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Random collisions on branched networks: How simultaneous diffusion prevents encounters in inhomogeneous structures

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A huge variety of natural phenomena, including prey-predator interaction, chemical reaction kinetics, foraging, and pharmacokinetics, are mathematically described as encounters between entities performing a random motion on an appropriate structure. On homogeneous structures, two random walkers meet with certainty if and only if the structure is recurrent, i.e., a single random walker returns to its starting point with probability 1. We prove here that this property does not hold on general inhomogeneous structures, and introduce the concept of two-particle transience, providing examples of realistic recurrent structures where two particles may never meet if they both move, while an encounter is certain if either stays put. We anticipate that our results will pave the way for the study of the effects of geometry in a wide array of natural phenomena involving interaction between randomly moving agents.

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I. INTRODUCTION

A huge variety of natural phenomena, including prey-predator interaction, chemical reaction kinetics, foraging, and pharmacokinetics, are mathematically described as encounters between entities performing a random motion on an appropriate structure. Independently of whether both are moving or only one, on all the regular structures on which such phenomena are usually studied, e.g., crystal lattices or plane surfaces, these entities will meet with certainty in one and two spatial dimensions, while in three and more spatial dimensions a finite probability exists that they will never meet. We prove here, both analytically and via computer simulations, that on ubiquitous natural structures different strategies bear qualitatively different results: in particular, if both agents move there is a finite probability that they will never meet, while if one stays put while the other moves they are bound to meet with certainty. Our results have possible applications to a huge variety of natural phenomena, as prey-predator interaction [1,2], chemical reactions kinetics [3], foraging [4,5], and pharmacokinetics [6,7], are mathematically described as encounters between entities performing a random motion on an appropriate structure. Immediate consequences are manifold: in pharmacokinetics, drugs will affect mobile and static targets differently; chemical reactions are favored when either of the reagents is immobilized; in prey-predator models, the prey is more likely to survive if it keeps moving.

II. MULTIPLE RANDOM WALKS: GENERAL RESULTS

At the moment, a general theory of multiple random walks is missing: several basic results have been obtained on regular structures (see, e.g., [8]), but only a handful of studies exist regarding inhomogeneous graphs. With this article we aim to contribute to closing the gap.

A *graph* $\mathcal{G}$ is a pair $(\mathcal{V},\mathcal{L})$, where $\mathcal{V}$ is a collection of vertices, and $\mathcal{L} \subset \mathcal{V} \times \mathcal{V}$ is a set of unoriented links between the vertices.

In a *simple random walk*, an agent at a vertex v moves to a vertex v' at discrete-time steps; v' is chosen with uniform probability among the first neighbors of v, i.e., the set $\{(v,v') \in \mathcal{L}\}$.

The probability that a walker starting from v at time $t = 0$ is at v' after t steps is

$$P_{vv'}(t) = (p^t)_{vv'},$$

where p is the one-step transition probability matrix. When considering two independent agents, starting at time 0 from the vertices v and w, the most straightforward quantity which one can compute is the joint probability of motion in t steps:

$$\mathcal{P}_{(vw)\to(v'w')}(t) = P_{vv'}(t)P_{ww'}(t).$$

If we let the final position be the same (i.e., $v' = w'$), we obtain the probability that the two walkers meet at time t.

In turn, it is possible to link this latter quantity to the probability that the first encounter between the walkers happens at time t at vertex v', which we write $\mathcal{F}_{(vw)\to(v')}(t)$: if the agents meet at t in v', either it is their first encounter, or they have already clashed somewhere else at an earlier time, so that the corresponding probability can be written, in the language of generating functions, as

$$\tilde{\mathcal{P}}_{(vw)\to(v')}(\lambda) = \sum_{l\in\mathcal{V}} \tilde{\mathcal{F}}_{(vw)\to(l)}(\lambda)\tilde{\mathcal{P}}_{(ll)\to(v')}(\lambda) + \delta_{vv'}\delta_{wv'}. \quad (1)$$

This rather cumbersome formula introduces a matrical relation between $\mathcal{P}$ and $\mathcal{F}$, a difficulty which is not met in the single-particle scenario and ultimately allows recurrent graphs to exhibit two-particle transience, which we define below.

