Random walk on disordered networks

Tomaso Aste

(April 19, 2018)
Equipe de Physique Statistique, LUDFC Université Louis Pasteur,
3, rue de l’Université, Strasbourg France
e-mail: tomaso@fresnel.u-strasbg.fr
PACS: 66.30.-h, 05.40.-j, 61.43.+j

Abstract

Random walks are studied on disordered cellular networks in 2-and 3-dimensional spaces with arbitrary curvature. The coefficients of the evolution equation are calculated in term 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 square displacement displays an enhancement at short time and a lowering at long ones, with respect to the ordered case. The asymptotic expression for the diffusion equation on hyperbolic cellular systems relates random walk on curved lattices to hyperbolic Brownian motion.

The simplest disordered networks are space-filling random partitions of space by cells. The cells are convex, irregular polygons in two dimension (2d) and irregular polyhedras in 3d. Disorder 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 (df) does not coincide with the dimension (d) of the embedding space.

Froths are the structures which characterizes a broad class of natural systems such as polycrystalline solids, foams, biological tissues etc. Moreover, froths and disordered packings are dual systems (see Fig.1). Therefore, amorphous materials, granular solids, metallic glasses etc. have structures which are dual of froths.

Many theoretical works, experiments, and computer simulations have been devoted to the study of random walk and transport phenomena on disordered and fractal systems. Random walk on Euclidean froths is a realistic model for diffusion in disordered systems, for signal propagation in granular media and it can be relevant in the study of
the evolution properties of natural foams and polycrystalline aggregates. Whereas, random walk on hyperbolic or elliptic froths can model transport phenomena in curved spaces.

Disordered structures are widespread in nature, and natural, disordered, two dimensional cellular structures can tile curved surfaces (e.g. amphiphilic membranes or epithelial tissues). The study of the effect of disorder and space-curvature on the diffusion phenomena is therefore of great physical interest and it is the aim of this paper.

In the present model, the walker starts at time $t = 0$ from a given cell, then, at each (finite) time-step it jumps with equal-probability to one of the neighbouring cells. The radial and angular components of the motion respect with the starting cell are decoupled. The radial component results the same as of the spherically symmetric model introduced recently in [11,12]. But, in the present case, the diffusion is on realistic cellular systems 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 studied 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 $2d$ (number of cells per layer and average coordination in the layer), and three parameter per layer in $3d$ (see [13] 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 of the cellular system. The intrinsic dimension $d_f$ coincide with the dimension $d$ of the embedding space in Euclidean froths (which are cellular tilings of flat spaces), whereas, $d_f > d$ in the hyperbolic case (tilings of negatively curves spaces) and $d_f < d$ in the elliptic one (tilings of positively curves spaces). A special case, discussed in [13], is a class of hyperbolic froths with $K(j) \propto \exp(\varphi j)$. Here the intrinsic dimension diverges.

Suppose the system being shell-structured-inflatable (SSI) around the central cell. (In SSI froths any cell in layer $(j)$ has neighbours in layer $(j-1)$, $(j)$ and $(j+1)$ and the layers make, concentric, closed rings of cells without “topological defects”. See Fig.1 and [16] for details.) 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, follows straightforward.

Let the central cell be the one where the walker starts at $t = 0$. Consider at time $t$ the walker being in a cell of layer $(j)$ (the cells in layer $j$ are supposed indistinguishable). At time $t+1$ it has moved outwards to layer $(j+1)$ or (for $j > 0$) inwards to layer $(j-1)$ or within the same layer $(j)$, with probabilities $p_{\text{out}}(j)$ or $p_{\text{in}}(j)$ or $p_{\text{stay}}(j)$, respectively. Note that, $p_{\text{in}}(j) + p_{\text{out}}(j) + p_{\text{stay}}(j) = 1$, 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 given by

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

for $j \geq 1$, (1)

and, for $j = 0$, by

$$P(0,t) = p_{\text{in}}(1)P(1,t-1)$$

(2)

With initial conditions $P(j,0) = \delta_{j,0}$. 

2
The probability \( p_{\text{out}}(j) \) is proportional to the number of paths connecting layer \((j+1)\) with layer \(j\). This number is equal to the number of interfaces (edges in \(2d\) and facets in \(3d\)) separating the two layers. Analogously, the probability \( p_{\text{in}}(j) \) is proportional to the number interfaces between layer \(j\) and \((j-1)\).

