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Random walks on disordered networks

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Random walks are studied on disordered cellular networks in two- and three-dimensional spaces with arbitrary curvature. The coefficients of the evolution equation are calculated in terms of the structural properties of the cellular system. The effects of disorder and space curvature on the diffusion phenomena are investigated. In disordered systems the mean squared displacement is increased at short times and decreased at long ones, with respect to the ordered case. The asymptotic expression for the diffusion equation on hyperbolic cellular systems relates random walks on curved lattices to hyperbolic Brownian motion. [S1063-651X(97)16605-3]

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The simplest disordered networks are space-filling random partitions of space by cells. The cells are convex, irregular polygons in two dimensions (2D) and irregular polyhedra in 3D. Topological stability imposes the incidence numbers at their minimum values ($d+1$ edges incident on a vertex in d dimensions). These cellular networks are also known in the literature as "froths," since the soap froth is the archetype of such structures. The space tiled by the froth can be curved. In this case, the intrinsic dimension of the cellular system (d_f) does not coincide with the dimension (d) of the embedding space. Froths are structures which characterize a broad class of natural systems such as polycrystalline solids, foams, biological tissues, amphiphilic membranes, epithelial tissues, etc., [1,2]. Moreover, froths and disordered packings are dual (see Fig. 1). Therefore, amorphous materials, granular solids, metallic glasses, etc., have structures which are dual to froths [3,4].

Many theoretical works, experiments, and computer simulations have been devoted to the study of random walks and transport phenomena on disordered [5–8] and fractal [9–15] structures. Random walks on Euclidean froths are a realistic models for diffusion in disordered systems, for signal propagation in granular media, and may be relevant to the evolution of natural foams and polycrystalline aggregates. Random walks on hyperbolic or elliptic froths can model transport phenomena in curved spaces.

In the present model, the walker starts at time $t=0$ from a given cell, and at each time step, jumps with equal probability to one of the neighboring cells. The radial and angular components of the motion with respect to the starting cell are decoupled. The radial component results the same as for the spherically symmetric model introduced recently in [11,12].

But, in the present case, the diffusion is on a realistic structure and all the parameters in the evolution equation are given in terms of the properties of the disordered cellular structure.

A d dimensional disordered cellular froth, can be viewed as structured in concentric layers of cells at the same topological distance (j) around a given central cell (where the topological distance between two cells is the minimum number of ($d-1$)-dimensional interfaces that a path must cross to connect the two cells). The structure is described topologically by two parameters per layer in two dimensions (number of cells per layer and average coordination in the layer), and three parameter per layer in three dimensions (see [16] for details). The number of cells in a layer at distance j from the central cell [$K(j)$], is related to the space curvature. One finds asymptotically, $K(j) \propto j^{d_f-1}$, where d_f is the intrinsic dimension; d_f coincides with the dimension d of the embedding space in Euclidean froths (tilings of flat spaces), whereas, $d_f > d$ in the hyperbolic case (tilings of negatively curved spaces) and $d_f < d$ in the elliptic one (tilings of positively curved spaces). A special case, discussed in [16], is a class of hyperbolic froths with $K(j) \propto \exp(\varphi j)$. Here the intrinsic dimension diverges.

Suppose the tiling is shell-structured inflatable (SSI) around the central cell. (In SSI froths any cell in layer (j) has neighbors in layer ($j-1$), (j), and ($j+1$). See Fig. 1 and [16] for details.) While, the number of paths connecting different layers can be more easily calculated in SSI froths, the extension to the general case of non-SSI froths is straightforward. Let the walker start at the central cell at $t=0$. Consider at time t, the walker to be in a cell of layer (j) (supposing the cells in layer j indistinguishable). At time $t+1$ it has moved outward to layer ($j+1$) or (for $j>0$) inward to layer ($j-1$) or stayed within the same layer (j), with probabilities $p_{out}(j)$ or $p_{in}(j)$ or $p_{stay}(j)$, respectively.