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Definition. A graph is *two-particle recurrent* if the probability that two particles will ever meet is 1, i.e.,

$$\sum_{t=0}^{\infty}\sum_{v'\in\mathcal{V}}\mathcal{F}_{(vw)\to v'}(t)=\sum_{v'\in\mathcal{V}}\tilde{\mathcal{F}}_{(vw)\to v'}=1,$$

for all (vw). Should the graph not satisfy this condition, we term it *two-particle transient*.

As it is an immediate extension of the type problem for a single random walker, we term the *two-particle type problem* the determination of whether a graph is two-particle recurrent.

From a complete knowledge of the two-particle probability $\mathcal{P}$, it is in principle possible to compute $\mathcal{F}$. Even though such complete knowledge is at best very difficult to achieve, several general conclusions can be drawn from the equation; in particular, for the case of homogeneous infinite graphs (i.e., all the points are equivalent), one can sum over the vertices v' and obtain

$$\tilde{\mathcal{F}}_{(vw)}(\lambda)=\frac{\tilde{P}_{(vw)}(\lambda)-1}{\tilde{P}_{(vv)}(\lambda)}, \tag{2}$$

where $\tilde{\mathcal{F}}_{(vw)}(\lambda)=\sum_{v'\in\mathcal{V}}\tilde{\mathcal{F}}_{(vw)\to v'}(\lambda)$, and similarly for $\tilde{\mathcal{P}}_{(vw)}$.

Since

$$\mathcal{P}_{(vw)}(t)=\sum_{v'\in\mathcal{V}}P_{vv'}(t)P_{wv'}(t)=P_{vw}(2t),$$

$\tilde{\mathcal{P}}(\lambda)$ has the same asymptotic behavior as $\tilde{P}(\lambda)$ for $\lambda\to 1$. For a recurrent graph this immediately entails $\tilde{\mathcal{F}}(\lambda=1)=1$, that is, *any homogeneous recurrent graph is two-particle recurrent*. It is thus guaranteed that, on homogeneous graphs, an infinite expected number of encounters and two-particle recurrence are one and the same thing.

What jumps to the eye is that on inhomogeneous graphs it need not be so, and indeed two-particle transient structures exist with an infinite expected number of encounters. In particular, we are going to prove in the following the existence of one-particle recurrent–two-particle transient graphs, using a specific mathematical property of some graphs, known as the finite collision property in the mathematical literature [9–11]):

Definition. A graph has the finite collision property if the probability that two random walkers will meet only a finite number of times is 1.

In a recurrent graph, the probability that the number of collisions is finite can only be either 1 or 0 [12] (it is sometimes called a trivial property in probability) and furthermore it has the same value for all the pairs of initial positions (vw) and $(v'w')$ such that

$$\mathcal{P}_{(vw)\to(v'w')}(t)\neq 0\quad\text{for some } t.$$

It should be stressed that the expected number of encounters of two particles, $\lim_{\lambda\to 1}\tilde{\mathcal{P}}_{(vw)}(\lambda)$, can diverge either because the graph has the infinite collision property, or because the probability that the number of encounters is less than N does not go to zero fast enough with growing N.

Under the formalism we have introduced above, the finite collision property for two particles starting from the same vertex v reads

$$\lim_{\lambda\to 1^-}\sum_{n=0}^{\infty}\sum_{l\in\mathcal{V}}(\tilde{\mathcal{F}}(\lambda))^n_{(vv)\to l}(1-\tilde{\mathcal{F}}(\lambda)_{(ll)})=1. \tag{3}$$

In fact, the finite collision property and the two-particle transience are one and the same thing. To prove this result, we perform a logical sidestep and consider the infinite matrix $\tilde{\mathcal{F}}_{(vv)\to l}$ at $\lambda=1$ as a transition matrix generating a random walk, in the same way as the single-particle transition matrix p_{vw} generates the random walk $P_{vw}(t)$.

