Random Walks on Bundled Structures

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Bundled structures (BS) are discrete structures obtained joining to each point of a "base" graph a copy of a "fiber" graph. In condensed matter physics BS are used as realistic models for the geometry and dynamics of nontranslationally invariant systems (polymers, inhomogeneous systems, etc.). We present an analytical solution for the random walk problem on these structures, which is possible when we know the solution for base and fiber separately. We obtain an expression for the spectral dimension of the BS as a function of the spectral dimensions of its components. Moreover, we discuss some applications of these results concerning anomalous diffusion laws, proving the existence of nondisordered structures with logarithmic and sublogarithmic diffusion laws due only to geometric features.

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Anomalous diffusion is one of the most studied and intriguing problems in contemporary statistical physics. Its applications concern a wide class of fields ranging from condensed matter to dynamical systems. Random walks on discrete structures give us a powerful and simple model to understand the microscopical origin of such phenomenon. The deviation from usual diffusion laws is due in general to the lack of translational invariance of transition probabilities. In fact, it has been known for many years that on translationally invariant lattices (TIL) the mean square displacement of a simple random walker (i.e., without bias) goes as

$$\langle r^2(t)\rangle \sim t\,, \tag{1}$$

and the probability of returning to the starting site goes as

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

for large t, where d is the Euclidean dimension, regardless of any other geometrical detail. Translational invariance can be lost in essentially two different ways, i.e., by introducing a random distribution of transition probabilities on a TIL and averaging over that, or by introducing discrete structures geometrically different from any TIL, without fluctuating probabilities. The first case has been studied by many authors and presents a wide collection of anomalous diffusion laws [1], including logarithmic behavior [2]. The second one, which we shall deal with, has become of primary importance since 1982, when Alexander and Orbach [3] realized that fractal geometry deeply affects diffusion phenomena, modifying the time exponents in (1) and (2). To describe such modifications, they introduced the spectral dimension $\tilde{d}$ and wrote (1) and (2) as

$$\langle r^2(t)\rangle \sim t^{d_f/\tilde{d}} \tag{3}$$

and

$$P_0(t) \sim t^{-\tilde{d}/2}, \tag{4}$$

where d_f is the fractal dimension. Later it became clear that this *fractal dynamics* is a much more general behavior, common not only to fractals, but also to other geometrical structures differing from TIL without being self-similar (e.g., comblattices [4], branched structures [5], etc.). Spectral dimension can be experimentally determined by measurements involving diffusion processes (e.g., time-resolved spectroscopy of nearest-neighbors energy transfer) but, in general, is quite difficult to obtain the theoretical prediction of such measures by analytical means. In fact, the only available general technique, i.e., the renormalization group approach, gives exact results only for a very small family of deterministic fractals, called exactly decimable fractals [5]. In particular, such a technique does not apply to structures with fractal dynamics and without self-similarity: in this case sometimes one can still obtain exact results, but always applying very particular tricks [4,6,7]. In this Letter we shall deal with a wide class of discrete structures (bundled structures), not necessarily fractals, different from TIL, of great interest from an experimental as well as a theoretical point of view. Bundled structures (BS) can be obtained joining to each point of a *base* structure, a copy of a *fiber* structure. Comb polymers [8] [Fig. 1(a)], brush polymers

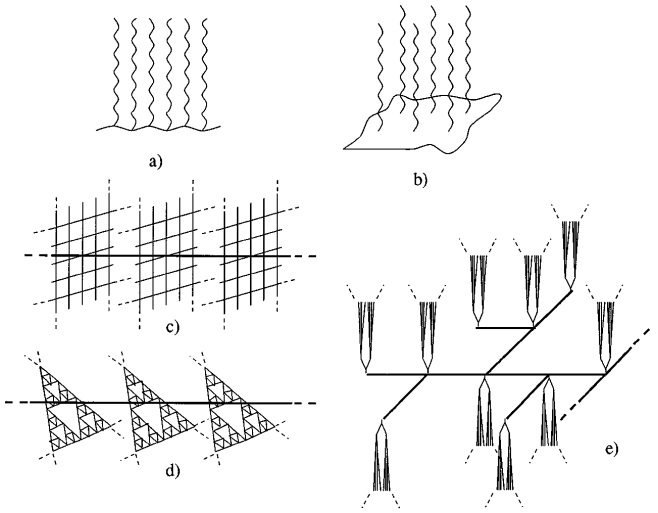

FIG. 1. (a) Comb polymer, (b) brush polymer, (c) kebab lattice, (d) Sierpinski-gasket kebab, and (e) BS with a T fractal as $\mathcal{B}$ and 2-NTD as $\mathcal{F}$.

