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MULTILINEAL RANDOM PATTERNS EVOLVING SUBDIFFUSIVELY IN SQUARE LATTICE

ADAM GADOMSKI
Institute of Mathematics and Physics, University of Technology and Agriculture, PL-85796 Bydgoszcz, Poland

Abstract

Stochastic multiline evolution in square lattice is studied. It turns out that the emerging patterns evolve subdiffusively, which is characterized by the $\frac{1}{4}$ exponent. Possible origin of such a slow behavior is discussed, and some elucidation, supporting the small fractional value is given. A notion of (dynamic) phase transition concept may sometimes help in understanding the presented random kinetic behavior.

1. INTRODUCTION

Retrospective view towards history of statistical physics shows that simple models are really worth developing. As a certain quite "out-of-date" general example, traced back to the twenties, the Ising model should be mentioned. A slightly younger "toy" model, known to almost everyone, appears to be the percolation model. After the era of applying the computer and its very capacities had emerged, they both have been visibly put forward, and stand nowadays for basis of many applications in microelectronics, materials engineering and technology, chemical processing, etc. Other examples of simple statistical-physical models can undoubtedly be the growth models, intensively explored since the early eighties, or even earlier. On the list of those models one can mostly find the following simple "computer-aided" phenomena, like e.g. diffusion-limited aggregation (first invented by Witten and Sander in 1981), and its variations; ballistic growth; Eden cluster formation or chemical reaction-limited growth. One has also to mention a large class of models, that may be named deposition models. They led to formation of random deposits on a plane (line), e.g. ballistic and/or diffusional deposits, just mentioning a few. They gave for sure rise to some intense theoretical understandings, leading to formulation of the conditions of surface dynamics, known as the Kardar-Parisi-Zhang (KPZ) system. This, in turn, initiated an eruption of theoretical approaches in surface science (thin film formation), crystal growth theory, polymer dynamics or turbulence studies, etc.[1–3]

It seems to be well-known that all the above mentioned dynamic processes deserved fruitful interpretation and description in terms of the random walk and/or phase transition concepts. As for the former, one may notice either the standard (normal) random walk or the anomalous (sub- or super-normal) one, realized possibly under some constrained conditions.[4] As for the latter, one easily checks the seminal literature and concludes thereafter, that either the continuous phase transition or that of order-disorder type should be considered while examining the above listed complex systems.[5] These notion will be used throughout this study, sometimes supported by certain kinetic arguments, *cf.* a review paper.[6]

The paper is structured as follows. In Sec. 2, a sketchy presentation of the algorithm, involving random evolution rules as well as initial conditions (IBCs) is given. In Sec. 3, some versatile physically-motivated explanation of the subdiffusive random motion of the evolving multiline is provided. In Sec. 4, one has to expect final remarks.

2. ALGORITHM, RULES AS WELL AS INITIAL AND BOUNDARY CONDITIONS

Because in Refs. 7 and 8, the algorithm of the random multiline evolution has been presented in sufficient detail, let us refer to its main points. Thus, let us start from a sketch of the algorithm. It is as follows:

- Initialize a starting configuration (a straight-line,[8] or a rectangular seed,[9] for example);
- Apply a set of random rules, i.e. choose a suitable one taken from 8 available rules (3 of reversible type, which means six forth and back rules in total, and some 2 remaining, being of irreversible nature), causing some evolution, or structural rearrangement, of the multilineal pattern(s) under investigation (the rules are specified below);
- Go permanently back to the above point unless desired statistics and/or other estimated quantities have been obtained; do not forget to refresh accordingly all the possible counters involved in the simulational process.

For introducing the rules in a possibly concise way, let us label four edges of the unit square on which the multiline may land by d, u, l and r, respectively, and assume for simplicity, that d-edge (lying on X-direction), being just occupied, will be shifted upwards along Y-direction, see Fig. 1 for some exemplified realization within a small system.

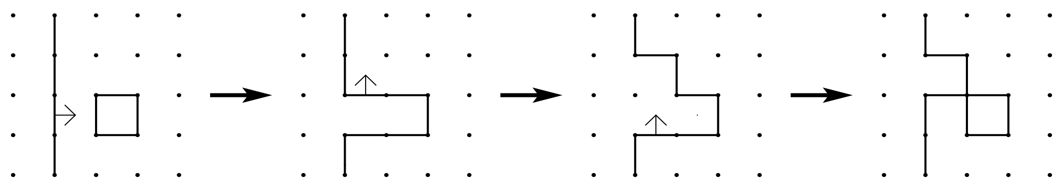

Fig. 1 A few snapshots taken from an evolution of the so-called small system, assumed that the first two steps are given as in Fig. 2 in Ref. 8, but the next few steps are accidentally realized in a different manner, just presented here.