As seen from Eq. (3), the finite collision property is linked to the matrix $\tilde{\mathcal{F}}_{(vv)\to l}$. The probability that the walkers meet no more than N times is a slight modification of Eq. (3):

$$\begin{aligned}\mathrm{Prob}_{(vv)}(n_{\mathrm{enc}}\leqslant N)&=\lim_{\lambda\to 1^-}\sum_{n=0}^{N}\sum_{l\in\mathcal{V}}(\tilde{\mathcal{F}}(\lambda))^n_{(vv)\to l}(1-\tilde{\mathcal{F}}(\lambda)_{(ll)})\\&=1-\left(\langle n\rangle^{(N+1)}_{(vv)}-\langle n\rangle^{(N)}_{(vv)}\right);\end{aligned} \tag{4}$$

here

$$\langle n\rangle^{(N)}_{(vv)}=\lim_{\lambda\to 1}\sum_{n=1}^{N}(\tilde{\mathcal{F}}(\lambda))^n_{(ll)}$$

is the expected number of steps performed in the random walk generated by $\tilde{\mathcal{F}}_{(vv)\to l}$.

Theorem. A graph has the infinite collision property if and only if it is two-particle recurrent.

Proof. If the graph is two-particle recurrent, i.e., $\tilde{\mathcal{F}}_{(vv)}=1$ for all vertices v, the random walk generated by $\tilde{\mathcal{F}}(\lambda)$ is conservative, so $\langle n\rangle^{(N)}_{(vv)}=N$, and from Eq. (4)

$$\lim_{N\to\infty}\mathrm{Prob}_{(vv)}(n_{\mathrm{enc}}\leqslant N)=0; \tag{5}$$

a two-particle recurrent graph thus has the infinite collision property. On the other hand, if the graph has the infinite collision property, Eq. (4) implies that

$$\lim_{N\to\infty}\left(\langle n\rangle^{(N+1)}_{(vv)}-\langle n\rangle^{(N)}_{(vv)}\right)=1;$$

this entails $\tilde{\mathcal{F}}_{(vv)}=1$ for all vertices v, since even a single $\tilde{\mathcal{F}}_{(vv)}<1$ is enough to achieve the absurd

$$\lim_{N\to\infty}\left(\langle n\rangle^{(N+1)}_{(vv)}-\langle n\rangle^{(N)}_{(vv)}\right)<1.$$

The infinite collision property thus implies two-particle recurrence, and the proof is complete. ■

III. THE COMB GRAPH

One graph that has been proved to possess the finite collision property [9] is the comb lattice [see Fig. 1(b)]; the

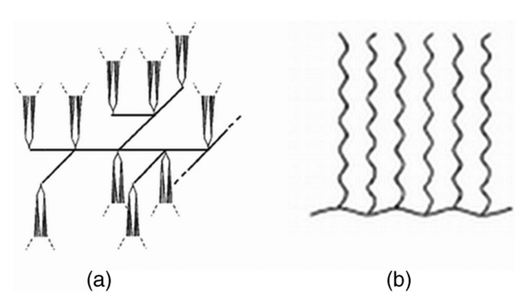

FIG. 1. *Two significant example graphs*. In (a) we show an example of a general bundled structure, a class of graphs made by attaching branches at each vertex of a base graph. In (b) the comb lattice, the simplest form of bundled graph, is depicted.

result from the previous section proves then that it is also two-particle transient. The most basic version of the comb graph can be obtained from the infinite square lattice by removing the horizontal edges everywhere but on a single line.

We explored the finite-size consequences of two-particle transience by means of simulations, some results of which are reported in Fig. 2. Since the comb graph is two-particle transient, even on its finite realizations the agents have a sizable probability of not meeting as long as they do not collide with the barriers of the system; this effect becomes more pronounced, with respect to the square lattice, as the system grows in size. For large (infinite) comb systems, one can see that, if the walkers have not already met at time $t > t_{\text{plateau}}$, it is less and less probable that they do so at any subsequent time [see Fig. 2(c)], while on the square lattice the probability of meeting remains sizable even at large times.

The next phase to examine is the proper finite-size effect, which kicks in when diffusion of the agents allows for a large probability of them hitting the walls of the structure; for the comb lattice, the consequent clash of the agents is more smeared than in the case of the square lattice. This fact is a reflection of the two-particle transience of the infinite comb lattice, which makes its finite realizations better compact labyrinths for the agents.