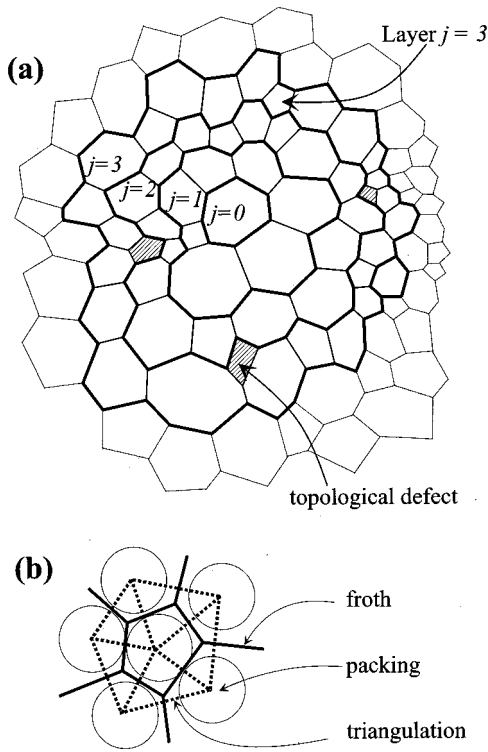*Electronic address: tomaso@fresnel.u-strasbg.fr

FIG. 1. A froth is a random partition of space by cells (a). Topological stability imposes minimal incidence number (three edges incident on a vertex in two dimensions). Froths are the dual structures of disordered packings (b). Such structures can be viewed as organized in concentric layers of cells at the same topological distance (j) from a given central cell ($j=0$). Some cells [hatched in (a)] have neighbors in the internal layer but not in the external one and are topological ''defects'' in the layered structure.

Note that, $p_{in}(j)+p_{out}(j)+p_{stay}(j)=1$, since the walker must move at each time step. The probability $P(j,t)$ of finding the walker in layer (j) at time t is

$$P(j,t)=p_{stay}(j)P(j,t-1)+p_{out}(j-1)P(j-1,t-1)$$
$$+p_{in}(j+1)P(j+1,t-1), \quad \text{for } j\geq 1 \quad (1)$$

and, $P(0,t)=p_{in}(1)P(1,t-1)$. The initial conditions are $P(j,0)=\delta_{j,0}$. The probability $p_{out}(j)$ is proportional to the number of paths connecting layer (j) with layer ($j+1$). This number is equal to the number of interfaces (edges in two dimensions and facets in three dimensions) separating the two layers. Analogously, the probability $p_{in}(j)$ is proportional to the number of interfaces between layer (j) and ($j-1$). In two dimensions, the number of edges separating layers (j) and ($j+1$) is $K(j)+K(j+1)$ (see Fig. 1). Thus,

$$p_{out}(j)=\frac{1}{\mathcal{N}_2(j)}[K(j)+K(j+1)]$$
$$\quad \text{(for } j\geq 1), \quad (2)$$
$$p_{in}(j)=\frac{1}{\mathcal{N}_2(j)}[K(j)+K(j-1)]$$

[and $p_{stay}(j)=1-p_{out}(j)-p_{in}(j)=2/e(j)$]. In Eq. (2) we defined, $K(0)=0$ and $\mathcal{N}_2(j)=e(j)K(j)$, with $e(j)$ the average number of edges per cell in layer (j). For $j=0$, one has $p_{out}(0)=1$ and $p_{in}(0)=0$. In three dimensions the layers

are separated by a system of faces which tile a spherical surface: the ''shell network'' [16]. The number of paths between two successive layers (j) and ($j+1$) is proportional to the number of facets of the shell network between these layers. This number is $2[K(j)+K(j+1)-8]/[n(j)-4]$ [16], where $n(j)$ is the average number of edges per face in the shell network. We have, therefore,