In \(2d\), the number of edges separating layers \((j)\) and \((j+1)\) is \(K(j)+K(j+1)\) (see fig.1). Thus,

\[
\begin{align*}
\text{out} &\quad p_{\text{out}}(j) = \frac{1}{N_2(j)}\left(K(j) + K(j+1)\right) \\
\text{in} &\quad p_{\text{in}}(j) = \frac{1}{N_2(j)}\left(K(j) + K(j-1)\right)
\end{align*}
\]

(for \(j \geq 1\)),

\[\text{out}\]

\[(\text{and } p_{\text{stay}}(j) = 1 - p_{\text{out}}(j) - p_{\text{in}}(j) = \frac{2}{e(j)})\]. In Eq.(3) we defined, \(K(0) = 0\) and \(N_2(j) = e(j)K(j)\), with \(e(j)\) the average number of edges per cell in layer \((j)\). For \(j = 0\), one has \(p_{\text{out}}(0) = 1\) and \(p_{\text{in}}(0) = 0\).

In \(3d\) the layers are separated by a system of faces which tile a spherical surface: the “shell-network” \(\Box\). 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 \(2^{K(j)+K(j+1)-8}\) \(\Box\), where \(n(j)\) is the average number of edges per face in the shell-network. We have therefore

\[
\begin{align*}
\text{out} &\quad p_{\text{out}}(j) = \frac{2}{N_3(j)}\left(K(j) + K(j+1) - 8\right) \\
\text{in} &\quad p_{\text{in}}(j) = \frac{2}{N_3(j)}\left(K(j) + K(j-1) - 8\right)
\end{align*}\]

(for \(j \geq 1\)),

\[\text{in}\]

where we defined: \(K(0) = 2\) and \(N_3(j) = f(j)K(j)\), with \(f(j)\) the average number of faces of the cells in layer \((j)\). For \(j = 0\), we have \(p_{\text{out}}(0) = 1\) and \(p_{\text{in}}(0) = 0\).

A quantity of interest is the probability \(\Pi\) that the walker ever returns to the origin. This quantity is associated with the mean time spent in the origin \((F(0) = \sum_{t=0}^{\infty} P(0,t))\) by the relation \(\Pi = 1 - \frac{1}{F(0)}\) \(\Box\). From Eq.(II) and by using Eqs.(3) and (II), we obtain

\[
\Pi = 1 - \frac{1}{F(0)} = 1 - \frac{1}{1 + K(1) \sum_{j=1}^{\infty} \frac{1}{N_3(j)p_{\text{out}}(j)}}.
\]

This expression is valid for any froth tiling an unbounded topological manifold. The quantity \(N_d(j)p_{\text{out}}(j)\) is related to the properties of the structure around the central cell, and asymptotically it scales as \(K(j)\) (see Eqs.(II) and (II)). In a cellular system with intrinsic dimension \(d_f\) the number of cells per layer have the asymptotic behaviour \(K(j) \propto j^{d_f-1}\), thus \(N_d(j)p_{\text{out}}(j) \sim K(j) \sim j^{d_f-1}\). By substituting into Eq.(II), we obtain \(\Pi = 1\) for \(d_f \leq 2\), and \(\Pi < 1\) for \(d_f > 2\). This result, already known for random walk on regular lattices, fractals, trees \(\Box\), and found here in froths, indicates the universality of this critical behaviour which is independent of the details of the structure. In Fig.2 the behaviour of \(\Pi\) vs. \(d_f\), given by equation (II) for \(2d\) SSI froths with \(K(j) = K(1)j^{d_f-1}\), is shown.

A quantity generally used to describe the diffusion phenomena is the mean square displacement \(\langle r^2 \rangle(t) = \sum_{j=0}^{\infty} j^2 P(j,t)\). The time-dependent diffusion coefficient \(D(t)\) is associated with this quantity by the relation \(2dD(t) = \frac{\partial}{\partial t} \langle r^2 \rangle\), and the usual diffusion coefficient \(D^\infty\) is the limit of \(D(t)\) at infinite time.
From Eq. (1) follows
\[
\langle r^2 \rangle (t + 1) - \langle r^2 \rangle (t) = \sum_{j=0}^{\infty} \left\{ \left[ p_{\text{out}}(j) + p_{\text{in}}(j) + 2j \left[ p_{\text{out}}(j) - p_{\text{in}}(j) \right] \right] P(j, t) \right\}.
\]

