Universal Properties of Spectral Dimension

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The infrared singularities of a Gaussian model on a general network are invariant under a local rescaling of the masses. This exact result leads to some interesting rigorous relations concerning diffusion and harmonic oscillations on fractals and inhomogeneous structures. We show that a generic distribution of waiting probabilities does not affect the spectral dimension in diffusive problems, neither does a change of masses in an oscillating network. In particular, we prove an exact relation between random walks and vibrational spectrum showing the possibility of noncoincidence of vibrational and usual diffusive spectral dimensions.

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The study of statistical properties in real structures by means of model systems is greatly stimulated and guided by the idea of universality. According to this idea, only a few very general features are sufficient to determine the physical behavior in a wide class of phenomena. In such a way we can group our systems in a limited number of universality classes. This is the case for crystalline solids undergoing magnetic phase transitions, where the lattice dimension and the symmetry of the Hamiltonian are the only information needed to determine critical exponents. In the same way many long range or low frequency properties depend only on the Bravais lattice dimensionality. This phenomenon allows us to study the simplest system in a given universality class to obtain general physical results common to all other members.

These universal properties would be even more important in noncrystalline and disordered structures, as amorphous solids, polymers, glasses, and fractals, for which a simple geometrical characterization based on dimension is not evident. In this case the determination of universality classes would suggest the most natural geometrical parameter generalizing the concept of dimension.

In recent years various definitions of generalized dimensions have been proposed, starting from Mandelbrot's fractal dimension [1]. The most useful in the study of dynamics and critical phenomena turned out to be the spectral dimension [2]. However, some different definitions of this parameter have been given and its universality properties are far from being evident. In this Letter we analyze these definitions and rigorously prove their universal features. The latter allow one in addition to deeply explore the relation between the definitions and to point out a highly nontrivial difference which could be fundamental in the study of inhomogeneous structures.

The idea of an anomalous dynamical dimension was first proposed by Dhar [3] in 1977, in connection with the behavior of statistical models on networks. Then in 1982 Alexander and Orbach [2] introduced the spectral dimension $\tilde{d}$ to describe low frequency vibrational spectrum and long time random walks (RW) properties on fractals, according to the asymptotic power laws

$$\rho(\omega) \sim \omega^{\tilde{d}-1}, \tag{1}$$

where $\rho(\omega)$ is the density of harmonic vibrational modes with frequency ω and

$$P_0(t) \sim t^{-\tilde{d}/2}, \tag{2}$$

where $P_0(t)$ is the probability of returning to the starting site after t steps for a random walker. These definitions were considered to be equivalent by physical arguments.

Then it became clear that the spectral dimension can be defined not only for fractals, but for generic networks. In this framework Hattori, Hattori, and Watanabe (HHW) [4] gave a rigorous mathematical definition of $\tilde{d}$ for an infinite discrete structure (graph) based on the infrared singularities of a Gaussian model defined on the same structure. Let us recall in a simplified way the main point of this definition. Given a connected graph G, its adjacency matrix A_{ij} has all elements equal to 0 except when the sites i and j are nearest neighbors (nn), where $A_{ij} = 1$. Then we can define a Gaussian model on G by the Hamiltonian

$$H(\{m_i^2\}) = \frac{1}{4} \sum_{\text{nn}} (\phi_i - \phi_j)^2 + \sum_i m_i^2 \phi_i^2$$
$$= \frac{1}{2} \sum_{ij} \phi_i (L_{ij} + m_i^2 \delta_{ij}) \phi_j\,, \tag{3}$$

where the square masses m_i^2 are all bounded from above and from below by positive numbers and L_{ij} is the Laplacian matrix defined by $L_{ij} \equiv z_i \delta_{ij} - A_{ij}$, with $z_i = \sum_j A_{ij}$ being the coordination number of site i. The correlation functions

$$\langle \phi_i \phi_j \rangle_{\{m_i^2\}} = (L + M)^{-1}_{ij}\,, \tag{4}$$

where $M_{ij} \equiv \delta_{ij} m_i^2$, can be defined by averaging with respect to the Boltzmann weight $\exp(-H)$. In the infrared limit $s \to 0^+$ the leading singular part of the correlation function $\langle \phi_i \phi_i \rangle_{\{sm_i^2\}}$ behaves as

$$\text{sing}\langle \phi_i \phi_i \rangle_{\{sm_i^2\}} \sim s^{(\tilde{d}/2)-1} (\ln s)^{I(\tilde{d}/2)}, \tag{5}$$

where $I(x) = 1$ for integer x and 0 otherwise. HHW showed that this definition has some universal properties: indeed it is independent of site i and, for a restricted class of graphs with $\tilde{d} < 2$, also of the particular distribution $\{m_i^2\}$. In addition, they proved the coincidence of their $\tilde{d}$ with the parameter defined in (2), in the case of continuous time RW.