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[Fig. 1(b)], and many kinds of branched aggregates are all examples of BS, as well as their theoretical models studied in [4,6,7]. By rigorous combinatorial methods, we relate the main random walk quantities for a generic BS to the corresponding ones for its base and its fiber. These relations allow us to obtain the exact spectral dimension and diffusion exponent for the BS simply knowing the same parameters for the base and the fiber, without any specific calculation. Moreover, we shall show that (3) and (4) are not the most general laws one can obtain for BS, but in many cases we have some important logarithmic corrections or even logarithmic laws, never obtained up to now without introducing bias or averaging on disorder.

Let us begin with some definitions. Given two graphs $\mathcal{B}$ and $\mathcal{F}$, not necessarily different, and a site F of $\mathcal{F}$, we call bundled graph with *base* $\mathcal{B}$ and *fiber* $\mathcal{F}$ the graph $(\mathcal{B}, \mathcal{F}, F)$, 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 (Fig. 2). Simple examples of bundled graphs are shown in Fig. 1. It is an easy exercise to show that the intrinsic fractal dimension (or connectivity dimension) of $(\mathcal{B}, \mathcal{F}, F)$ is given by $d_{(\mathcal{B},\mathcal{F},F)} = d_{\mathcal{B}} + d_{\mathcal{F}}$; i.e., it is simply the sum of the base and fiber intrinsic fractal dimensions. Moreover, it can be shown that it always exists a natural embedding in an Euclidean space of suitable dimension, such that these connectivity dimensions coincide with the corresponding fractal ones. In the following we shall drop the subscript $(\mathcal{B}, \mathcal{F}, F)$ for quantities referring to the whole BS where no confusion is possible.

Now let us introduce discrete time random walks on the bundled graph defining the jumping probabilities $p_{ij} = 1/z_i$ if i and j are nearest neighbors and $p_{ij} = 0$ otherwise [z_i is the coordination number of site i in $(\mathcal{B}, \mathcal{F}, F)$]. In the following we describe the main steps of the derivation of our results together with some applications; more details and examples will be given in a forthcoming paper [9]. We shall first calculate the probability $P_0(t)$.

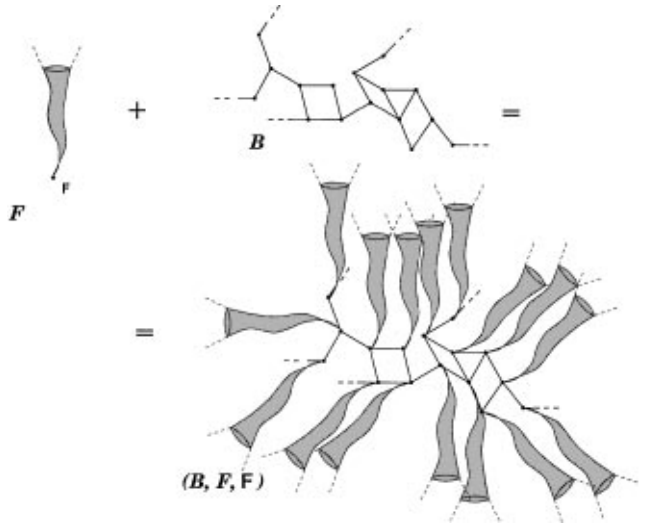

FIG. 2. Building of a bundled structure.

Although the explicit functional form of such a quantity depends in general on the chosen starting site, it has been shown [6] that its asymptotic behavior and the spectral dimension in particular are independent of this choice. This is why, for simplicity's sake, we shall deal with walkers starting from a point belonging to the base. Moreover, for the first time we shall restrict ourselves to base graphs with constant coordination number $z_{\mathcal{B}}$. This constraint will then be easily removed. If a walker returns to 0 in t steps, in general $t_{\mathcal{B}}$ among them have been spent on the base and $t_{\mathcal{F}} = t - t_{\mathcal{B}}$ on the fibers. Let us divide the latter into groups of successive steps on a fiber, separated by a step on the base. In such a way we obtain $t_{\mathcal{B}} + 1$ groups of $t_1, \ldots, t_{t_{\mathcal{B}}+1}$ steps, respectively, with $t_i \geq 0$ and $\sum_i t_i = t_{\mathcal{F}}$. Each group corresponds to a walk on the fiber starting and returning in F, with a decay probability in F equal to $z_{\mathcal{B}}/(z_{\mathcal{B}} + z_F)$, z_F being the coordination number of F on the fiber, due to the possibility of escaping along the base. This allows us to write