Now, one can draw 8 basic annihilation-creation (or, neutral) rules, driving the system, schematically by means of a single formula:

$$X_i^d + X_j^u + Y_k^l + Y_l^r \rightleftharpoons Y_{1-l}^r + Y_{1-k}^l + X_{1-j}^u + X_{1-i}^d \,, \tag{1}$$

where: i, j, k, l can be equal to 0 (means: empty edge) or 1 (means: non-empty edge), and where the following elementary local rearrangements of the multilineal (discrete) patterns are possible to occur:

- Rule No. 1: Eq. (1) for $i = 1$, $j = k = l = 0$, i.e. with ± 2 gain/loss of elementary units (creative/annihilative); note, that the multiline is composed of elementary units, and that the length of the elementary unit is always equal to the square lattice constant
- Rule No. 2: Eq. (1) for $i = l = 1$, $j = k = 0$, i.e. with 0 gain/loss of elementary units (neutral)
- Rule No. 3: Eq. (1) for $i = j = 1$, $k = l = 0$, i.e. with 0 gain/loss of elementary units (neutral); see remarks on indirect reversibility in[7]
- Rule No. 4: Eq. (1) for $i = j = k = 1$, $l = 0$, i.e. with $+2$ loss of elementary units (moderately annihilative)
- Rule No. 5: Eq. (1) for $i = j = k = l = 1$, i.e. with $+4$ loss of elementary units (strongly annihilative),

where the last two cases listed above have to be taken irreversibly, so that one has to put "$\rightharpoonup$" into Eq. (1) instead of the double arrows indicating reversibility, valid exclusively for the three first points mentioned above. To get wider outlook about the (ir)reversibility in question, *cf.* Refs. 7–9. (For another realization, but presenting a large system, see Fig. 2.)

As to the IBCs applied, let as ascertain the following. In a study,[7] some nearly periodic boundary conditions (BCs), i.e. vertically periodic, but horizontally free, have been applied. The IC was a vertical straight-line, usually placed in the middle of the lattice. In another work,[8] the IC remained the same, but the BCs have been changed subject to physical reality (constraints, see Ref. 4), which implies, that some reflecting BCs have been assumed. In Ref. 9, the authors decided to use fully periodic (on-torus-concept based) BCs. Quite versatile ICs have also been probed, like the rectangular seed(s) or two parallel lines, constituting an interfacial stripe, as a certain extension of the single-line IC concept.

The performed simulations, *cf.* Refs. 7–9, enable to arrive at some elucidations, mostly in terms of the subdiffusive (random walk) behavior, shown in the simulation time scale, measured in Monte Carlo steps. (Note, however, that another time scale applied, mostly

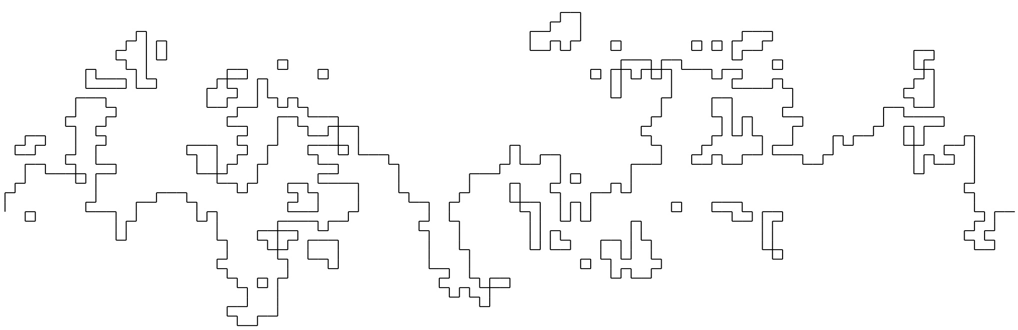

Fig. 2 A large configuration, resulting from simulation of the random multiline (*Courtesy of Martin Schönhof and Lutz Schimansky-Geier*).

motivated by some real or Gillespie time scale concept,[9b] may result in slightly different time behavior.) It will be explained in the next section.