When, \( j \gg 1 \), 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 behaviour), Eqs. (3) and (4) give
\[
p_{\text{out}}(j) + p_{\text{in}}(j) = 1 - p_{\text{stay}}(j) = \begin{cases} \frac{\langle e \rangle - 2}{\langle e \rangle} & \text{for } d = 2 \\ \frac{\langle f \rangle - 6}{\langle f \rangle} & \text{for } d = 3 \end{cases} = 2C_d,
\]
and, for \( d_f \) finite, \( j \left[ p_{\text{out}}(j) - p_{\text{in}}(j) \right] = (d_f - 1)C_d \). Thus, from Eq. (3)
\[
\langle r^2 \rangle (t) \sim 2d_fC_dt.
\]

The diffusion coefficient is therefore, \( D^\infty = d_fC_d \). Numerical solutions of Eq. (1) for 2d and 3d structures with different intrinsic dimensions and coordinations give diffusion coefficients in very good agreement with Eq. (8). Note that, \( \langle r^2 \rangle \) in Eq. (8) is expressed in term of topological distances. The metric quantities can be retrieved from the topological ones by multiplying the topological distance \( \rho \) by the average asymptotic distance \( \rho_0 \) between layers. For instance, in the hexagonal lattice, \( \rho_0 = \sqrt{3}a \), with \( a \) the lattice spacing. From Eq. (8), one gets therefore \( \langle r^2 \rangle = \rho_0^2\langle r^2 \rangle = a^2t \), which is the known expression for the mean square displacement in the hexagonal lattice.

The linear dependence on \( t \) of \( \langle r^2 \rangle \) in Eq. (8), indicates a diffusive behaviour. In this case, the spectral dimension \( d_s \) (defined from the exponents \( \langle r^2 \rangle \sim t^{d_s/d_f} \) and \( P(0, t) \sim t^{-d_s/2} \)) coincide 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 neighbours in layer \( j + 1 \) (see fig.1 and [14]). Asymptotically, the number of defective cells in layer \( j \) is a fraction \( \delta \) of the total number of cells \( K(j) \). Typically, 2d Euclidean, disordered froths have \( 0.1 < \delta < 0.2 \) [17]. In 2d, the number of paths connecting layer \( j \) with non-defective 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 \( \eta \delta K(j + 1) \), with \( \eta \) the average number of interfaces added by a defect to the shell between two successive layers (typically, \( 1 < \eta < 1.3 \) in 2d [17]). Therefore, asymptotically, Eqs. (8) and (9) can be extended to the non-SSI case by multiplying expression (7) by the factor \( (1 - \delta + \frac{\delta}{2}) \). The same result holds in 3d.

The non-SSI defects have important effects on the froth structure. In particular, it has been found in [14] that, in 2d non-SSI Euclidean froths, the number of cells per layer increases with the distance following a linear law \( K(j) = Cj + B \), with a slope \( C \sim 9 \). This slope is higher than the both values, \( C = 2\pi \) expected from simple geometrical consideration and \( C = 6 \) of the SSI hexagonal lattice. An higher increment in the number of cells per layer, must correspond to a faster diffusion (higher number of paths to go outward). On the other hand, in typical 2d disordered systems, one has \( (1 - \delta + \frac{\delta}{2}) < 1 \), which indicate asymptotically, a slower diffusion in non-SSI froths compared with the ordered SSI case. These two opposite behaviours are not in contradiction. 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. \( < \delta < \frac{\delta}{2} \)).
the intrinsic dimension - 1), and not on the slope. Therefore, we expect the diffusion in disordered structures compared with ordered SSI lattices, being faster at small distances (where the slope of $K(j)$ is relevant) and then becoming slower in the asymptotic part (where only the exponent of $K(j)$ is relevant). Fig. 3 shows $\langle r^2 \rangle / t$ calculated numerically for a non-SSI 2d Euclidean froth (a) and for the SSI hexagonal lattice (b). The diffusion in the disordered structure is faster than in the SSI hexagonal lattice in the first stage ($t < 15$ and $j < 4$), then it slows down to reach an asymptotic behaviour where the mean square displacement grows with $t$ more slowly in the disordered than in the ordered system.