$$P_0(t) = \sum_{t_{\mathcal{B}}=0}^{\infty} \sum_{t_1=0}^{\infty} \cdots \sum_{t_{\mathcal{B}}+1=0}^{\infty} P_{\mathcal{B}}(t_{\mathcal{B}}) \left(\frac{z_{\mathcal{B}}}{z_{\mathcal{B}} + z_F} \right)^{t_{\mathcal{B}}} \times P'_{\mathcal{F}}(t_1) \cdots P'_{\mathcal{F}}(t_{t_{\mathcal{B}}+1}) \delta_{t, t_{\mathcal{B}} + \sum_i t_i}, \quad (5)$$

where $P_{\mathcal{B}}(t)$ is the probability of returning to the origin on the base graph and $P'_{\mathcal{F}}(t)$ is the probability of returning to the starting point on the fiber with the given decay probability in F.

Introducing the generating functions $\tilde{P}(\lambda) \equiv \sum_{t=0}^{\infty} \lambda^t P(t)$, we obtain

$$\tilde{P}_0(\lambda) = \tilde{P}'_{\mathcal{F}}(\lambda) \tilde{P}_{\mathcal{B}} \left(\frac{\lambda z_{\mathcal{B}}}{z_{\mathcal{B}} + z_F} \tilde{P}'_{\mathcal{F}}(\lambda) \right). \quad (6)$$

Notice that the constant coordination number requirement was introduced in order to have a probability of escaping on the fiber independent of the base point. The same condition can be reached even if the base points have a different coordination number z_i, simply by adding a staying probability on the site equal to $(z_{\mathcal{B}} - z_i)/z_{\mathcal{B}}$, where $z_{\mathcal{B}}$ is the largest value of z_i. Now it can be shown that on a generic graph the addition of a staying probability bounded from above does not affect the asymptotic behavior of Green functions at large times, so that the following results still hold for general base graphs (the only condition being the boundedness of z_i).

In order to calculate the spectral dimension of the bundled graph $\tilde{d}$, notice that (4) implies the following behavior for the singular part of $\tilde{P}_0(\lambda)$:

$$S[\tilde{P}_0(\lambda)] \sim \begin{cases} (1 - \lambda)^{\tilde{d}/2-1} & \text{for } \tilde{d} \neq 2n, \\ (1 - \lambda)^{\tilde{d}/2-1} \ln(1 - \lambda) & \text{otherwise}, \end{cases} \quad (7)$$

for $\lambda \to 1^-$, where n is any natural number.

By an asymptotic development of (6) and the introduction of (7) we obtain the following expression for $\tilde{d}$:

$$\tilde{d} = \begin{cases} \tilde{d}_{\mathcal{F}} & \text{if } \tilde{d}_{\mathcal{F}} \geq 2\,, \\ 4 - \tilde{d}_{\mathcal{F}} & \text{if } \tilde{d}_{\mathcal{F}} \leq 2 \text{ and } \tilde{d}_{\mathcal{B}} \geq 4\,, \\ \tilde{d}_{\mathcal{F}} + \tilde{d}_{\mathcal{B}} - \frac{\tilde{d}_{\mathcal{F}}\tilde{d}_{\mathcal{B}}}{2} & \text{if } \tilde{d}_{\mathcal{F}} \leq 2 \text{ and } \tilde{d}_{\mathcal{B}} \leq 4\,, \end{cases} \quad (8)$$

where $\tilde{d}_{\mathcal{F}}$ and $\tilde{d}_{\mathcal{B}}$ are the spectral dimensions of the fiber and of the base, respectively. It is remarkable that the result is independent of the point F where the fibers are joined to the base.

Notice that in (8) the cases $\tilde{d}_{\mathcal{F}} = 2$ and $\tilde{d}_{\mathcal{B}} = 4$ play a particular role. These are indeed critical dimensions, involving logarithmic corrections. In order to deal with them we now introduce a more general expression for $P_0(t)$ allowing logarithmic corrections to the main power law as well as a compact notation to deal with them.