$$p_{out}(j)=\frac{2}{\mathcal{N}_3(j)}\frac{K(j)+K(j+1)-8}{n(j)-4}$$
$$\quad \text{(for } j\geq 1),$$
$$p_{in}(j)=\frac{2}{\mathcal{N}_3(j)}\frac{K(j)+K(j-1)-8}{n(j-1)-4}$$
$$(3)$$

where we defined: $K(0)=2$ and $\mathcal{N}_3(j)=f(j)K(j)$, with $f(j)$ the average number of faces per cell in layer (j). For $j=0$, we have $p_{out}(0)=1$ and $p_{in}(0)=0$.

A quantity of interest is the probability Π that the walker ever returns to the origin. This quantity is associated with the mean time spent at the origin $[F(0)=\Sigma_{t=0}^{\infty}P(0,t)]$ via the relation, $\Pi=1-[1/F(0)]$ [18]. From Eq. (1) and using Eqs. (2) and (3), we obtain,

$$\Pi=1-\frac{1}{F(0)}=1-\frac{1}{1+K(1)\Sigma_{j=1}^{\infty}\frac{1}{\mathcal{N}_d(j)p_{out}(j)}}. \quad (4)$$

This expression is valid for any froth tiling an unbounded topological manifold. The quantity $\mathcal{N}_d(j)p_{out}(j)$ is related to the properties of the structure around the central cell, and asymptotically scales as $K(j)$ [see Eqs. (2) and (3)]. In a cellular system with intrinsic dimension d_f, the number of cells per layer has the asymptotic behavior $K(j)\propto j^{d_f-1}$, thus $\mathcal{N}_d(j)p_{out}(j)\sim K(j)\sim j^{d_f-1}$. Substituting into Eq. (4), we obtain $\Pi=1$ for $d_f\leq 2$, and $\Pi<1$ for $d_f>2$. This result, also holds for random walks on regular lattices, fractals and trees [18], indicating the universality of this critical behavior. Figure 2 shows Π vs d_f, for two dimensional SSI froths with $K(j)=K(1)j^{d_f-1}$.

A quantity generally used to describe diffusion is the mean squared displacement $\langle r^2\rangle(t)=\Sigma_{j=0}^{\infty}j^2P(j,t)$. The time-dependent diffusion coefficient $D(t)$ is associated with this quantity by the relation $2dD(t)=(\partial/\partial t)\langle r^2\rangle$, and the usual diffusion coefficient D^{∞} is the limit of $D(t)$ at infinite time. Equation (1) implies

$$\langle r^2\rangle(t+1)-\langle r^2\rangle(t)=\sum_{j=0}^{\infty}\{p_{out}(j)+p_{in}(j)+2j[p_{out}(j)$$
$$-p_{in}(j)]\}P(j,t). \quad (5)$$

When, $j\geq 1$, and the parameters $e(j)=\langle e\rangle$, $f(j)=\langle f\rangle$, and $n(j)=\langle n^N\rangle$ are independent of j (this is the expected asymptotic behavior), Eqs. (2) and (3) give,

$$p_{out}(j)+p_{in}(j)=1-p_{stay}(j)=\begin{cases}\dfrac{\langle e\rangle-2}{\langle e\rangle} & \text{for } d=2 \\ \dfrac{\langle f\rangle-6}{\langle f\rangle} & \text{for } d=3\end{cases}=2\mathcal{C}_d.$$
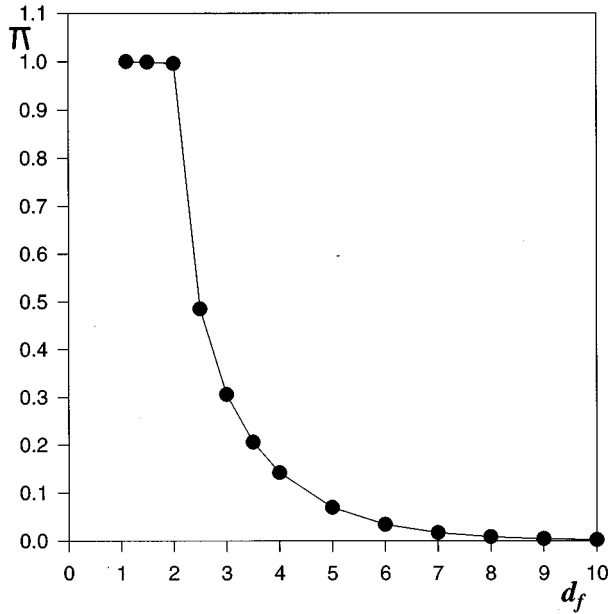$$(6)$$