Here we prove that the HHW definition is independent of the $\{m_i\}$ distribution for *any* graph. This result allows in turn to prove the following fundamental properties: (i) The coincidence of HHW definition with the corresponding one for discrete time RW; (ii) the independence of RW $\tilde{d}$ of any waiting probabilities distribution; (iii) an explicit relation between vibrational $\tilde{d}$ and the average of $P_0(t)$ over all sites; and (iv) the independence of vibrational $\tilde{d}$ of any bounded mass distribution.

Let us begin by the generalization of universality with respect to mass rescaling. HHW proved that if $m_i'^2 \leq m_i^2$ for any i, then $\langle \phi_i \phi_i \rangle_{\{m_i^2\}} \leq \langle \phi_i \phi_i \rangle_{\{m_i'^2\}}$. Because of the divergence of $\langle \phi_i \phi_j \rangle_{\{sm_i^2\}}$ for vanishing s when $\tilde{d} < 2$ and to the boundedness conditions on the squared masses, this allows us to prove the independence of $\tilde{d}$ of a specific mass distribution. Notice that the divergence of the correlation function is necessary in this proof, in order to get significant inequalities between asymptotic behaviors. If these functions do not diverge, in the infrared limit the singular part containing the information about $\tilde{d}$ cannot be separated by a generic nonsingular finite part. However, it is possible to get divergent quantities by taking derivatives up to a suitable order of $\langle \phi_i \phi_j \rangle_{\{sm_i^2\}}$ with respect to s. In this way we obtain a function diverging according to a power law with exponent depending on $\tilde{d}$. Then it has been proven [4] that

$$\left(-\frac{d}{ds}\right)^N \langle \phi_i \phi_i \rangle_{s\{m_i^2\}} = N! \sum_{k_1 \ldots k_n} m_{k_1}^2 \cdots m_{k_N}^2 \langle \phi_i \phi_{k_1} \rangle_{s\{m_i^2\}} \langle \phi_{k_1} \phi_{k_2} \rangle_{s\{m_i^2\}} \cdots \langle \phi_{k_N} \phi_j \rangle_{s\{m_i^2\}} . \tag{6}$$

Now notice that, by straightforward steps, one can also prove that if $m_i'^2 \leq m_i^2$ for any i, then $\langle \phi_i \phi_j \rangle_{\{m_i^2\}} \leq \langle \phi_i \phi_j \rangle_{\{m_i'^2\}}$, for $i \neq j$. Applying the last inequalities to the correlation functions appearing in (6), and considering the boundedness by positive numbers of mass distributions, it is easy to prove the independence of $\tilde{d}$ of $\{m_i^2\}$ for a generic graph.

Now consider discrete time RW on a graph, defined by the hopping probabilities matrix

$$P_{ij} = \frac{A_{ij}}{z_i} . \tag{7}$$

The probability $P_{ii}(t)$ of returning to a starting site i after t steps is given by

$$P_{ii}(t) = (P^t)_{ii} . \tag{8}$$

If we introduce the generating functions $\tilde{P}_{ii}(\lambda) \equiv \sum_t \lambda^t P_{ii}(t)$, it holds

$$\tilde{P}_{ii}(\lambda) = (1 - \lambda P)_{ii}^{-1} = (L + M)_{ii}^{-1} \frac{z_i}{\lambda} = \langle \phi_i \phi_i \rangle_{\{m_i^2\}} \frac{z_i}{\lambda} , \tag{9}$$

with $m_i^2 = z_i(1 - \lambda)/\lambda$. Considering that, from Tauberian and Abelian theorems, the conditions $P_{ii}(t) \sim t^{-\tilde{d}/2}$ for $t \to \infty$ and $\text{sing}[\tilde{P}_{ii}(\lambda)] \sim (1 - \lambda)^{(\tilde{d}/2)-1}$ for $\lambda \to 1^-$ are equivalent [5], it follows also that the Gaussian and the discrete time RW definitions of $\tilde{d}$ are equivalent.

Now let us introduce a waiting probability distribution w_i modifying the hopping probabilities matrix P to

$$P'_{ij} = \frac{A_{ij} + \delta_{ij} w_i}{z_i + w_i} . \tag{10}$$

The modified generating functions are given by

$$\tilde{P}'_{ii}(\lambda) = (1 - \lambda P')_{ii}^{-1} = (L + M')_{ii}^{-1} \frac{z_i + w_i}{\lambda} = \langle \phi_i \phi_i \rangle_{\{m_i'^2\}} \frac{z_i + w_i}{\lambda} , \tag{11}$$

with $m_i'^2 = (z_i + w_i)(1 - \lambda)/\lambda$ and, from the mass independence, they have the same singular part as $\tilde{P}_{ii}(\lambda)$. This proves that the RW asymptotic behavior and consequently the RW spectral dimension are independent of the introduction of waiting probabilities.