A special behaviour 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 $\varphi = \cos(\frac{(e-4)}{2})$. In this case, from Eqs. (3), (4) and (6), one derives the asymptotic expression

$$\langle r^2 \rangle(t) \sim \frac{(\langle e \rangle - 6)(\langle e \rangle - 2)}{\langle e \rangle^2} t^2 \quad \text{for } t \gg 1.$$  \hspace{1cm} (9)

Numerical solutions of Eq. (11) for SSI 2d hyperbolic froths with various $\langle e \rangle > 6$, give time-dependent diffusion coefficient in excellent agreement with expression (9). The quadratic exponent in Eq. (11) indicates a ballistic diffusion and $d_s = 2d_f$.

We now write the evolution equation (1) in the continuous limit. Let introduce the continuous variables $\rho = \rho_0$ and $\tau = t\tau_0$, where $\rho_0$ is the average distance between two layers and $\tau_0$ 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, equation (1) can be written in the continuous form

$$\frac{\partial}{\partial \tau} P(\rho, \tau) = \frac{\rho^2}{\tau_0} C_d \frac{\partial}{\partial \rho} \left\{ \frac{\partial}{\partial \rho} P(\rho, \tau) - \frac{4}{(s + 2)} \frac{1}{K(\rho)} \frac{\partial}{\partial \rho} K(\rho) \right\} P(\rho, \tau),$$  \hspace{1cm} (10)

where $s$ is the inflation parameter ($s = \langle e \rangle - 4$ in 2d, and $s = \frac{1}{2} (\langle f \rangle - 6)(\langle n^N \rangle - 4) - 2$ in 3d [16]), which is a quantity associated with the curvature of the manifold tiled by the froth ($s = 2$ Euclidean, $s > 2$ hyperbolic and $s < 2$ elliptic froths). Expression (10) is the diffusion equation, for a $d$-dimensional spherically symmetric cellular system, written in polar coordinate. All the information about the structure, its intrinsic dimension, the disorder, are contained in the term in the square brackets and in the parameter $C_d$.

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 (10) becomes $\frac{d_f - 1}{\rho}$, and Eq. (10) has the solution

$$P(\rho, \tau) = \frac{2\rho^{d_f - 1}}{\Gamma \left( \frac{d_f}{2} \right)(4\varepsilon_0^2 C_d \tau)^{d_f/2}} \exp \left( - \frac{\rho^2}{4\varepsilon_0^2 C_d \tau} \right).$$  \hspace{1cm} (11)

The probability $P(\rho, \tau)$ increases with $\rho$ until a maximum at $\rho_{\max} = (2(d_f - 1)\varepsilon_0^2 C_d \tau)^{1/2}$, then it decreases exponentially. From solution (11), the mean square displacement results

$$\langle r^2 \rangle \sim \int_0^\infty \frac{\rho^2}{\tau_0} P(\rho, \tau) d\rho = 2d_f \rho_0^{d_f} C_d \tau,$$

which is already obtained in Eq. (8).

In a previous paper [16], it was found a class of 2d and 3d hyperbolic SSI froths which can be generated iteratively by using a simple recursive equation. These froths have $K(\rho) = \cos(\frac{(e-4)}{2})$. In this case, one can write the evolution equation (1) in the continuous form

$$\frac{\partial}{\partial \tau} P(\rho, \tau) = \frac{\rho^2}{\tau_0} C_d \frac{\partial}{\partial \rho} \left\{ \frac{\partial}{\partial \rho} P(\rho, \tau) - \frac{4}{(s + 2)} \frac{1}{K(\rho)} \frac{\partial}{\partial \rho} K(\rho) \right\} P(\rho, \tau),$$
\[ C \sinh(\varphi \rho_0), \] where \( \varphi = \cosh^{-1}(\kappa) \) is a constant associated with the space curvature (in simple 2d cases one can show the equivalence \( \varphi = \sqrt{-k} \), with \( k \) the Gaussian curvature. Here, \( s > 2 \) and \( k < 0 \). For these froths, the term in the square brackets in Eq.(10) is \( \frac{4}{(s+2) \rho_0} \coth(\varphi \rho_0) \). Therefore, the evolution equation (10) takes the form

\[
\frac{\partial}{\partial \tau} P(\rho, \tau) = \frac{\rho_0^2 C_d}{\tau_0} \frac{\partial}{\partial \rho} \left\{ \frac{\partial}{\partial \rho} P(\rho, \tau) - \left[ \frac{4}{(s+2) \rho_0} \coth(\varphi \rho_0) \right] P(\rho, \tau) \right\} .
\] (12)