FIG. 2. Probability Π that the walker ever returns to the origin for several values of the intrinsic dimension d_f. The walker always returns to the origin when $d_f \leq 2$, whereas the probability is less than 1 and decreases with d_f when $d_f > 2$. This critical behavior is independent of the details of the structure. (The line is a guide for the eyes.)

For d_f finite, $j[p_{out}(j) - p_{in}(j)] = (d_f - 1)\mathcal{C}_d$. Thus, from Eq. (5),

$$\langle r^2 \rangle (t) \sim 2 d_f \mathcal{C}_d t. \tag{7}$$

The diffusion coefficient is therefore, $D^\infty = (d_f/d)\mathcal{C}_d$. Numerical solutions of Eq. (1) for two-dimensional and three-dimensional structures with different intrinsic dimensions and coordination numbers give diffusion coefficients in very good agreement with Eq. (7). Note that, $\langle r^2 \rangle$ in Eq. (7) is expressed in term of topological distances (j). The metric quantities can be retrieved by multiplying j by the average asymptotic distance ρ_0 between layers. For instance, in the hexagonal lattice, $\rho_0 = (\sqrt{3}/2)a$, with a the lattice spacing. From Eq. (7), one gets, therefore, $\langle \rho^2 \rangle = \rho_0^2 \langle r^2 \rangle = a^2 t$, which is the known expression for the mean squared displacement in the hexagonal lattice. The linear dependence of $\langle r^2 \rangle$ on t in Eq. (7), indicates normal diffusion. The spectral dimension d_s (defined from the exponents $\langle r^2 \rangle \sim t^{d_s/d_f}$ and $P(0,t) \sim t^{-d_s/2}$ [19]) coincides with the intrinsic dimension d_f.

In disordered froths, topological non-SSI defects are always present. Defects, in layer (j), are cells which have no neighbors in layer ($j+1$) (see Fig. 1 and [16]). Asymptotically, the number of defective cells in layer (j) is a fraction δ of the total number of cells $K(j)$ (typically, $0.1 < \delta < 0.2$ in two dimensions [17]). In two dimensions, the number of paths connecting layer (j) with nondefective cells in layer ($j+1$) is $(1-\delta)[K(j) + K(j+1)]$ (see Fig. 1), whereas, the number of paths ending in a defective cell is $\eta \delta K(j+1)$,
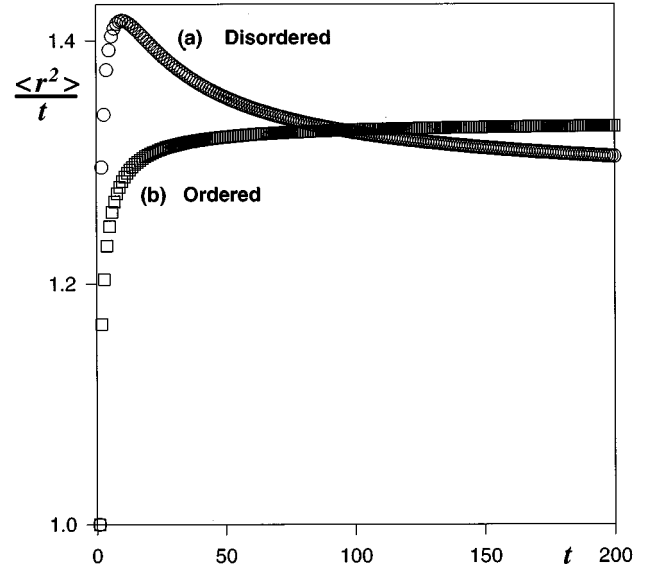