Let us define the logarithmic dimensions $\beta(i)$ by

$$P_0(t) \sim \prod_{i=0}^{\infty} {}^{i}\ln^{\beta(i)}(t) \quad (9)$$

for $t \to \infty$, where ${}^{i}\ln x \equiv \ln^{i-1}\ln x$, with ${}^{0}\ln x \equiv x$ and $\beta(0) = -\tilde{d}/2$.

According to such notation, by similar techniques and standard Tauberian theorems, it is possible to obtain the following complete composition formulas:

$$\beta(i) = \begin{cases} -1 & \text{for } 0 < i < m\,, \\ (1 - \frac{\tilde{d}_{\mathcal{B}}}{2})[\beta_{\mathcal{F}}(m_{\mathcal{F}}) + I(\frac{\tilde{d}_{\mathcal{F}}}{2})] - I(\frac{\tilde{d}_{\mathcal{F}}}{2}) & \text{for } i = m = m_{\mathcal{F}}\,, \\ (1 - \frac{\tilde{d}_{\mathcal{B}}}{2})\beta_{\mathcal{F}}(i) + \theta(i - m_{\mathcal{F}} - m_{\mathcal{B}})\beta_{\mathcal{B}}(i - m_{\mathcal{F}}) & \\ +\delta_{i-m_{\mathcal{F}},m_{\mathcal{B}}} I(\frac{\tilde{d}}{2}) - \delta_{i,m} I(\frac{\tilde{d}}{2}) & \text{otherwise}\,, \end{cases} \quad (10)$$

holding for $\tilde{d}_{\mathcal{B}} < 4$, $\tilde{d}_{\mathcal{F}} < 2$, where $m = \min[i \geq 0, |\beta(i) \neq -1]$, $m = m_{\mathcal{F}} + \delta_{\tilde{d}_{\mathcal{B}},2} m_{\mathcal{B}}$, and $I(x) = 1$ for integer x and 0 otherwise. For $\tilde{d}_{\mathcal{F}} > 2$, $\beta(i) = \beta_{\mathcal{F}}(i)$ for each i. For $\tilde{d}_{\mathcal{F}} < 2$ and $\tilde{d}_{\mathcal{B}} > 4$ the expression of $P_0(t)$ for the bundled structure can be easily obtained from the expression of the correspondent quantity of the fiber alone by replacing each $\beta_{\mathcal{F}}(i)$ with $\beta(i) \equiv -\beta_{\mathcal{F}}(i) - 2\delta_{i,m_{\mathcal{F}}} I(\tilde{d}_{\mathcal{F}}/2)$ for $i \geq m_{\mathcal{F}}$ while $\beta(i) = \beta_{\mathcal{F}}(i)$ for $0 < i < m_{\mathcal{F}}$. Finally the case $\tilde{d}_{\mathcal{F}} < 2$ and $\tilde{d}_{\mathcal{B}} = 4$ is the same as the case $\tilde{d}_{\mathcal{F}} < 2$ and $\tilde{d}_{\mathcal{B}} > 4$ if $m_{\mathcal{B}} < -1$ and the same as the case $\tilde{d}_{\mathcal{F}} < 2$ and $\tilde{d}_{\mathcal{B}} < 4$ if $m_{\mathcal{B}} > -1$. The case $\tilde{d}_{\mathcal{F}} = 2$ must be treated as the case $\tilde{d}_{\mathcal{F}} < 2$ if the fiber is a recursive lattice, and as the case $\tilde{d}_{\mathcal{F}} > 2$ when the fiber is transient.

Following similar steps we can obtain the expression of the diffusion law on BS of the projection x on the base of the position of the random walker at time t, x being the chemical distance of the projection from the starting point. Once we know that on the base alone the diffusion law has the expression

$$\langle x^2 \rangle_{\mathcal{B}}(t) \sim \prod_{i=0}^{\infty} {}^{i}\ln^{\gamma_{\mathcal{B}}(i)}(t)\,, \quad (11)$$

we can prove that on BS with $\tilde{d}_{\mathcal{F}} \leq 2$ we have the expression (11) with exponents given by