The finite-size effect can thus be divided into three qualitatively different phases: an initial rapid growth, followed by a slowly rising (square graph) or almost flat (comb) plateau, and finally a transient, in which the finite-size effects are first experienced by the agents, culminating in the saturation to 1 of the encounter probability. This simple time structure hints at possible applications whenever the real system has a time scale which is comparable to the time the random walk needs to reach the transient, e.g., an antibody, which has not been able to locate a corresponding randomly moving ligand before

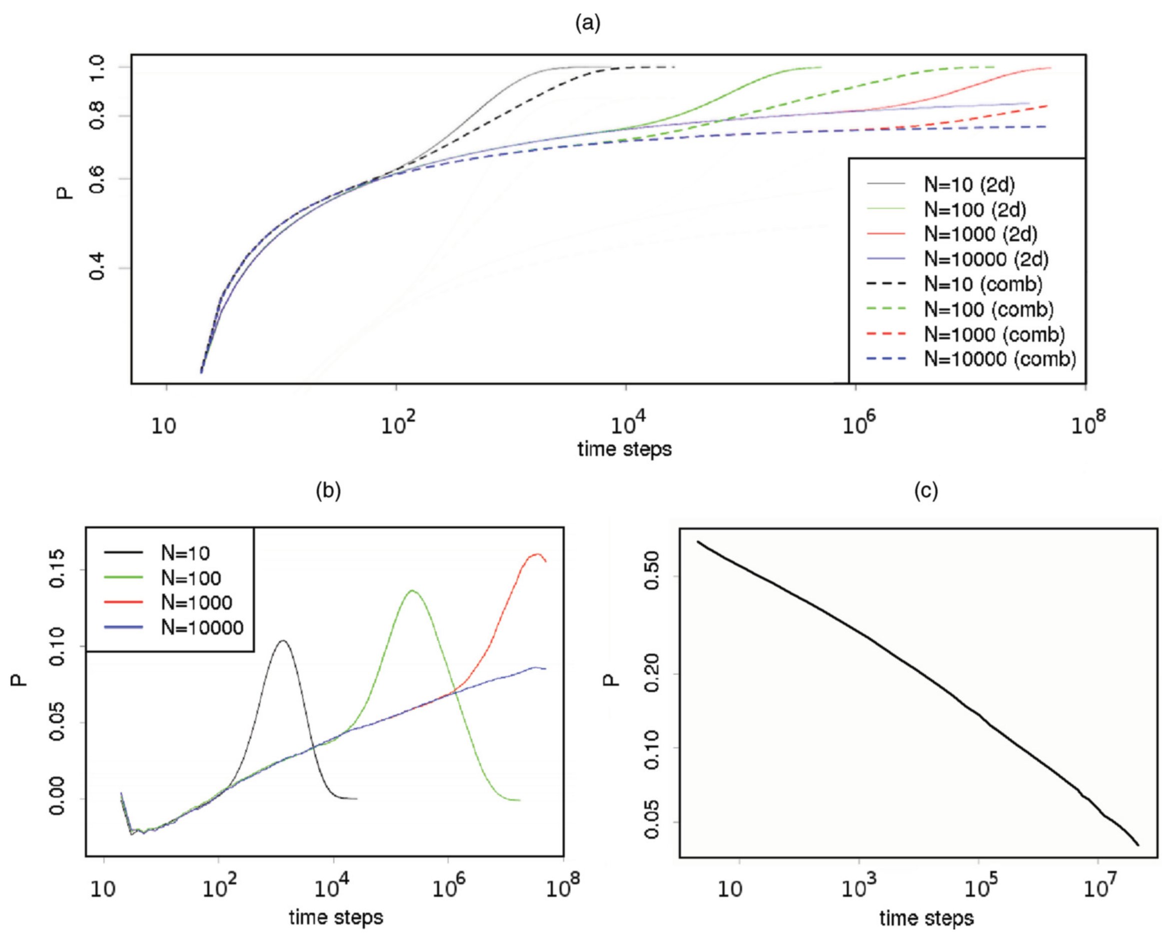

FIG. 2. (Color online) *Finite-size behavior.* In (a) the encounter probability $D_v(t) = \sum_{\tau=0}^{t} \mathcal{F}_v(\tau)$ is plotted for several realizations of finite combs and square lattices of $N \times N$ vertices. In the realizations with $N = 10, 10^2, 10^3$ (solid and dashed lines corresponding to maxima from left to right), one can clearly identify the three phases of steep increase, slow convergence (which lasts until the agents perceive the finite size of the structure), and saturation of $D_v(t)$, as discussed in the main text. In the $N = 10^4$ cases (never-rising solid and dashed lines), the simulation time has not been long enough to exhibit the finite-size characteristics of the graph. In (b) the difference $\Delta_v(t) = D_v^{\text{comb}}(t) - D_v^{\text{square}}(t)$ between the comb and square lattices is plotted, highlighting that for long times it tends to a constant. The peaks correspond, from left to right, to $N = 10, 100, 1000$; $N = 10\,000$ corresponds to the monotonic line. Last, in (c) the conditional probability that an encounter happens if the agents have not yet met at time t is plotted for the extrapolated infinite comb lattice, using a probability of survival $D_v(\infty) = 0.228$. As expected it rapidly tends to zero, reflecting the fact that, if they have not yet met at time t, they are likely to be far from each other, and thus less and less prone to ever meeting.

reaching the plateau will definitely fail to do so if its expected lifetime expires before it hits the walls of the finite structure inside which it diffuses.

The difference between two-particle transient and recurrent structures becomes qualitative, not only quantitative, when their size becomes large: the transient phase disappears for two-particle recurrent graphs, as the probability that an encounter has already happened approaches 1 as the time grows large.

IV. DISCUSSION

