$ is known for a wide class of structures [7,10,11]: for lattices it coincides with the usual Euclidean dimension and for exactly decimable graph (the Sierpinski gasket [10] and the T-fractal are illustrated in figure 2) it can be proven [7] that $\bar{d} < 2$.

A more important model, relevant for real condensed matter structures, is a pure hopping of non-interacting bosons on graphs. This has been considered in [8] for the description of the Josephson junction arrays in the weak coupling limit. In this case the Hamiltonian matrix is given by $h_{ij} = -t A_{ij}$. A relevant point about the application of our result to real systems concerns the effects of the introduction of a fluctuating local potential. Indeed it can be shown [12] that in presence of a hidden spectrum giving rise to BEC, the existence of a condensate is not affected by the introduction of a small enough potential.

Let us now focus on the pure hopping model described by the Hamiltonian $h_{ij} = -t A_{ij}$ where the only effects are due to topology, to show how the general theorem can be applied to a wide class of discrete structures. Condensation at finite temperature due to the presence of low-energy hidden states is typical of bundle structures [11]. These graphs are obtained by a 'fibring' procedure, i.e. attaching the origin site of copy of a graph we will call the 'fibre' graph, to every point of another graph called 'base'. An example is the brush graph, shown in figure 3, where the base (the two-dimensional lattice) is fibred by a linear chain. On bundled structures

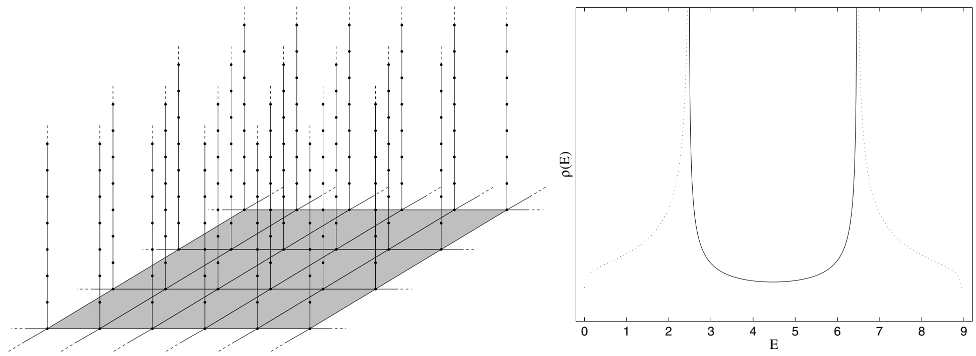

Figure 3. The brush graph and the spectrum of the pure hopping model on this graph (obtained from the diagonalization of a structure of $200 \times 200 \times 200$ sites). The dotted curves represent the hidden spectrum which gives rise to condensation even if the spectral dimension is 1.

the spectrum $\rho(E)$ is simply given by the spectrum of the pure hopping model on the fibre but the inhomogeneities due to the base give rise to a low-energy hidden spectrum. Moreover, the wavefunction of the condensate is localized along the base and presents a fast decay along the fibres. This result can be in general obtained by first diagonalizing the Hamiltonian of a pure hopping model defined on the base and then solving the eigenvalues problem of the Hamiltonian of the fibre with a suitable impurity in the origin, whose form depends on the result of the previous diagonalization (see [8] for a detailed application of this techniques to the comb graph). In the case of the brush graph $E_m = \sqrt{(20)} - 2 \approx 2.47 > E_0 = 0$ (in all figures the energy is measured in t units and the energy zero has been chosen so that $E_0 = 0$), so that we can apply the general result for low-energy hidden spectra. In the figure the continuous curve is $\rho(E)$ and it coincides with the density of states of the hopping model on a linear chain (the fibre). The dotted curve represents the hidden spectral region, which is filled continuously by the hidden states. Since on the comb graph the fraction of states in the hidden spectral region goes to zero as $1/N_r^{1/3}$ for $r \to \infty$, in order to obtain the dotted curves we have to normalize $\rho^r(E)$ dividing by $N_r^{2/3}$ and not by the total number of sites in the sphere.

Graphs with constant coordination number z_i are typical examples in which the pure hopping model do not present hidden low energy regions ($E_0 = E_m$). This is due to the fact that for this class of graphs the spectrum of the model can be obtained from that of the Laplacian matrix by a shift of the zero in the energy. The existence of BEC is therefore determined by the spectral dimension $\bar{d}$ of the graph. This parameter can be exactly calculated for a wide class of discrete structures. On lattices, $\bar{d} = d$ is the usual Euclidean dimension and one recovers the classical result for BEC on translation invariant structures. The d-dimensional Sierpinski gaskets [10] (see figure 2) are example of exactly decimable graphs with constant coordination number. Since for these graphs $\bar{d} < 2$, our general result proves that in these cases no BEC occurs.