FIG. 3. Mean squared displacement $\langle r^2 \rangle$ over t vs time for disordered (a) and ordered (b) cellular lattices. The average distance of the walker from the starting point is $j \simeq \langle r^2 \rangle^{1/2}$. At short distances ($j < 5$) the walker diffuses faster in the disordered than in the corresponding ordered lattice. Then diffusion in disordered lattice slows down to reach an asymptotic regime where the walker propagates more slowly in the disordered system than in the ordered one.

with η the average number of interfaces added by a defect to the shell between two successive layers (typically, $1 < \eta < 1.3$ in two dimensions [17]). Therefore, asymptotically, Eqs. (7) and (6) can be extended to the non-SSI case by multiplying expression (6) by the factor $[1 - \delta + (\eta\delta/2)]$. The same result holds in three dimensions. Non-SSI defects have important effects on the froth structure. In particular, in two-dimensional non-SSI Euclidean froths, the number of cells per layer increases linearly with the distance, $K(j) = Cj + B$, with slope $C \sim 9$ [17]. This slope is higher than the $C = 2\pi$ expected from simple geometrical considerations and the $C = 6$ of the SSI hexagonal lattice. Larger increments in the number of cells per layer, correspond to *faster diffusion* (more paths outward). On the other hand, in typical two-dimensional disordered systems, $[1 - \delta + (\eta\delta/2)] < 1$, which indicates asymptotically, *slower diffusion* in non-SSI froths. These two opposite behaviors are not contradictory. Indeed, for $j \gg 1$, the ratio between the number of paths in successive layers depends only on the exponent of $K(j)$ vs j (i.e., the intrinsic dimension -1), and not on the slope. Therefore, we expect the diffusion in disordered structures, compared with ordered SSI lattices, to be *faster at small distances* [where the slope of $K(j)$ is relevant] and then *slower at large distances* [where only the exponent of $K(j)$ is relevant]. Figure 3 shows $\langle r^2 \rangle / t$, calculated from Eq. (1), for a non-SSI two-dimensional Euclidean froth 3(a) and for the SSI hexagonal lattice 3(b).

A special behavior of $\langle r^2 \rangle$ is obtained for the 2D SSI hyperbolic froth, studied in Ref. [16], which has $e(j) = \langle e \rangle > 6$ and $K(j) = C \exp(\varphi j)$, with $\varphi = \cosh^{-1}[(\langle e \rangle - 4)/2]$. In this case, from Eqs. (2), (3), and (5), one derives the asymptotic expression

$$\langle r^2 \rangle(t) \sim \frac{(\langle e \rangle - 6)(\langle e \rangle - 2)}{\langle e \rangle^2} t^2 \quad \text{for } t \gg 1. \qquad (8)$$

Numerical solutions of Eq. (1) for SSI two-dimensional hyperbolic froths with various $\langle e \rangle > 6$, give time-dependent diffusion coefficient in excellent agreement with expression (8). The quadratic exponent in Eq. (8) indicates ballistic diffusion and $d_s = 2 d_f$.