3. $\frac{1}{4}$-EXPONENT DRIVEN SUBDIFFUSIVE BEHAVIOR

Since a subdiffusive time-behavior has been checked quite thoroughly for many different realizations,[7–9] even quite irrespective of the BCs applied (mentioned in the preceding section), but preferentially for the single-line IC condition, it is certainly worth elucidating why and when such a behavior survives. It is interesting to note that such $\frac{1}{4}$ exponent driven characteristics are observed even if we use slightly different measures,[7,8] though they are chosen to describe some linear characteristics of the multilineal evolution in the course of time. To be more specific, let us state explicitly, that in Ref. 7 we studied the overall averaged length of that interline (termed also a diffusion-reaction front), whereas in Ref. 8 one has to notice, that we considered the problem of survival of the multiline, since boundary conditions under use (reflecting BCs) helped the multiline to disappear. We simply wanted to know how those disappearence events are related to a linear measure of the available evolution space, which in this particular case means the overall lattice (square or triangular)[8] size. All the characteristics obtained, but measured for long enough simulation times as well as averaged over a set of single simulations for each lattice size, L, end up with the following asymptotic formula, namely

$$\mathrm{L} \sim t^{\alpha}, \tag{2}$$

where $\alpha \approx \frac{1}{4}$; here L means a characteristic length, while t stands for the simulation time, see above. Such a dependency has also been revealed for the fully periodic BCs.[9] Let us then try to explain it briefly in the subsequent subsections.

3.1 Line-Tension Controlled Expansion Behavior

In the following, we wish to rationalize, what we have done in computer simulations, that we performed. First, we are willing to rely on some simple, or even verbal argumentation, supporting the evolution in question. Second, we are trying to utilize a proportionality law, quite well-known while offering a stochastic description of grain growth, e.g. in metals or ceramics. A common denominator of both of them appears to be everypresence of the line tension, which is a factor controlling (damping) multiline expansion process.

As for the former, we have to observe that based on our numerical study of random multilineal pattern evolution, one can quite firmly risk to state[9] that we may have to do with a competition process. We checked accurately the statistics coming from our simulations, *cf.* another unpublished study[10] (also another study[9] can be invoked), and we may state that the rules No. 1 (but creative, i.e. the forth rule) and No. 2 (neutral, but acting forth and back) as well as the irreversible multiline tension[7] rule No. 4 support to very large extent the statistics. The rules No. 1 and No. 2 are much responsible for random expansion of the line, characterized by the random motion exponent, say $\nu \approx \frac{1}{2}$, which is a value commonly assigned to standard diffusional behavior. The countereffect (a "contraction" case, or a case of preservation of the change in time of area, A, covered instantanously in the lattice by the line, must be given by roughly the same exponent, denoted however by μ, where $\mu \approx \frac{1}{2}$, just for underlying that two different mechanisms are involved in the evolution. This is because a change in time of the area A, scavenged (swept) by the evolving multiline, is given by

$$\frac{dA}{dt} \simeq const., \tag{3}$$

which is fulfilled if we realize that the overall multilineal expansion-contraction process is readily going to proceed purely at random (this is just the case!), so that none of the major competition forces can be *a priori* priviledged, and the competition, because of every present random circumstances ("random mixing"), can be thought of to be a kind of liazon, which must then be expressed by the fact, that $\nu \times \mu$ is the overall characteristic exponent of the evolution, so that any L has to follow

$$\mathrm{L} \sim t^{\nu \times \mu}, \tag{4}$$

where $\nu \times \mu \approx \frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$, and where L has to be measured for sufficiently large times.

As for the latter (read: more sophisticated elucidation will appear), let us present the following reasoning. To do so, however, let us start with the following question. What is possible to ascertain while trying to get a relative change of that variable $A \equiv A(t)$ in two consecutive time instants t as well as $t + \Delta t$? Our observations, much confirmed by systematic numerical investigations[9] reveal, that

$$\frac{A(t+\Delta t) - A(t)}{A(t)} \propto \varepsilon\,, \tag{5}$$

where ε is a random fraction, *cf.* a study on polycrystals and their boundaries,[11] being independent of time. (By the way, Eq. (5) is called the law of proportionate effects, or simply a proportionality law. It appears often to be a signature of the log-normal behavior in the system.[11]) But we do not have to forget that from Eq. (3) a constancy of changes of the area A in time follows, and that this way a line tension effect is manifested.

Following Eq. (3) we have crudely to assume that $A \sim N\Delta t$ holds, where $\Delta t \ll 1$ (but, unfortunately $\Delta t \to 0$ is not guaranteed) and $N \gg 1$ is expected, where N (a positive constant) can be the number of the simulation steps, or some quantity very related to it.