A fundamental property of the low eigenvalues spectral density of the Laplacian matrix is its independence from the local details of the graph, i.e. geometrical universality [5]. The value of $\bar{d}$ is not changed under a wide class of transformations, called isospectralities, which can strongly modify the geometry of the graph. A simple consequence of this property is that if we consider the pure hopping model on a graph with constant coordination number, which differs from a graph of known dimension $\bar{d}$ by an isospectrality, BEC occurs only if $\bar{d} > 2$. An example of this behaviour is given by the ladder graph (figure 4) which can be obtained

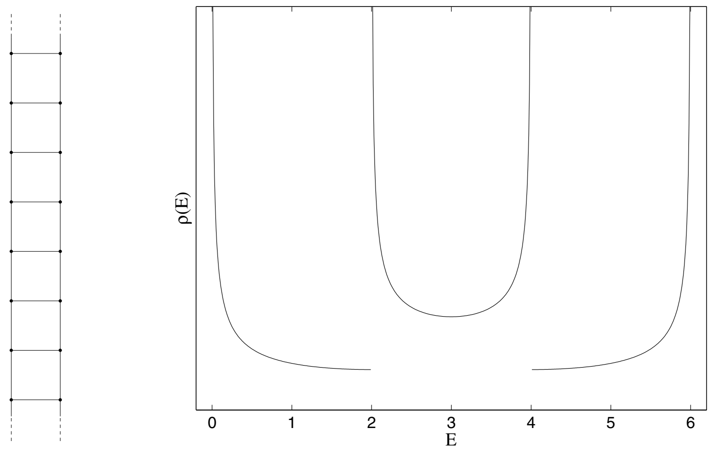

Figure 4. The ladder graph and the spectrum of the pure hopping model obtained from an exact diagonalization in the thermodynamic limit. Here there is no hidden spectrum and $\rho(E) \to \infty$ when $E \to E_m = E_0$ ($\bar{d} = 1$), then there is no condensation at finite temperature.

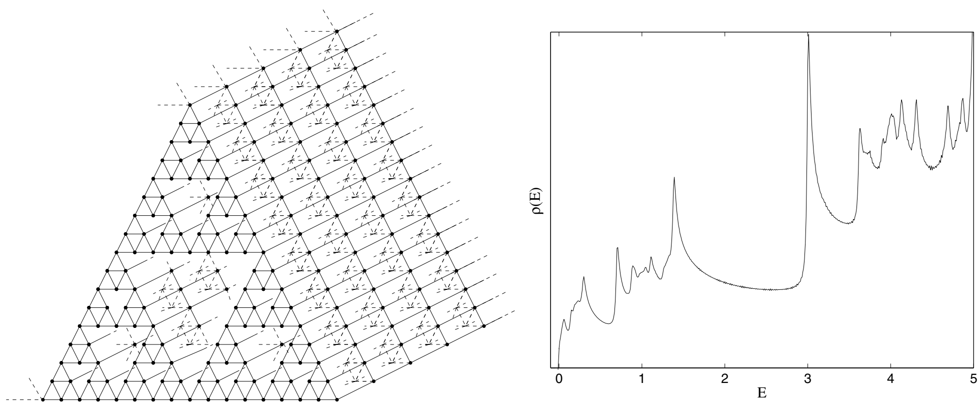

Figure 5. The graph obtained as a product of the Sierpinski gasket and a linear chain. Here the spectrum of the pure hopping model is obtained from the diagonalization of a graph of 840 192 sites. Here condensation occurs since $\bar{d} = 1 + 2\ln(3)/\ln(4) > 2$ (indeed the spectral vanishes for $E \to E_m = E_0$).

from the linear chain by the addition of finite-range links, which is one of the simplest cases of isospectralities. On this structure then there is no low-energy hidden spectrum, $\bar{d} = 1$ and the pure hopping model does not exhibit BEC.

An important property of $\bar{d}$ is that the dimension of the graph obtained as a direct product of two graphs is the sum of the dimensions of the original structures. An example is illustrated in figure 5, where we show the direct product of a linear chain and a well known fractal, a Sierpinski gasket. In this case the coordination number z_i is constant. Applying this property of $bard$ it is easy to show that $\bar{d} = 1 + 2\ln(3)/\ln(4) > 2$, and therefore one immediately infers that BEC occurs on this graph. Interestingly, in this case we do not know the analytical form of the spectrum of the Hamiltonian (the spectral density in the figure is obtained by a numerical diagonalization), nevertheless we can prove the existence of BEC from the general theorem and from the properties of $\bar{d}$.

References

[1] Dalfovo F, Giorgini S, Pitaevskii L and Stringari S 1999 *Rev. Mod. Phys.* **71** 463
[2] See e.g. Hohenberg P C 1967 *Phys. Rev.* **158** 383
[3] Fisher M P A, Weichman P B, Grinstein G and Fisher D S 1989 *Phys. Rev.* B **40** 546
Bruder C, Fazio R, Kampf A, vanOtterlo A and Schön G 1992 *Phys. Sci.* **42** 159
Scalettar R T, Batrouni G G, Kampf A P and Zimanyi G T 1995 *Phys. Rev.* B **50** 8467
[4] Alexander S and Orbach R 1987 *J. Physique Lett.* **92** 108
[5] Burioni R and Cassi D 1996 *Phys. Rev. Lett.* **76** 1091
Burioni R and Cassi D 1997 *Mod. Phys. Lett.* B **11** 1095
[6] For a review see: Nakayama T, Yakubo K and Orbach R L 1994 *Rev. Mod. Phys.* **66** 381
[7] Hattori K, Hattori T and Watanabe H 1987 *Prog. Theor. Phys. Suppl.* **92** 108
[8] Burioni R, Cassi D, Meccoli I, Rasetti M, Regina S, Sodano P and Vezzani A 2000 *Europhys. Lett.* **52** 251
[9] Burioni R, Cassi D and Vezzani A 2000 *Eur. Phys. J.* B **15** 665
[10] Rammal R 1984 *J. Physique* **45** 191
[11] Cassi D and Regina S 1997 *Mod. Phys. Lett.* B **11** 997
[12] Buonsante P, Burioni R, Cassi D and Vezzani A 2002 in preparation