We now write the evolution equation (1) in the continuous limit. Introduce the continuous variables $\rho = j \rho_0$ and $\tau = t \tau_0$, where ρ_0 is the average distance between two layers and τ_0 is the average time between two jumps. In the asymptotic limit ($j = \rho/\rho_0 \to \infty$ and $t = \tau/\tau_0 \to \infty$), when the average topological arrangements of the cells is independent of the layer number, Eq. (1) can be written in the continuous form

$$\frac{\partial}{\partial \tau} P(\rho, \tau) = \frac{\rho_0^2}{\tau_0} \mathcal{C}_d \frac{\partial}{\partial \rho} \left\{ \frac{\partial}{\partial \rho} P(\rho, \tau) \right. $$
$$\left. - \left[\frac{4}{(s+2)} \frac{1}{K(\rho)} \frac{\partial}{\partial \rho} K(\rho) \right] P(\rho, \tau) \right\}, \qquad (9)$$

where s is the inflation parameter ($s = \langle e \rangle - 4$ in two dimensions, and $s = \frac{1}{2}(\langle f \rangle - 6)(\langle n^N \rangle - 4) - 2$ in three dimensions [16]), which is associated with the curvature of the manifold tiled by the froth ($s = 2$ in Euclidean, $s > 2$ in hyperbolic, and $s < 2$ in elliptic froths). Expression (9) is the diffusion equation for a d-dimensional spherically symmetric system written in polar coordinates. All the information about the cellular structure, its intrinsic dimension, and its disorder, are contained in the term in square brackets and in the parameter $\mathcal{C}_d$. For a random cellular system with finite intrinsic dimension, d_f we have asymptotically, $K(\rho) \sim \rho^{d_f - 1}$ and $s \to 2$. Therefore the coefficient inside the square brackets in Eq. (9) becomes $(d_f - 1)/\rho$, and Eq. (9) has the solution

$$P(\rho, \tau) = \frac{2 \rho^{d_f - 1}}{\Gamma\left(\dfrac{d_f}{2}\right) \left(4 \dfrac{\rho_0^2}{\tau_0} \mathcal{C}_d \tau \right)^{d_f/2}} \exp\left(- \frac{\rho^2}{4 \dfrac{\rho_0^2}{\tau_0} \mathcal{C}_d \tau} \right). \quad (10)$$

The probability $P(\rho, \tau)$ increases with ρ until a maximum at $\rho_{max} = [2(d_f - 1)(\rho_0^2/\tau_0)\mathcal{C}_d \tau]^{1/2}$, then decreases exponentially. From solution (10), the mean squared displacement is $\langle r^2 \rangle \simeq \int_0^\infty (\rho^2/\tau_0) P(\rho, \tau) d\rho = 2 d_f (\rho_0^2/\tau_0) \mathcal{C}_d \tau$, as in Eq. (7).

A previous paper [16], described a class of two- and three-dimensional hyperbolic SSI froths where, $K(\rho) = C \sinh[\varphi(\rho/\rho_0)]$, with $\varphi = \cosh^{-1}(s/2)$ a constant associated with the space curvature (in simple two-dimensional cases $\varphi = \sqrt{-k}$, with k the Gaussian curvature, here, $s > 2$ and $k < 0$). For these froths, the evolution equation (9) takes the form

$$\frac{\partial}{\partial \tau} P(\rho, \tau) = \frac{\rho_0^2}{\tau_0} \mathcal{C}_d \frac{\partial}{\partial \rho} \left\{ \frac{\partial}{\partial \rho} P(\rho, \tau) \right.$$
$$\left. - \left[\frac{4}{(s+2)} \frac{\varphi}{\rho_0} \coth\left(\varphi \frac{\rho}{\rho_0} \right) \right] P(\rho, \tau) \right\}. \quad (11)$$

Equation (11) is the diffusion equation in hyperbolic spaces with constant, negative curvature [15,20]. Here the equation has been obtained from a tessellation model, linking therefore diffusion in curved lattices to hyperbolic Brownian motion. At large distances, the coefficient in the square brackets in Eq. (11) tends to a constant, and the solution is a Gaussian which moves ballistically outward with its maximum at $\rho_{max} = [4/(s+2)] \varphi (\rho_0/\tau_0) \mathcal{C}_d \tau$. This behavior is consistent with Eq. (8).

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