If the above is accepted, we may, loosing a bid on accuracy, write down a Langevin-like equation of the form

$$\frac{dA}{dt} \propto \chi\,, \tag{6}$$

where χ equals $N\varepsilon$, and stands for a random but uncorrelated "force", having a constant average value, χ_o. Note that A scales with some $t = N \times \Delta t$, so that a characteristic line tension influenced scaling behavior can be detected this way, presumed that N would remain constant or insensitive to such a time scale; notice that if $A \propto \mathrm{L}^2$ one automatically provides the known standard relation, namely $\mathrm{L}^2 \propto t$ (in fact, characteristic for both typical line (surface) tension-driven as well as standard diffusional behaviors, but argued just for the latter).

The above physical picture notwithstanding, and knowing that such a Langevin-like equation has its counterpart in the so-called Fokker-Planck-Kolmogorov representation,[12a] we conclude that this is exactly the standard diffusion equation

$$P_t(\mathrm{L}^2, t) = D\Delta P(\mathrm{L}^2, t)\,, \tag{7}$$

[a]One may certainly argue whether such a continuous representation may stand for some argumentation for supporting discretized pictures, that usually come from the computer experiment. Nevertheless, we are of the opinion, that it can provide at least another direction of how to deal with problems of such types in approximate way.

where P_t and Δ (Laplacian) have their usual meanings; here D is the strength of the noise (or, the diffusion coefficient, but assumed that the diffusion process in the space of the quantity L^2, proportional to the instantaneous area swept by the multiline, but not in the position space is provided). The mean squared displacement, $\langle(\mathrm{L}^2)^2(t)\rangle$, evaluated as the second (statistical) moment of the stochastic process, namely

$$\langle(\mathrm{L}^2)^2(t)\rangle = \int_0^\infty (\mathrm{L}^2)^2 P(\mathrm{L}^2, t) d\mathrm{L}^2, \tag{8}$$

reads

$$\langle(\mathrm{L}^2)^2(t)\rangle \propto t\,, \tag{9}$$

so that the $\frac{1}{4}$ exponent behavior has this way been recovered, based on the above continuum approximation. Summing up, one has to consider the evolution in question as a nonstandard random walk behavior, where such a nonstandard (decelerated) kinetic character is anticipated because the line tension effect somehow balances random (standard diffusional) expansion of the multilineal pattern (it is clearly not in contradiction to define that random walk as self-avoiding, which comes directly from computer simulation[7,9]).

3.2 Back to Smoluchowski: Diffusion-Controlled Annihilation Problem Revisited

In Ref. 7 it was mentioned that some most elementary "chemical reactions" in our model phenomenon are the following

$$\begin{aligned} X^* + X &\rightharpoonup 0 \\ Y^* + Y &\rightharpoonup 0 \\ X^* + 0 &\rightleftharpoons X \\ Y^* + 0 &\rightleftharpoons Y\,, \end{aligned}$$

where X means a horizontal "particle", whereas Y represents a vertical one; notice that the superscript "$*$" means that a corresponding "particle" will be chosen (shifted; movable). It was stated therein,[7] that the two first reactions are far from being trivial. Even more, following seminal literature one has to argue that they constitute a theoretical framework for the diffusion-controlled annihilation process, e.g. characteristic of self-segregation phenomena, which in one dimension obeys the $\frac{1}{4}$ temporal law,[4] when presumed that X^* (shifted along Y-direction), or Y^* (shifted along X-direction, accordingly), do realize a one-dimensional random walk (time t stands here for a survival time) until they are trapped by unmovable (not selected at random for being shifted!) traps X and/or Y, respectively. While looking at the formula 5.57 in Ref. 4a (Chap. 5), one sees, that for sufficiently long times, namely $t \gg 1$, one gets similarly to Eq. (9)

$$\langle \mathrm{L}(t)\rangle \propto t^{1/4}, \tag{10}$$

where here $\langle \mathrm{L}(t)\rangle$ stands for the average nearest distance between X (or, Y) "particle" and another of the same type, just before meeting it at random (in the above equation a certain prefactor may appear, which depends upon details of the model[4a]); notice, that according to the rule No. 3 both of them are annihilated, but some two new counterparticles Y (or, X), respectively, emerge. This scenario agrees well with our simulational observations.

It touches also visibly the problem of determining the mean first passage time for the multiline,[9b] since the above distance quantity is defined as

$$\langle \mathrm{L}(t) \rangle = \int_0^\infty Q(\mathrm{L},\, t) dt \,, \tag{11}$$

where $Q(\mathrm{L},\, t)$ stands for a survival probability.[4] It is, by the way, noteworthy that such a kinetic anomaly, concerning the exploration of $X^* + X \rightharpoonup 0$ (or, $Y^* + Y \rightharpoonup 0$) reactions, has first been pointed out by Marian Smoluchowski (also, later touched upon by Ovchinnikov and Zeldovich[3]), who showed, that it can be fully manifested in a restricted (e.g. two-dimensional) geometry, where effective stirring, controlled by diffusion, seems to fail.[4] Finishing this subsection, let us underscore that the annihilation process in a $1D$ system described is not only thought of when a single unmovable trap stands for sink for randomly walking individuals, but also under a set of more relaxed conditions. We believe, that our conditions belong also to such a group. (Notice that in such problems all the realizations have to be averaged over the available set of ICs, and a thorough confirmation of the above reasonable suppositions needs just a repetition of the experiment towards satisfying this ascertion.)[4]