Now let us consider our graph G as an oscillating network with point masses $\mathcal{M}_i$, bounded by positive numbers, joined by springs of elastic constant $k = 1$ when $A_{ij} = 1$.

The normal modes of this system are the solutions of the eigenvalue equations

$$\sum_j L_{ij} x_j = \omega^2 \mathcal{M}_i x_i , \tag{12}$$

with ω being the frequency and x_i the displacement from equilibrium position at site i. Let us pose $\omega^2 = l$ and define the density $\rho_l(l)$ of eigenstates with eigenvalue l, and $\rho_\omega(\omega)$ the density of modes with frequency ω. If $\rho_\omega(\omega) \sim \omega^{\tilde{d}-1}$ for $\omega \to 0$, then $\rho_l(l) \sim l^{\tilde{d}/2-1}$ for $l \to 0$. Now notice that, in this case,

$$\int \frac{\rho_l(l)}{l + \epsilon} \, dl \sim \epsilon^{(\tilde{d}/2)-1} \tag{13}$$

for $\epsilon \to 0$. But

$$\int \frac{\rho_l(l)}{l + \epsilon} \, dl = \bar{\text{T}}\text{r}[(\mathcal{M}^{-1} L + \epsilon)^{-1}] = \bar{\text{T}}\text{r}[(L + \mathcal{M}\epsilon)^{-1} \mathcal{M}] , \tag{14}$$

with $\mathcal{M}$ being the diagonal matrix of oscillating masses $\mathcal{M}_i$ and $\bar{\mathrm{T}}\mathrm{r}[C] \equiv \lim_{N\to\infty} N^{-1} \sum_{i=1}^{N} C_{ii}$. Now we can observe that the latter expression, due to the mass boundedness, has the same singular part as the average over all sites of G of $\langle \phi_i \phi_i \rangle_{\{\epsilon m_i^2\}}$ with $m_i^2 \equiv \mathcal{M}_i$. Because of the generalized HHW inequalities we considered at the beginning of this Letter, it follows the mass independence of the asymptotic behavior of $\rho_\omega(\omega)$ and consequently of the vibrational spectral dimension.

The latter, as one can see from (14), is also related to RW. However, it depends on the average over all sites of the probabilities $P_{ii}(t)$ and not on a specific one. Although all $P_{ii}(t)$ have always the same asymptotic behavior, it is not possible to conclude that even their average should behave in the same way. So, in principle, the vibrational $\tilde{d}$ is independent and possibly different from all the other definition of spectral dimension.

Although it seems rather difficult to give a general geometrical condition leading to different asymptotic behaviors of $P_{ii}(t)$ and $\bar{\mathrm{T}}\mathrm{r}[P(t)]$, in some specific structures where they can be explicitly calculated such a difference is indeed found. This is the case of the class of graphs known as comb lattices [6]. There, by direct computation, one can verify that, due to the very particular geometry, $\bar{\mathrm{T}}\mathrm{r}[P(t)]$ coincides with the probability of returning to the starting point on a linear chain and goes as $t^{-1/2}$ for large t, while $P_{ii}(t) \sim t^{-q/2}$, with $q = 2 - 2^{-d+1}$, where the integer number d is the Euclidean dimension of the natural embedding space [6].

Notice that the boundedness of oscillating masses as well as the boundedness of the weights w_i are sufficient conditions for universality. It is a hard task to prove a weaker necessary condition, since in absence of boundedness the asymptotic behavior could in principle depend on the spatial mass (or w_i) distribution. However, on a linear chain one can argue that the boundedness of the mean value of m_i and the finiteness of the mean value of w_i are necessary and sufficient to preserve universality. The validity of this criterion for more complex structures, although likely, is still an open problem.

In conclusion, the results obtained clarify the universal properties of the spectral dimension and show that this parameter is a good generalization of the usual dimension in the description of a large class of physical phenomena. The coincidence of Gaussian and RW definitions suggests that the long range geometry affects in the same way two classes of problems that are in principle very different: indeed the Gaussian model is deeply related to statistical models for phase transitions, while discrete time RW are usually introduced to describe diffusion on real structures. Moreover, the fact that the possibility for a random walker of staying on each site with different probabilities does not affect its long time properties clearly shows that the latter are related only to large scale geometry and largely independent of any local detail. In a similar way, the result obtained for the harmonic spectrum, meaning the independence of its low frequencies regime of any changes in the masses (such as, e.g., the presence of different isotopes with any distribution), underline the fundamental role played by the geometrical structures with respect to other physical ingredients. Finally, the possibility of difference between the vibrational spectral dimension and the RW and Gaussian ones, which will be further studied in a forthcoming paper [7], is a sign of the need to distinguish between local and bulk parameters on inhomogeneous structures [8] where, due to the lack of invariance properties, local quantities do not contain a complete information about the whole system.

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