The dichotomy between one-particle and two-particle type problems needs a thorough inquiry in several fields, in order to ascertain its real-world consequences. *Diffusion-limited* (or diffusion-controlled) *reactions* are reactions that happen as soon as the reactants collide; the collision between two random walkers can be seen as a schematic view of such processes, and several papers have already addressed this problem (see, e.g., [13–15]). In particular, we can now provide a counterexample to the so-called Pascal principle, which states, *mutatis mutandis*, that the best strategy to avoid destruction is standing still: Moreau *et al*. [16] have in fact proved that the survival probability for a particle, performing a simple random walk in a d-dimensional hypercubic lattice and surrounded by a set of moving traps, is greater at all times if the particle does not move. Since on two-particle transient graphs the probability of the particle surviving tends to a nonzero constant, the Pascal principle fails, highlighting that geometry, together with the symmetry of the model, has the last word on what the winning strategy turns out to be.

A full characterization of graphs possessing two-particle transience is yet to come: some small steps forward have been taken, with a few specific cases solved [9,11] and a straightforward necessary condition laid down [12], but general criteria to assess two-particle transience are still lacking. Comblike graphs, or bundled structures, constructed by engrafting a separate branch on each vertex of a base graph [see Fig. 1(a)], are probably the most interesting candidate class of two-particle transient structures: they are recurrent for several choices of base and branches [17] and it has been conjectured [9] that they have the finite collision property, and hence are two-particle transient, whenever both base and branches are recurrent; a counterexample was provided in Ref. [11], using, however, pathological structures as branches.

Many real-world structures are not as regular as combs. However, it has been proved that the long-time behavior of every single random walker on disordered comblike structures depends only upon their long-range geometry, while it is unaffected by local details [18]. Therefore, we also expect the two-particle transience to be independent of local details and disorder.

A real-world example of comblike graphs is provided by microtubules [19], a component of the cytoskeleton, as organized around a centrosome. More general branched structures are ubiquitous in biological systems; the circulatory system, lungs, lymphatic system, and endoplasmic reticulum all fall into this category. It may prove interesting to explore the kinetics of diffusion-limited reactions on such structures, in order to examine the role of two-particle transience in a real system. Similar studies, using agent-based simulations, have recently been conducted for the whole intracellular environment [3].

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