3.3 Naive Renormalization Group Considerations

The most naive (probably, oversimplified) explanation for the $\frac{1}{4}$ exponent driven temporal multiline behavior may come from real space renormalization[5] considerations presented below, and valid preferentially for certain $2D$ systems, like XY model. We may also refer to Fig. 3, where the most primitive as well as self-consistent configurations (say directly, most essential) both for the square lattice[7,8] but also for a triangular one[8] are depicted.

The number of them, M_n, on each level of the renormalization (designated by n, being in general not mismatched with N) equals

$$M_n = 4^n = 2^{2n}, \tag{12}$$

whereas the (square root) "renormalization length" or factor, l_n, typically reads[13]

$$l_n = 2^{n/2}. \tag{13}$$

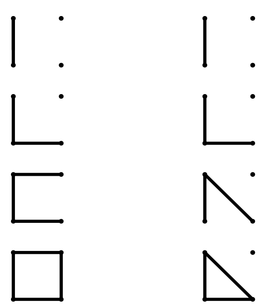

Fig. 3 Most primitive configurations, constituting the random multiline for square as well as triangular lattices, respectively (*cf.* Figs. 3 and 4 in Ref. 8).

Defining the critical exponent for the proposed renormalization procedure, namely

$$\bar{\nu} = \frac{\ln(l_n)}{\ln(M_n)} \tag{14}$$

taken for $n \to \infty$, one gets immediately the desired value of $\bar{\nu} = \frac{1}{4}$. Such a value can mostly be met while inspecting certain numerical investigations on the $2D$ Ising system dynamics near equilibrium.[14,15] (We may also find interesting to perform quite simple calculations, according to what is done in Ref. 13, Chap. 5 for the $2D$ bond percolation problem, i.e. to derive the so-called renormalization group equation. The result can be that we get, as in the percolation problem two seemingly different limits, namely the low- as well as high-temperature ones at the rearrangement probability equal to 0 and 1. Moreover, instead of one intermediate probability point somewhere in between, as in the bond percolation problem, one provides now two such points: A certain one closer to 0, and another one closer to 1. This result may indicate that in our system, instead of the continuous order first transition, or that of the second type according to Landau,[5] one would have to do with the order-disorder phase change of Kosterlitz-Thouless-like type, with an intermediate, or "hexatic" (tetratic) phase, placed just in between, *cf.* Refs. 5, 13 and 16. This attractive supposition must however be checked, perhaps in another study.)

4. CONCLUSIONS

The following final remarks, based on what has been presented before, can be juxtaposed. These are:

- The multilineal evolution under study can be analyzed on three levels of description, and by applying three seemingly different approaches, *cf.* Sec. 3.
- The first description presented (Subsec. 3.1) seems to be most physically motivated, and is readily realized in two-dimensional space. It takes into account that the evolution studied can be understood in terms of cooperation of two randomly acting processes. The first process is due to random expansion (random walk in the area space) whereas its "*alter ego*" is the surface tension (random contraction), which in the case of line tension effect, present in the system, causes mostly a continuous (dynamic) phase transition,[17] quite differently than in a $3D$ case, where some first order phase transition effects are present. (Phases can be differentiated in our problem as sets of points inside and outside the area covered by the line(s), so that a problem of intermingled phases, like in biomembranes, may likely arise.)
- The second description (Subsec. 3.2) is realized in a $1D$ space, and borrows something from the concept of mean first passage or survival time.[4]
- Last but hopefully not the least, the third description (Subsec. 3.3) is most general, and refers to the problem in question as being renormarizable,[5,15] or statistically self-similar (or, even more, *e.g.* self-affine); its shortage seems to be that no straightforward physical argumentation is observed to stay behind it.
- It is interesting to note, that a common denominator of all of the above presented descriptions appears to be confirmation of subdiffusional random motion of the multiline, characterized by $\frac{1}{4}$ exponent (in the domain of simulation times, and surely, within the accuracy level of computer experiments performed[7–10]).
- Finally, let us state clearly, that the problem studied has been treated on kinetic level,[6–10] and that no dynamic assignements[14] have so far been proposed.

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