Equation (12) was already known in literature as the diffusion equation in hyperbolic spaces with constant, negative curvature \([15,20]\). Here the same equation have been obtained starting from a tessellation model, making therefore a link between diffusion in curved lattices and hyperbolic Brownian motion. At long distances, the coefficient in the square brackets in Eq.(12) tends to a constant and the corresponding solution is a Gaussian with a constant drift. Here, the probability distribution move ballistically outward with the maximum at \( \rho_{\text{max}} = \frac{4}{s+2} \varphi \rho_0 \tau_0 C_d \tau \). This ballistic diffusion is consistent with the result for the mean square displacement for hyperbolic froth given in Eq.(9).

The author acknowledges discussions and correspondence with A. Comtet, D.J. Durian, E. Galleani d’Agliano, J.F. Joanny, F. Napoli and N. Rivier. This work was partially supported by EU, HCM contract ERBCHRXT940542 and by TMR contract ERBFMBICT950380.
REFERENCES

[1] D. Weaire and N. Rivier, Contemp. Phys. 25, 59 (1984).
[2] J. Stavans, Rep. Prog. Phys. 54, 733 (1993).
[3] J.F. Sadoc and R. Mosseri, J. Physique 46, 1809 (1985).
[4] N. Rivier and J. F. Sadoc, Phil. Mag. B 55, 537 (1987).
[5] Y. Limoge and J. L. Bocquet, Phys. Rev. Lett. 65, 60 (1990).
[6] D. H. Zanette and P. A. Alemany, Phys. Rev. Lett. 75, 366 (1995).
[7] D.J. Durian, Phys. Rev. E 50, 857 (1994). M.U. Vera and D.J. Durian, Phys. Rev. E 53, 3215 (1996).
[8] S. McMurry, D. Weaire, J. Lunney and S. Hutzler, Opt. Eng. 33, 3849 (1994). D. J. Durian, Opt. Eng. 34, 3344 (1995).
[9] A. Bunde and S. Havlin, Fractals and Disordered Systems (Springer-Verlag, Heidelberg, 1991).
[10] A. Comtet and C. Monthus, J. Phys. A 29, 1331 (1996).
[11] S. Boettcher and M. Moshe, Phys. Rev. Lett. 74, 2410 (1995).
[12] C. M. Bender, S. Boettcher and P. N. Meisinger, Phys. Rev. Lett. 75, 3210 (1995).
[13] D. Cassi and S. Regina, Phys. Rev. Lett. 76, 2914 (1996).
[14] P. C. Bressloff, V. M. Dwyer and M. J. Kearney, J. Phys. A 29, 1881 (1996).
[15] C. Monthus and C. Texier, J. Phys. A 29, 2399 (1996).
[16] T. Aste, D. Boose and N. Rivier, Phys. Rev. E 53, 6181 (1996).
[17] T. Aste, K. Y. Szeto and W. Y. Tam, Phys. Rev. E (1996), to appear.
[18] C. Itzykson and J.M. Drouffe, Statistical Field Theory (Cambridge University Press 1988) vol.1, chap.1 and vol.2, chap.11.
[19] S. Alexander and R. Orbach, J. Physique Lett. 43, L635 (1982).
[20] E. B. Davies, Heat kernels and spectral theory (Cambridge University Press) chap.5.
FIG. 1. A froth is a random partition of space by cells (a). Disorder imposes the incidence number at the minimum value (3 edges incident on a vertex in 2d). Froths are the dual structures of disordered packings (b). Such structures can be analysed as organized in concentric layers of cells at the same topological distance \( j \) from a given central cell \( (j = 0) \). Some cells (brought out by hatcheries in (a)) have neighbours in the internal layer but not in the external one and are topological inclusion or “defects” in the layered-structure.
FIG. 2. Probability $\Pi$ that the walker ever return to the origin for several values of the intrinsic dimension $d_f$. The walker always return in 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 behaviour is independent of the details of the structure. (The line is a guide for eyes.)
FIG. 3. Mean square displacement $\langle r^2 \rangle$ over $t$ vs. time for disordered (a) and ordered (b) cellular systems. 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 disordered system than in the corresponding ordered lattice. Then diffusion in disordered system slows down to reach an asymptotic regime where the walker propagates more slowly in disordered system than in the ordered case.