$$\gamma(i) = \begin{cases} \gamma_{\mathcal{B}}(0)\,(1 - \frac{\tilde{d}_{\mathcal{F}}}{2}) & \text{for } i = 0\,, \\ 0 & \text{for } 0 < i < m_{\mathcal{F}}\,, \\ \gamma_{\mathcal{B}}(0)\,[\beta_{\mathcal{F}}(i) + I(\frac{\tilde{d}_{\mathcal{F}}}{2})] & \text{for } i = m_{\mathcal{F}} > 0\,, \\ \gamma_{\mathcal{B}}(0)\beta_{\mathcal{F}}(i) + \gamma_{\mathcal{B}}(i - m_{\mathcal{F}}) & \text{for } i > m_{\mathcal{F}}\,, \end{cases} \quad (12)$$

while for $\tilde{d}_{\mathcal{F}} > 2$ the expression of $\langle x^2 \rangle$ tends to a constant independent of t which means localization.

Now let us see how the recipes previously obtained work treating in detail a few cases. Let us first consider a BS where $\mathcal{B}$ and $\mathcal{F}$ are both linear chains; it is easy to realize that we have built a two-dimensional comb lattice. To find out that the spectral dimension of the comb is $\tilde{d} = 3/2$ it is sufficient to put $\tilde{d}_{\mathcal{F}} = \tilde{d}_{\mathcal{B}} = 1$ in (8); then we easily obtain that $\langle x^2 \rangle(t) \sim t^{1/2}$ since $\gamma_{\mathcal{B}}(0) = 1$; following similar steps we can recover, in a much simpler way, all the results that we found after direct calculation in a previous work [10]. If we use a 2D hypercubical lattice for the base and a linear chain for the fiber, we obtain a "brush lattice" where $P_0(t) \sim t^{-1}$ and $\langle x^2 \rangle(t) \sim t^{1/2}$. A curious result is represented by the class of lattices with $\tilde{d}_{\mathcal{B}} \geq 4$ and $\tilde{d}_{\mathcal{F}} = 2$; in this case we have BS which result to be transient lattices [i.e., $\tilde{P}_0(\lambda)$ is finite for $\lambda \to 1^-$] while their spectral dimension is $\tilde{d} = 2$, a value usually considered typically of recursive lattices [$\tilde{P}_0(\lambda)$ infinite in the considered limit].

To find logarithmic corrections we can, for example, build up a BS with a linear chain as $\mathcal{B}$ and a 2D TIL as $\mathcal{F}$; in a previous paper [7] we studied in detail these structures, we called "kebab lattices," and found out that $P_0(t) \sim t^{-1}\ln^{-1/2}(t)$ and $\langle x^2 \rangle(t) \sim \ln(t)$. Now these results come straightforward as a result of (12). This example suggests that we can find, by a suitable choice of $\mathcal{B}$ and $\mathcal{F}$, BS with logarithmic corrections at every order. If both $\mathcal{B}$ and $\mathcal{F}$ are 2D TIL, we have $P_0(t) \sim t^{-1}\ln^{-1}(t)$; these lattices used as fibers for another 2D TIL give $P_0(t) \sim t^{-1}\ln^{-1}(t)$ and, iterating this procedure n times, we get $P_0(t) \sim \prod_{i=0}^{n} {}^{i}\ln^{-1}(t)$. On these structures we have $\langle x^2 \rangle(t) \sim {}^{n}\ln(t)$.

Notice that, even if the structures considered in all the previous examples cannot be embedded in 3D space, if we use the fractal trees called NTD with integer $\tilde{d}$ [11] instead of d-dimensional TIL, we obtain BS with the same asymptotic laws, which are not only embeddable, but even realistic models for a wide class of branched polymers. So we can predict the existence of real systems showing sublogarithmic diffusion. Not only polymers can be described by BS but this is also the case of disordered solid materials showing anisotropic transport such as some cuprates [12]. Using our results we can obtain BS with different diffusion laws along the base and fiber directions. This is the case, e.g., of kebab lattices [7] where we have $\langle x^2 \rangle \sim \ln t$ along the axis and $\langle x^2 \rangle \sim t$ along the orthogonal directions, so that it behaves as an insulating or a conducting system depending on the particular direction.

But maybe the most interesting feature of all these results is that, since they relate the properties of a whole structure to those of its components, we cannot only predict the behavior of existing systems by decomposing them in simpler parts, but also we can project complex systems with required diffusion properties by composing simpler existing structures. This aspect of "diffusion engineering" could be easily exploited by chemists and material scientists building up polymers and noncrystalline solids with predefined anomalous diffusion and transport properties, simply by joining more common existing "bricks."

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